4D-Var or Ensemble Kalman Filter?

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Chaos/Weather group at the University of Maryland:

Profs. **Hunt, Szunyogh, Kostelich,Ott**, Sauer, Yorke, Kalnay Graduated Ph.D. students: Drs. Patil, Corazza, Zimin, Gyarmati, Peña, Oczkowski, Yang, Miyoshi, Danforth, Harlim, Fertig, Li, Liu

Current Ph.D. students: Merkova, Kuhl, Baker, Kang, Hoffman, Satterfield, Penny, Singleton, Greybush

Google: chaos weather umd, or www.atmos.umd.edu/^ekalnay

Outline

- 4D-Var or EnKF? Lorenc (2003, 2004)
- Local Ensemble Transform Kalman Filter (Hunt et al.)
- Examples and some new ideas (inspired by 4D-Var):
 - QG model: 3D-Var, Hybrid, 4-DVar, LETKF (Yang et al.)
 - Estimation of model errors (Li et al.)
 - Estimation of inflation and R online (Li et al.)
 - Forecast and analysis sensitivity to observations (Liu et al.)
 - Comparison of LETKF and operational 4D-Var at JMA (Miyoshi et al.), typhoon forecasts
 - Other comparisons with real obs: current status
- Summary: Both methods give similar results
 - LETKF can benefit from ideas developed in 4D-Var research

Lorenc (2004): "Relative merits of 4DVar

He concluded: "Use both (hybrid)"

and EnKF"

+ Var

Summary of (dis-)advantages

EnKF+

Simple to design & code.

Needs smooth forecast model. Needs PF & Adjoint models. Needs a covariance model.

Generates an ensemble forecast.

Sampled covariances noisy. Can only fit N data.

Can extract info from tracers.

Nonlinear obs operators & non-Gaussian errors modelled.

Complex obs operators (eg rain) coped with automatically, but sample is then fitted by Gaussian.

Incremental balance easy

External initialisation of each forecast needed?

Accurate modelling of time-covariances only within 4D-Var window.

Covariances evolved indefinitely only if represented in ensemble.

Lorenc (2004): "Relative merits of 4DVar and EnKF"

He concluded: "Use both (hybrid)"

Questionable disadvantages of EnKF



Summary of (dis-)advantages

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Local Ensemble Transform Kalman Filter (Ott et al, 2004, Hunt et al, 2004, 2007)

Model

Observation operator

ensemble

ensemble

"observations"

ensemble

analyses

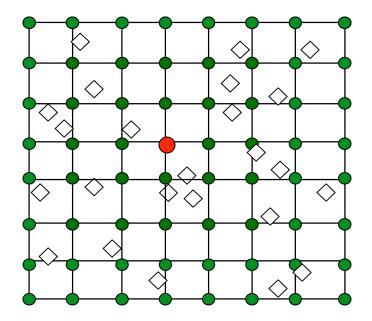
ensemble forecasts

- Model independent (black box)
- Obs. assimilated simultaneously at each grid point
- 100% parallel: very fast
- 4D LETKF extension

Localization based on observations

Perform data assimilation in a local volume, choosing observations

The state estimate is updated at the central grid red dot

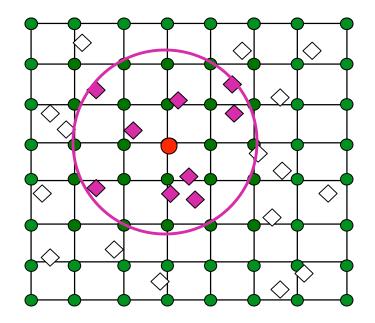


Localization based on observations

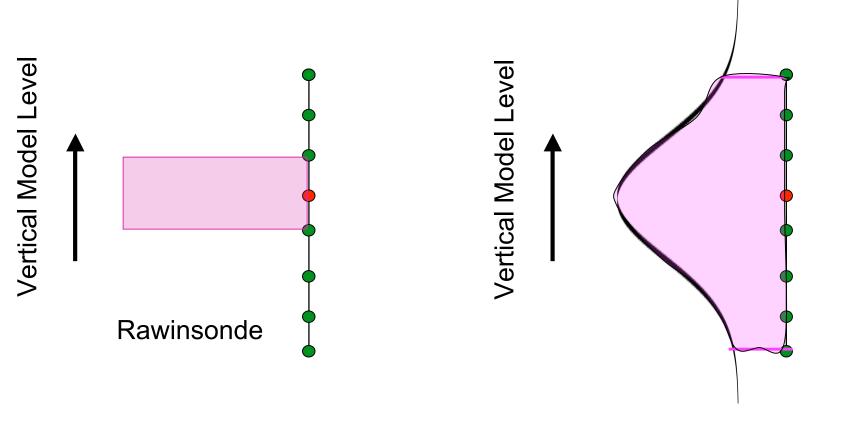
Perform data assimilation in a local volume, choosing observations

The state estimate is updated at the central grid red dot

All observations (purple diamonds) within the local region are assimilated



The localization is based on observations and can be different, e.g., satellite radiances vs. rawinsondes (Fertig et al. 2007)



Radiance weighting function

Local Ensemble Transform Kalman Filter (LETKF)

Globally:

Forecast step:
$$\mathbf{x}_{n,k}^b = M_n \left(\mathbf{x}_{n-1,k}^a \right)$$

Analysis step: construct $\mathbf{X}^b = \left[\mathbf{x}_1^b - \overline{\mathbf{x}}^b, ..., \mathbf{x}_K^b - \overline{\mathbf{x}}^b \right];$
 $\mathbf{y}_i^b = H(\mathbf{x}_i^b); \, \mathbf{Y}_n^b = \left[\mathbf{y}_1^b - \overline{\mathbf{y}}^b, ..., \mathbf{y}_K^b - \overline{\mathbf{y}}^b \right]$

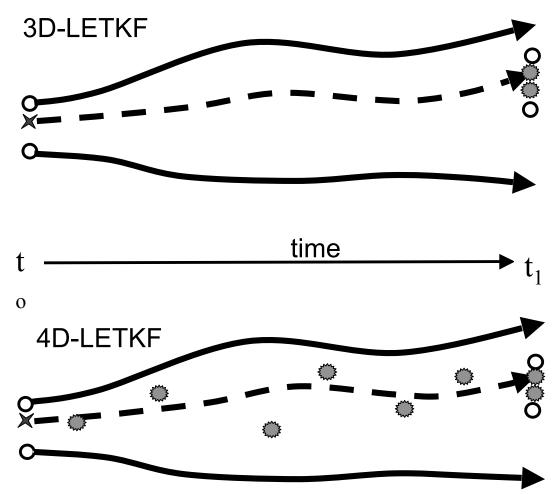
Locally: Choose for each grid point the observations to be used, and compute the local analysis error covariance and perturbations in ensemble space:

$$\tilde{\mathbf{P}}^a = \left[\left(K - 1 \right) \mathbf{I} + \mathbf{Y}^{bT} \mathbf{R}^{-1} \mathbf{Y}^b \right]^{-1}; \mathbf{W}^a = \left[\left(K - 1 \right) \tilde{\mathbf{P}}^a \right]^{1/2}$$

Analysis mean in ensemble space: $\overline{\mathbf{w}}^a = \tilde{\mathbf{P}}^a \mathbf{Y}^{bT} \mathbf{R}^{-1} (\mathbf{y}^o - \overline{\mathbf{y}}^b)$ and add to \mathbf{W}^a to get the analysis ensemble in ensemble space

The new ensemble analyses in model space are the columns of $\mathbf{X}_n^a = \mathbf{X}_n^b \mathbf{W}^a + \overline{\mathbf{x}}^b$. Gathering the grid point analyses forms the new global analyses.

LETKF chooses the linear combination of the ensemble forecasts that best fits the observations (stars)



No-cost LETKF smoother (cross): apply at t₀ the same weights found to be optimal at t₁ This works for both 3D- and 4D-LETKF

Analysis sensitivity study with LETKF (Liu) (inspired by Cardinali et al. 2004 in 4D-Var)

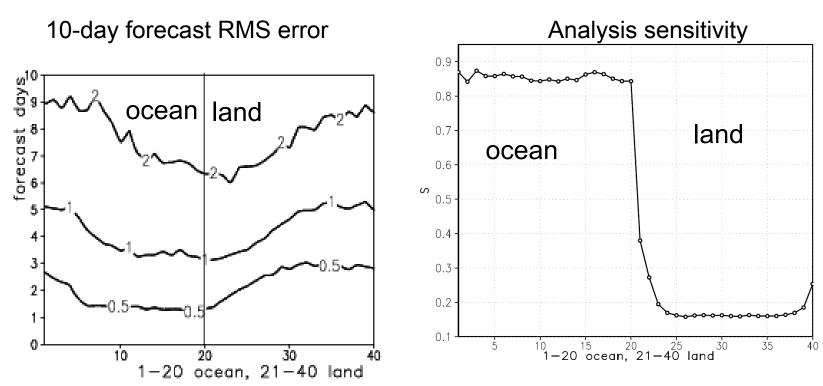
$$\mathbf{S} = \frac{\partial \mathbf{H} \mathbf{x}_a}{\partial \mathbf{y}} = \mathbf{R}^{-1} \mathbf{H} \mathbf{P}^a \mathbf{H}^T$$

It shows the analysis sensitivity with respect to:

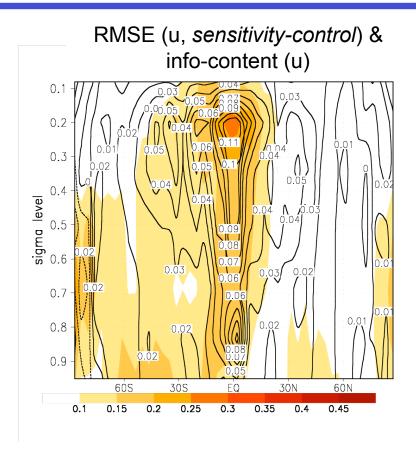
- a) different types of observations (e.g., rawinsonde, satellite)
- b) the observations in different areas (e.g., SH, NH)

Easy to compute within LETKF since Pa is known

Analysis sensitivity of adaptive observation (one obs. selected from ensemble spread method over ocean) and routine observations (every grid point over land) in Lorenz-40 variable model



- Over land, the analysis information coming from observations is only 17%.
- Over ocean, the analysis accepts about 85% of the information from the single observation.
- The analysis knows that a single adaptive observation over ocean is more important than a single observation over land.

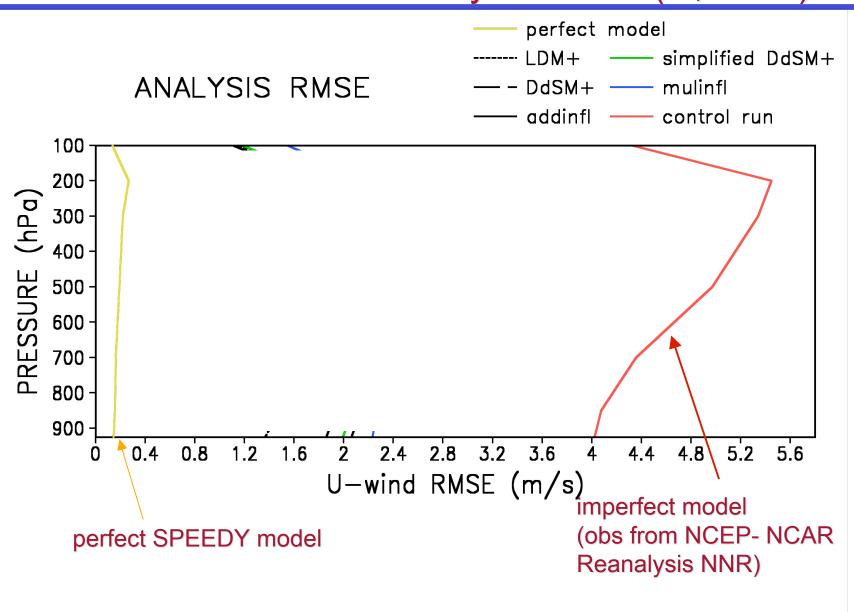


Information content qualitatively reflects the actual observation impact from datadenial experiments.

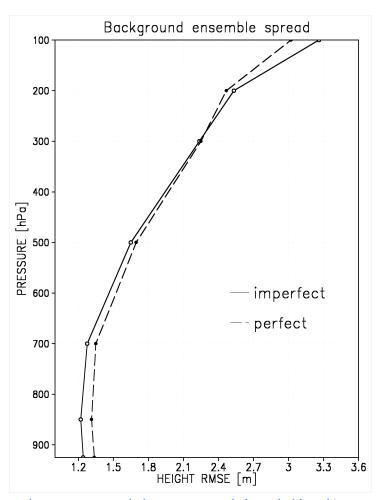
Model error: comparison of methods to correct model bias and inflation

Hong Li, Chris Danforth, Takemasa Miyoshi, and Eugenia Kalnay

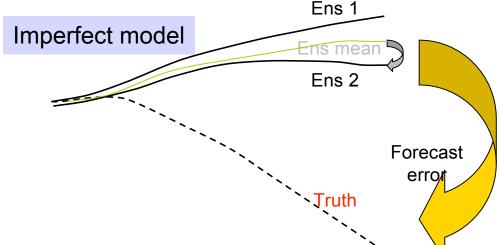
Model error: If we assume a perfect model in EnKF, we underestimate the analysis errors (Li, 2007)



— Why is EnKF vulnerable to model errors?



The ensemble spread is 'blind' to model errors



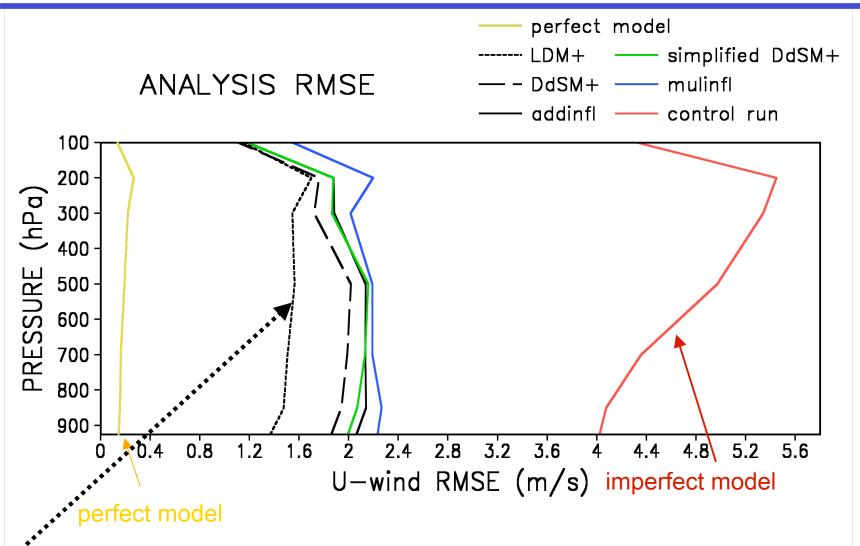
In the theory of Extended Kalman filter, forecast error is represented by the growth of errors in IC and the model errors.

$$\mathbf{P}_{i}^{f} = \mathbf{M}_{\mathbf{x}_{i-1}^{a}} \mathbf{P}_{i-1}^{a} \mathbf{M}_{\mathbf{x}_{i-1}^{a}}^{T} + \mathbf{Q}$$

➤ However, in ensemble Kalman filter, error estimated by the ensemble spread can only represent the first type of errors.

$$\mathbf{P}_i^f \in \frac{1}{k-1} \sum_{i=1}^K (x_i^f - \overline{x^f}) (x_i^f - \overline{x^f})^T$$

We compared several methods to handle bias and random model errors

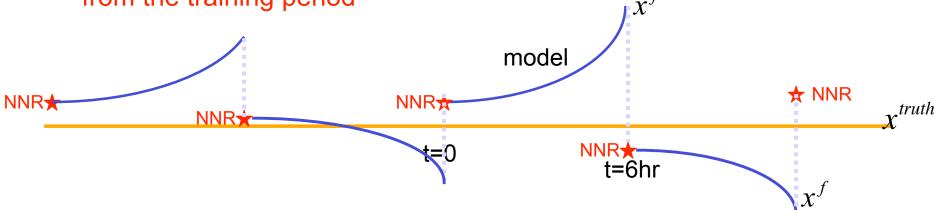


Low Dimensional Method to correct the bias (Danforth et al, 2007) combined with additive inflation

Bias removal schemes (Low Dimensional Method)

2.3 Low-dim method (Danforth et al, 2007: Estimating and correcting global weather model error. *Mon. Wea. Rev, J. Atmos. Sci., 2007*)

• Generate a long time series of model forecast minus reanalysis x_{6hr}^e from the training period

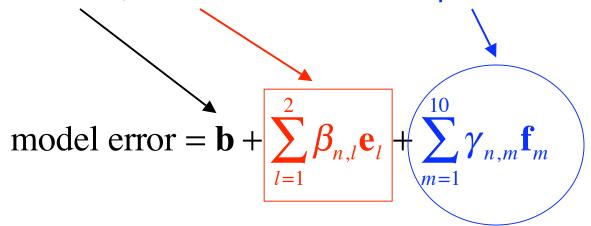


We collect a large number of estimated errors and estimate from them bias, etc.

$$\mathcal{E}_{n+1}^f = \mathbf{x}_{n+1}^f - \mathbf{x}_{n+1}^t = M(\mathbf{x}_n^a) - M(\mathbf{x}_n^t) + \mathbf{b} + \sum_{l=1}^L \beta_{n,l} \mathbf{e}_l + \sum_{m=1}^M \gamma_{n,m} \mathbf{f}_m$$
Forecast error Time-mean Diurnal due to error in IC model bias model error model error

Low-dimensional method

Include Bias, Diurnal and State-Dependent model errors:



Having a large number of estimated errors allows to estimate the global model error beyond the bias

SPEEDY 6 hr model errors against NNR (diurnal cycle)

1987 Jan 1~ Feb 15

Error anomalies

$$x_{6hr(i)}^{e} = x_{6hr}^{e} - \overline{x_{6hr}^{e}} - pc1$$

$$pc2$$

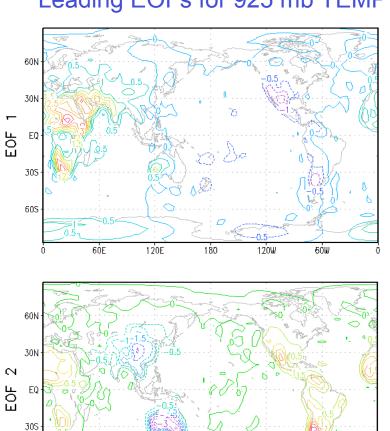
$$x_{6hr(i)}^{e} = x_{6hr}^{e} - \overline{x_{6hr}^{e}} - pc1$$

$$pc3$$

$$x_{6hr(i)}^{e} = x_{6hr}^{e} - \overline{x_{6hr}^{e}} - pc1$$

 For temperature at lower-levels, in addition to the time-independent bias, SPEEDY has diurnal cycle errors because it lacks diurnal radiation forcing

Leading EOFs for 925 mb TEMP

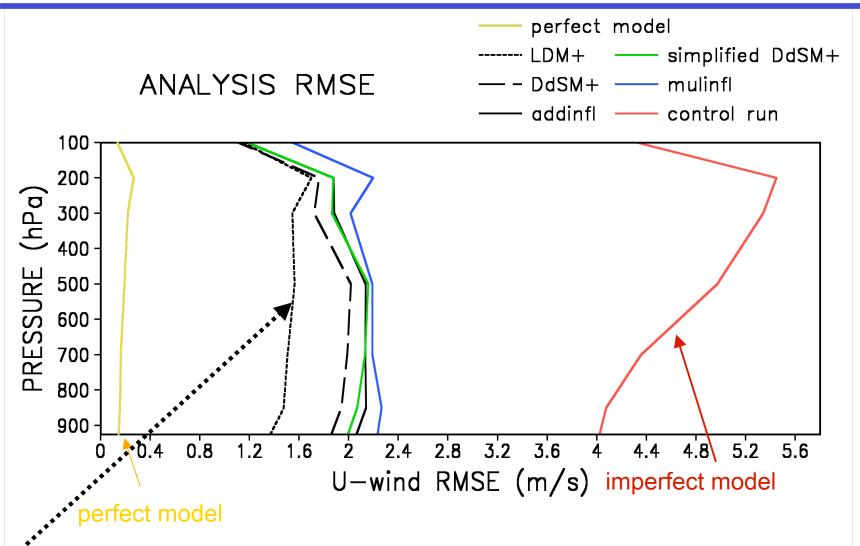


120E

180

120W

We compared several methods to handle bias and random model errors



Low Dimensional Method to correct the bias (Danforth et al, 2007) combined with additive inflation

Simultaneous estimation of EnKF inflation and obs errors in the presence of model errors

Eugenia Kalnay¹
Hong Li^{1,2}
Takemasa Miyoshi³

¹University of Maryland

²Typhoon Institute of Shanghai

³Numerical Prediction Division, JMA

We use the "observation" of inflation to update the inflation online with a simple KF (adaptive regression)

$$\Delta^{o} = \frac{(\mathbf{d}_{o-b}^{T} \mathbf{d}_{o-b}) - Tr(\mathbf{R})}{Tr(\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T})} - 1 \qquad (OMB^{2}) \qquad \begin{array}{l} \text{Assumption: } \mathbf{R} \text{ is known} \\ \text{This gives an "observation"} \\ \text{of } \Delta \end{array}$$

Online estimation: use scalar KF (adaptive regression), Kalnay 2003, App. C:

$$\Delta^a = \frac{v^o \Delta^f + v^f \Delta^o}{v^o + v^f} \qquad v^a = (1 - \frac{v^f}{v^f + v^o})v^f$$

where
$$\Delta^{f}_{t+1} = \Delta^{a}_{t}$$
 $v^{f}_{t+1} = (1+0.03)v^{a}$

This scalar KF is used for all the online estimation experiments discussed here

The method works very well to estimate the optimal inflation if \mathbf{R} is correct, but it fails if \mathbf{R} is wrong: one equation (1a) with two unknowns...

Diagnosis of observation error statistics

(Desroziers et al, 2005, Navascues et al, 2006)

Desroziers et al, 2005, introduced two new statistical relationships:

$$OMA*OMB < \mathbf{d}_{o-a}\mathbf{d}_{o-b}^T >= \mathbf{R}$$

correct if the **R** and **B** statistics are correct and errors are uncorrelated!

$$AMB*OMB < \mathbf{d}_{a-b}\mathbf{d}_{o-b}^{T} > = \mathbf{HP}^{b}\mathbf{H}^{T}$$

Writing their inner products we obtain two more equations which we can use to "observe" \mathbf{R} and Δ :

$$(\tilde{\sigma}_o)^2 = \mathbf{d}_{o-a}^T \mathbf{d}_{o-b} / p = \sum_{j=1}^p (y_j^o - y_j^a)(y_j^o - y_j^b) / p$$
 OMA*OMB

$$\Delta^{o} = \mathbf{d}_{a-b}^{T} \mathbf{d}_{o-b} / Tr(\mathbf{H} \mathbf{P}^{b} \mathbf{H}^{T}) - 1 = \sum_{j=1}^{p} (y_{j}^{a} - y_{j}^{b}) (y_{j}^{o} - y_{j}^{b}) / Tr(\mathbf{H} \mathbf{P}^{b} \mathbf{H}^{T}) - 1$$
 AMB*OMB

Diagnosis of observation error statistics

(Desroziers et al, 2005, Navascues et al, 2006)

$$\Delta^{o} = \frac{(\mathbf{d}_{o-b}^{T} \mathbf{d}_{o-b}) - Tr(\mathbf{R})}{Tr(\mathbf{H} \mathbf{P}^{b} \mathbf{H}^{T})} - 1$$

 OMB^2

$$\Delta^{o} = \sum_{j=1}^{p} (y_{j}^{a} - y_{j}^{b})(y_{j}^{o} - y_{j}^{b}) / Tr(\mathbf{HP}^{b}\mathbf{H}^{T}) - 1$$

AMB*OMB

$$(\tilde{\sigma}_o)^2 = \mathbf{d}_{o-a}^T \mathbf{d}_{o-b} / p = \sum_{j=1}^p (y_j^o - y_j^a)(y_j^o - y_j^b) / p$$

OMA*OMB

Desroziers et al. (2005) and Navascues et al. (2006) have used these relations in a diagnostic mode, from past 3D-Var/4D-Var stats. Here we use a simple KF to estimate both Δ and σ_o^2 online.

Tests within LETKF with Lorenz-40 model

Perfect model experiments. True ob error $\sigma_{o(true)}^2 = 1$ Optimally tuned $\Delta = 0.046$ rms=0.201

Right σ_o^2 , estimate inflation using OMB² or AMB*OMB: **both work**

Δ method	$oldsymbol{\sigma}^2_{o(\mathit{specified})}$	Δ	rms
OMB ²	1	0.044	0.202
AMB*OMB	1	0.042	0.202

Wrong σ_0^2 , estimate inflation using OMB² or AMB*OMB: **both fail**

$_{\Delta}$ method	$\sigma^2_{o(specified)}$	Δ	rms
OMB ²	4.0	0.021	1.635
AMB*OMB		0.033	1.523

Tests with LETKF with perfect L40 model

Now we estimate ob error and inflation simultaneously using OMB² or AMB*OMB and OMA*OMB : it works great!

R method	Δ method	Initial σ_o^2	Estimated σ_o^2	Estimated Δ	rms
	OMB^2	0.25	1.002	0.046	0.208
OMA*OMB	AMB*OMB		1.003	0.043	0.205
	OMB^2	4.0	1.000	0.046	0.202
	AMB*OMB		1.000	0.043	0.203

The question is: will this method work if the model is not perfect, i.e., if it has either random errors or biases?

Tests with LETKF with imperfect L40 model: added random errors to the model

Error	A: true $\sigma_o^2 = 1.0$		B: true $\sigma_o^2 = 1.0$		C: adaptive σ_o^2		
amplitude (random)	(tuned) constant Δ		adaptive Δ		adaptive Δ		
а	Δ	RMSE	Δ	RMSE	Δ	RMSE	σ_o^2
4	0.25	0.36	0.27	0.36	0.39	0.38	0.93
20	0.45	0.47	0.41	0.47	0.38	0.48	1.02
100	1.00	0.64	0.87	0.64	0.80	0.64	1.05

The method works quite well even with very large random errors!

Tests with LETKF with imperfect L40 model: added biases to the model

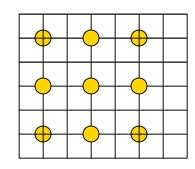
Error	A: true	$\sigma_o^2 = 1.0$	B: true	$e \sigma_o^2 = 1.0$	C: a	daptive σ_o^2	2
amplitude (bias)	(tuned) constant Δ		adaptive Δ		adaptive Δ		
α	Δ	RMSE	Δ	RMSE	Δ	RMSE	σ_o^2
1	0.35	0.40	0.31	0.42	0.35	0.41	0.96
4	1.00	0.59	0.78	0.61	0.77	0.61	1.01
7	1.50	0.68	1.11	0.71	0.81	0.80	1.36

The method works well for low biases, but fails for large biases: Model bias needs to be accounted by a separate bias correction method, not by multiplicative inflation

Tests within LETKF with SPEEDY

OBSERVATIONS

• Generated from the 'truth' plus "random errors" with error standard deviations of 1 m/s (u), 1 m/s(v), 1K(T), 10⁻⁴ kg/kg (q) and 100Pa(Ps).

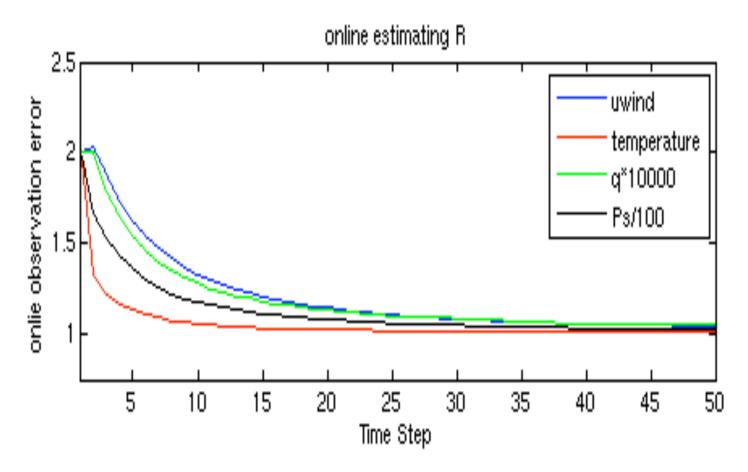


 Dense observation network: 1 every 2 grid points in x and y direction

EXPERIMENTAL SETUP

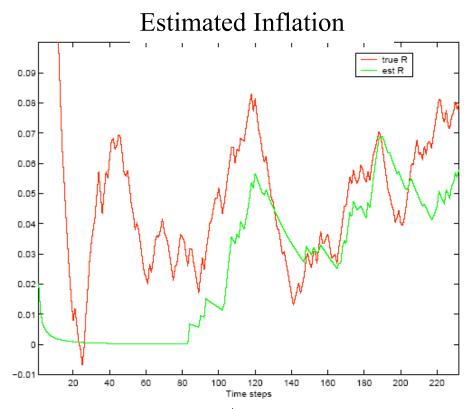
- Run SPEEDY with LETKF for two months (January and February 1982), starting from wrong (doubled) observational errors of 2 m/s (u), 2 m/s(v), 2K(T), 2*10⁻⁴ kg/kg (q) and 200Pa(Ps).
- Estimate and correct the observational errors and inflation adaptively.

online estimated observational errors



The original wrongly specified R converges to the right R quickly (in about 5-10 days)

Estimation of the inflation



Using an initially wrong R and $\,\Delta\,$ but estimating them adaptively Using a perfect R and estimating $\,\Delta\,$ adaptively

After **R** converges, they give similar inflation factors (time dependent)

2008/1/31 WCRP Conference on Reanalysis, Tokyo

Developments of a local ensemble transform Kalman filter at JMA

Takemasa Miyoshi (NPD/JMA)

Shozo Yamane (CIS, JAMSTEC), Takeshi Enomoto (ESC/JAMSTEC), Yoshiaki Sato (NCEP and NPD/JMA), Takashi Kadowaki (NPD/JMA), Ryouta Sakai (NPD/JMA), and Masahiro Kazumori (NPD/JMA)

A core concept of EnKF

Complementary relationship between data assimilation and ensemble forecasting



This cycle process = EnKF

Analyze with the flow-dependent forecast error, ensemble forecast with initial ensemble reflecting the analysis error

Advantages of EnKF

- Automatic estimation of flow-dependent error covariance (background and analysis)
 - Automatic adjustment to observing density in each era
 - Large **B** in the past (sparse observations)
 - Small **B** in the present (dense observations)
 - Quantitative information of analysis uncertainties
- Generally model-independent
 - Relatively easy application to many kinds of dynamical models

EnKF vs. 4D-Var

	EnKF	4D-Var		
"advanced" method?	Y	Y		
Simple to code?	Y	N (e.g., Minimizer)		
Adjoint model?	N	Y		
Observation operator	Only forward	Adjoint required		
	(e.g., TC center)			
Asynchronous obs?	Y (4D-EnKF)	Y (intrinsic)		
Initialization after analysis?	N?	Y		
Analysis errors?	Y (ensemble ptb)	N		
Limitation	ensemble size	Assim. window		
		EnKF with infinite ensemble size and 4D-Var with infinite window would be equivalent (linear perfect model).		

ALERA

(AFES-LETKF Experimental Ensemble Reanalysis)

data are now available online for free!!

http://www3.es.jamstec.go.jp/

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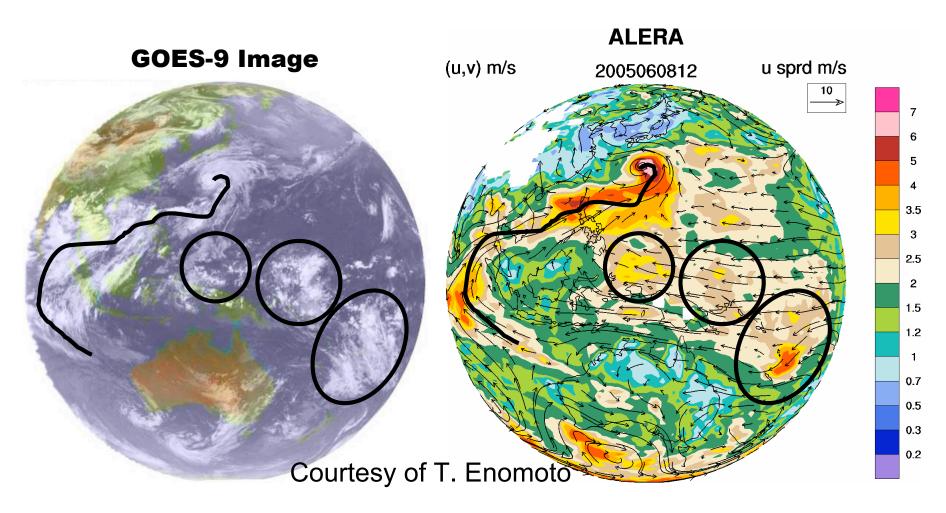
Ensemble reanalysis dataset for over 1.5 years since May 1, 2005

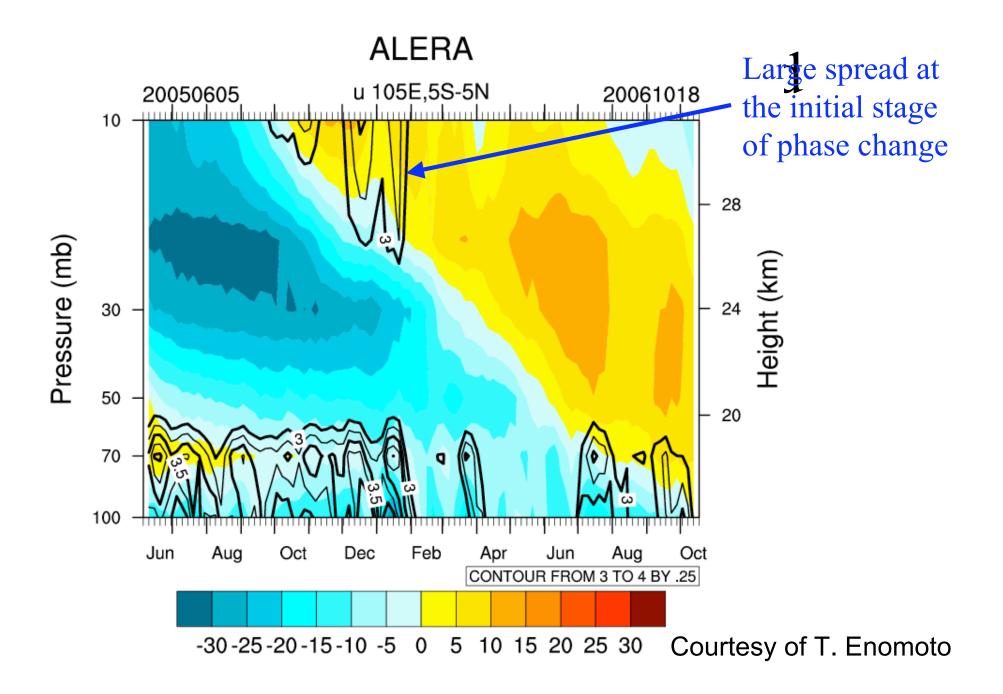
- >40 ensemble members
- >ensemble mean
- >ensemble spread

Available 'AS-IS' for free ONLY for research purposes Any feedback is greatly appreciated.

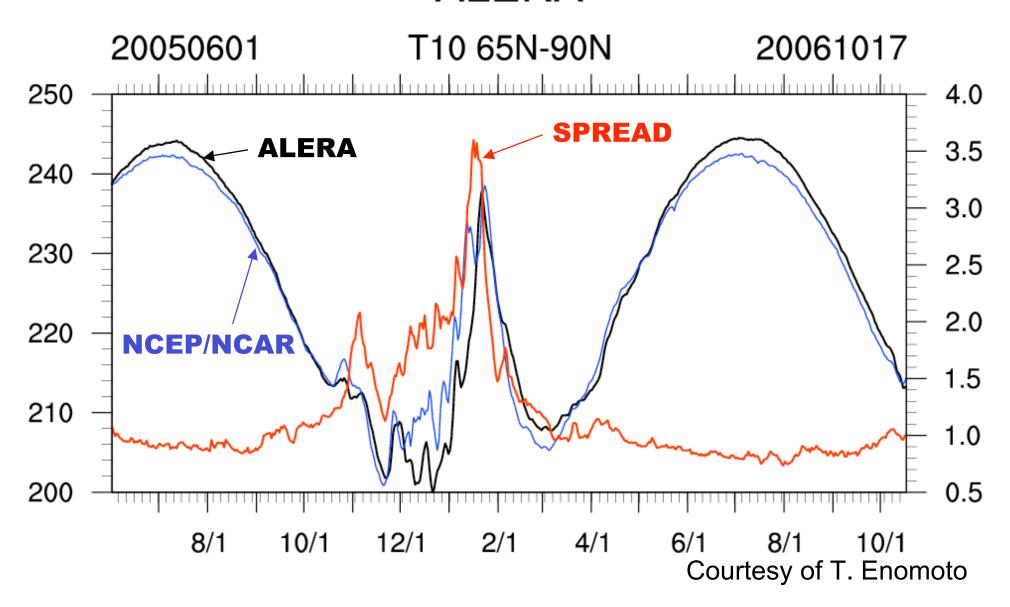
Analyzing the analysis errors

- EnKF provides not only analysis itself but also the analysis errors (or uncertainties of the analysis)
- What is the dynamical meaning of the analysis errors?

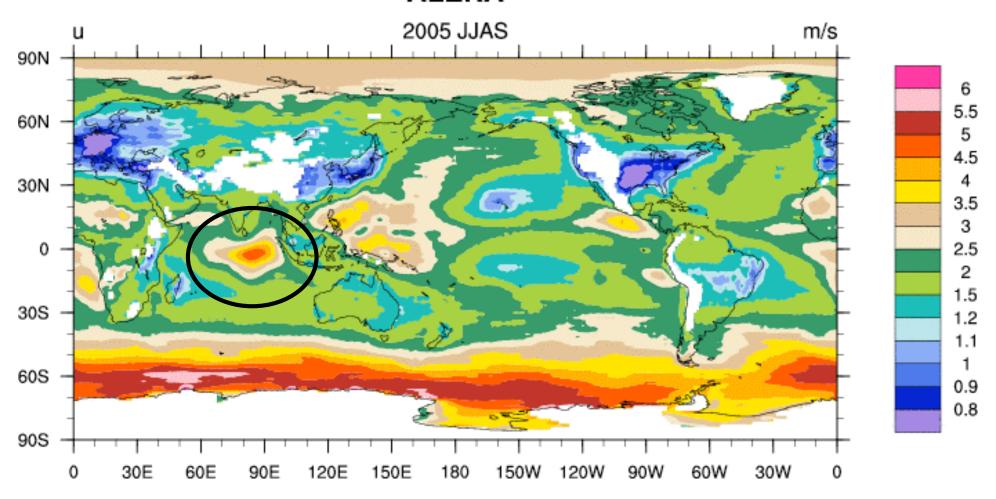




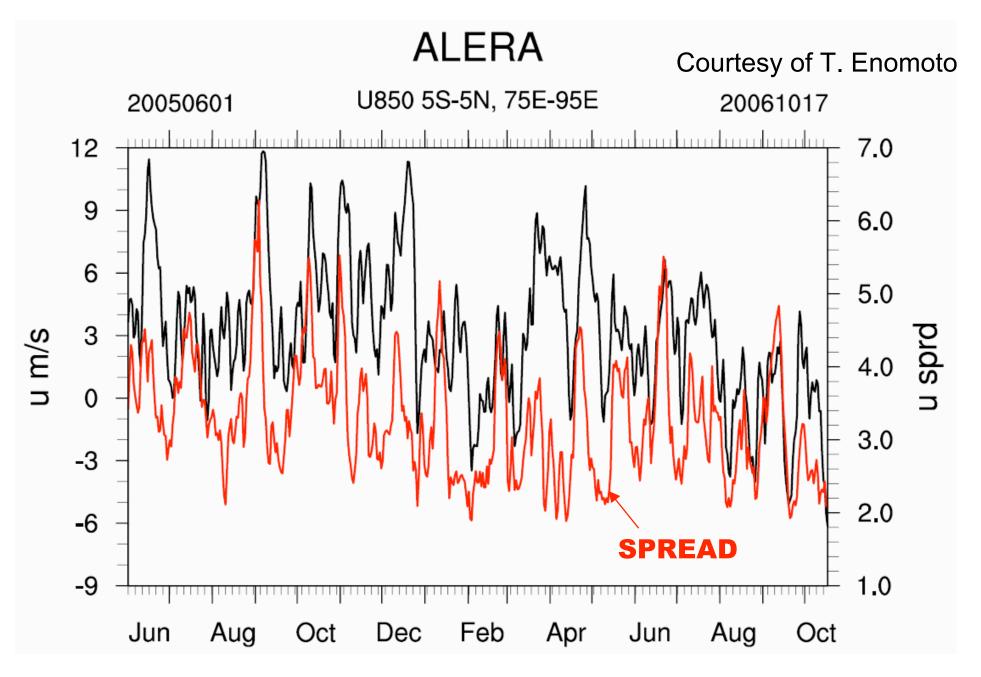
ALERA



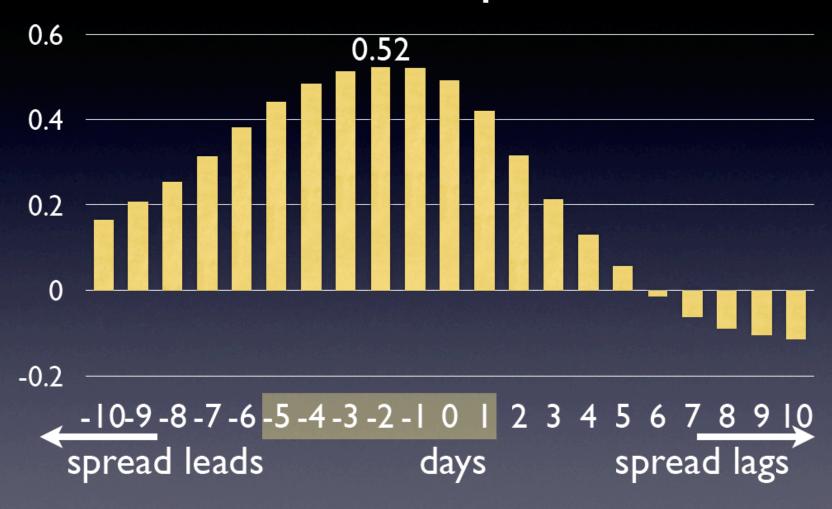
Large spread in tropical lower



Tropical lower wind and the spread



Lag correlation between mean and spread



Courtesy of T. Enomoto

Summary so far (Miyoshi)

- Ensemble spread represents errors well.
- There seems to be dynamical meanings of analysis ensemble spread, which could be investigated in various scales.
- Long-term ensemble reanalysis...
 - would be more accurate because of the automatic adaptation of
 B appropriate for each observing system
 - would have a great potential to promote research using the analysis errors
- It is important to develop with a quasi-operational environment

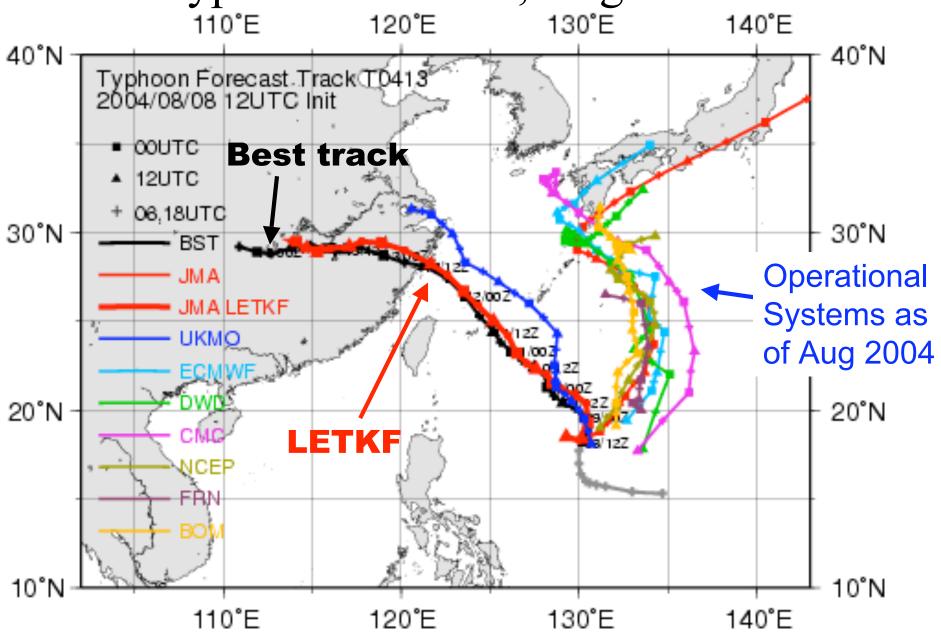
LETKF developments at JMA

- LETKF (Local Ensemble Transform Kalman Filter, U of MD, Hunt et al. 2007; Ott et al. 2004) has been applied to 3 models
 - AFES (AGCM for the Earth Simulator)
 Miyoshi and Yamane, 2007: Mon. Wea. Rev., 3841-3861.
 - Miyoshi, Yamane, and Enomoto, 2007: SOLA, 45-48.

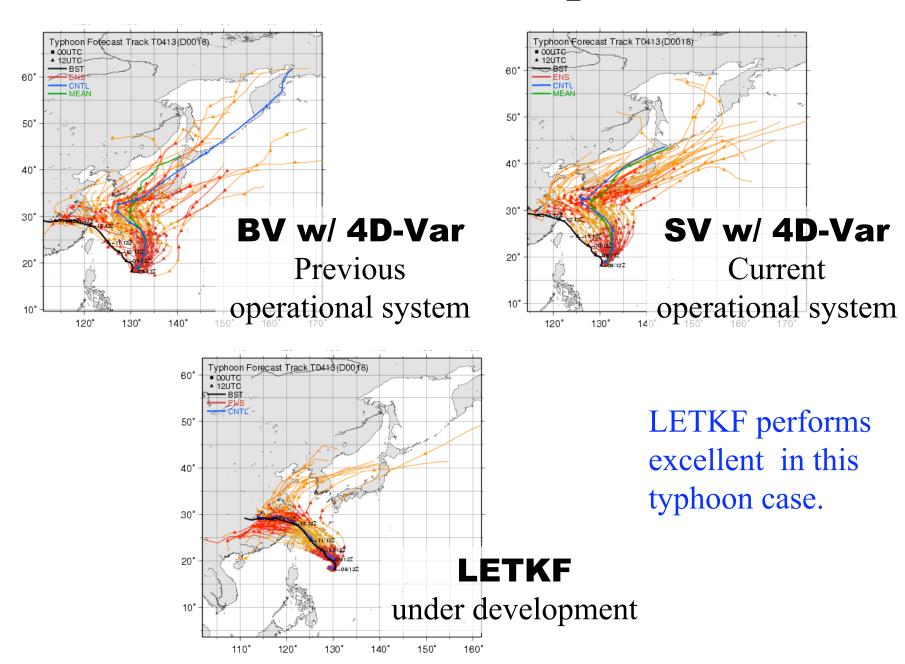
 NHM (JMA nonhydrostatic model)
 - GSM (JMA global spectral model)
 Miyoshi and Aranami, 2006: SOLA, 128-131

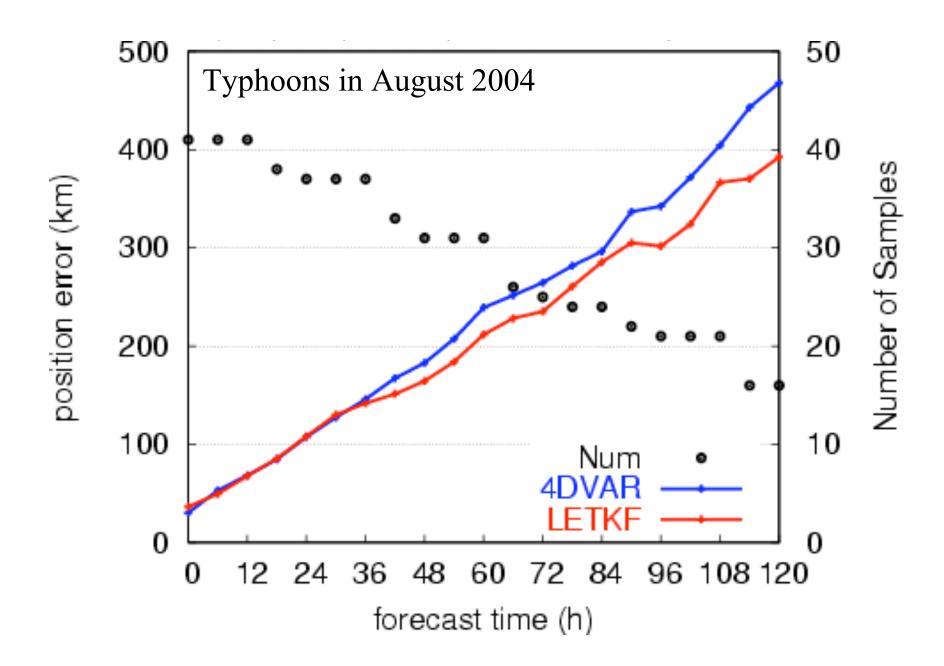
Miyoshi and Sato, 2007: SOLA, 37-40.

Typhoon Rananim, August 2004



TC track ensemble prediction





Improvement (%) relative to 4D-Var

	PseaSurf	T850	Z500	Wspd850	Wspd250
Global	-9.00	-10.45	-10.64	2.38	0.13
N. Hem.	-4.47	-2.95	-1.72	3.74	0.66
Tropics	0.48	_11.66	_17.60	11.69	9.88
S. Hem.	-10.90	-14.51	-13.00	-1.52	-3.81

Apply adaptive bias correction

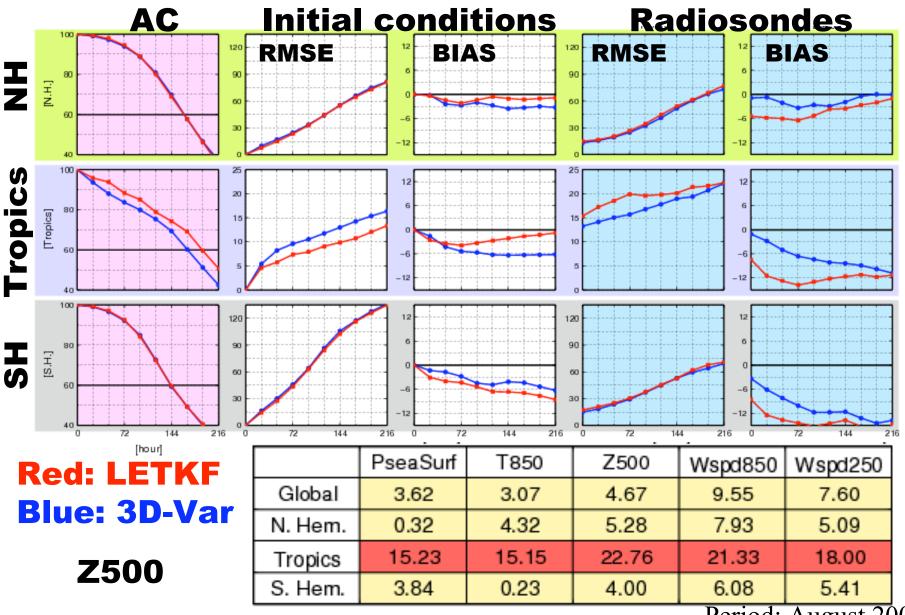
	PseaSurf	T850	Z500	Wspd850	Wspd250
Global	-6.19	-4.36	-5.71	3.66	1.32
N. Hem.	-4.18	1.12	0.91	3.98	0.57
Tropics	6.86	3.39	3.09	14.07	10.21
S. Hem.	-7.60	-8.91	-7.91	-0.08	-1.62

Some bugs fixed in surface emissivity calculation

	PseaSurf	T850	Z500	Wspd850	Wspd250
Global	-5.21	-2.33	-4.21	3.94	1.73
N. Hem.	-3.89	2.06	1.32	4.30	1.30
Tropics	7.05	6.49	7.44	13.58	9.57
S. Hem.	-6.35	-6.47	-6.20	0.39	-1.14

Period: August 2004

Comparison with 3D-Var



Period: August 2004

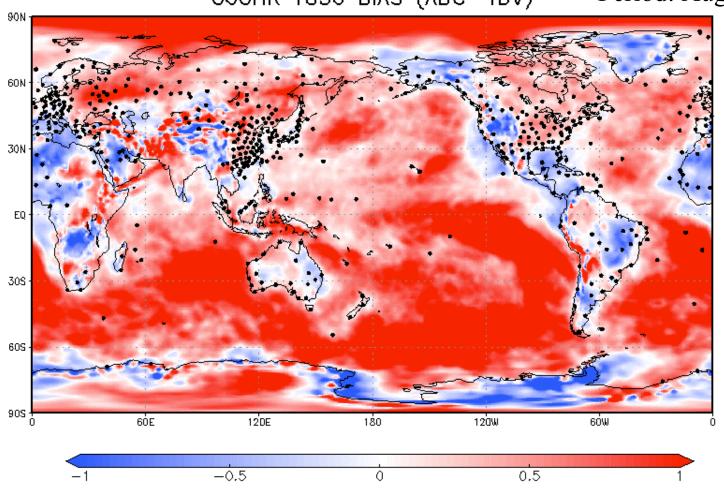
Computational time

LETKF	4D-Var
11 min x 60 nodes	17 min x 60 nodes
5 min for LETKF	
6 min for 9-hr ensemble forecasts	
TL319/L60/M50	Inner: T159/L60
	Outer: TL959/L60

Estimated for a proposed next generation operational condition 6 min (measured) x 8 nodes for LETKF with TL159/L40/M50

Computation of LETKF is reasonably fast, good for the operational use.

850 hPa Temperature bias of (LETKF – 4D-Var) 000HR T850 BIAS (ABC-4DV) Period: August 2004



Summary (Miyoshi)

• Relative forecast scores (August 2004)

NH	LETKF \sim or $>$ 4D-Var $>>$ 3D-Var
Tropics	LETKF >> 4D-Var >> 3D-Var
SH	4D-Var >> LETKF > 3D-Var

- Surface pressure forecasts in the extratropics need to be improved
- SH forecasts need to be improved
 - Positive bias in lower tropospheric temperature over ocean

Summary

- Both 4D-Var and EnKF are similar and better than 3D-Var
- 4D-Var with perfect model and long windows is better than EnKF (but expensive).
- A 3D-Var hybrid with BVs improves at low cost.
- LETKF can assimilate asynchronous obs just as 4D-Var, simple no-cost smoother.
- EnKF does not require adjoint of the NWP model (or the observation operator), or simplifications of the physics.
- Can estimate R and inflation online
- Ideal for adaptive observations. Can compute obs sensitivity
- Methods developed for 4D-Var can be adapted to LETKF
- Free 6 hr forecasts in an ensemble operational system
- Provides optimal initial ensemble perturbations: $\sum \delta \mathbf{x}_i^a \delta \mathbf{x}_i^{aT} = \mathbf{A}$
- More operational testing is needed

Discussion: 4D-Var vs. EnKF "war"

- Correcting the bias with a simple low-dim method (Danforth et al. 2007) and combining it with additive inflation should effectively deal with both systematic and random model errors. But it needs an "unbiased" reanalysis.
- We should be able to adopt some simple strategies to capture the advantages of 4D-Var:
 - Smoothing and running in place
 - A simple outer loop to deal with nonlinearities
 - Adjoint sensitivity without adjoint model
 - Coarse resolution analysis without degradation
 - **–** ...
- It seems like there is nothing that 4D-Var can do that 4D-LETKF cannot do as well, usually simpler, cheaper and better.