

The Ensemble of Data Assimilations

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Outline

- KF, EKF, Reduced-rank KF, EnKF
- Hybrid methods
- The Ensemble of Data Assimilations (EDA) method
- Applications of the EDA

The EDA method

For a linear system the data assimilation update is:

$$\begin{aligned}\mathbf{x}_a^k &= \mathbf{x}_b^k + \mathbf{K}_k (\mathbf{y}^k - \mathbf{H}_k \mathbf{x}_b^k) \\ \mathbf{x}_b^{k+1} &= \mathbf{M}_k \mathbf{x}_a^k\end{aligned}$$

Under the assumptions of statistically independent background (\mathbf{P}^b), observation (\mathbf{R}) and model errors (\mathbf{Q}), the evolution of the system error covariances is given by:

$$\begin{aligned}\mathbf{P}_k^a &= (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_k^b (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)^T + \mathbf{K}_k \mathbf{R}_k \mathbf{K}_k^T \\ \mathbf{P}_{k+1}^b &= \mathbf{M}_k \mathbf{P}_k^a \mathbf{M}_k^T + \mathbf{Q}_k\end{aligned}$$

The EDA method

Consider now the evolution of the same system where we perturb the observations and the forecast model with random noise drawn from the respective error covariances:

$$\begin{aligned}\tilde{\mathbf{x}}_a^k &= \tilde{\mathbf{x}}_b^k + \mathbf{K}_k \left(\mathbf{y}^k + \boldsymbol{\eta}_k - \mathbf{H}_k \tilde{\mathbf{x}}_b^k \right) \\ \tilde{\mathbf{x}}_b^{k+1} &= \mathbf{M}_k \tilde{\mathbf{x}}_a^k + \boldsymbol{\zeta}_k\end{aligned}$$

where $\boldsymbol{\eta}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$, $\boldsymbol{\zeta}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{Q})$.

If we define the **differences between the perturbed and unperturbed state** $\boldsymbol{\varepsilon}_a \equiv \tilde{\mathbf{x}}_a - \mathbf{x}_a$ and $\boldsymbol{\varepsilon}_b \equiv \tilde{\mathbf{x}}_b - \mathbf{x}_b$, their evolution is obtained by subtracting the unperturbed state evolution equations from the perturbed ones:

$$\begin{aligned}\boldsymbol{\varepsilon}_a^k &= \boldsymbol{\varepsilon}_b^k + \mathbf{K}_k \left(\boldsymbol{\eta}_k - \mathbf{H}_k \boldsymbol{\varepsilon}_b^k \right) \\ \boldsymbol{\varepsilon}_b^{k+1} &= \mathbf{M}_k \boldsymbol{\varepsilon}_a^k + \boldsymbol{\zeta}_k\end{aligned}$$

The EDA method

$$\boldsymbol{\varepsilon}_a^k = \boldsymbol{\varepsilon}_b^k + \mathbf{K}_k (\boldsymbol{\eta}_k - \mathbf{H}_k \boldsymbol{\varepsilon}_b^k)$$

$$\boldsymbol{\varepsilon}_b^{k+1} = \mathbf{M}_k \boldsymbol{\varepsilon}_a^k + \boldsymbol{\zeta}_k$$

- i.e., the perturbations evolve with the same update equations of the state (Kalman gain and model operator).

What about the **errors**?

If we take the statistical expectation of the outer product of the perturbations:

$$\left\langle \boldsymbol{\varepsilon}_k^a (\boldsymbol{\varepsilon}_k^a)^T \right\rangle = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \left\langle \boldsymbol{\varepsilon}_k^b (\boldsymbol{\varepsilon}_k^b)^T \right\rangle (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)^T + \mathbf{K}_k \mathbf{R}_k \mathbf{K}_k^T$$

$$\left\langle \boldsymbol{\varepsilon}_{k+1}^b (\boldsymbol{\varepsilon}_{k+1}^b)^T \right\rangle = \mathbf{M}_k \left\langle \boldsymbol{\varepsilon}_k^a (\boldsymbol{\varepsilon}_k^a)^T \right\rangle \mathbf{M}_k^T + \mathbf{Q}_k$$

The EDA method

$$\left\langle \boldsymbol{\varepsilon}_k^a (\boldsymbol{\varepsilon}_k^a)^T \right\rangle = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \left\langle \boldsymbol{\varepsilon}_k^b (\boldsymbol{\varepsilon}_k^b)^T \right\rangle (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)^T + \mathbf{K}_k \mathbf{R}_k \mathbf{K}_k^T$$

$$\left\langle \boldsymbol{\varepsilon}_{k+1}^b (\boldsymbol{\varepsilon}_{k+1}^b)^T \right\rangle = \mathbf{M}_k \left\langle \boldsymbol{\varepsilon}_k^a (\boldsymbol{\varepsilon}_k^a)^T \right\rangle \mathbf{M}_k^T + \mathbf{Q}_k$$

- These are the same equations for the evolution of the system error covariances:

$$\mathbf{P}_k^a = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_k^b (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k)^T + \mathbf{K}_k \mathbf{R}_k \mathbf{K}_k^T$$

$$\mathbf{P}_{k+1}^b = \mathbf{M}_k \mathbf{P}_k^a \mathbf{M}_k^T + \mathbf{Q}_k$$

provided that:

1. The applied perturbations $\boldsymbol{\eta}_k, \boldsymbol{\zeta}_k$ have the right covariances (\mathbf{R}, \mathbf{Q}) ;
2. At some stage in time $\left\langle \boldsymbol{\varepsilon}_k^b (\boldsymbol{\varepsilon}_k^b)^T \right\rangle = \mathbf{P}_k^b$

The EDA method

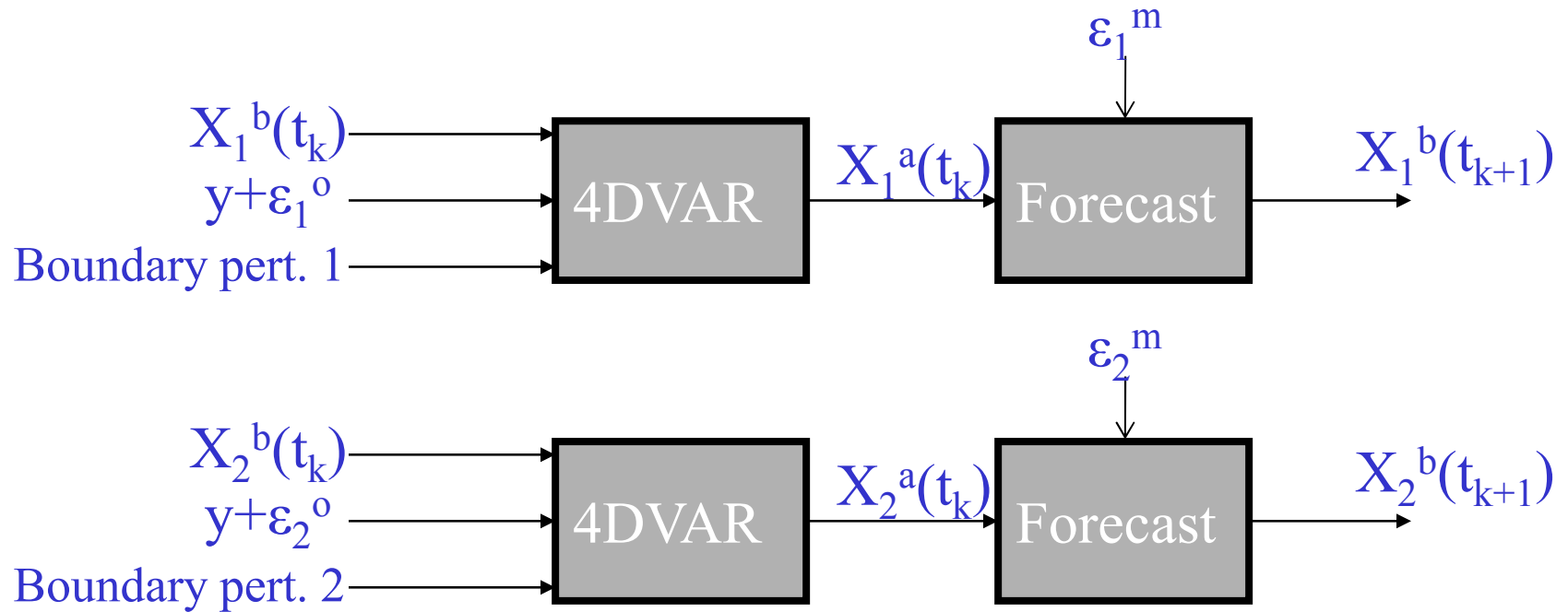
What does all this mean in practice?

- We can use an ensemble of perturbed assimilation cycles to simulate the errors of our reference assimilation cycle;
- The ensemble of perturbed DAs should be as similar as possible to the reference DA (i.e., same or similar \mathbf{K} matrix)
- The applied perturbations $\boldsymbol{\eta}_k, \boldsymbol{\zeta}_k$ must have the required error covariances (\mathbf{R}, \mathbf{Q});
- There is no need to explicitly perturb the background \mathbf{x}_b

The EDA method

- **25** ensemble members using 4D-Var assimilations at reduced resolution
- **T399** outer loop, **T95/T159** inner loops. (Reference DA: **T1279** outer loop, **T159/T255/T255** inner loops)
- Observations randomly perturbed according to their estimated errors
- SST perturbed with climatological error structures
- Model error represented by stochastic methods (**SPPT**, Leutbecher, 2009)

The EDA method

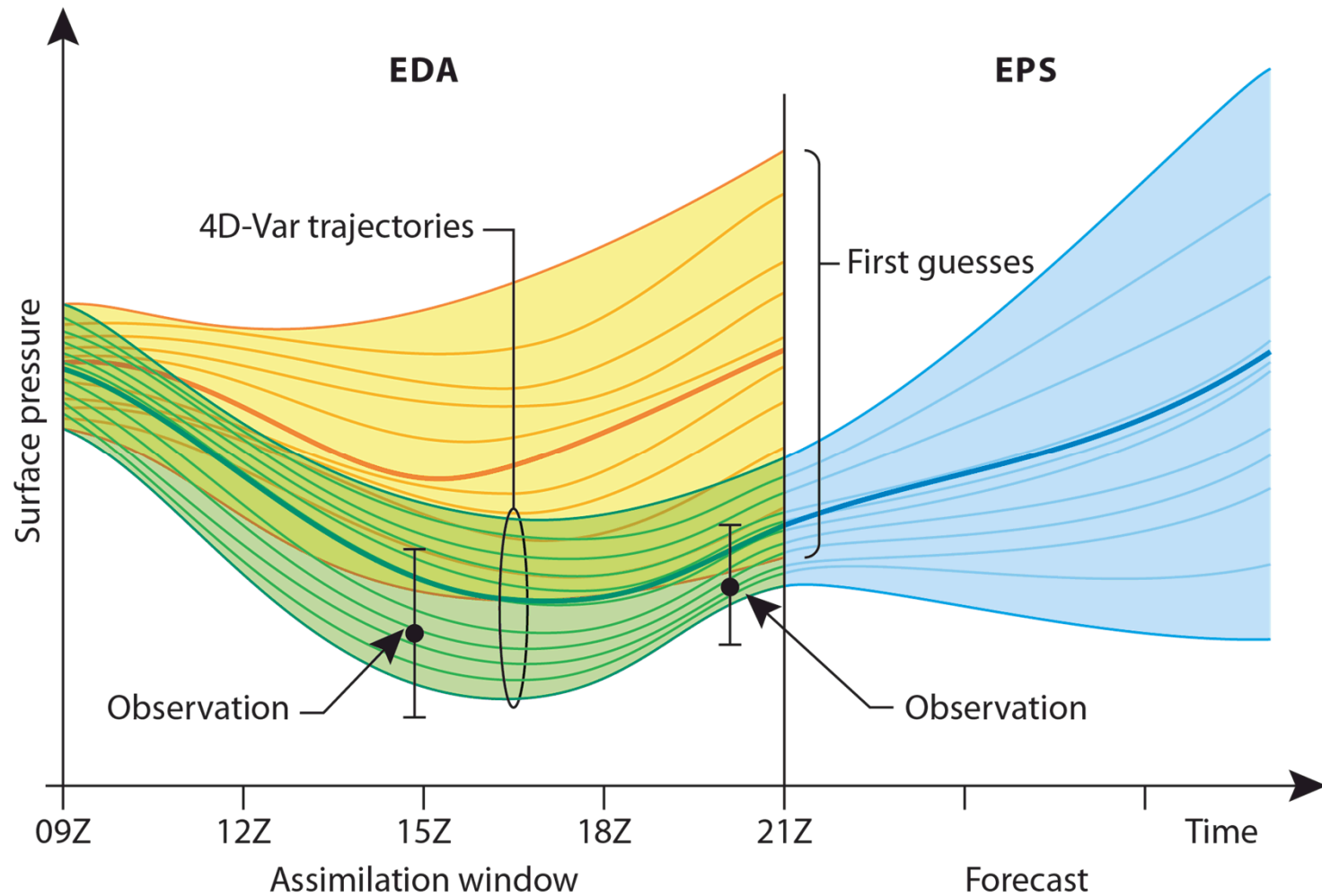


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Applications of the EDA

- The EDA simulates **the error evolution** of the 4DVar analysis cycle. As such it has two main applications:
 1. Provide a **flow-dependent estimate of analysis errors** to initialize the ensemble prediction system (EPS)
 2. Provide a **flow-dependent estimate of background errors** for use in 4D-Var assimilation

Applications of the EDA



Applications of the EDA

- **Note that the EDA impacts the EPS in two distinct ways:**
 1. **Directly**, by providing a **flow-dependent estimate of the initial perturbations** of the ensemble prediction system (EPS)
 2. **Indirectly**, through the provision of a **flow-dependent estimate of background errors** for use in the 4D-Var deterministic (HRES) assimilation cycle: **this improves the deterministic analysis around which the EPS initial perturbations are re-centered**

Applications of the EDA

1. **Directly**, by providing a **flow-dependent estimate of the initial perturbations** of the ensemble prediction system (EPS)
2. **Indirectly**, through the provision of a **flow-dependent estimate of background errors** for use in the 4D-Var deterministic (HRES) assimilation cycle: **this improves the deterministic analysis around which the EPS initial perturbations are re-centered**

The second effect is arguably the more important:

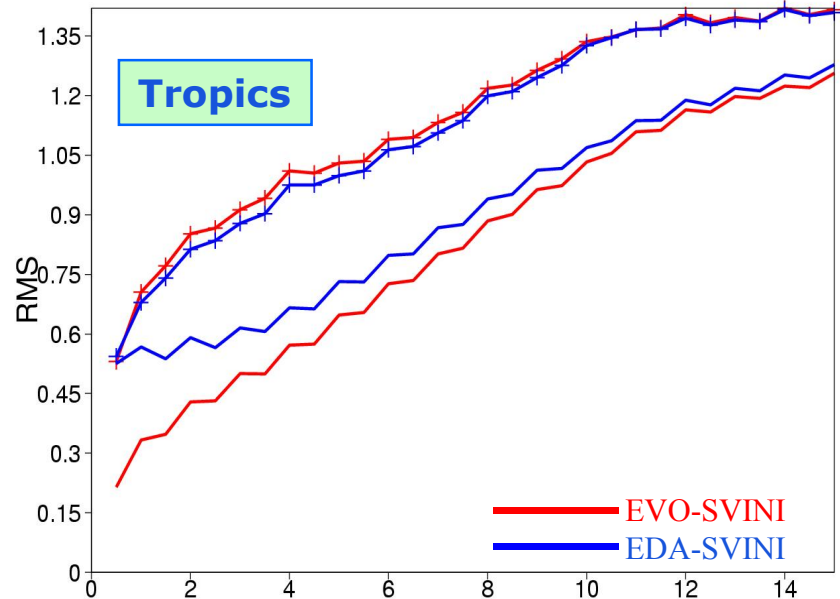
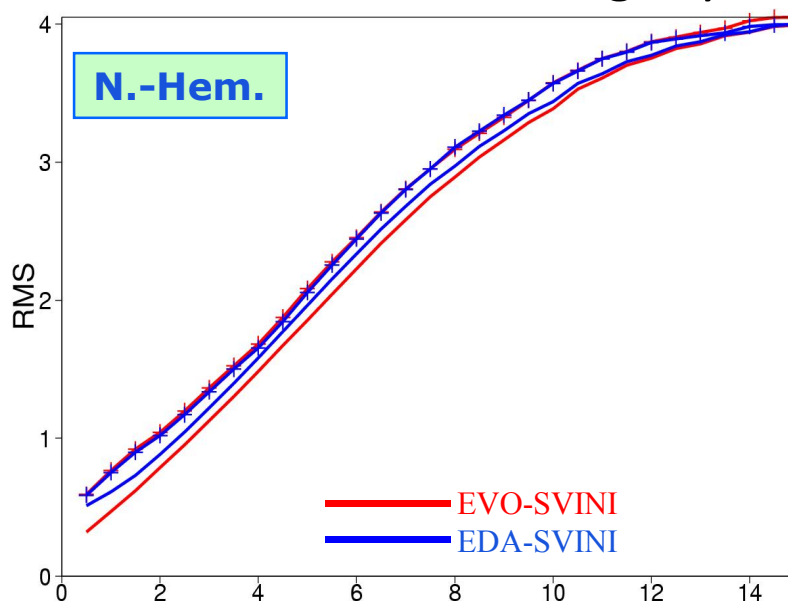
“... the main reason for the better performance of the EC-EPS in terms of the RMS, PAC, ROC and Brier Skill Score measures is the superiority of the ECMWF data assimilation (and perhaps numerical forecast modelling) system, and not necessarily the strategy used to simulate initial value and model related uncertainties in the EC-EPS.” Buizza et.al., 2005

Applications of the EDA

Improving Ensemble Prediction System by including EDA perturbations for initial uncertainty (implemented June 2010)

The Ensemble Prediction System (EPS) benefits from using EDA based perturbations. Replacing evolved singular vector perturbations by EDA based perturbations improve EPS spread, especially in the tropics.

The Ensemble Mean has slightly lower error when EDA is used.



Ensemble spread and Ensemble mean RMSE for 850hPa T

Applications of the EDA

- The EDA simulates **the error evolution** of the 4DVar analysis cycle. As such it has two main applications:
 1. Provide a flow-dependent estimate of analysis errors to initialize the ensemble prediction system (EPS)
 2. Provide a flow-dependent estimate of background errors for use in 4D-Var assimilation

Hybrids: EDA

In the ECMWF 4D-Var, the \mathbf{B} matrix is defined implicitly in terms of a transformation from the background departure ($\mathbf{x}-\mathbf{x}_b$) to a control variable χ :

$$(\mathbf{x}-\mathbf{x}_b) = \mathbf{L}\chi$$

So that the implied $\mathbf{B}=\mathbf{L}\mathbf{L}^T$.

In the current [wavelet formulation](#) (Fisher, 2003), the variable transform can be written as:

$$(\mathbf{x} - \mathbf{x}_b) = \mathbf{T}^{-1} \boldsymbol{\Sigma}_b^{1/2} \sum_j \psi_j \otimes [\mathbf{C}_j^{1/2}(\lambda, \phi) \chi_j]$$

\mathbf{T} is the balance operator, i.e. the operator that links the control variables to the model variables

$\boldsymbol{\Sigma}_b$ is the gridpoint variance of background errors

$\mathbf{C}_j(\lambda, \phi)$ is the vertical covariance matrix for wavelet index j

ψ_j are the set of radial basis function that define the wavelet transform.

Hybrids: EDA

$$(\mathbf{x} - \mathbf{x}_b) = \mathbf{T}^{-1} \boldsymbol{\Sigma}_b^{1/2} \sum_j \psi_j \otimes [\mathbf{C}_j^{1/2}(\lambda, \phi) \chi_j]$$

$\mathbf{C}_j(\lambda, \phi)$ are full vertical covariance matrices, function of (λ, ϕ) . They determine both the horizontal and vertical background error *correlation structures*;

In standard 4D-Var \mathbf{T} and \mathbf{C}_j are computed off-line using **a climatology** of EDA perturbations.

$\boldsymbol{\Sigma}_b$ is computed by random sampling of the static \mathbf{B} matrix (**randomization procedure**, Fisher and Courtier, 1995)

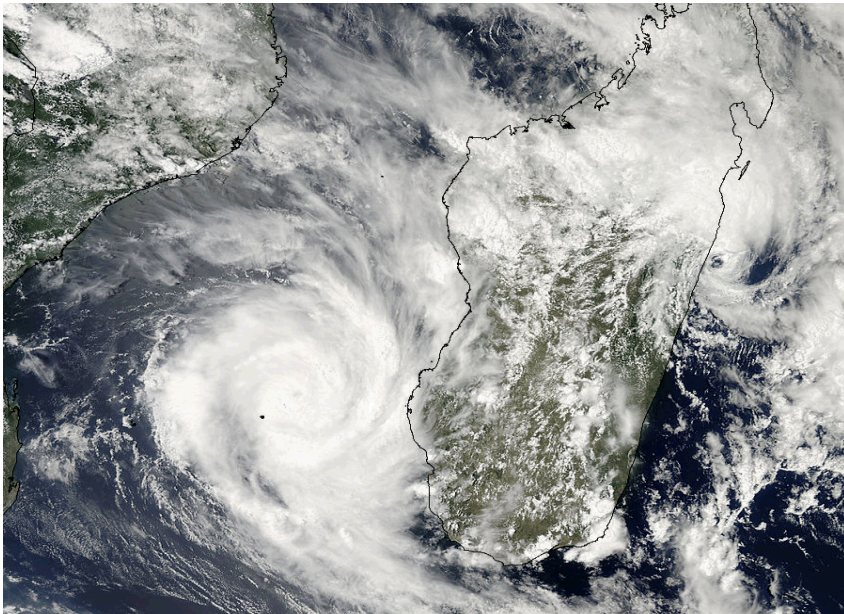
How do we make this error covariance model flow-dependent?

We look for **flow-dependent EDA estimates** of $\boldsymbol{\Sigma}_b$ and $\mathbf{C}_j(\lambda, \phi)$

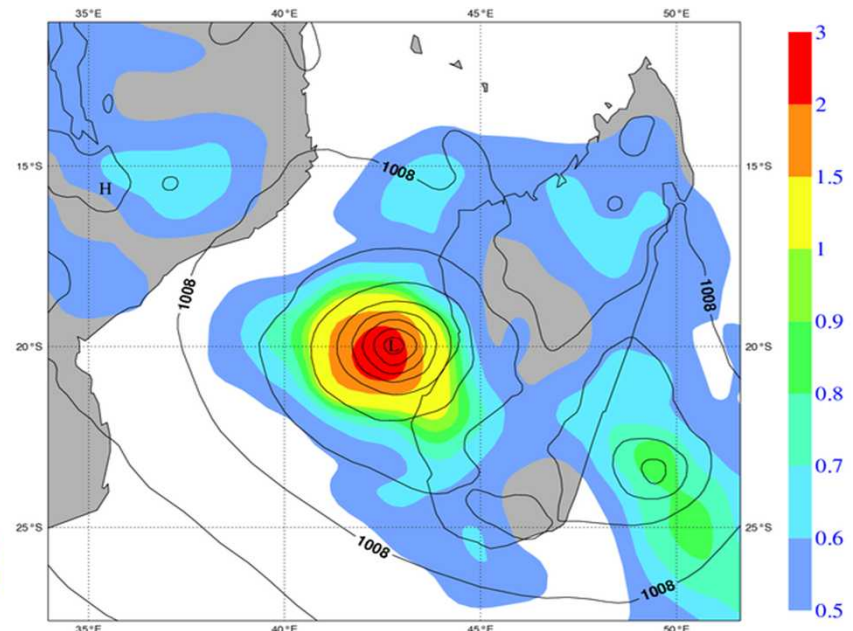
Applications of the EDA

- We want to use EDA perturbations to simulate 4DVar **flow-dependent background error covariance evolution**
- We start with the EDA flow-dependent estimates of **background error variances** (diagonal of the B matrix, Σ_b)

Hurricane Fanele, 20 January 2009



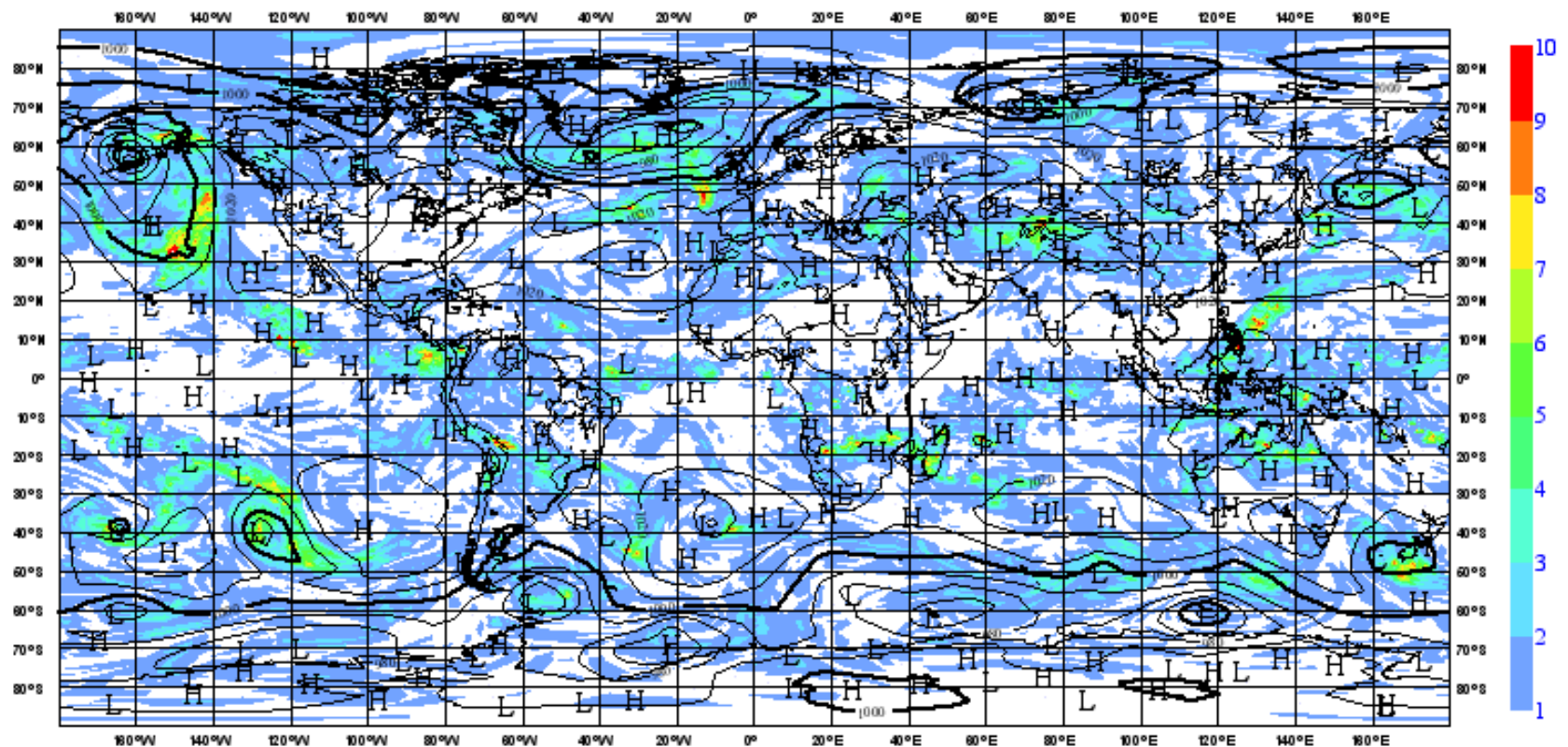
EDA based background error variance for surface pressure



Applications of the EDA

What do raw ensemble variances look like?

Spread of Vorticity t+9h 500hPa



Applications of the EDA

- Noise level is due to sampling errors: 25 member ensemble
- EDA is a **stochastic** system: error variance of variance estimator $\sim 1/N_{\text{ens}}$
- We need a system to effectively filter out noise from first guess ensemble forecast variances: Reduce the random component of the estimation error

Applications of the EDA

Mallat *et al.*: 1998, Annals of Statistics, 26,1-47

Define $G^e(i)$ as the random component of the sampling error in the estimated ensemble variance at gridpoint i :

$$G^e(i) \equiv \tilde{B}_{ii} - E[\tilde{B}_{ii}]$$

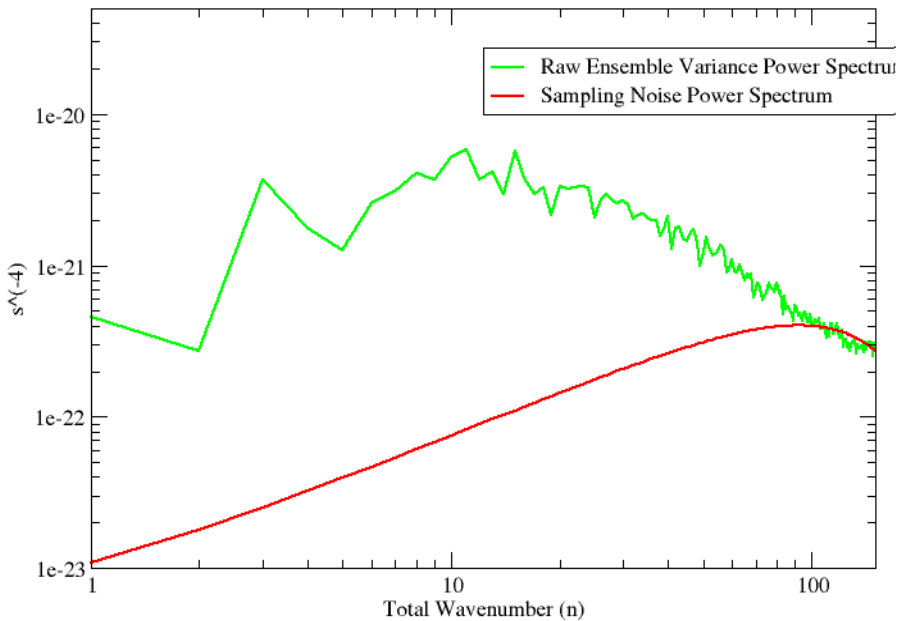
Then the **covariance of the sampling noise** can be shown to be a simple function of the expectation of the ensemble-based covariance matrix:

$$E[G^e(i)G^e(j)] = \frac{2}{N-1} \left(E[\tilde{B}_{ij}] \right)^2 \quad (1)$$

Applications of the EDA

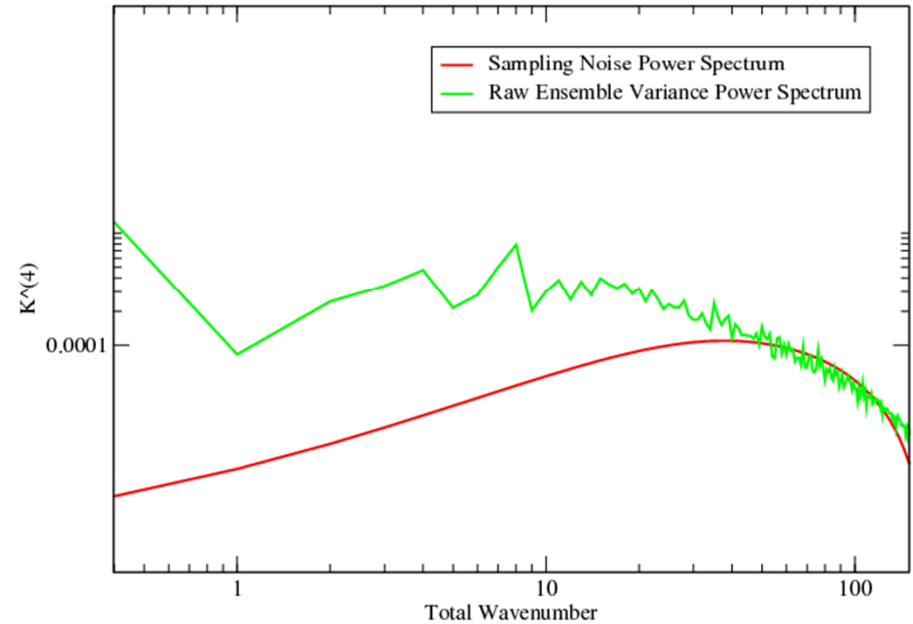
Vorticity

ml 64 (~500hPa)



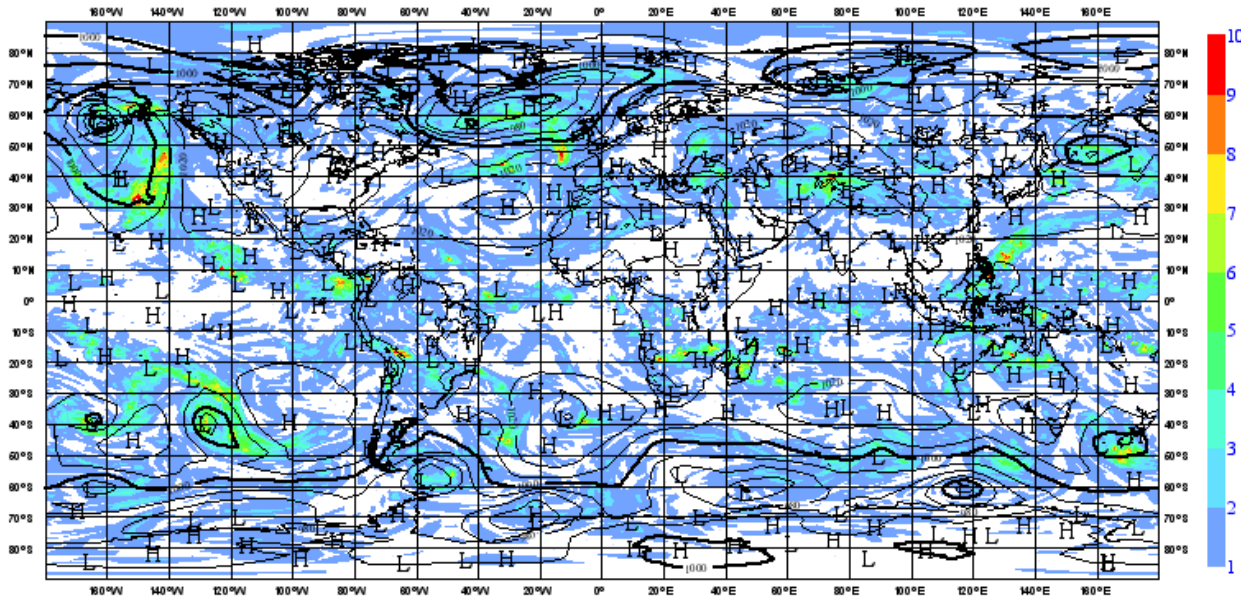
Temperature

ml49 (~200hPa)



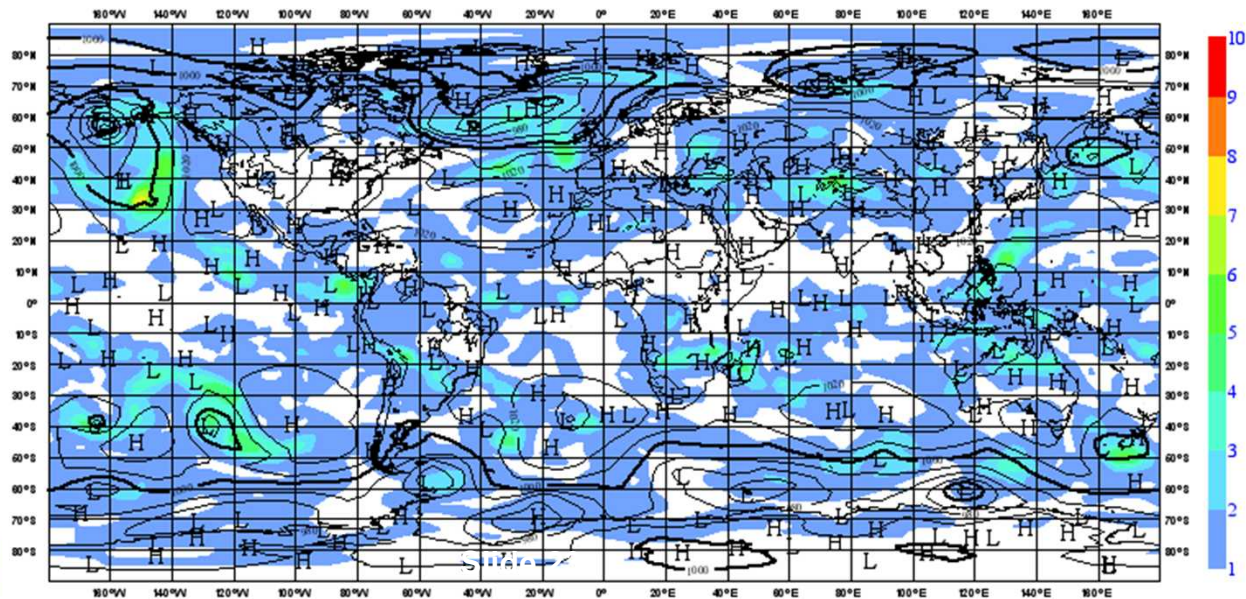
- We can use a **spectral filter** to disentangle noise from signal
- Truncation wavenumber is determined by **maximizing signal-to-noise** ratio of filtered variances (Raynaud *et al.*, 2009; Bonavita *et al.*, 2011)

Applications of the EDA

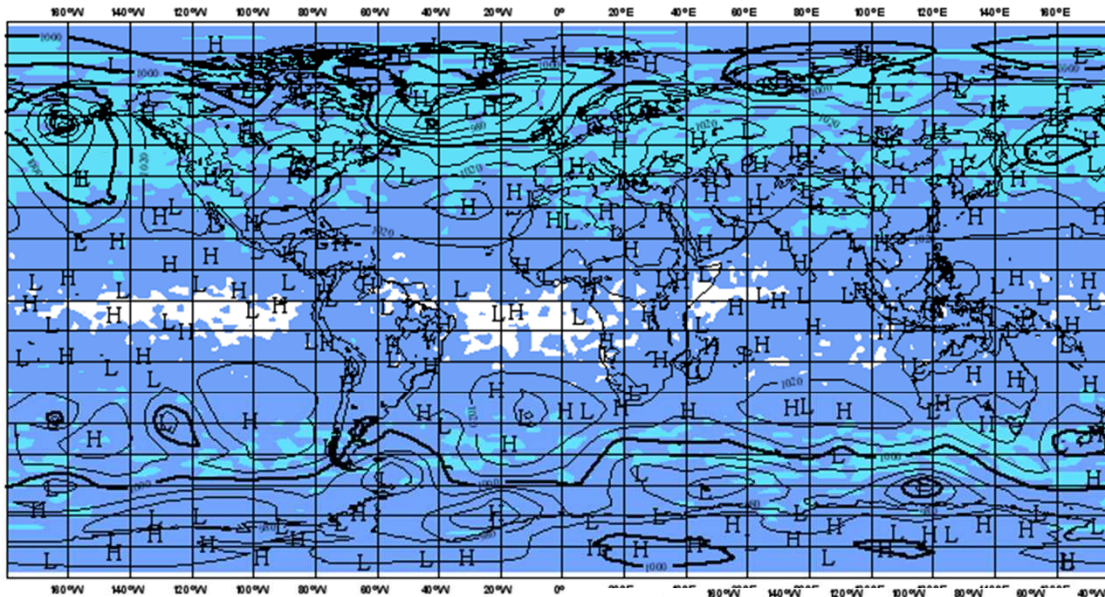


Raw EDA StDev
Vorticity 500 hPa

Filtered EDA StDev
Vorticity 500 hPa

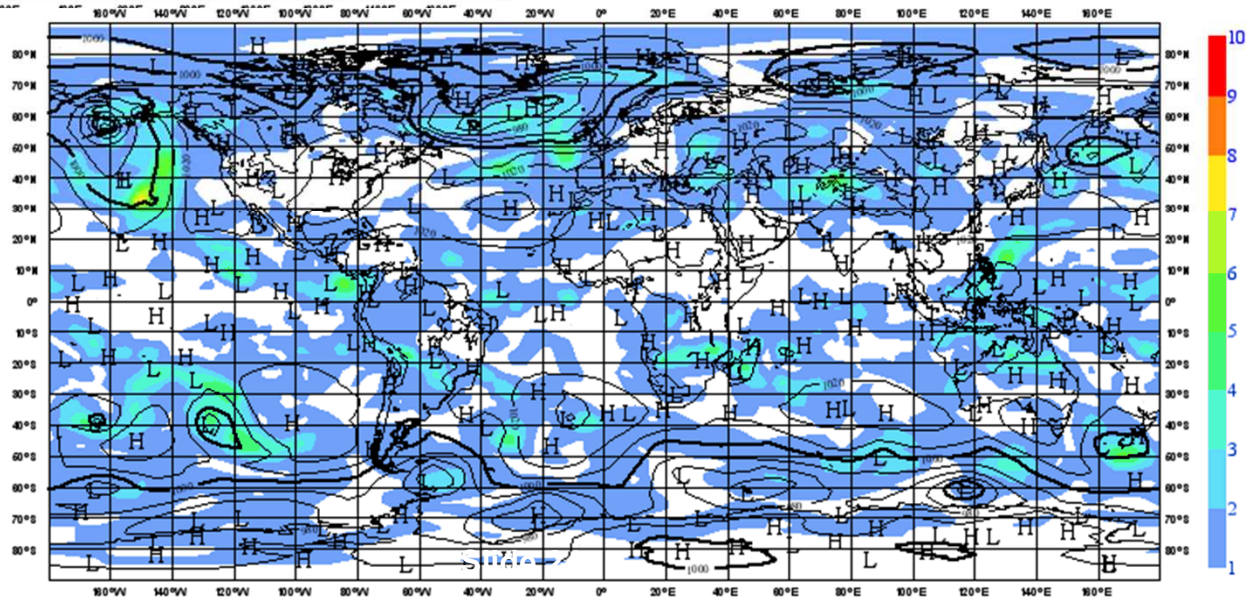


Applications of the EDA



StDev of Vorticity at 500 hPa
estimated from **static B**
Random. Method
(Fisher & Courtier, 1995)

Filtered EDA estimate of
StDev of Vorticity 500 hPa



Applications of the EDA

Is there also a systematic error in our EDA
sampled variances?

A statistically consistent ensemble satisfies:

$$(1-1/N_{ens})^{-1}\langle\text{Ens_Var}\rangle = (1+1/N_{ens})^{-1}\langle\text{Ens_Mean_Square_Error}\rangle$$

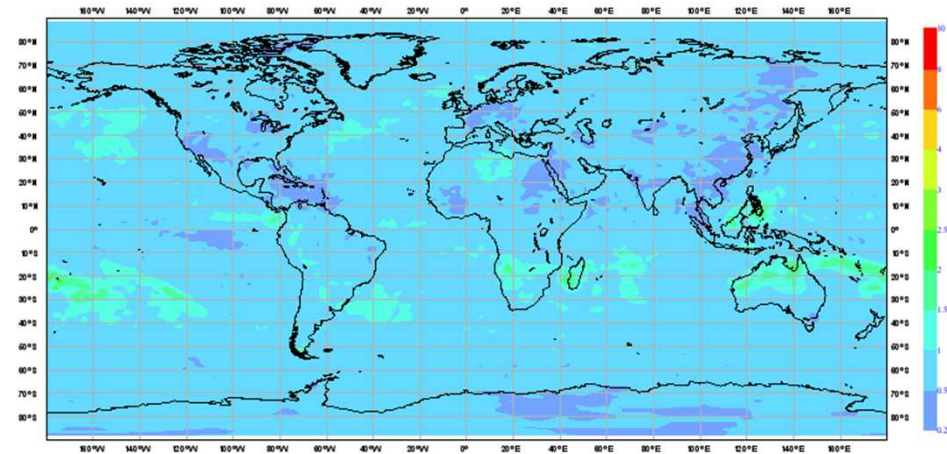
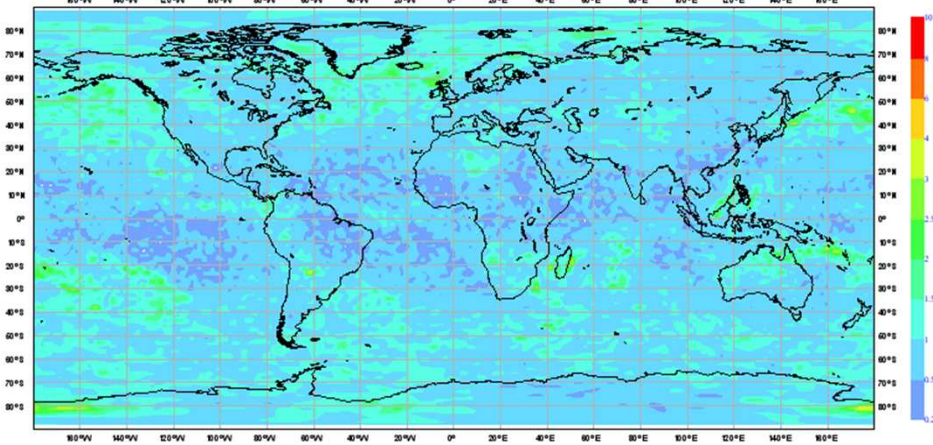
Applications of the EDA

Vorticity ml 78 (~850hPa)

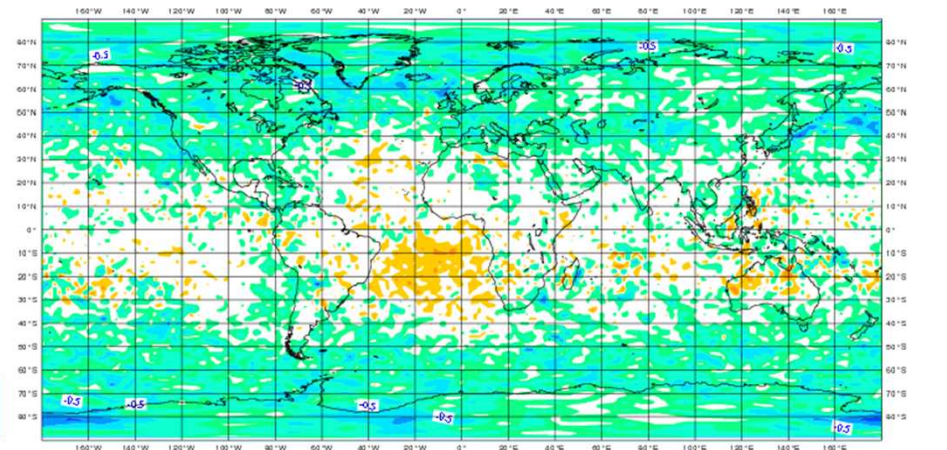
Ensemble Error

Ensemble Spread

Tuesday 6 January 2009 12UTC ECMWF Forecast t+9 VT: Tuesday 6 January 2009 21UTC Model Level 78 "Vorticity (relative)

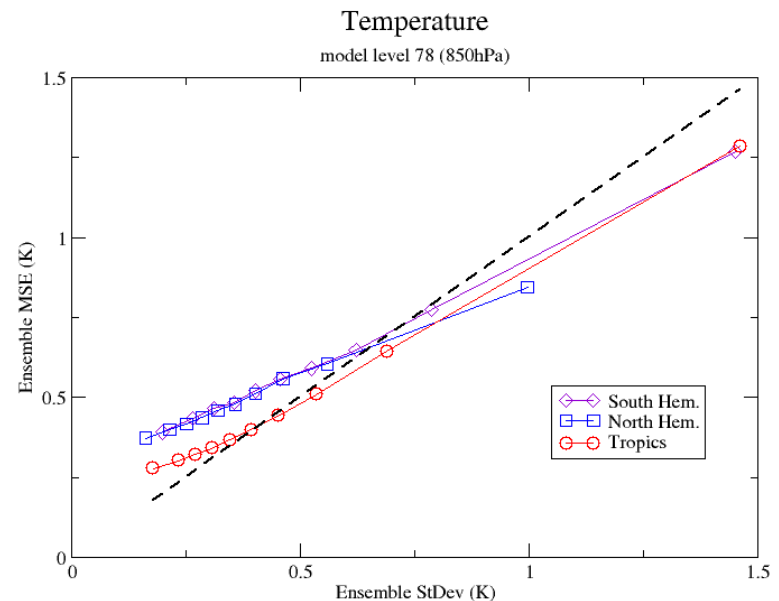
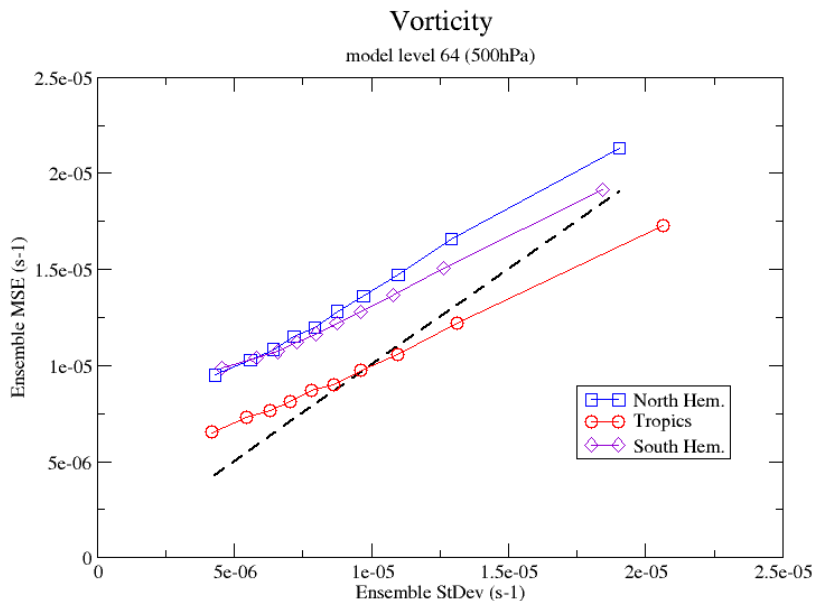


Spread - Error

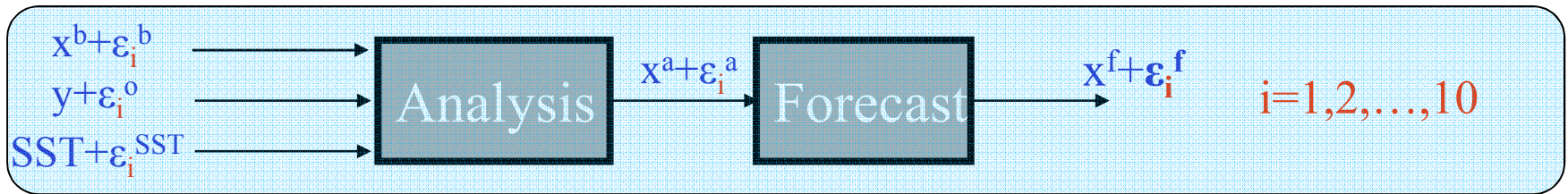


Applications of the EDA

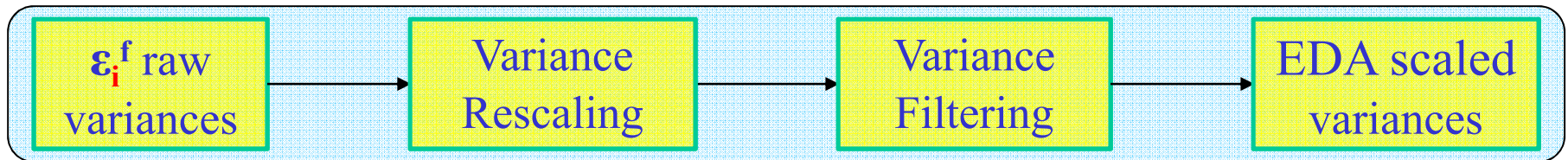
- To get statistically consistent EDA variances we need to perform an **online calibration** (**Ensemble Variance Calibration**; Kolczynsky et al., 2009, 2011; Bonavita et al., 2011)
- Calibration factors are also **state-dependent**, i.e. depend on the size of the expected error
- Need to perform calibration of variances reflects underlying problem in **Q** and **R** models, system non-linearities, ensemble size



EDA Cycle



Variance post-process



4DVar Cycle



Use of EDA variances in 4DVar

- How does the flow-dependent structure of the EDA variances affect the 4DVar analysis?
- Two mechanisms:
 1. Inside 4DVar EDA variances change the **shape and size of analysis increments**
 2. Before 4DVar they affect the **observation quality control decisions**

Use of EDA variances in 4DVar

1. Inside 4DVar EDA variances change the **shape and size of analysis increments**
- Tropical Cyclone Aere, Philippines 8-9 May 2011.

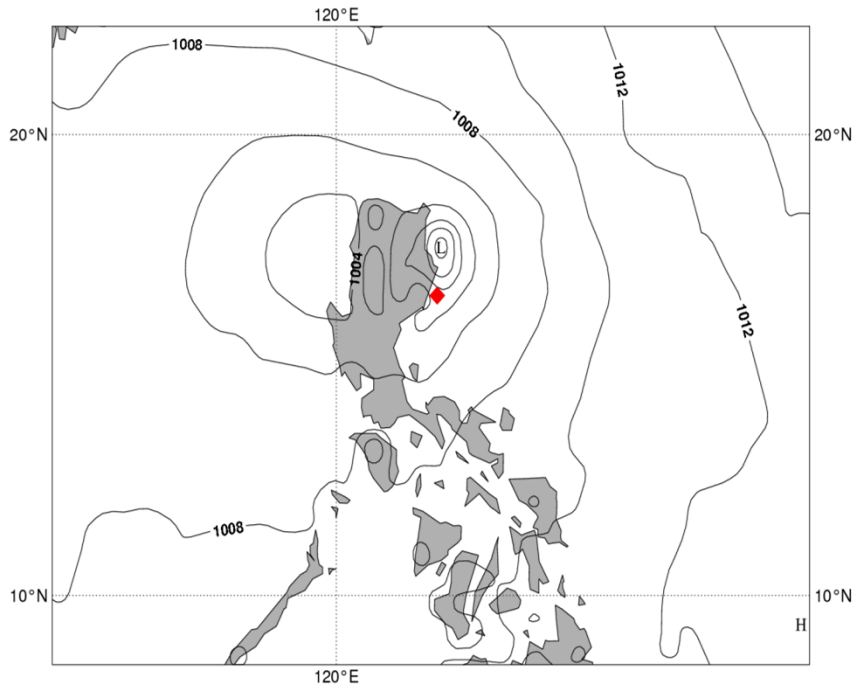


Use of EDA variances in 4DVar

1. Inside 4DVar EDA variances change the **shape and size of analysis increments**
- Significant operational analysis error, corrected by 4DVar with EDA variances

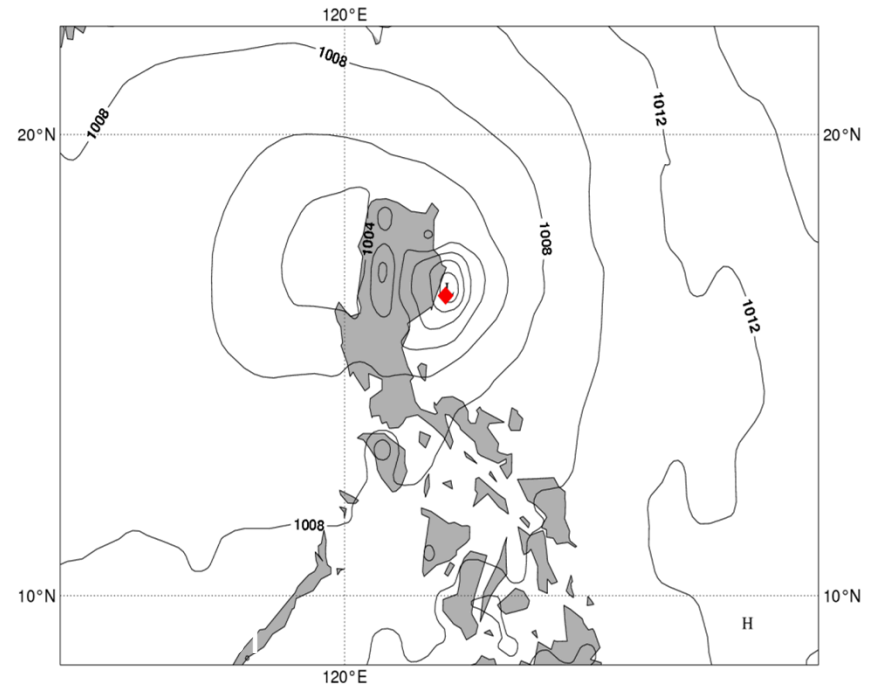
4DVar with Static errors

ECMWF Analysis VT:Monday 9 May 2011 00UTC Surface: Mean sea level pressure



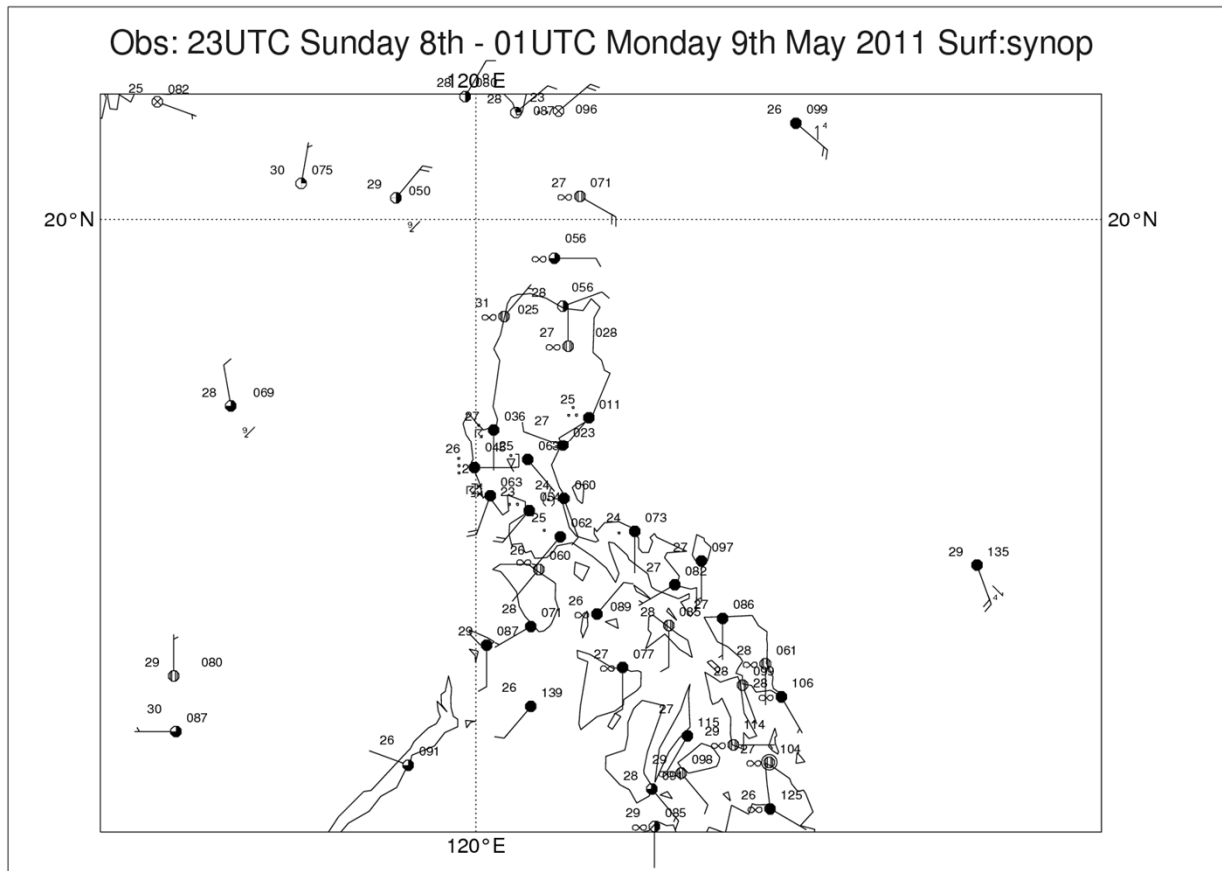
4DVar with EDA errors

ECMWF Analysis VT:Monday 9 May 2011 00UTC Surface: Mean sea level pressure

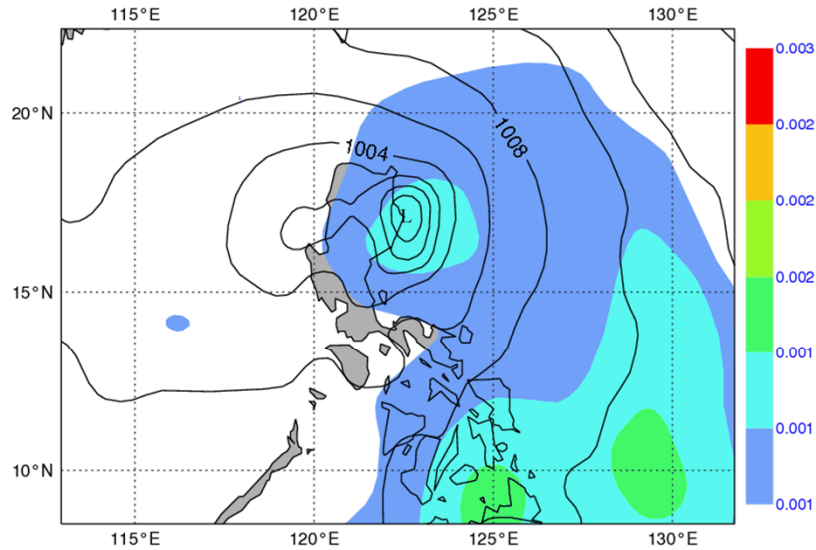


Use of EDA variances in 4DVar

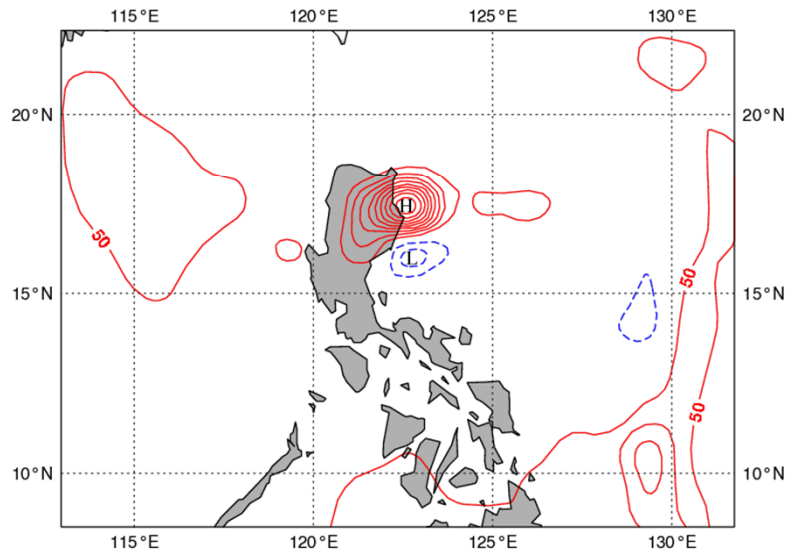
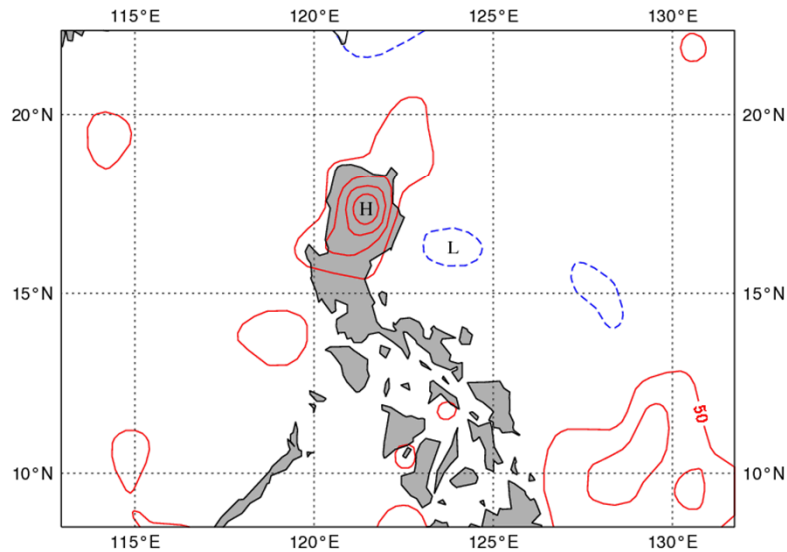
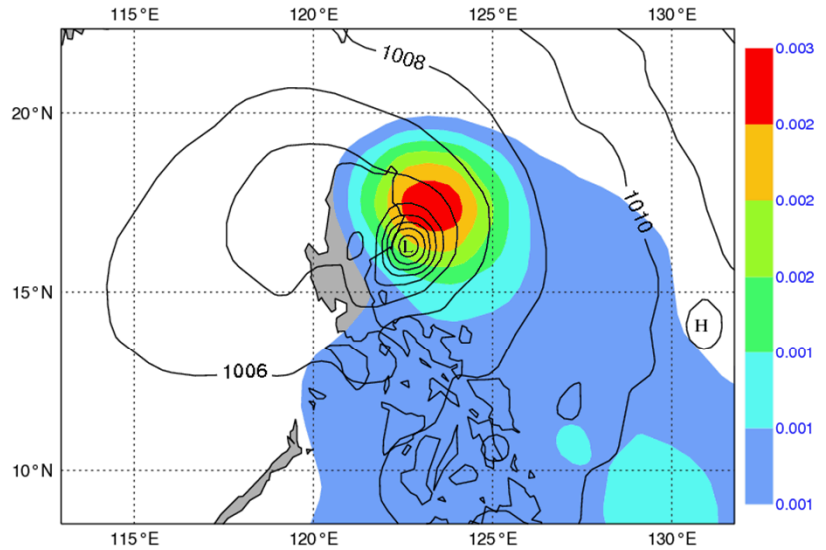
1. Inside 4DVar EDA variances change the **shape and size of analysis increments**



log(P_s) Static errors



log(P_s) EDA errors



Static mslp ana incr.

EDA mslp ana incr.

Use of EDA variances in 4DVar

- Flow-dependent EDA errors have been used operationally since May 2012 (CY37R2)
- The effect of using flow-dependent EDA estimated errors is large on average skill scores

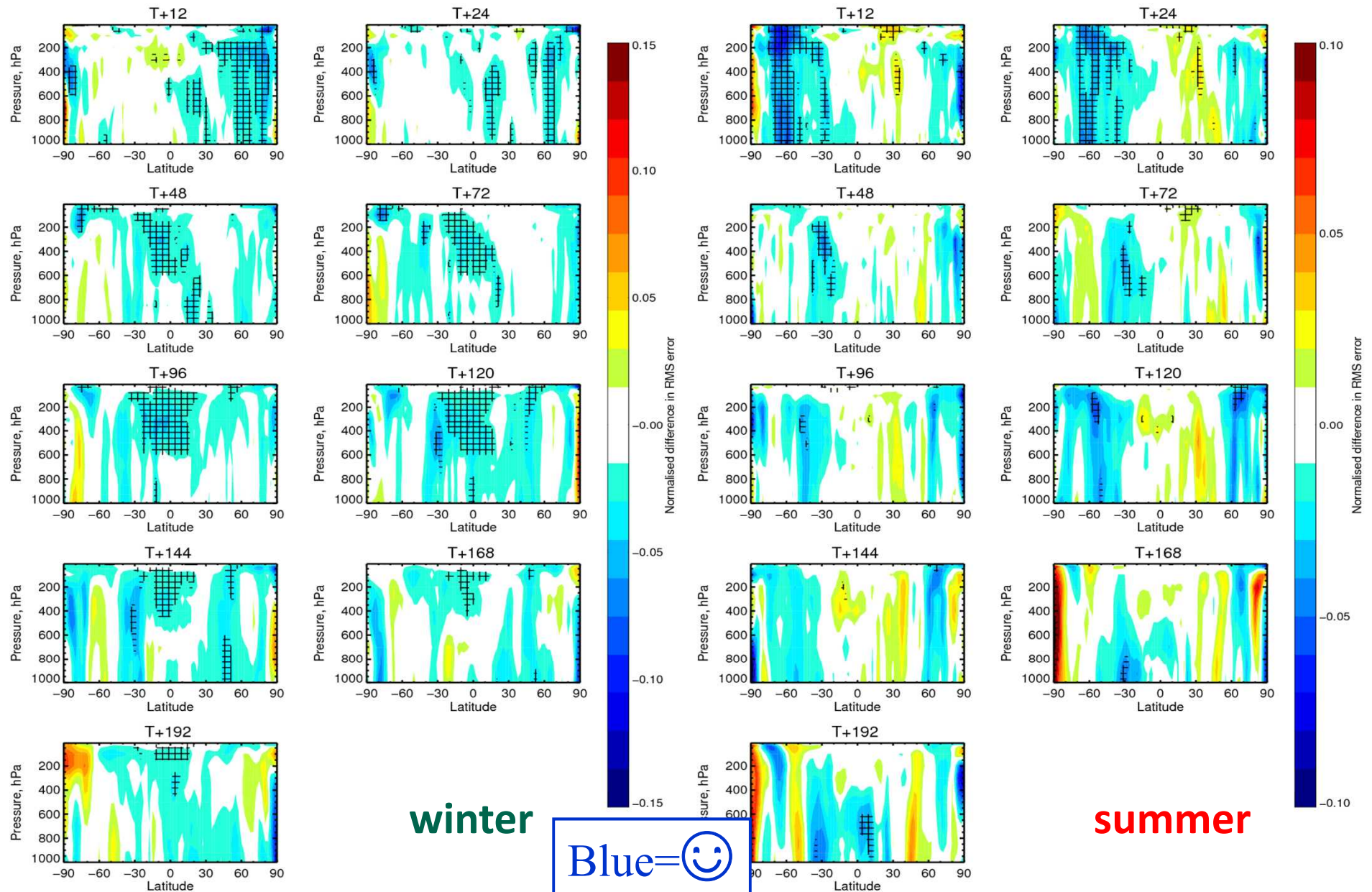
Geopotential RMSE reduction

RMS forecast errors in Z(ffg8-fezj), 11-Jan-2010 to 30-Mar-2010, from 72 to 79 samples.

Point confidence 99.5% to give multiple-comparison adjusted confidence 90%. Verified against own-analysis.

RMS forecast errors in Z(ffge-0051), 2-Aug-2010 to 30-Oct-2010, from 83 to 90 samples.

Point confidence 99.5% to give multiple-comparison adjusted confidence 90%. Verified against own-analysis.



winter

summer

Blue = 😊

Use of EDA covariances in 4DVar

$$(\mathbf{x} - \mathbf{x}_b) = \mathbf{T}^{-1} \boldsymbol{\Sigma}_b^{1/2} \sum_j \psi_j \otimes [\mathbf{C}_j^{1/2}(\lambda, \phi) \chi_j]$$

\mathbf{T} is the balance operator

$\boldsymbol{\Sigma}_b$ is the gridpoint variance of background errors

$\mathbf{C}_j(\lambda, \phi)$ is the vertical covariance matrix for wavelet index j

ψ_j are the set of radial basis function that define the wavelet transform

$\mathbf{C}_j(\lambda, \phi)$ are fields of full vertical covariance matrices, defined for each wavelet band. They determine both the horizontal and vertical background error correlation structures.

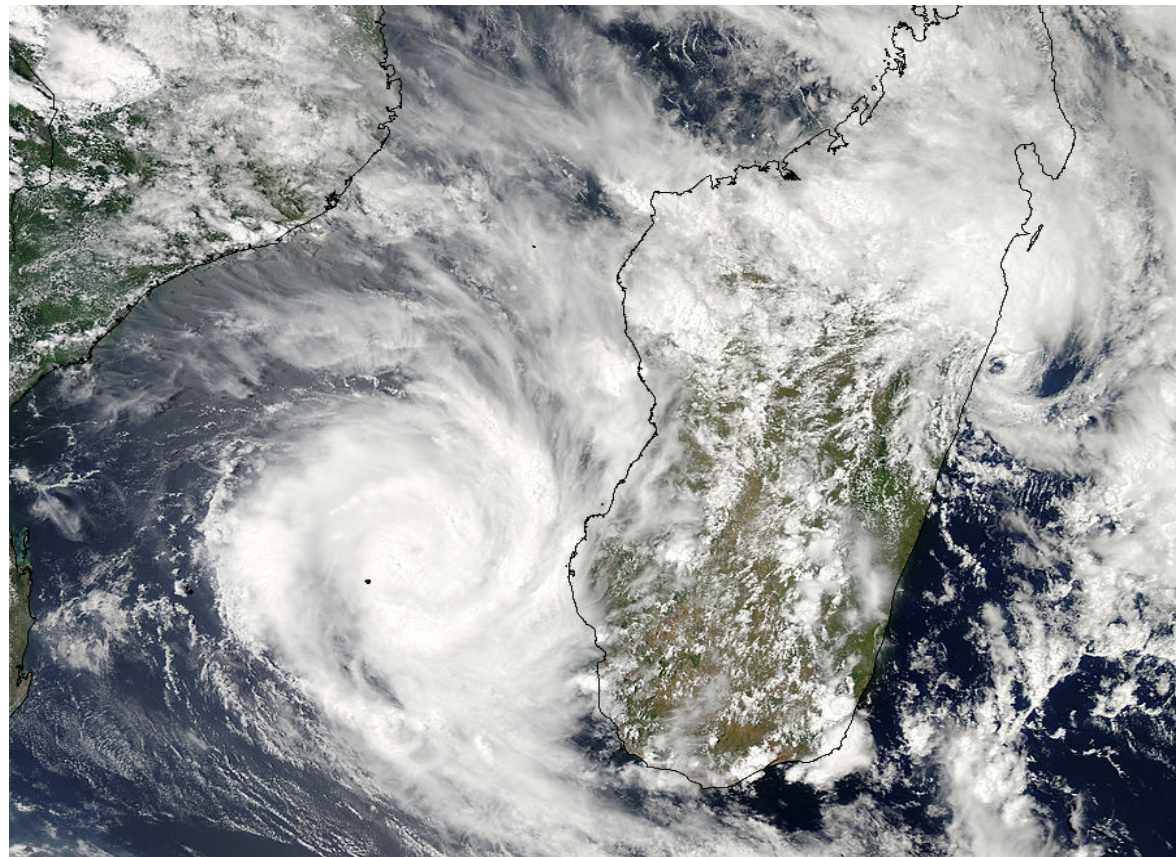
In order to get flow-dependent error covariances we need flow-dependent estimates of $\mathbf{C}_j(\lambda, \phi)$.

Use of EDA covariances in 4DVar

Diagnosing the Background Error Correlation Length-Scales

$$L \equiv \sqrt{-\frac{\rho(r)}{\partial^2 \rho(r) / \partial r^2} \Big|_{r=0}}$$

Hurricane Fanele
20 January 2009

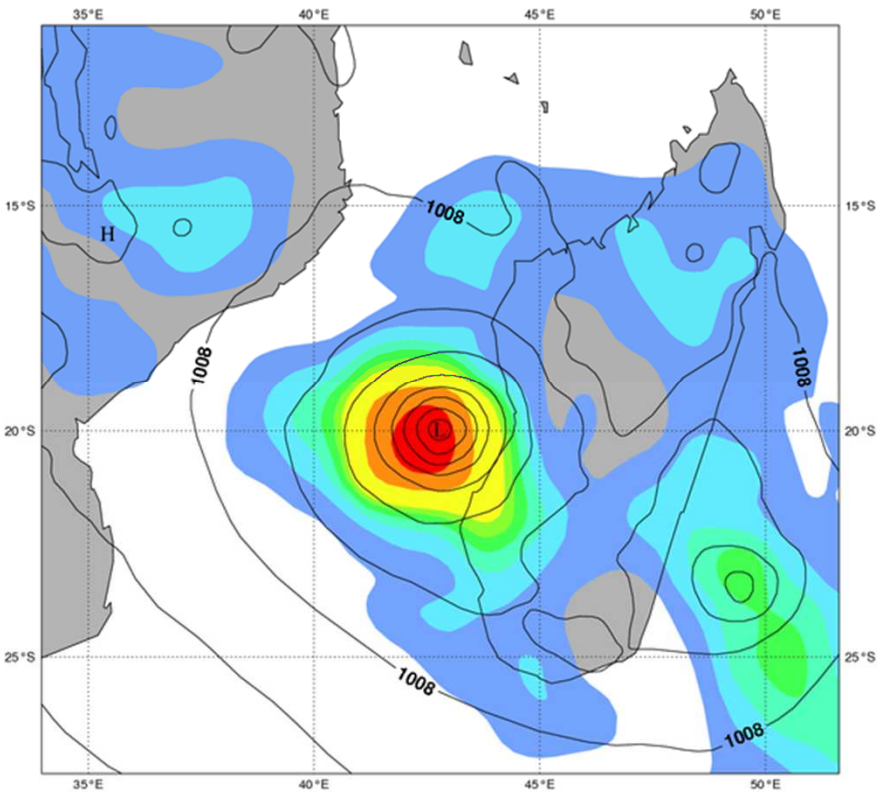


Use of EDA covariances in 4DVar

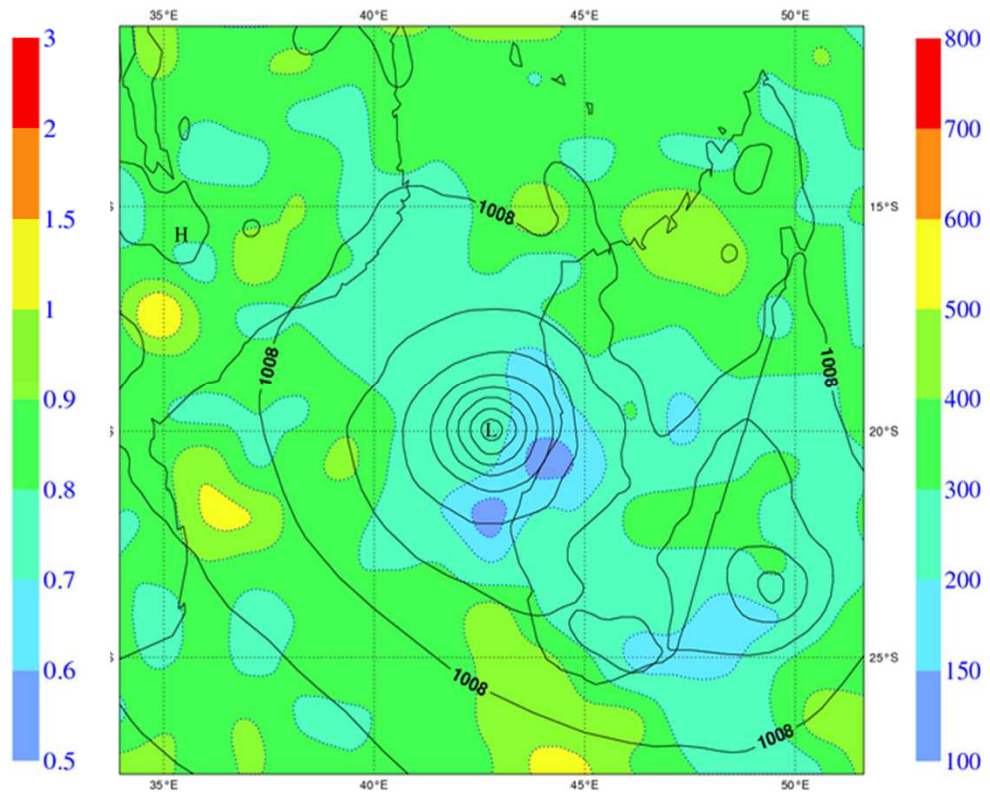
20 member EDA

Surf. Press. Background Err. St.Dev. Surf. Press. BG Err. Correlation L. Scale

Tuesday 20 January 2009 00UTC ECMWF Forecast t+9 VT: Tuesday 20 January 2009 09UTC Surface: Mean sea level pressure



Tuesday 20 January 2009 00UTC ECMWF Forecast t+9 VT: Tuesday 20 January 2009 09UTC Surface: Mean sea level pressure

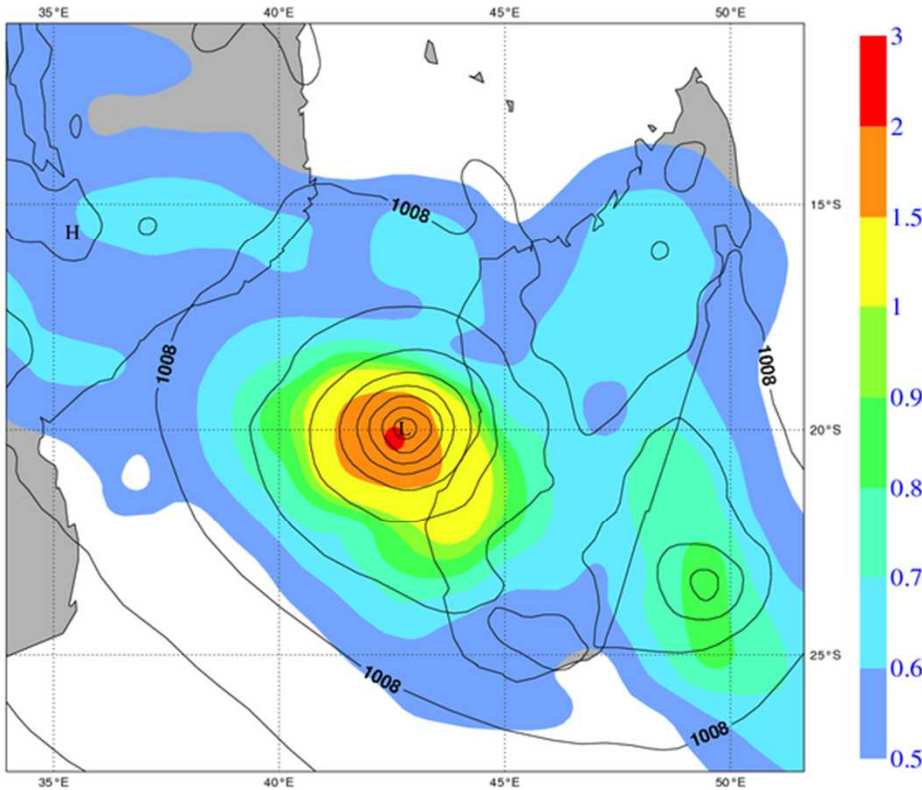


Use of EDA covariances in 4DVar

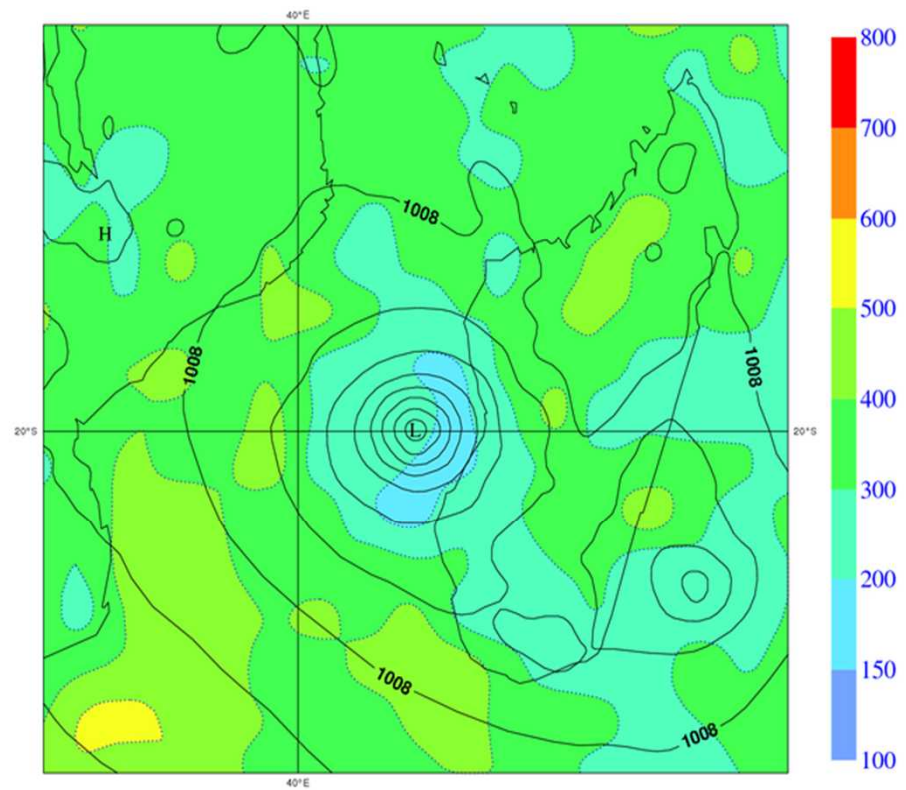
50 member EDA

Surf. Press. Background Err. St.Dev. Surf. Press. BG Err. Correlation L. Scale

Tuesday 20 January 2009 00UTC ECMWF Forecast t+9 VT: Tuesday 20 January 2009 09UTC Surface: Mean sea level pressure



Tuesday 20 January 2009 00UTC ECMWF Forecast t+9 VT: Tuesday 20 January 2009 09UTC Surface: Mean sea level pressure



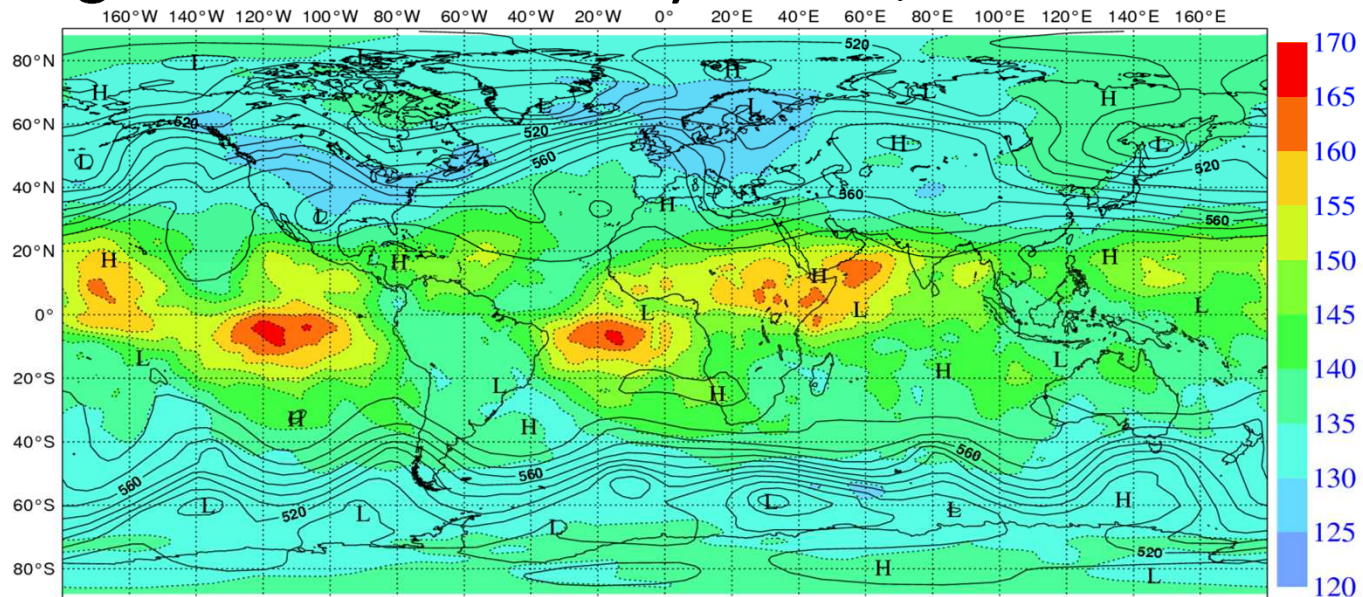
Use of EDA covariances in 4DVar

- a) From November 2013 (CY40R1) background error covariances (wavelet JB) are computed online, i.e. they are updated at every assimilation time (00, 12 UTC)
- b) EDA perturbations from the past **12 days** are used, with an exponential decay factor (i.e., reduce noise at the cost of losing some flow-dependent detail)
- c) Continuously updated JB is used in High Resolution 4D-Var

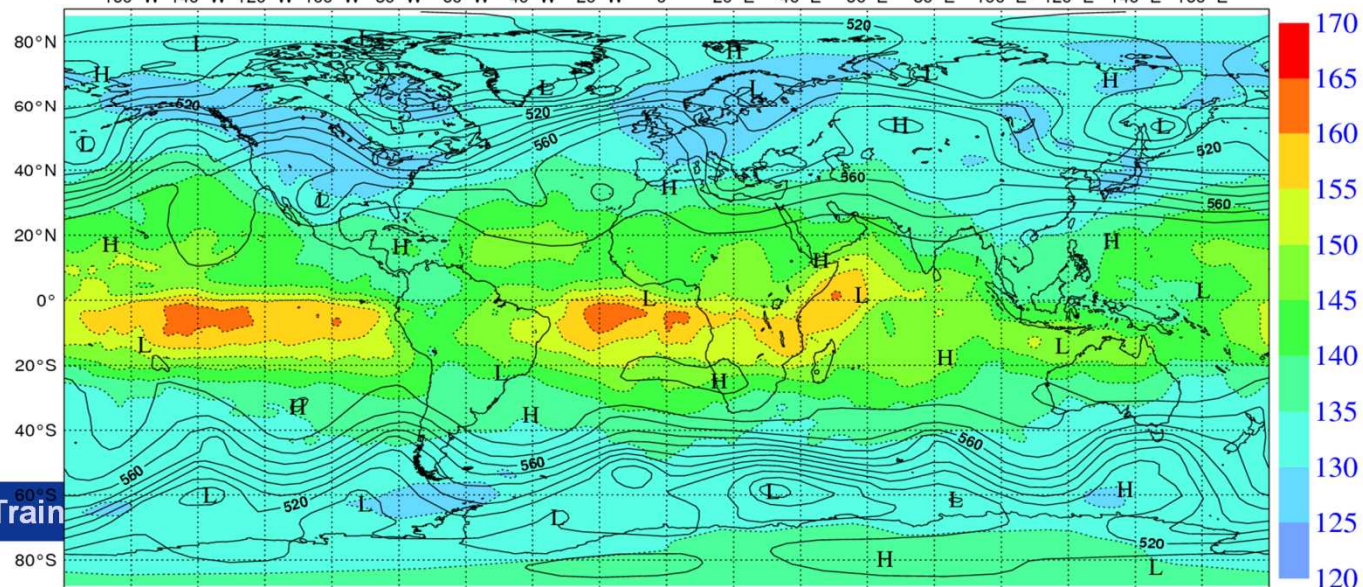
Why is a flow-dependent JB better?

Correlation length scale of Vorticity errors, ~500 hPa

*Online wavelet JB,
valid 20120110 00Z*

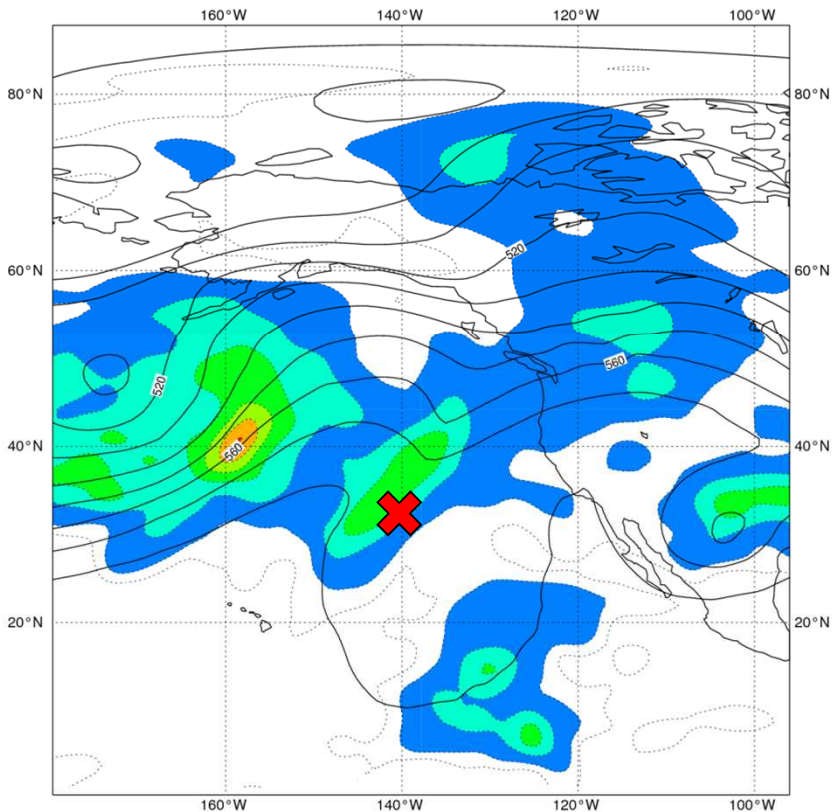
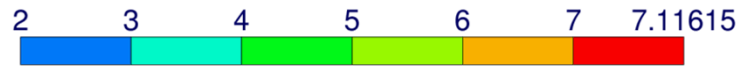


Static wavelet JB

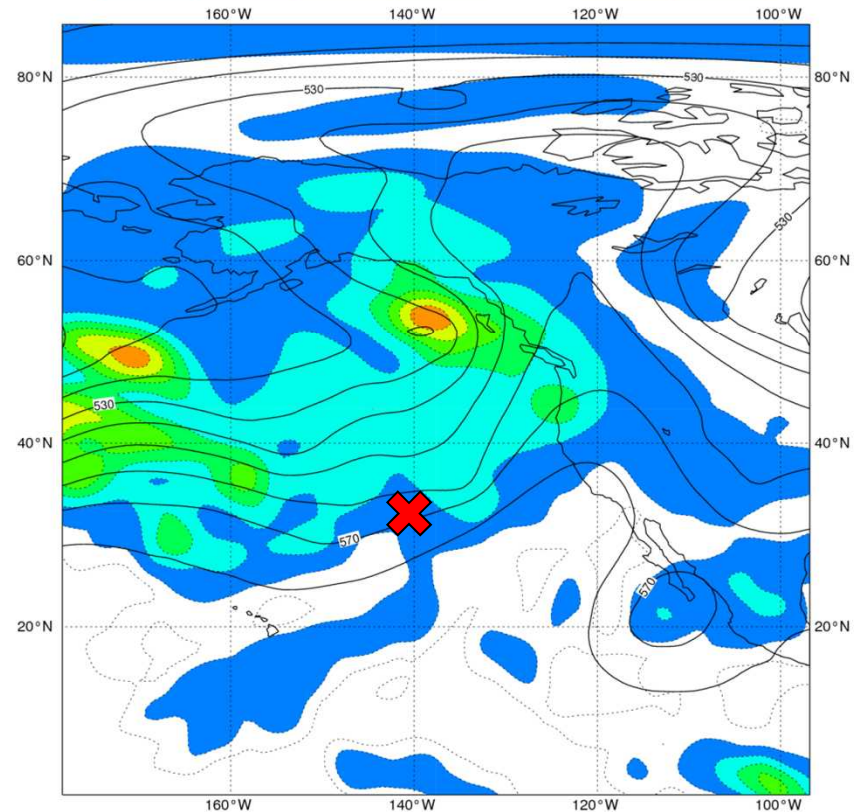
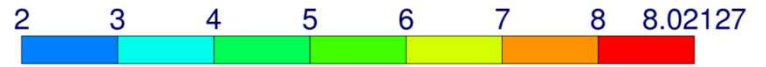


Why is a flow-dependent JB better?

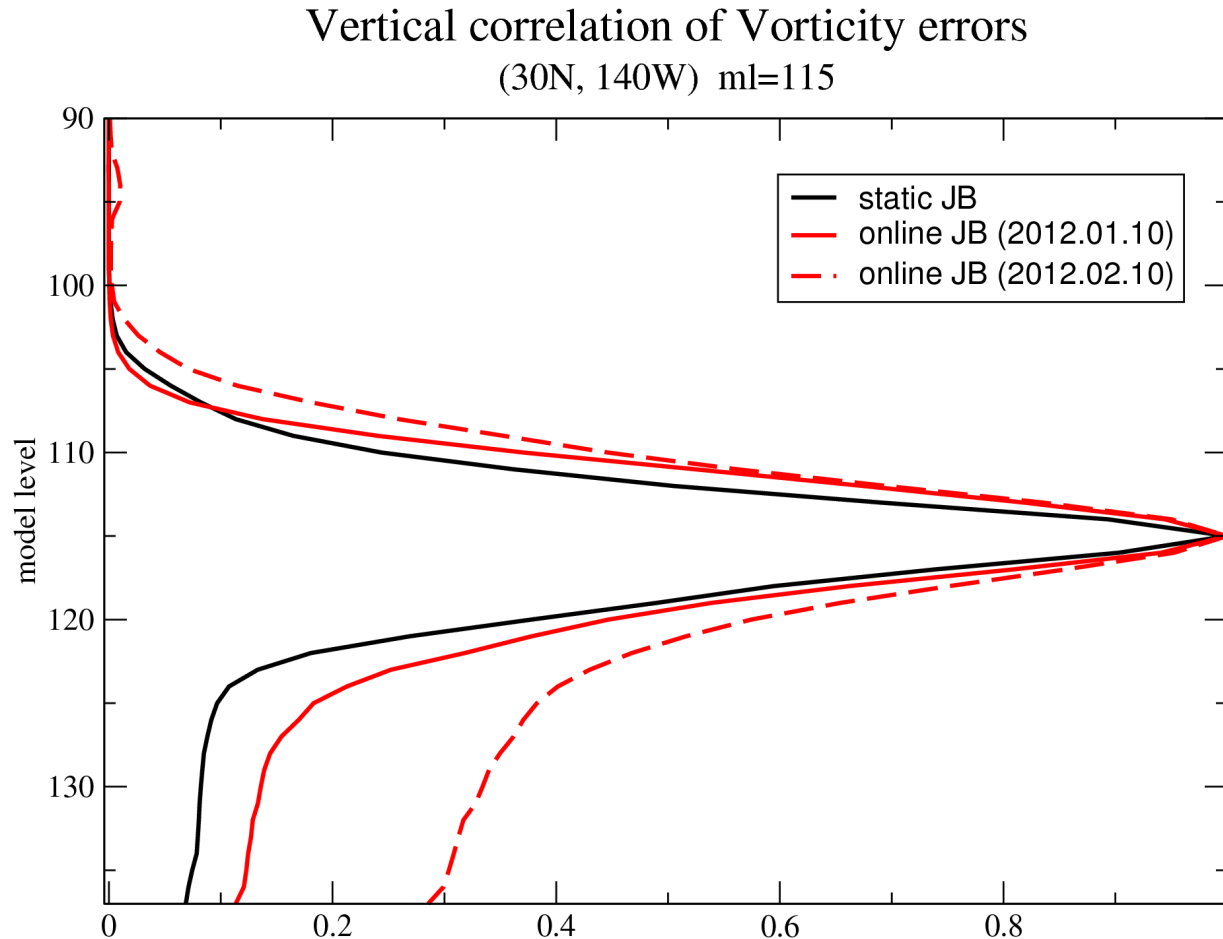
2012-01-01 00Z



2012-02-01 00Z

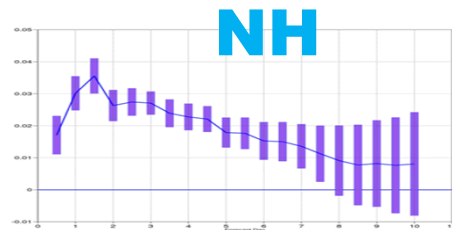


Why is a flow-dependent JB better?

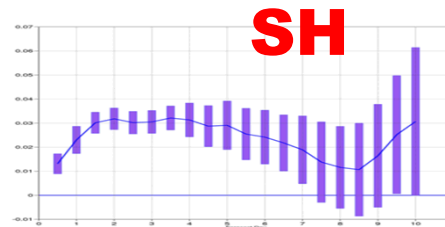


Impact of online JB

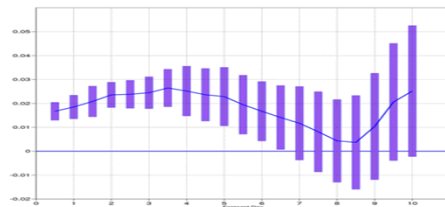
Reduction in Geopotential RMSE - 95% confidence



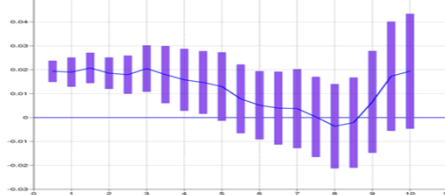
50 hPa



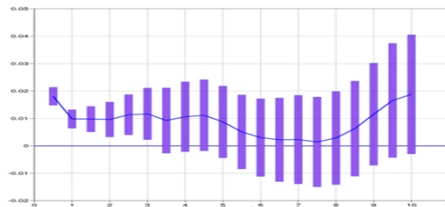
100 hPa



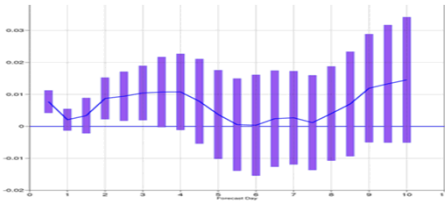
200 hPa



500 hPa



1000 hPa



Period: Feb - June 2012

T511L91, 3 Outer Loops
(T159/T255/T255)

Verified against operational
analysis

Summary

- The **EDA** is the best available tool at ECMWF to estimate **analysis and background errors of the ECMWF analysis**
- The EDA derived **analysis errors** contribute to the estimation of **initial perturbations of the Ensemble Prediction System (EPS)**
- The EDA **background perturbations** provide flow-dependent estimates of **background errors variances and covariances for use in the High-Resolution 4DVar analysis**

Summary

- The use of EDA **background perturbations** in a variational analysis is currently done in two ways:
 - a) adding an ensemble, flow-dependent component to the static **B** used in 4D-Var (UK MetO, NCEP; **alpha control variable method**: Lorenc, 2003)
 - b) using EDA perturbations to get an on-line, flow-dependent estimate of parameterised **B** (ECMWF, Meteo France; **EDA approach**)

Summary

- Flow-dependent background errors from EDA variances have been used in ECMWF 4D-Var since April 2011 (Cycle 37R2)
- They benefit the analysis and forecast skill by:
 - a) changing the weight given to observations near dynamically active zones;
 - b) introducing a level of flow-dependency in the analysis increments
 - c) Allowing a state and flow-dependent QC of observations
- Increase in ensemble size will benefit the system allowing less aggressive filtering of raw variances (Bonavita *et al.*, 2011)

Summary

- Flow-dependent background error covariances (**B**) estimated from **EDA perturbations** has been implemented recently (CY40R1, November 2013)
- They also have an important effect on the analysis by providing **flow-dependent, non homogeneous, correlation structures**
- The introduction of flow-dependent background errors and covariances estimated from the EDA has been one of the largest source of improvement in recent years in the analysis and forecast skill of the IFS

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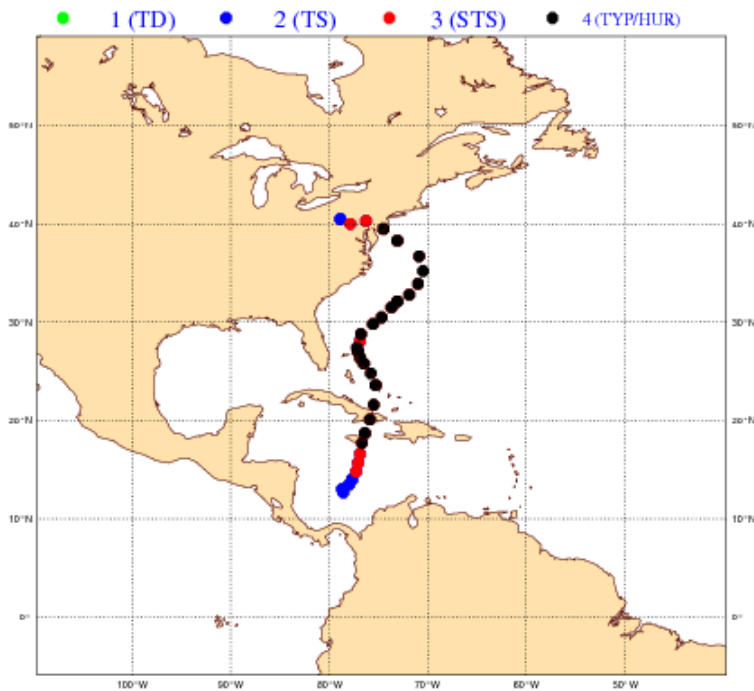
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Additional Slides

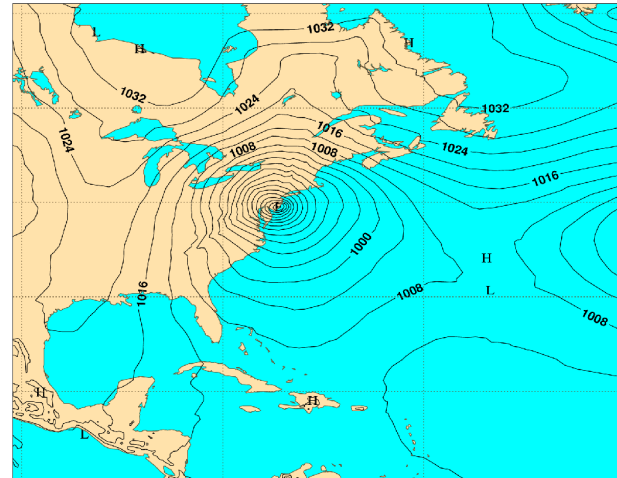
Use of EDA variances in 4DVar

2. Before 4DVar they affect the **observation quality control** decisions

- Super Storm Sandy

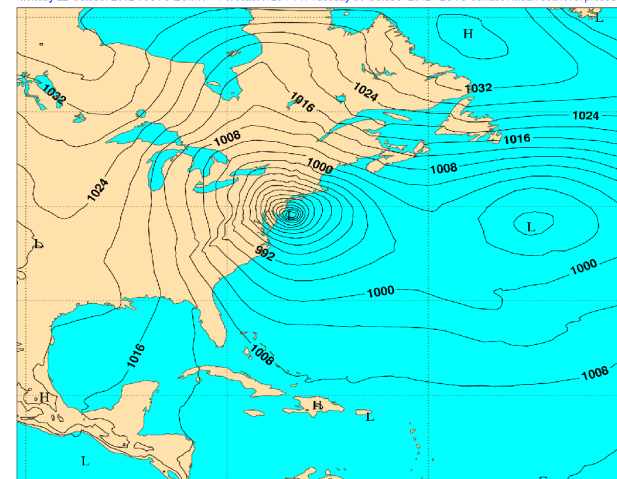


ECMWF Analysis VT: Tuesday 30 October 2012 00UTC Surface: Mean sea level pressure



Mslp **Ana**
30/10/2012
00UTC

Monday 22 October 2012 00UTC ECMWF Forecast I+204 VT: Tuesday 30 October 2012 12UTC Surface: Mean sea level pressure



Mslp **t+204h**
Fcst valid at
30/10/2012
00UTC

Use of EDA variances in 4DVar

What happens if we **withhold polar-orbiters observations** (i.e., approx. 90% of obs. counts)?

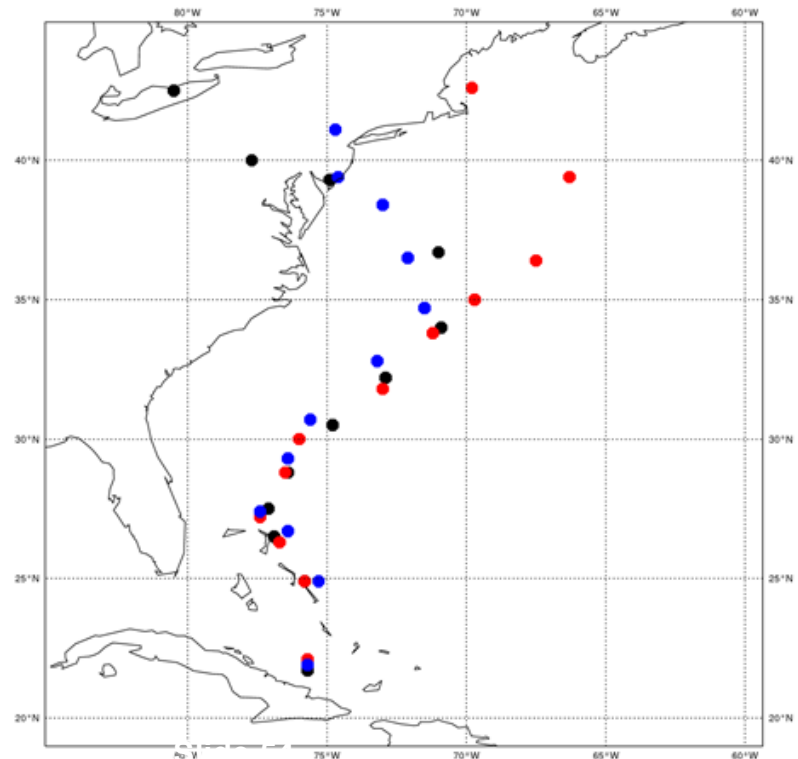
The forecast performance is obviously degraded, and only 5 days before landfall the system recovers the correct track

Sandy's forecast tracks 25 Oct
2013 00UTC

Operational forecast

Forecast from HRES assimilation
cycle without polar orbiters and
errors from operational EDA

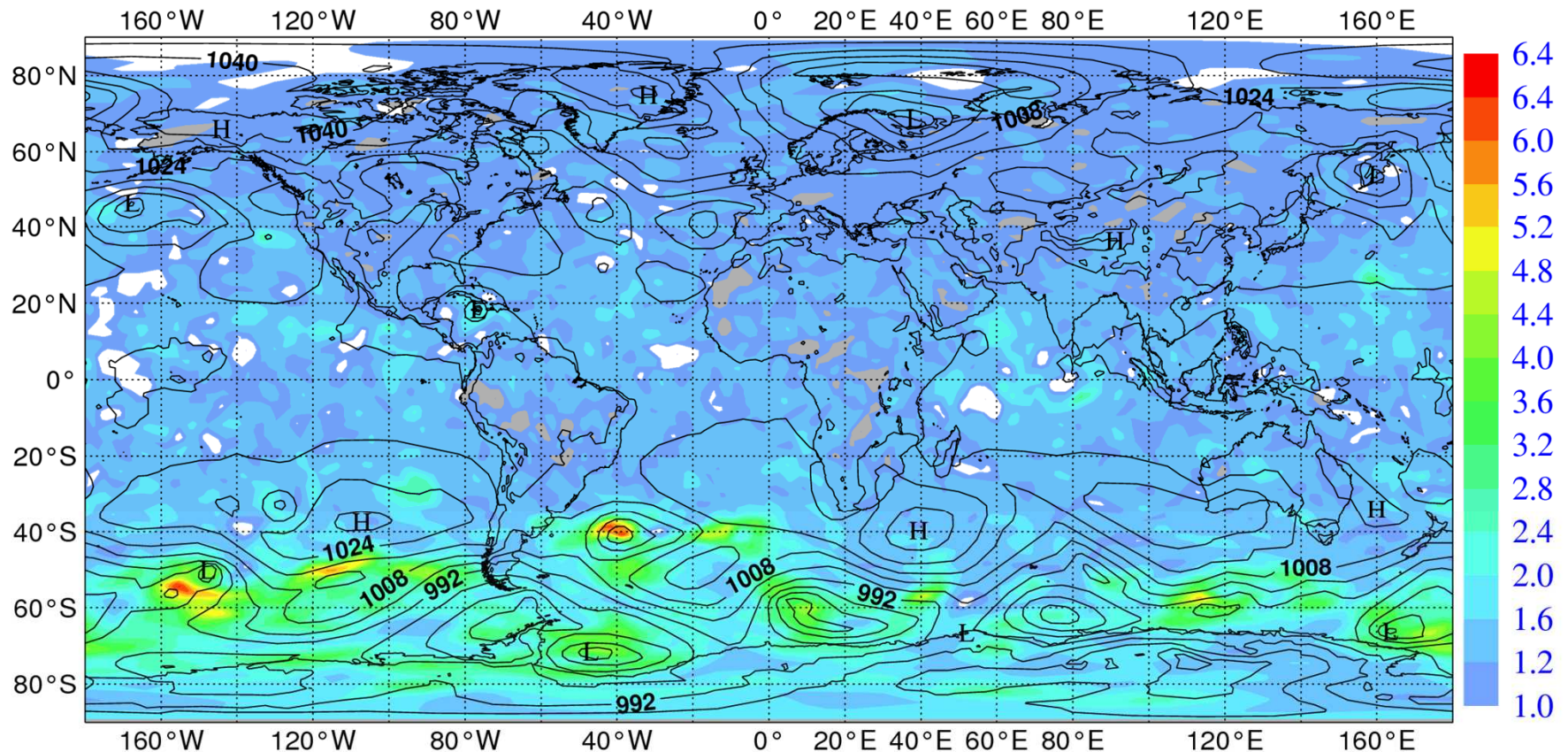
Forecast from HRES assimilation
cycle and EDA both without polar
orbiters data



Use of EDA variances in 4DVar

EDA without polar orbiters' data has larger spread than operational EDA

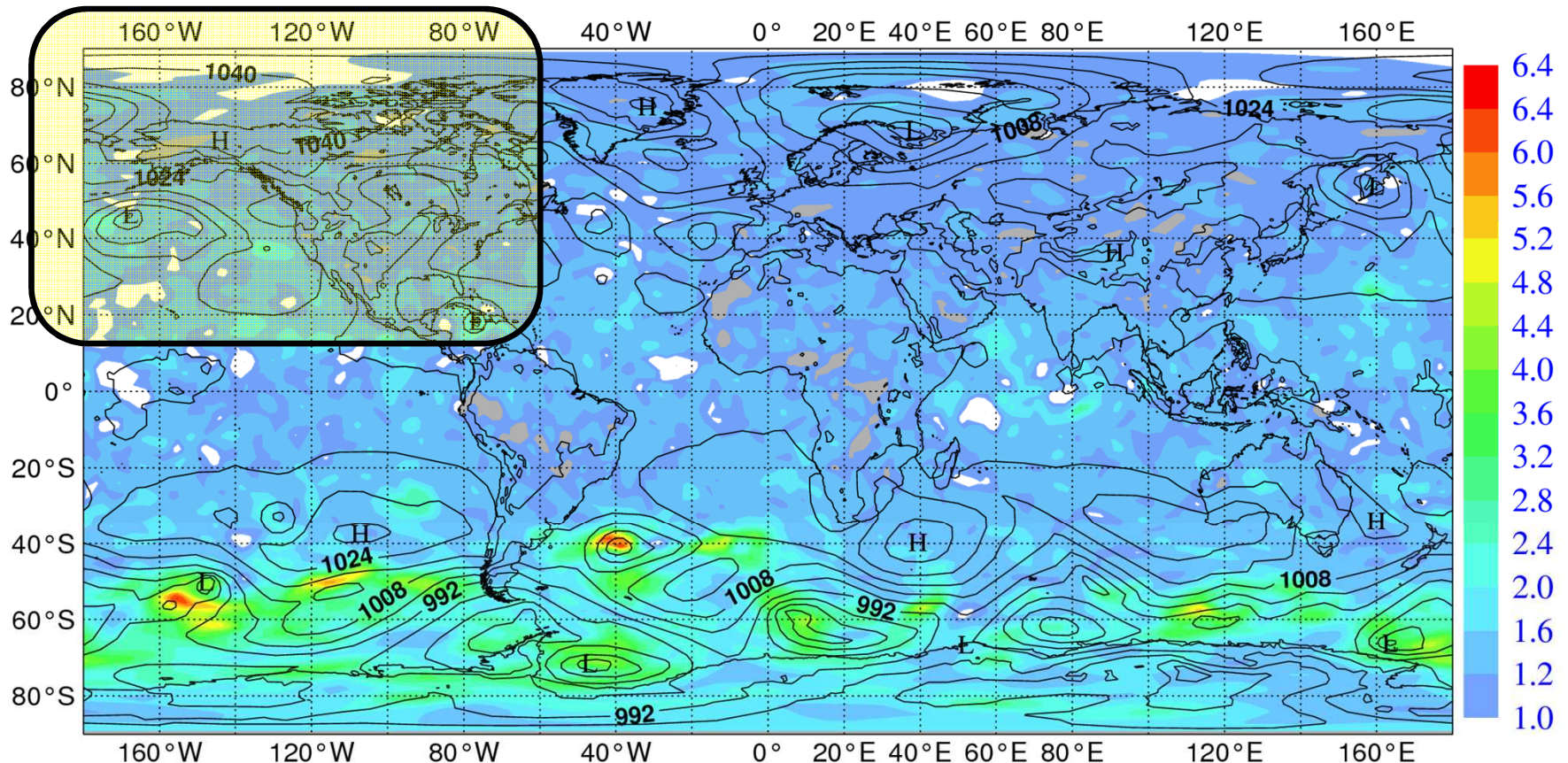
EDA spread for u-wind component at 850 hPa: No-Polar/Oper ratio



Use of EDA variances in 4DVar

EDA without polar orbiters' data has larger spread than operational EDA

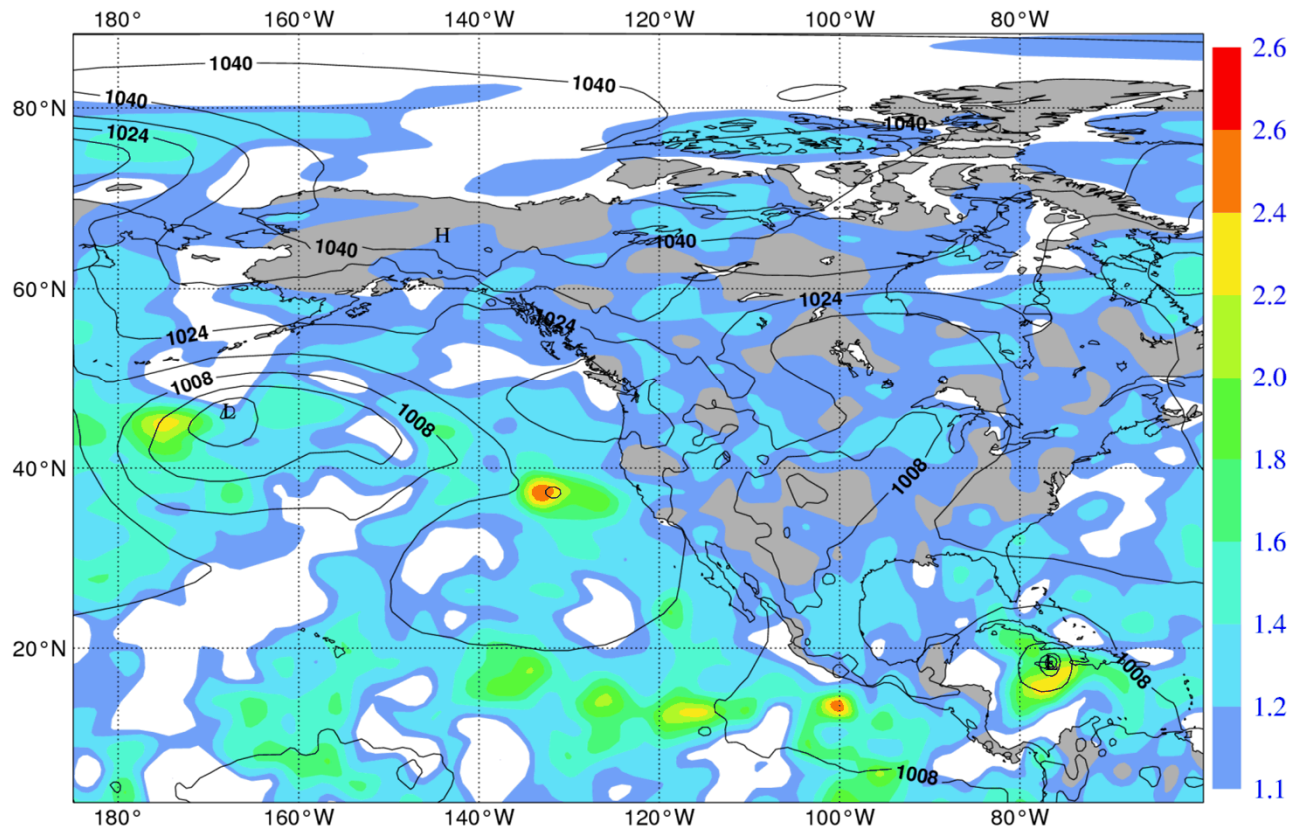
EDA spread for u-wind component at 850 hPa: No-Polar/Oper ratio



Use of EDA variances in 4DVar

EDA without polar orbiters' data has larger spread than operational EDA

EDA spread for u-wind component at 850 hPa: No-Polar/Oper ratio

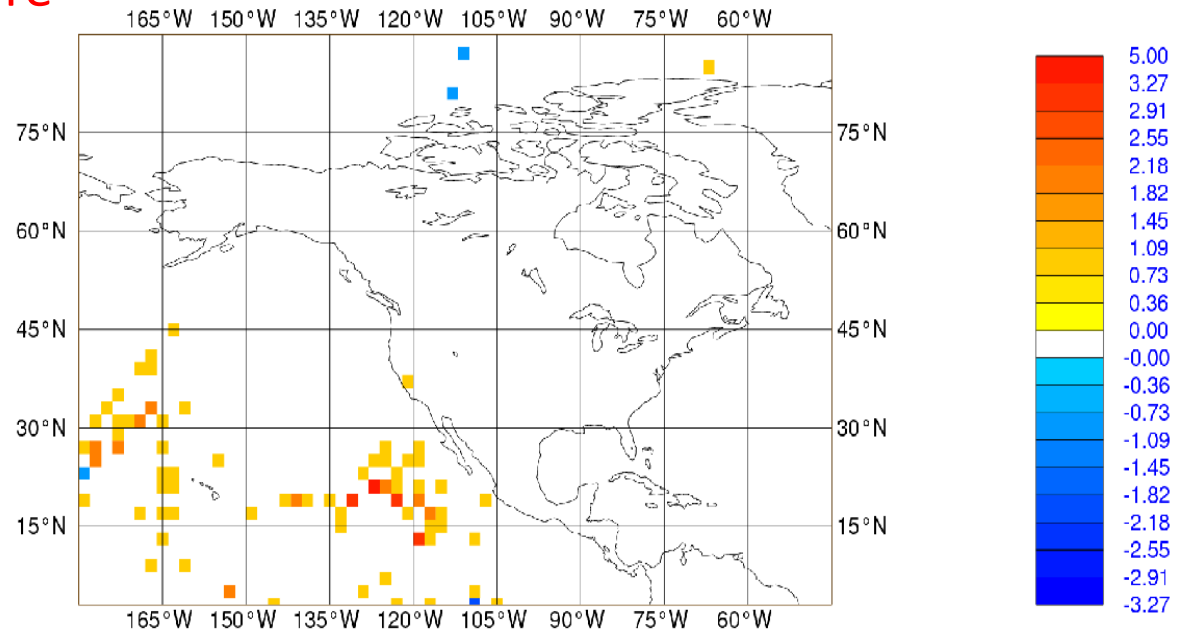


Use of EDA variances in 4DVar

EDA without polar orbiters' data has larger spread than operational EDA

This has two effects: a) Observations are more closely fit and b) More observations pass first guess quality control: $(y - \mathcal{H}(x))^2 \leq \alpha(\sigma_b^2 + \sigma_o^2)$

In this case more AMVs from geostationary satellites are assimilated



In this case more AMVs
from geostationary
satellites are assimilated

