





Uncertainty characterisation in Data Assimilation

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Introduction

- Data Assimilation combines :

  - several **sources of information** : observations, background state ;
  - specific **operators** : error covariance matrices and observation operators ;
  - specific **cycling process** : succession of analysis and forecast steps.

- How do these different components contribute to information & uncertainties in DA ?

  - knowledge & understanding of **information & error dynamics** in DA ;
  - develop adequate **error simulation & estimation** methods for DA & EPS.

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Outline

- From **innovation-based estimates** to EDA

- **Expansion** of error contributions in cycled DA

- Damping of **old background errors**,
  accumulation of **recent observation errors**

- Compensation between **old and recent errors**,
  building of **information** in DA cycling

- Estimation and simulation of **model errors**

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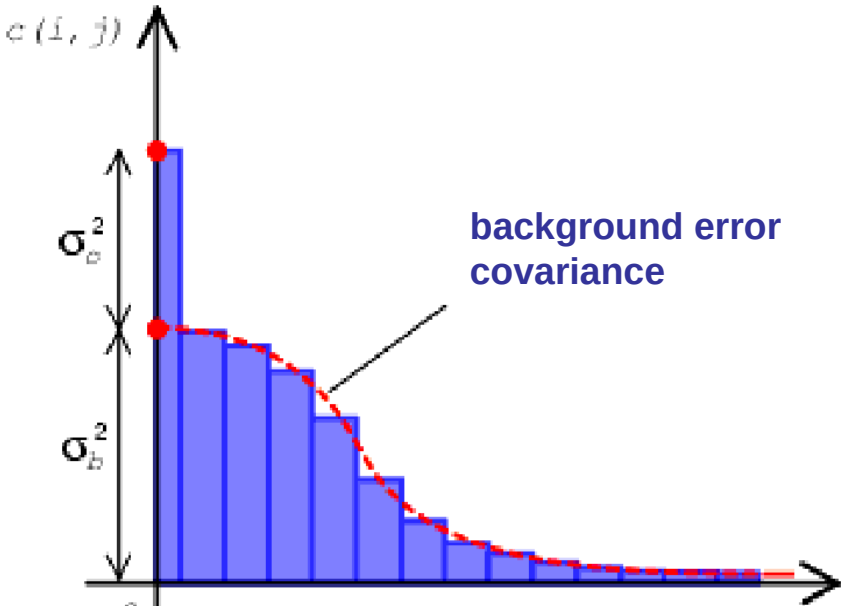
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Innovation-based diagnostics



$$E[(\mathbf{y}^o - H(\mathbf{x}^b))(\mathbf{y}^o - H(\mathbf{x}^b))^T] = \mathbf{R} + \mathbf{HBH}^T$$

=> For spatially uncorrelated observation errors,
- at non zero separation : innovation covariances = background error covariances ;
- extrapolate them to zero separation distance, to estimate σ_b^2, σ_o^2 and background error correlations.

(e.g. Hollingsworth and Lönnberg 1986)

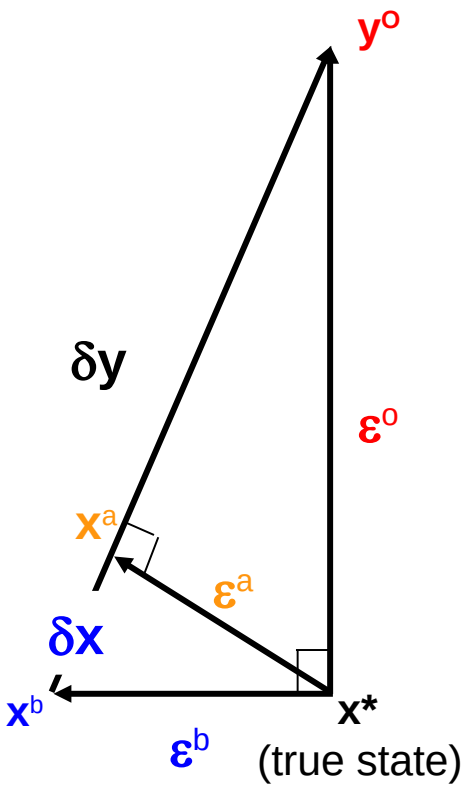
Diagnosis of space-averaged error covariances in observation space

$\delta \mathbf{y} = \mathbf{y}^o - H(\mathbf{x}^b)$ (innovation)

$\mathbf{H}\,\delta\mathbf{x} = H(\mathbf{x}^a) - H(\mathbf{x}^b)$ (increment)

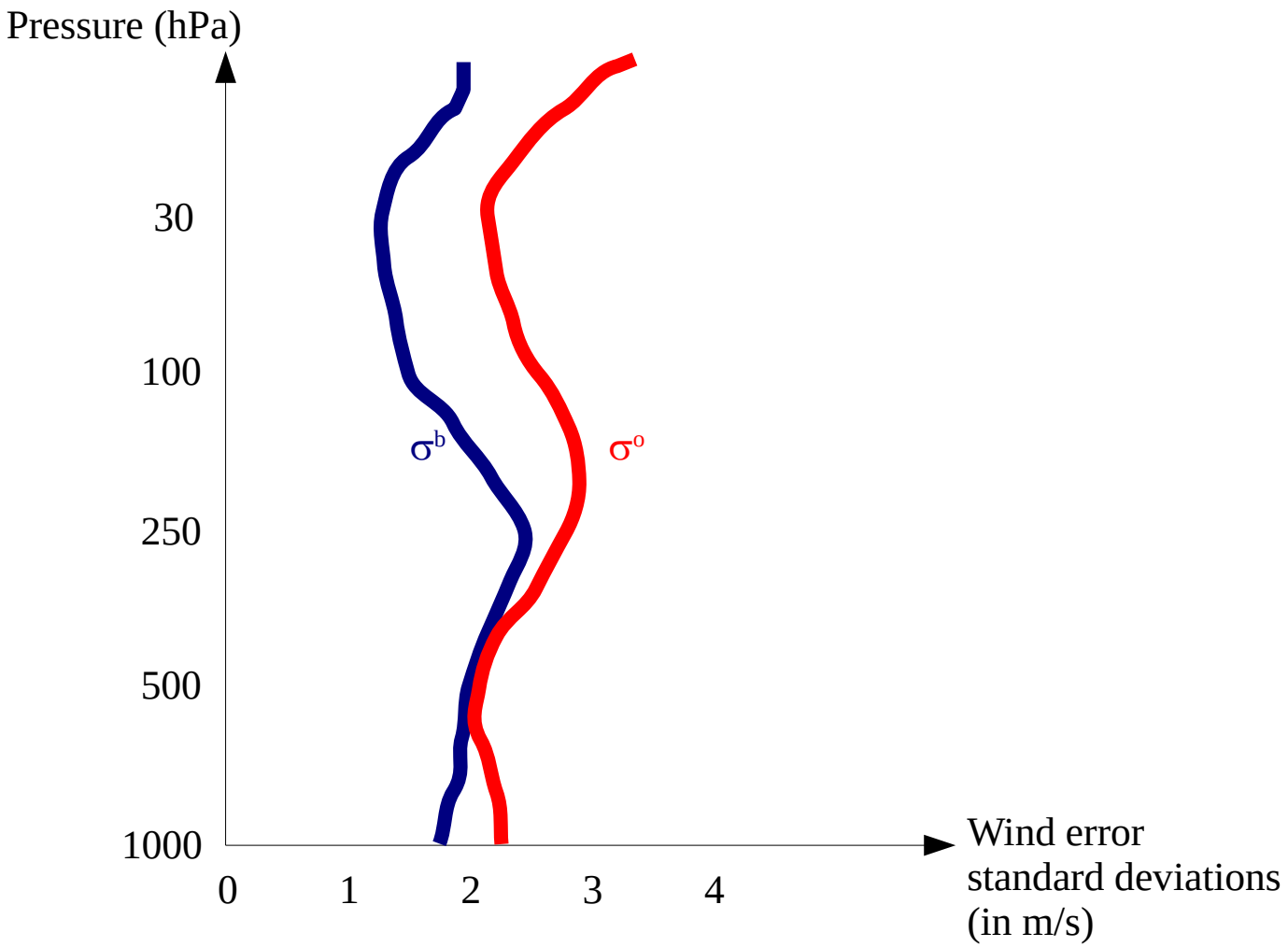
$E[\mathbf{H}\,\delta\mathbf{x}\ \ \delta\mathbf{y}^T] \simeq \mathbf{H}\mathbf{B}\mathbf{H}^T$

$E[(\mathbf{y}^o - H(\mathbf{x}^a))\ \delta\mathbf{y}^T] \simeq \mathbf{R}$



(Desroziers et al 2005)

Vertical profiles of standard deviations of background errors and observation errors



(Desroziers et al 2005)

From innovation-based diagnostics to EDA

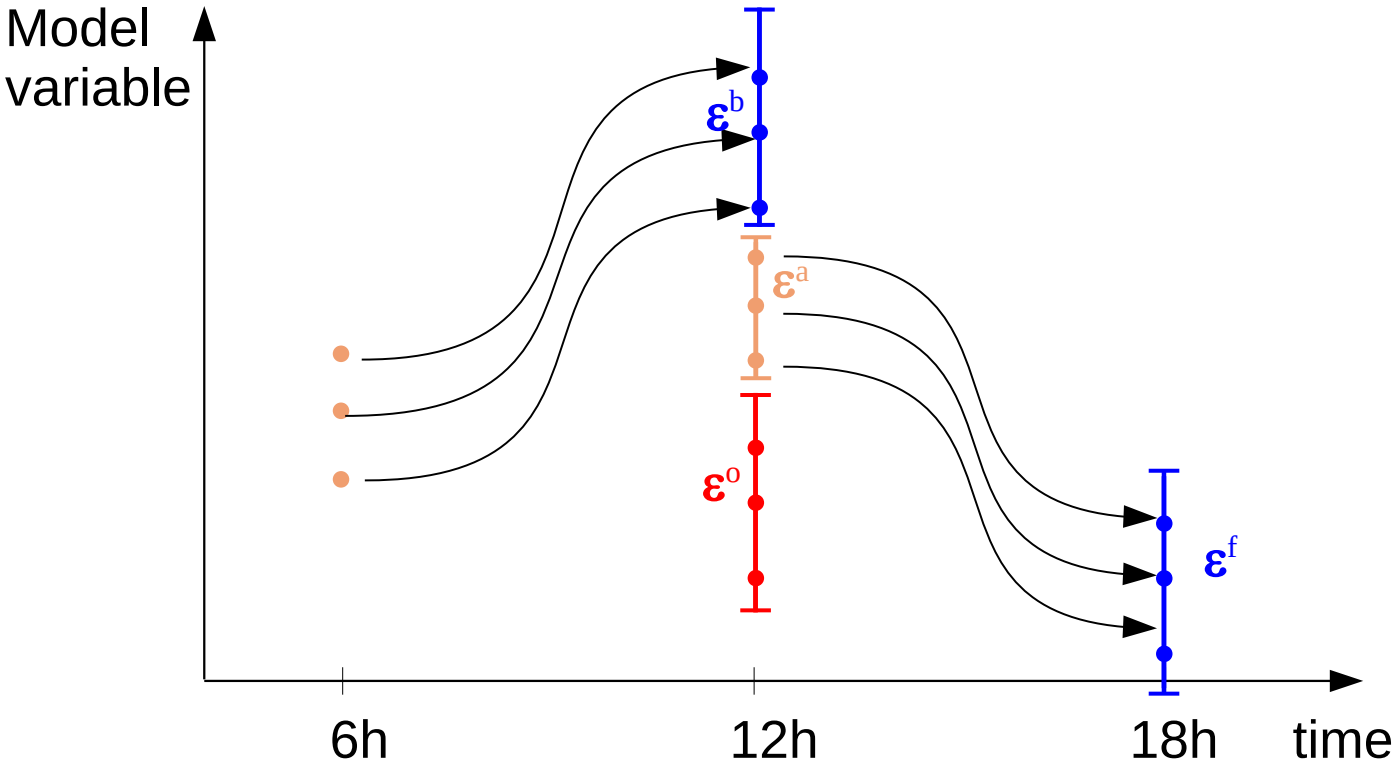
For a given time & location, only 1 realisation (innovation) is available :
use space- and time-averages to estimate mathematical expectations (ergodicity).

=> **Innovation-based diagnostics** to estimate
space- and time-averaged covariances in observation space.

=> **Ensemble** approach (ex: EDA) to estimate
space- and time-dependent covariances in model space.

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Ensemble of Data Assimilations (EDA)

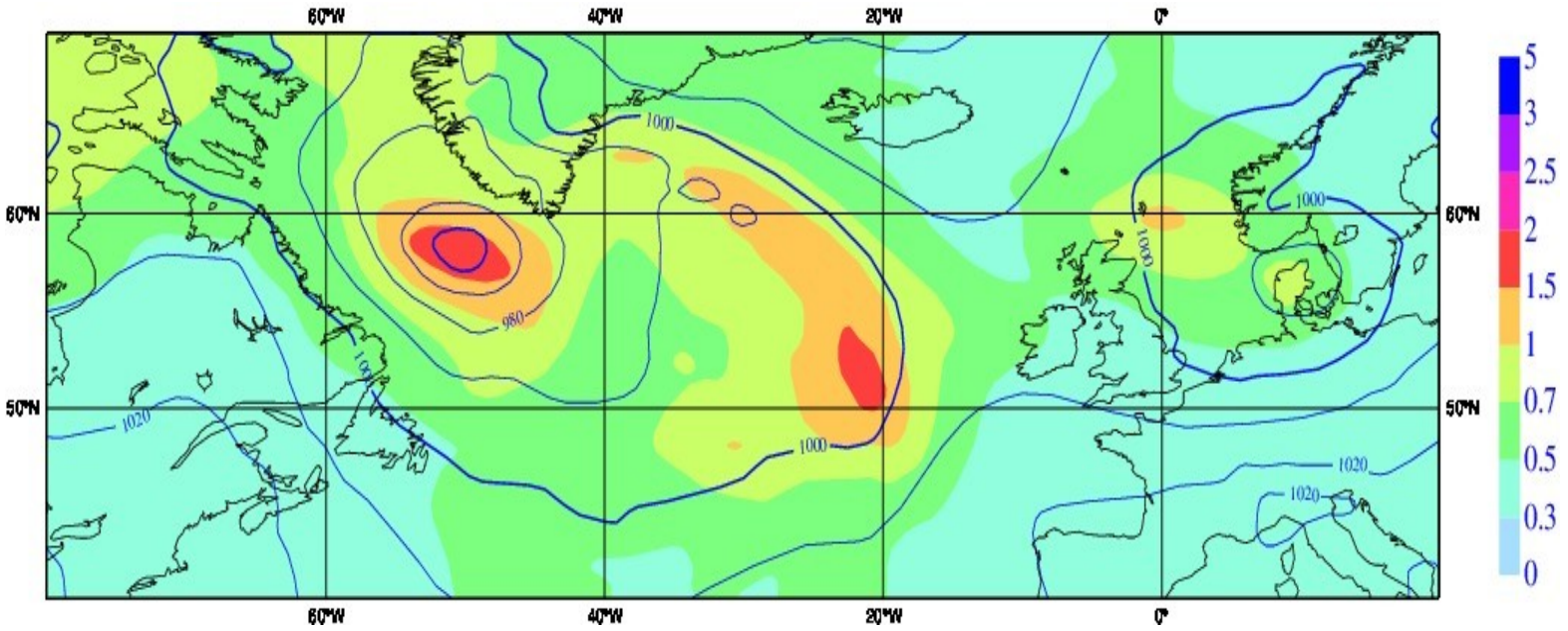


Observation perturbations (random draws of **R**) to simulate observation errors,
model perturbations (ex : SPP) to mimic model errors.

Propagation of perturbations in DA allows error cycling to be simulated.
=> flow-dependent covariances for DA and initial perturbations for EPS.

(e.g. Houtekamer et al 1996, Fisher 2003, Buehner 2005, Berre et al 2006, 2015, Bonavita et al 2012, ...)

Dynamics of background error variances (EDA)

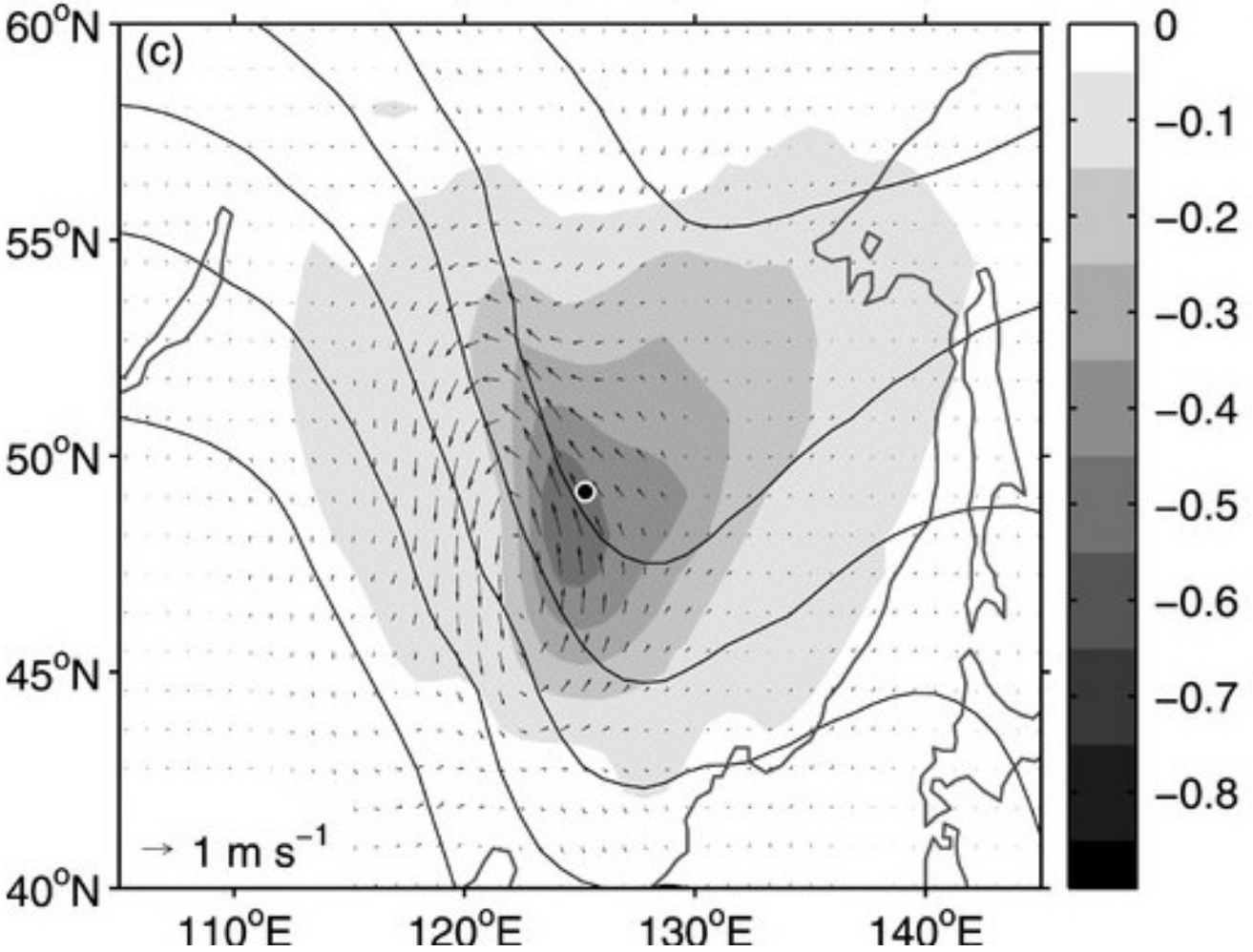


Standard deviations of surface pressure errors (hPa)
(superimposed with MSLP analysis, in hPa).

=> Larger weight given to observations in regions
where the background is particularly uncertain
(intense weather events and/or previous lack of observations)

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Spatial and multivariate spreading of observed information, through B

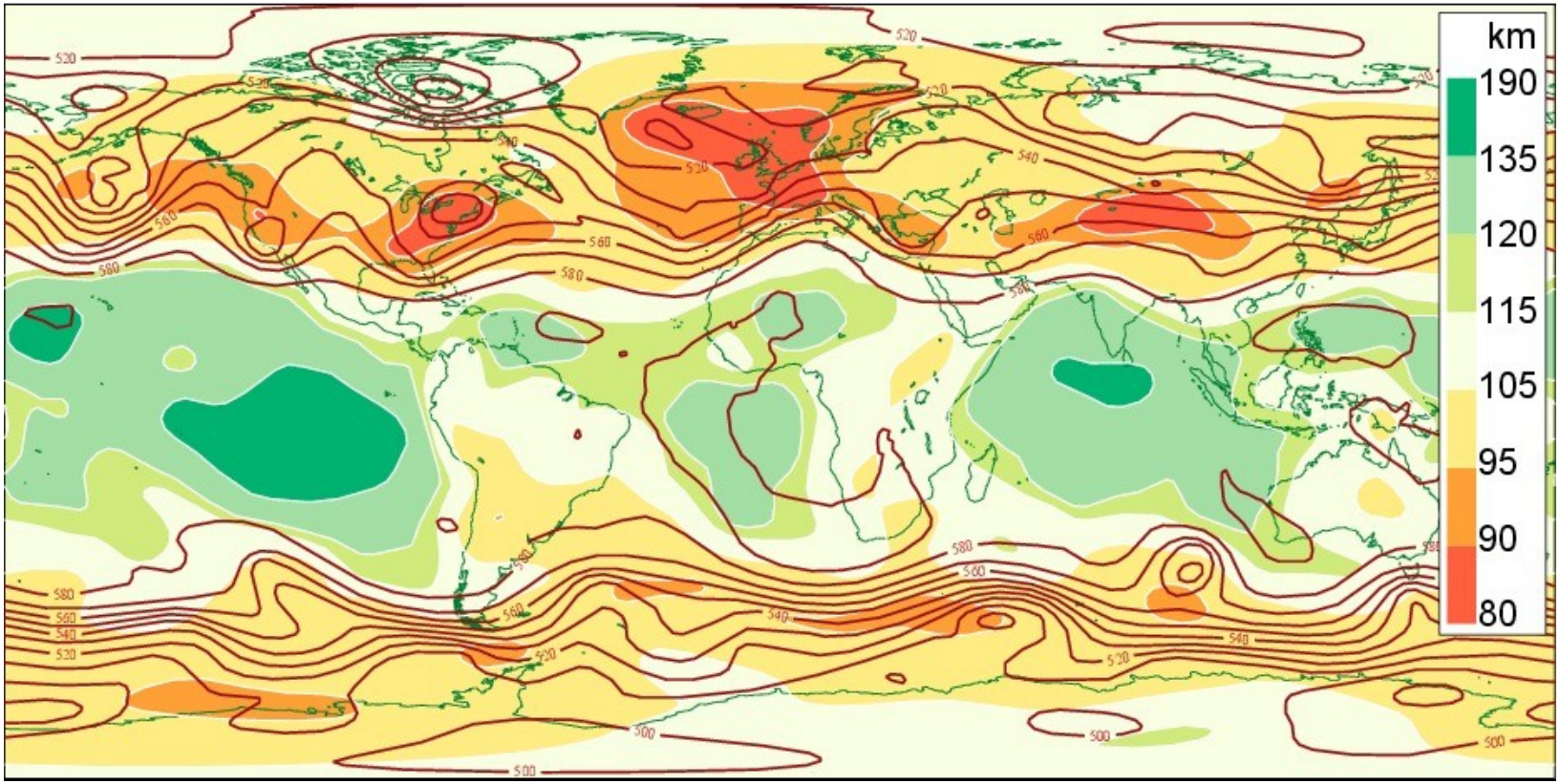


Impact of one temperature observation on temperature and wind analysis

(thermal wind law = geostrophy + hydrostatism)

(Buehner et al 2010)

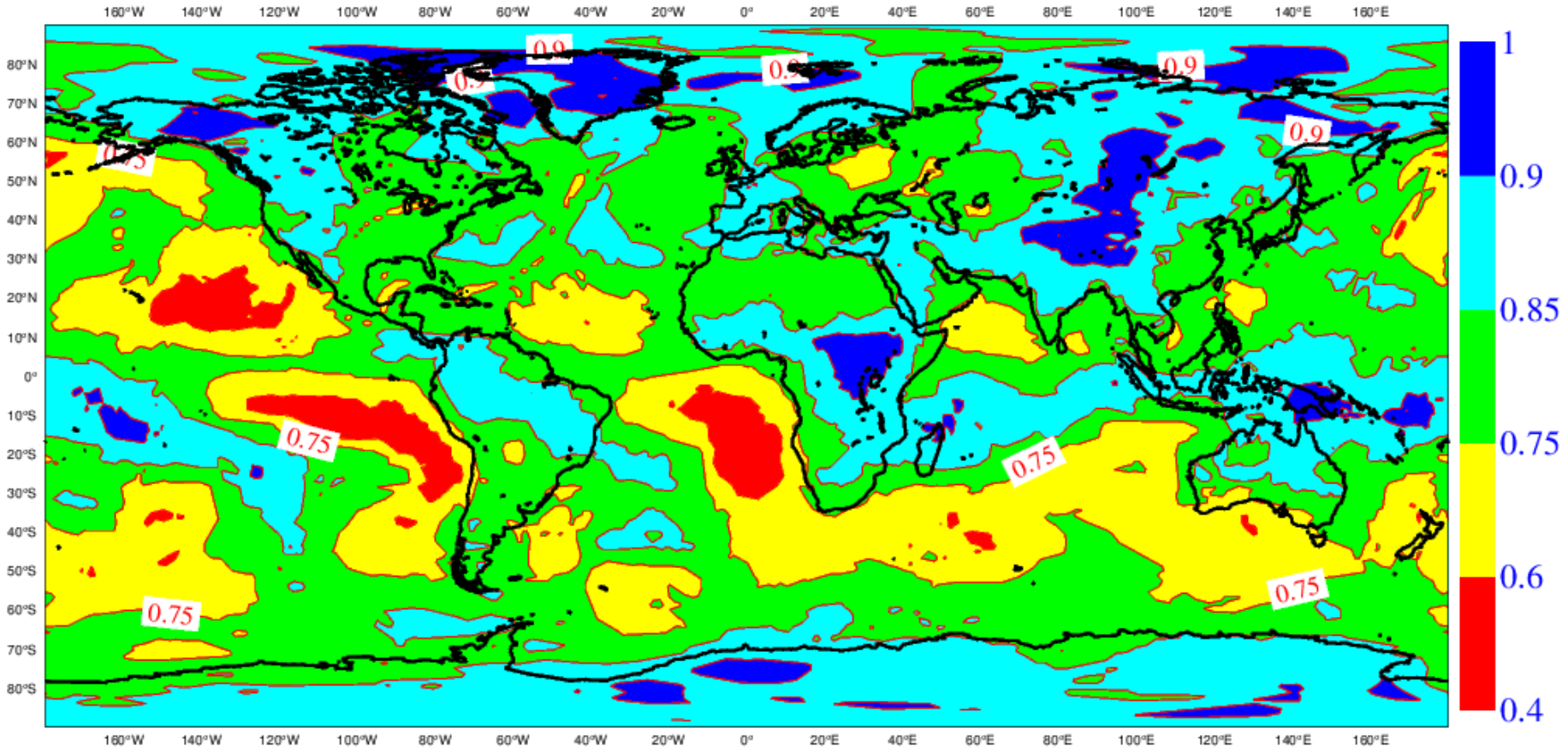
Dynamics of horizontal correlations (EDA)



Horizontal length-scales (in km) of wind errors near 500 hPa,
superimposed with geopotential

=> Observation spreading more local in areas with large spatial gradients.

Dynamics of vertical correlations (EDA)

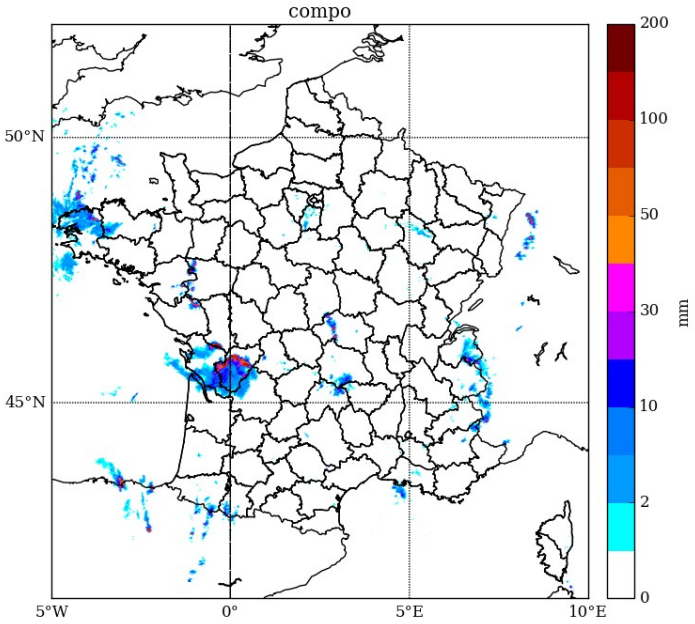


Vertical correlations of temperature errors
between 850 & 870 hPa

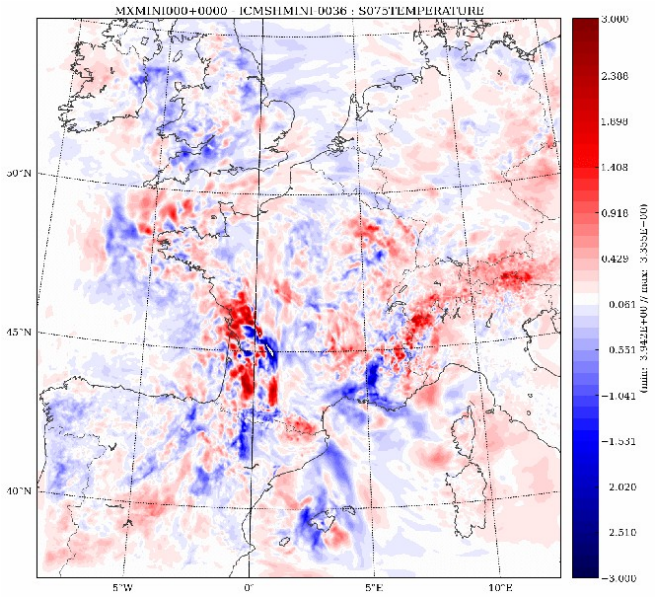
=> Lesser amount of vertical propagation in vertically stable areas.

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4D ensemble covariances at high resolution



« Observed 1h rain rates »
(from radar & rain gauges)



4DEnVar increments
(T, 850 hPa, 3.2 km)
13h30-14h30

4D ensemble covariances in 4DEnVar allow
4D analysis increments to be provided consistently at different times,
in accordance with ongoing processes in such a convective situation at high resolution.

(4DEnVar will be made operational for AROME at Météo-France within the next weeks)

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(P. Brousseau)

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Linearised analysis & forecast error equations

ANALYSIS STEP $$\varepsilon^a \simeq (\mathbf{I} - \mathbf{KH})\varepsilon^b + \mathbf{K}\varepsilon^o$$

=> The analysis dampens background errors (ε^b) & adds dampened new observation errors (ε^o).

FORECAST STEP $$\varepsilon^f \simeq \mathbf{M}\varepsilon^a + \varepsilon^m$$

=> Propagation of « previous » (analysis) errors (ε^a) & addition of « new » model errors (ε^m).

COMBINATION of ANALYSIS & FORECAST STEPS :

$$\varepsilon^f \simeq \mathbf{M}(\mathbf{I} - \mathbf{KH})\varepsilon^b + \mathbf{MK}\varepsilon^o + \varepsilon^m$$

=> Since DA is cycled sequentially,
how does this depend on previous errors in observations & model ?

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Contributions to forecast errors : backward linearised expansion at cycling step t_i

$$\begin{aligned} \boldsymbol{\varepsilon}_i^f &= \mathbf{M}_i \boldsymbol{\varepsilon}_i^a + \boldsymbol{\varepsilon}_i^m \\ &= \mathbf{M}_i(\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\boldsymbol{\varepsilon}_i^b + \mathbf{M}_i\mathbf{K}_i\boldsymbol{\varepsilon}_i^o + \boldsymbol{\varepsilon}_i^m \end{aligned}$$

Contributions to forecast errors : backward linearised expansion at cycling step t_i

$$
\begin{aligned}
\boldsymbol{\varepsilon}_i^f &= \mathbf{M}_i \boldsymbol{\varepsilon}_i^a + \boldsymbol{\varepsilon}_i^m \\
&= \mathbf{M}_i(\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\boldsymbol{\varepsilon}_i^b + \mathbf{M}_i\mathbf{K}_i\boldsymbol{\varepsilon}_i^o + \boldsymbol{\varepsilon}_i^m \\
&= \mathbf{M}_i(\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)[\mathbf{M}_{i-1}(\mathbf{I} - \mathbf{K}_{i-1}\mathbf{H}_{i-1})\boldsymbol{\varepsilon}_{i-1}^b + \mathbf{M}_{i-1}\mathbf{K}_{i-1}\boldsymbol{\varepsilon}_{i-1}^o + \boldsymbol{\varepsilon}_{i-1}^m] + \mathbf{M}_i\mathbf{K}_i\boldsymbol{\varepsilon}_i^o + \boldsymbol{\varepsilon}_i^m
\end{aligned}
$$

Contributions to forecast errors : backward linearised expansion at cycling step t_i

$$
\begin{aligned}
\boldsymbol{\varepsilon}_i^f = & \quad \mathbf{M}_i \boldsymbol{\varepsilon}_i^a & + \boldsymbol{\varepsilon}_i^m \\
= & \quad \mathbf{M}_i(\mathbf{I}-\mathbf{K}_i\mathbf{H}_i)\boldsymbol{\varepsilon}_i^b & + \mathbf{M}_i\mathbf{K}_i\boldsymbol{\varepsilon}_i^o + \boldsymbol{\varepsilon}_i^m \\
= & \; \mathbf{M}_i(\mathbf{I}-\mathbf{K}_i\mathbf{H}_i)[\mathbf{M}_{i-1}(\mathbf{I}-\mathbf{K}_{i-1}\mathbf{H}_{i-1})\boldsymbol{\varepsilon}_{i-1}^b & + \mathbf{M}_{i-1}\mathbf{K}_{i-1}\boldsymbol{\varepsilon}_{i-1}^o + \boldsymbol{\varepsilon}_{i-1}^m] + \mathbf{M}_i\mathbf{K}_i\boldsymbol{\varepsilon}_i^o + \boldsymbol{\varepsilon}_i^m \\
= & \quad \mathbf{T}_2 \; \boldsymbol{\varepsilon}_{i-1}^b & + \sum_{j=i-1}^{i} \mathbf{T}_{i-j}(\mathbf{M}_j\mathbf{K}_j\boldsymbol{\varepsilon}_j^o + \boldsymbol{\varepsilon}_j^m) \\
- &
\end{aligned}
$$

Contributions to forecast errors : backward linearised expansion at cycling step t_i

$$
\begin{aligned}
\boldsymbol{\varepsilon}_i^f &= \mathbf{M}_i \boldsymbol{\varepsilon}_i^a + \boldsymbol{\varepsilon}_i^m \\
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&= \mathbf{M}_i(\mathbf{I}-\mathbf{K}_i\mathbf{H}_i)[\mathbf{M}_{i-1}(\mathbf{I}-\mathbf{K}_{i-1}\mathbf{H}_{i-1})\boldsymbol{\varepsilon}_{i-1}^b + \mathbf{M}_{i-1}\mathbf{K}_{i-1}\boldsymbol{\varepsilon}_{i-1}^o + \boldsymbol{\varepsilon}_{i-1}^m] + \mathbf{M}_i\mathbf{K}_i\boldsymbol{\varepsilon}_i^o + \boldsymbol{\varepsilon}_i^m \\
&= \mathbf{T}_2\ \boldsymbol{\varepsilon}_{i-1}^b + \sum_{j=i-1}^{i} \mathbf{T}_{i-j}(\mathbf{M}_j\mathbf{K}_j\boldsymbol{\varepsilon}_j^o + \boldsymbol{\varepsilon}_j^m) \\
&= \dots \\
&= \mathbf{T}_{i+1}\ \boldsymbol{\varepsilon}_0^b + \sum_{j=0}^{i} \mathbf{T}_{i-j}(\mathbf{M}_j\mathbf{K}_j\boldsymbol{\varepsilon}_j^o + \boldsymbol{\varepsilon}_j^m)
\end{aligned}
$$

where, for $j < i$,

$$\mathbf{T}_{i-j} = \prod_{k=j+1}^{i} \mathbf{M}_k(\mathbf{I}-\mathbf{K}_k\mathbf{H}_k)$$

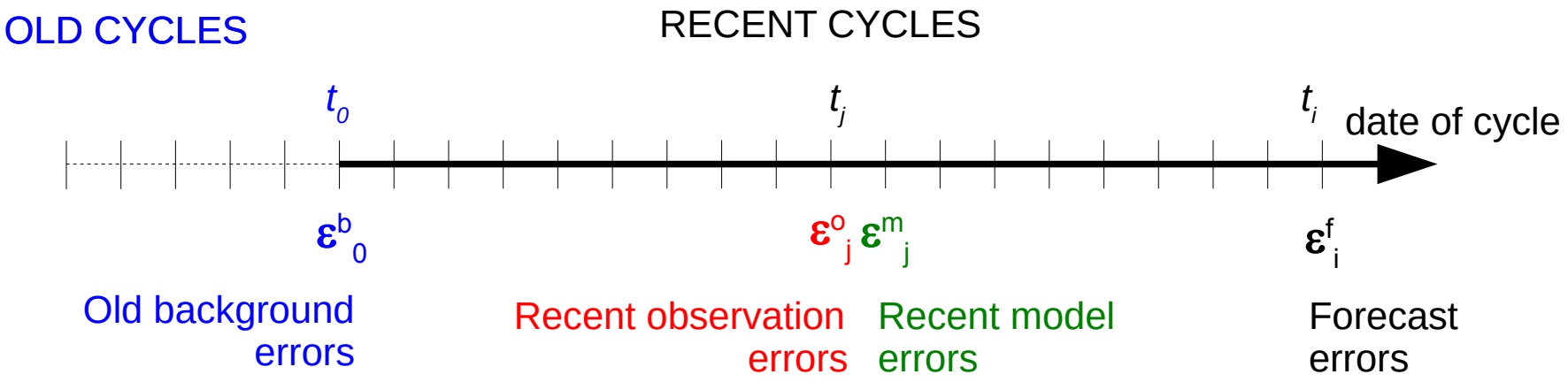
and t_0 is the beginning of the considered cycling period.

(e.g. El Ouaraini and Berre 2011, Berre 2019)

Old and recent error contributions

$$\boldsymbol{\varepsilon}_i^f \simeq \mathbf{T}_{i+1}\ \boldsymbol{\varepsilon}_0^b + \sum_{j=0}^{i} \mathbf{T}_{i-j}(\mathbf{M}_j\mathbf{K}_j\boldsymbol{\varepsilon}_j^o + \boldsymbol{\varepsilon}_j^m)$$

$$\text{with } \mathbf{T}_{i-j} = \prod_{k=j+1}^{i} \mathbf{M}_k(\mathbf{I} - \mathbf{K}_k\mathbf{H}_k) \quad (= \text{cycling operator}).$$



Forecast errors = accumulation, propagation & damping
of old & recent errors.

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Simulation of old and recent error contributions

- Baseline Ensemble DA experiment (**EDA**) : ARPEGE 4D-Var (global NWP), observation perturbations (random draws of **R**) and multiplicative inflation, 6h cycling over 2 weeks ; same $\mathbf{B}_j$ (provided by operational EDA) for all xp's.

- **Simulation of old background errors ε^b_0 :**

  warm start of EDA at t_0 from perturbed $\mathbf{x}^b$'s of the operational EDA,
  + deactivation of observation and model perturbations during next EDA cycles.

- **Accumulation of recent observation errors ε^o_j :**

  cold start of EDA at t_0 from the same $\mathbf{x}^b$ (control run),
  + activation of observation perturbations during next EDA cycles.

- Propagation of states is done **non linearly** (4D-Var + NL model) ; propagation of perturbations is interpreted using linearised formalism.

- Evolution of global variance of error contributions for temperature (500 hPa) from corresponding ensemble variance.

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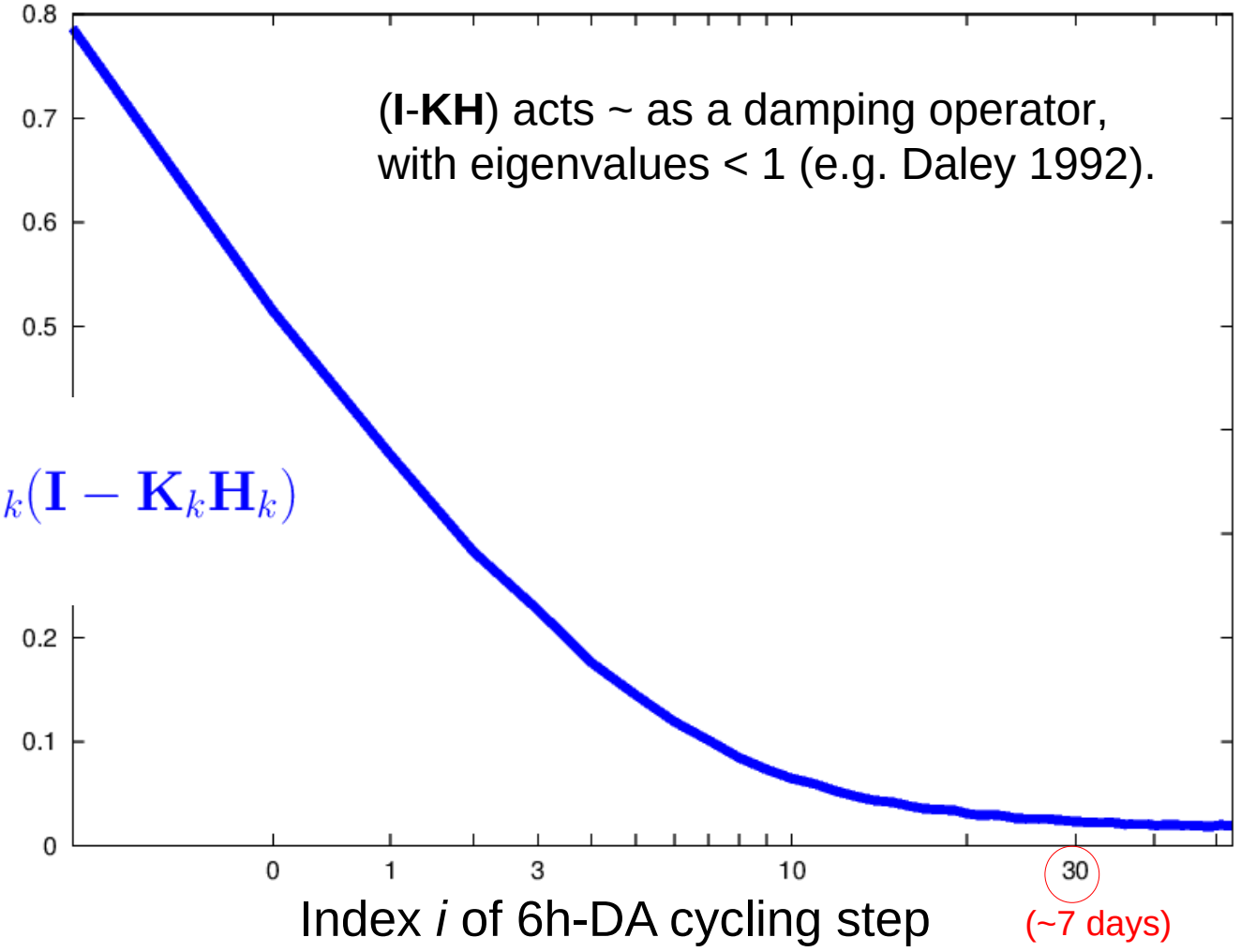
Damping of old background errors

$$\mathrm{Var}(\mathbf{T}_{i+1}\ \boldsymbol{\varepsilon}_0^b)$$

with

$$\mathbf{T}_{i+1} = \prod_{k=0}^{i} \mathbf{M}_k(\mathbf{I} - \mathbf{K}_k\mathbf{H}_k)$$

(**I-KH**) acts ~ as a damping operator,
with eigenvalues < 1 (e.g. Daley 1992).



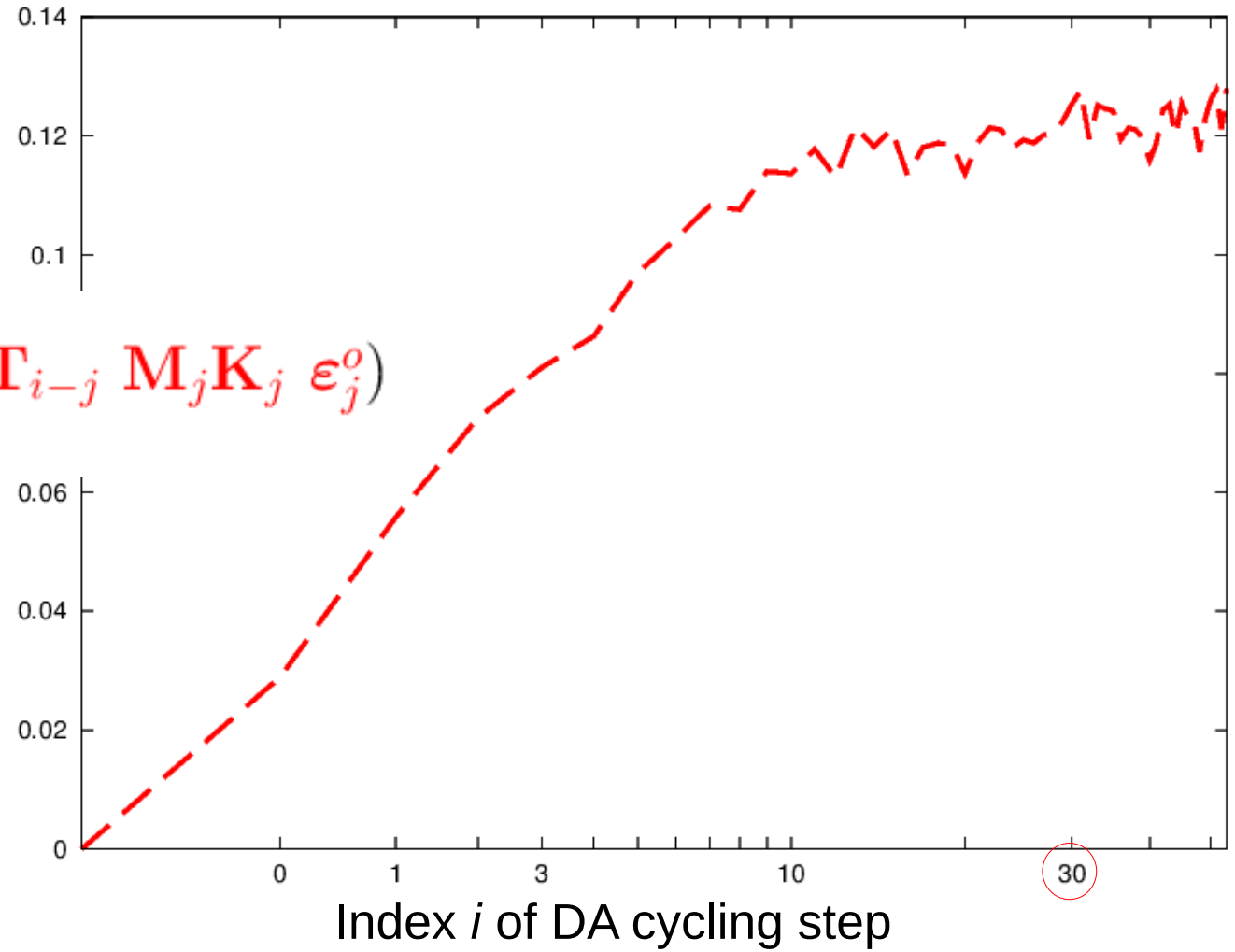
Old background errors are dampened but persist during several days, before vanishing after ~7 days.

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Accumulation of recent observation errors

$$\mathrm{Var}\Big(\sum_{j=0}^{i} \mathbf{T}_{i-j}\,\mathbf{M}_j\mathbf{K}_j\,\boldsymbol{\varepsilon}_j^o\Big)$$

(K²)



Starting from the same $\boldsymbol{x}^b$ *(cold start ensemble), recent observation perturbations are accumulated and dampened by successive DA steps.*

Accumulated error amplitude is stabilised after ~ 7 days.

Why does it stabilise like this ?

Spectral interpretation of the convergence in terms of power series

$$\mathrm{Var}\Big(\sum_{j=0}^{i} \mathbf{T}_{i-j}\,\mathbf{M}_j\mathbf{K}_j\,\boldsymbol{\varepsilon}_j^o\Big)$$

Spectral variance (for a given wave vector $\vec{m}$) :

for homogeneous and static covariances, etc.

$$V[e_{i,\vec{m}}^{f,o_{rct}}] = \sum_{j=0}^{i}(|T_{\vec{m}}|^2)^{i-j}\,V[\tilde{e}_{\vec{m}}^{f,o_j}]$$

$$= V[\tilde{e}_{\vec{m}}^{f,o}]\sum_{j=0}^{i}(|T_{\vec{m}}|^2)^{i-j}$$

Convergence of power series :

(if $|T_m|^2 < 1$)

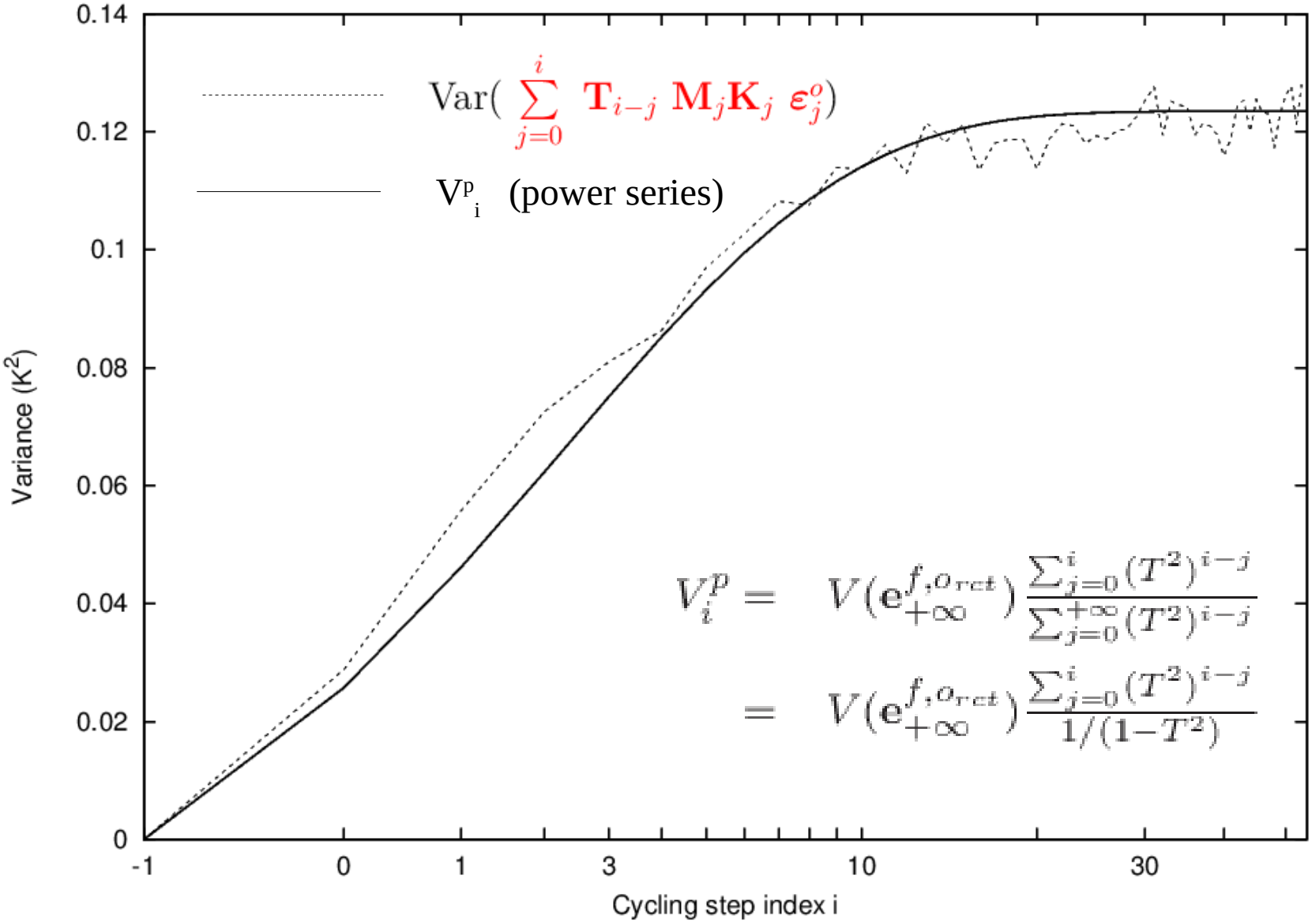
$$\lim_{i\to+\infty}\sum_{j=0}^{i}(|T_{\vec{m}}|^2)^{i-j} = \sum_{j'=0}^{+\infty}(|T_{\vec{m}}|^2)^{j'} = \frac{1}{1-|T_{\vec{m}}|^2}$$

Weighted sum of power series

(with **K'** = **I** – **KH**)

$$V(e_{+\infty}^{f,o_{rct}}) = \sum_{\vec{m}}\frac{|(MK)_{\vec{m}}|^2}{1-|(MK')_{\vec{m}}|^2}V(e_{\vec{m}}^{o})$$

Spectral interpretation of the convergence as a power series



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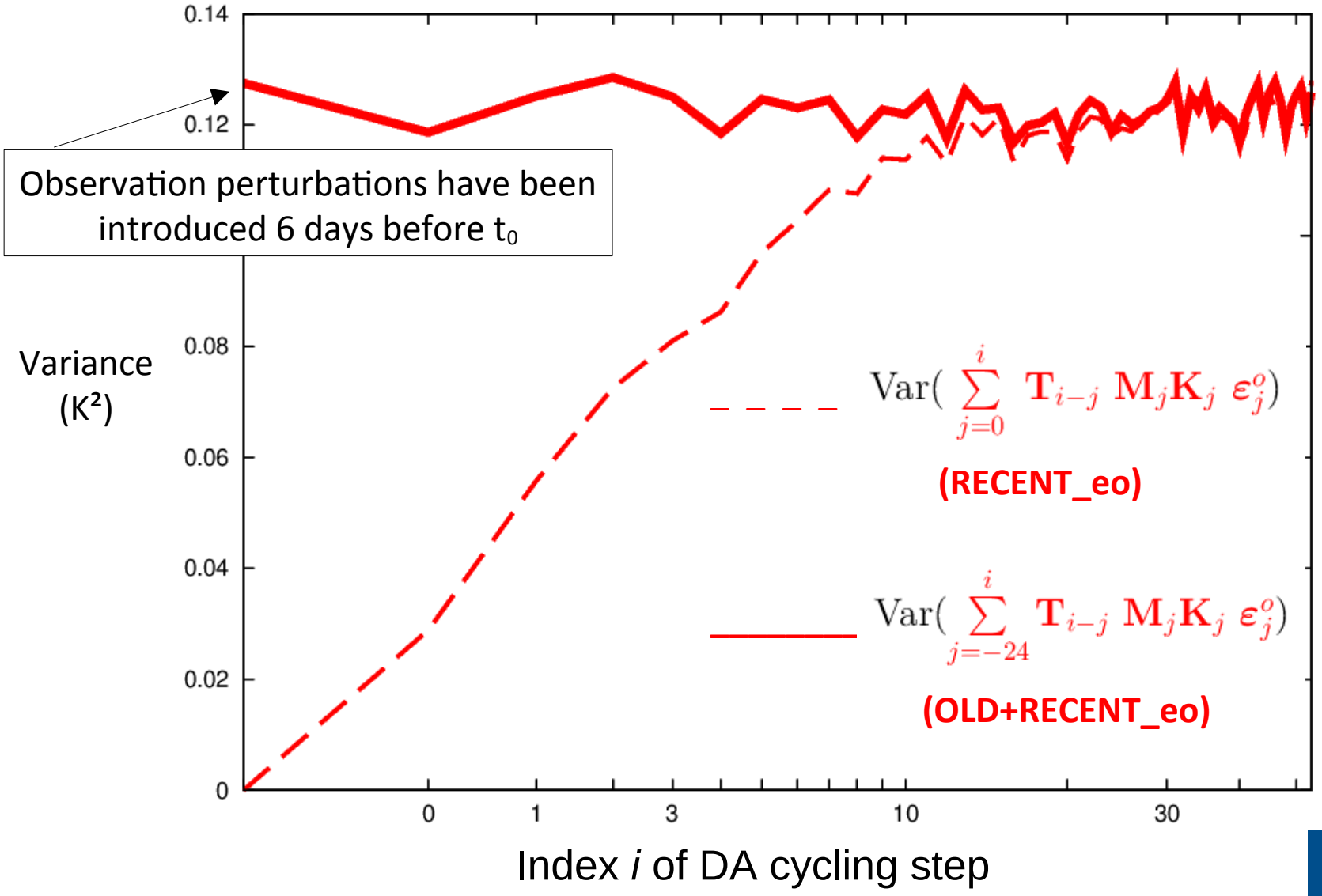
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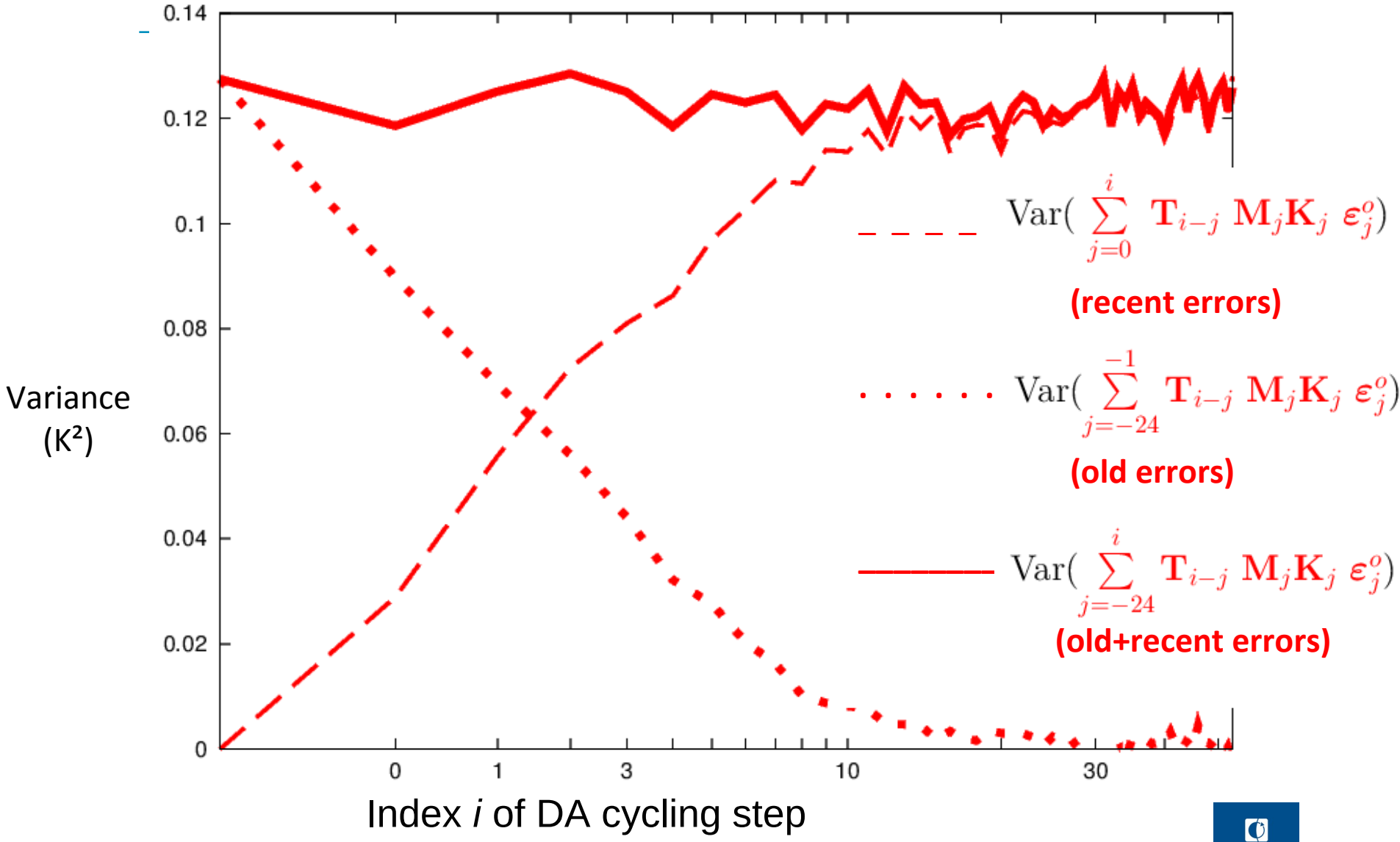
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Accumulation and propagation of old+recent observation errors



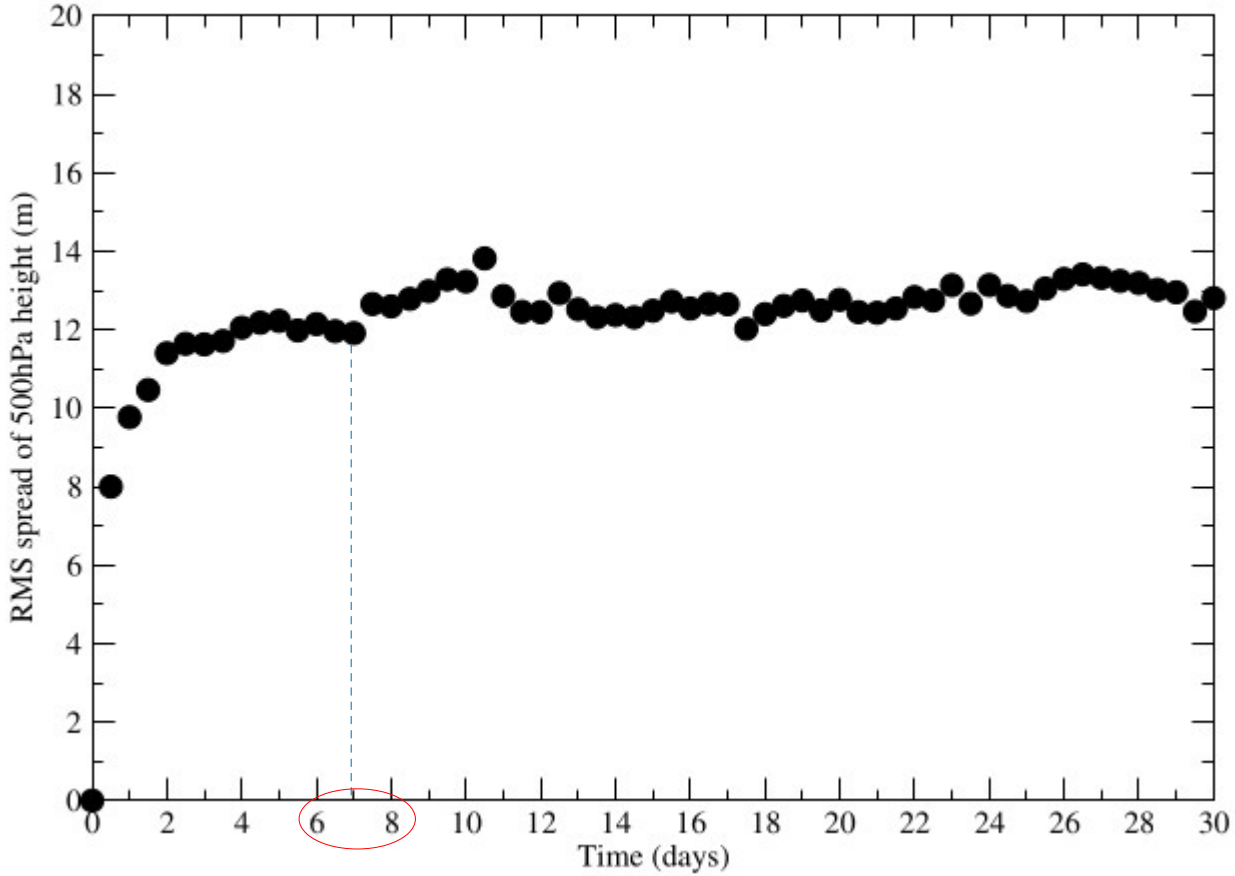
Global error variance (old+recent) is stable.

Evolution of old & recent observation error contributions



Global error variance is stable : accumulation of recent errors is compensated by damping of old errors.

Example of similar results in IFS-EDA



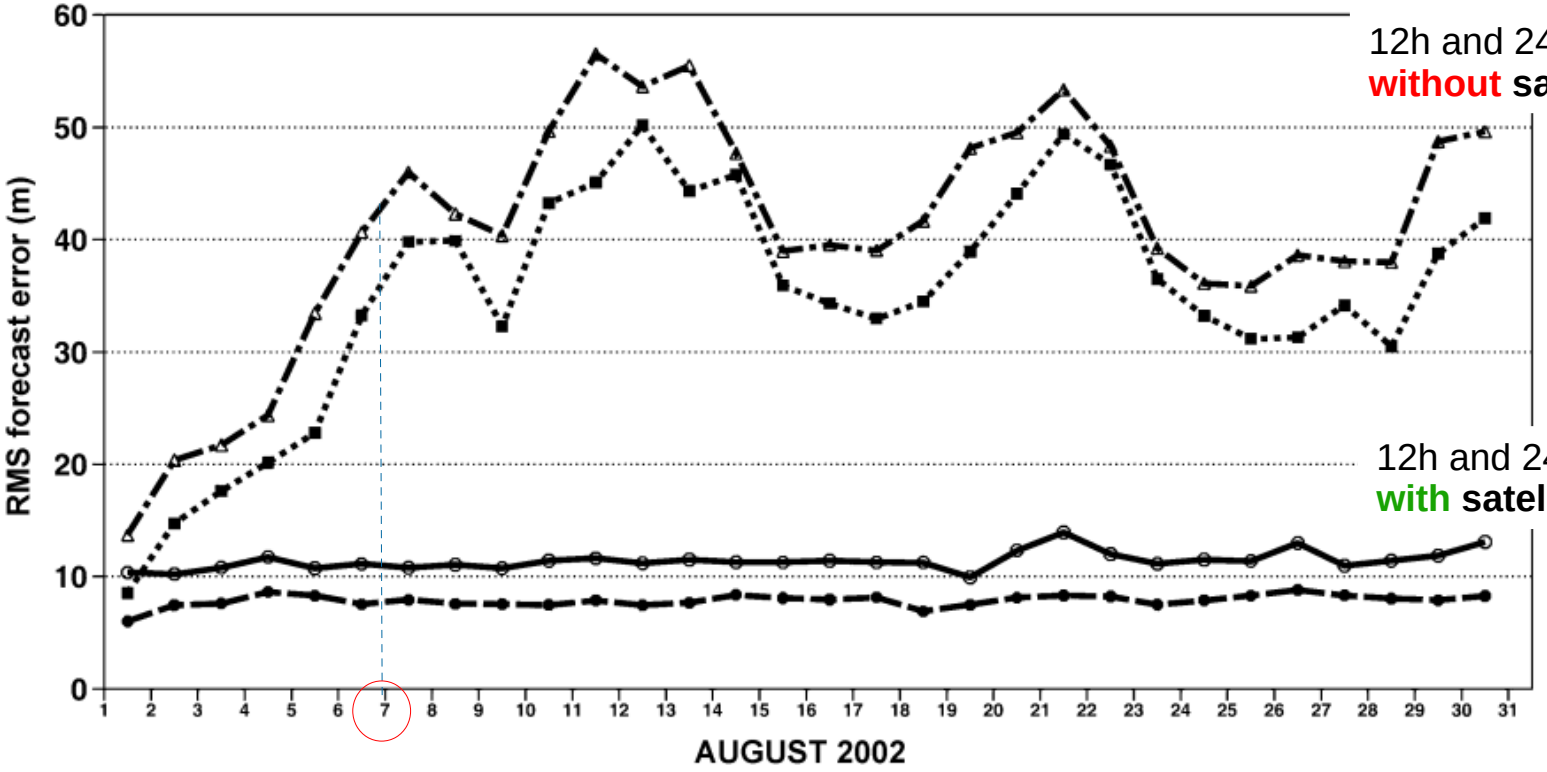
(Fisher 2005)

Starting from the same $\boldsymbol{x}^b$ (cold start), IFS-EDA ensemble spread increases and stabilises within a similar 7-day period.

Similar results also e.g. at ECCC in Houtekamer et al (1996).

=> Somewhat « universal » results for global NWP ?

Example of related results in IFS-DA (no EDA results here)



Withdraw of satellite data in IFS-DA leads to increased errors = lesser damping of model & obs errors in DA cycling, which stabilizes after ~7 days of cycling.

(Fisher 2005)

Building & propagation of information in cycled DA

Similar equations may be derived for model states,
e.g. for state anomalies $\mathbf{x}' = \mathbf{x} - \mathbf{x}^c$ and observed anomalies $\mathbf{y}'^o = \mathbf{y}^o - H[\mathbf{x}^c]$
i.e. deviations from a fixed climatologic state $\mathbf{x}^c$:

$$\boldsymbol{x}_i'^f \simeq \mathbf{T}_{i+1}\, \boldsymbol{x}_0'^b + \sum_{j=0}^{i} \mathbf{T}_{i-j}\, \mathbf{M}_j \mathbf{K}_j\, \boldsymbol{y}_j'^o + \sum_{j=0}^{i} \mathbf{T}_{i-j}\, (\mathcal{M}_j[\boldsymbol{x}^c] - \boldsymbol{x}^c)$$

=> Analysis & forecast states typically built from several days of observed information, propagated by **K** and **M** to « fill the gaps » of $\mathbf{y}^o$ (spatial locations and model variables) ?

with likely variations for different geographical regions, model variables, spatial scales, etc. ?

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Diagnosis of recent model error contributions

Contributions to forecast error variance :

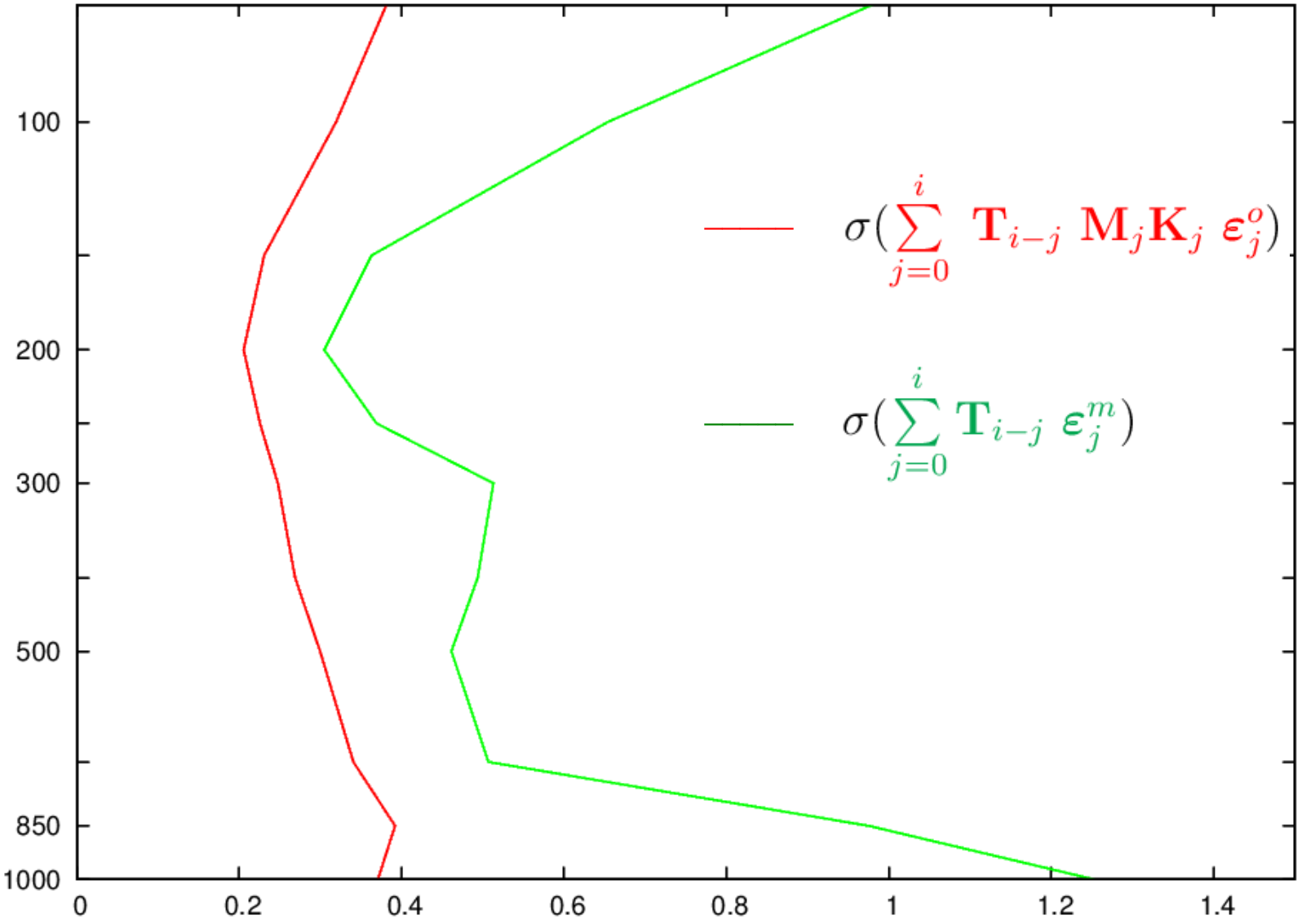
$$\mathrm{Var}(\boldsymbol{\varepsilon}_i^f) \simeq \mathrm{Var}(\sum_{j=0}^{i} \mathbf{T}_{i-j}\ \mathbf{M}_j\mathbf{K}_j\ \boldsymbol{\varepsilon}_j^o) + \mathrm{Var}(\sum_{j=0}^{i} \mathbf{T}_{i-j}\ \boldsymbol{\varepsilon}_j^m)$$

which leads to the following estimation approach

- $\mathrm{Var}(\boldsymbol{\varepsilon}_i^f)$ estimated by innovation-based diagnostics (e.g. Desroziers et al 2005);
- $\mathrm{Var}(\sum_{j=0}^{i} \mathbf{T}_{i-j}\ \mathbf{M}_j\mathbf{K}_j\ \boldsymbol{\varepsilon}_j^o)$ estimated by EDA with observation perturbations only ;
- $\mathrm{Var}(\sum_{j=0}^{i} \mathbf{T}_{i-j}\ \boldsymbol{\varepsilon}_j^m) \simeq \mathrm{Var}(\boldsymbol{\varepsilon}_i^f) - \mathrm{Var}(\sum_{j=0}^{i} \mathbf{T}_{i-j}\ \mathbf{M}_j\mathbf{K}_j\ \boldsymbol{\varepsilon}_j^o)$

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Diagnosis of model error contributions versus observation error contributions

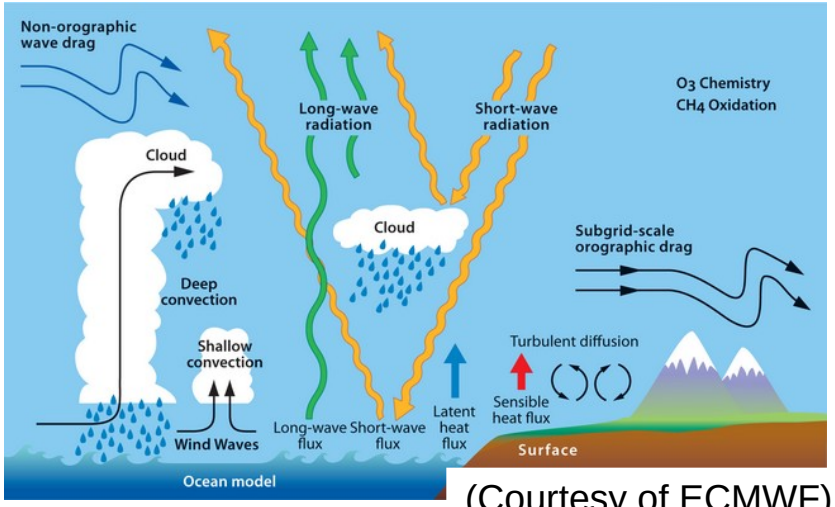


Height (hPa)

Standard deviations of error contributions (K)

(Berre 2019)

Simulation of model error contributions



(Courtesy of ECMWF)

- **Neglect of model errors in EDA leads to an underestimation of errors by a factor 2,** underlining the importance of model errors in cycled DA! (e.g. Houtekamer et al 2009, Berre 2019)

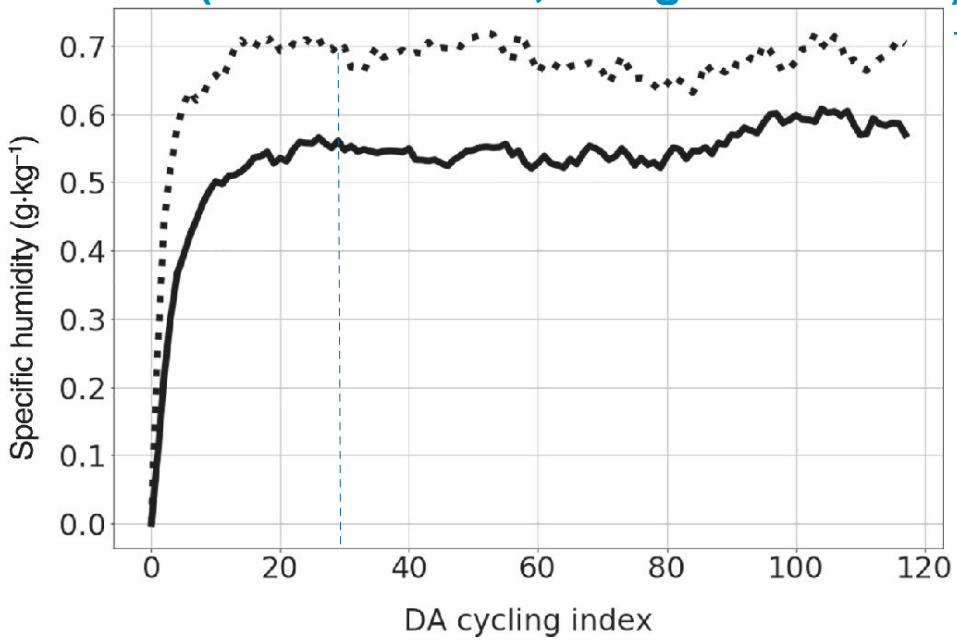
- **Model errors can be simulated in different ways in EDA**, e.g. :
  - multi-model approach (e.g. Houtekamer et al 1996, 2009, Hubans et al 2022) ;
  - stochastic perturbation of physical tendencies (SPPT, e.g. Buizza et al 1999) ;
  - stochastic perturbations of model parameters (SPP, e.g. Ollinaho et al 2017).

- The **accumulation of model errors** can be simulated and diagnosed in EDA, in a similar way as for observation errors.

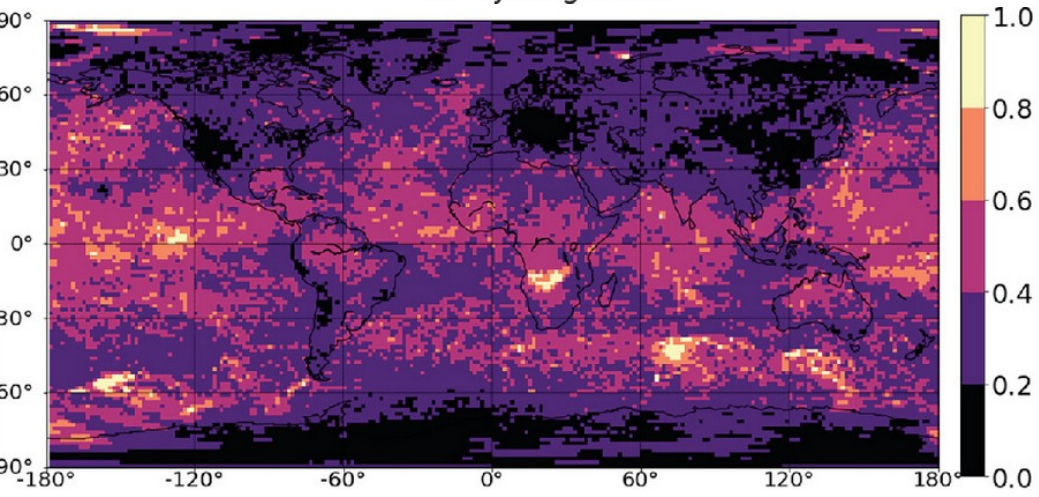
- **Comparison with innovation-based estimates** suggests that simulation of model errors remains a significant challenge.

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Spread effect of differences between 2 parametrisations of deep convection (Tiedtke = TDK, Bougeault = BGT)



Standard deviations of
cycled simulated obs errors (---------) &
cycled simulated model errors (▬▬▬ , TDK-BGT)
both converge within ~7 days
(~ 28 DA cycling steps).

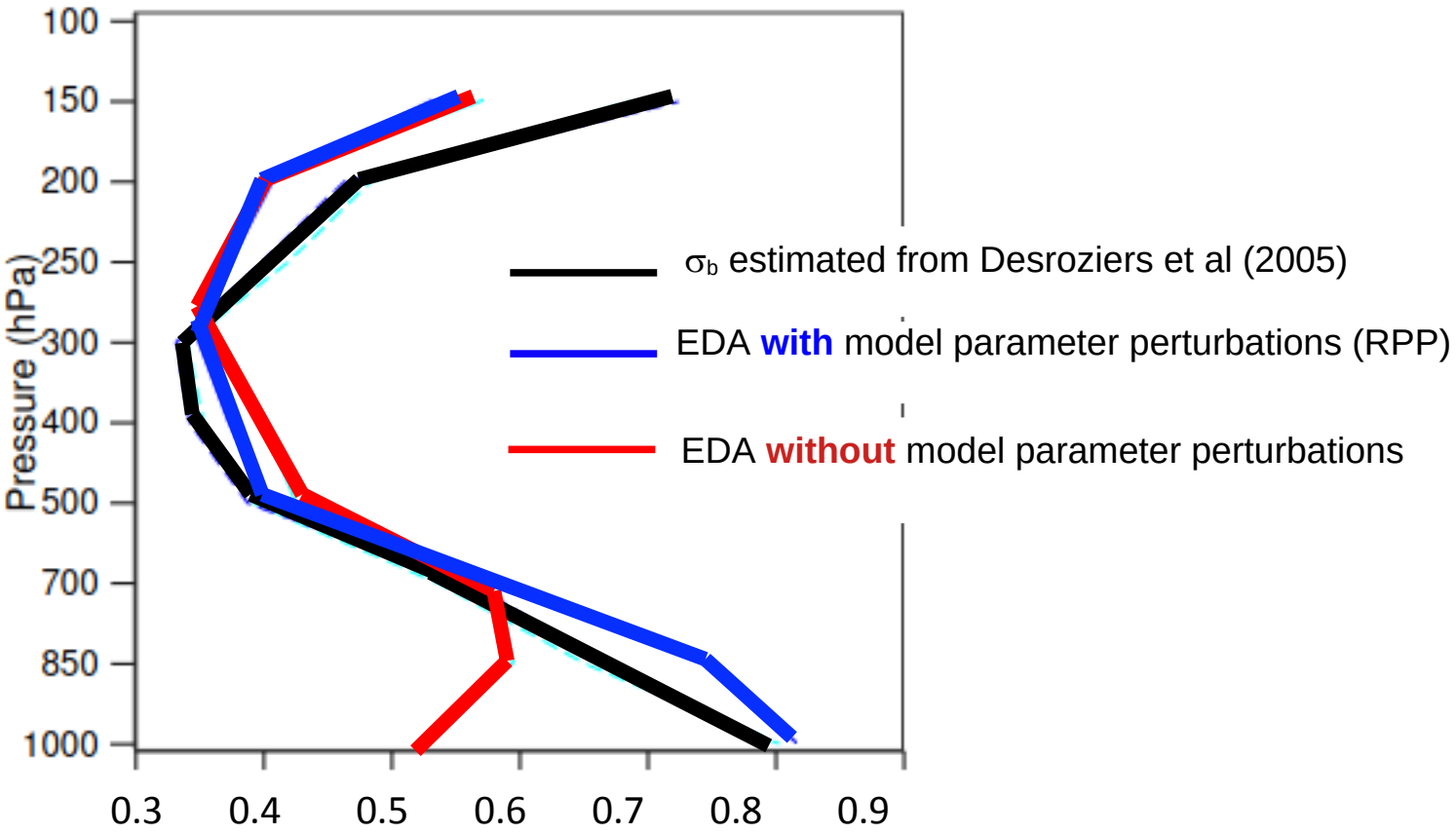


Cycled simulated model errors (TDK-BGT) increase analysis spread in convective areas, especially where observation density is low.

Analysis spread from cycled TDK-BGT differences

(Hubans et al, 2022)

Impact of Random Parameters (RPP) on EDA (model perturbations)



Estimates of ***background error standard deviations***
in observation space (AIREP)
(temperature, in K)

With model parameter perturbations,
EDA spread is more realistic in the Boundary Layer

(N. Girardot)

Conclusions & perspectives

- **Innovation-based diagnostics** for space-averaged covariance estimates,
  ensemble approaches (**EDA**) for flow-dependent 3D/4D covariances.

- Linearised **expansion of contributions** to gain more insight
  on the accumulation and damping of old & recent error contributions in cycled DA, and maybe also

  about how information is built in DA cycling from several days of observations typically,
  through propagation by gain matrix & model.

- **EDA** is a powerful method to **simulate error contributions** in DA cycling,
  arising from observations, model and background.

- **Estimation of observation and model error covariances** remains a significant challenge,
  especially for model errors.

- Combination of **model expertise, ensemble methods and innovation-based diagnostics**
  is crucial in order to reach further progress.

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Thanks for listening