

Accounting for an imperfect model in 4D-Var

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- Introduction
- Weak constraint 4D-Var
- Model error covariance matrix
- Some results
- Future work

4D Variational Data Assimilation

Variational data assimilation is based on the minimisation of:

$$\begin{aligned} J(x) &= \frac{1}{2} [\mathcal{H}(x) - y]^T R^{-1} [\mathcal{H}(x) - y] \\ &+ \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \frac{1}{2} \mathcal{F}(x)^T C^{-1} \mathcal{F}(x) \end{aligned}$$

- x is the 4D state of the atmosphere over the assimilation window.
- \mathcal{H} is a 4D observation operator, accounting for the time dimension.
- \mathcal{F} represents the remaining theoretical knowledge after background information has been accounted for (balance, DFI...).
- Control variable reduces to x_0 using the relation: $x_i = \mathcal{M}_i(x_{i-1})$.
- Used in operational 4D-Var implementations.
- Model \mathcal{M} verified exactly although it is not perfect...

Weak constraint 4D-Var

- The model can be imposed as a constraint in the cost function, in the same way as other sources of information:

$$\mathcal{F}_i(x) = x_i - \mathcal{M}_i(x_{i-1})$$

- Model error η is defined as: $\eta_i = x_i - \mathcal{M}_i(x_{i-1})$
- The cost function becomes:

$$\begin{aligned} J(x) &= \frac{1}{2} \sum_{i=0}^n [\mathcal{H}(x_i) - y_i]^T R_i^{-1} [\mathcal{H}(x_i) - y_i] \\ &+ \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \frac{1}{2} \sum_{i=1}^n \eta_i^T Q_i^{-1} \eta_i \end{aligned}$$

- Model error covariance matrix Q has to be defined.
- Strong constraint 4D-Var is $\mathcal{F}_i(x) \equiv 0$ i.e. $\eta \equiv 0$ (perfect model).

Control Variable in 4D-Var

4D-Var
 x_0
 $x_i = \mathcal{M}_i(x_{i-1})$
 \Downarrow
 3D Initial
 Condition

4D-Var $_x$
 x
 $x_i \approx \mathcal{M}_i(x_{i-1})$
 \Downarrow
 4D Model
 Trajectory

4D-Var $_{\eta}$
 x_0, η
 $x_i = \mathcal{M}_i(x_{i-1}) + \eta_i$
 \Downarrow
 3D I.C. + Model
 Error Forcing

4D-Var $_{\beta}$
 x_0, β
 $x_i = \mathcal{M}_{i,0}(x_0) + \beta_i$
 \Downarrow
 3D I.C. + Model
 Bias

Model Error Forcing Control Variable

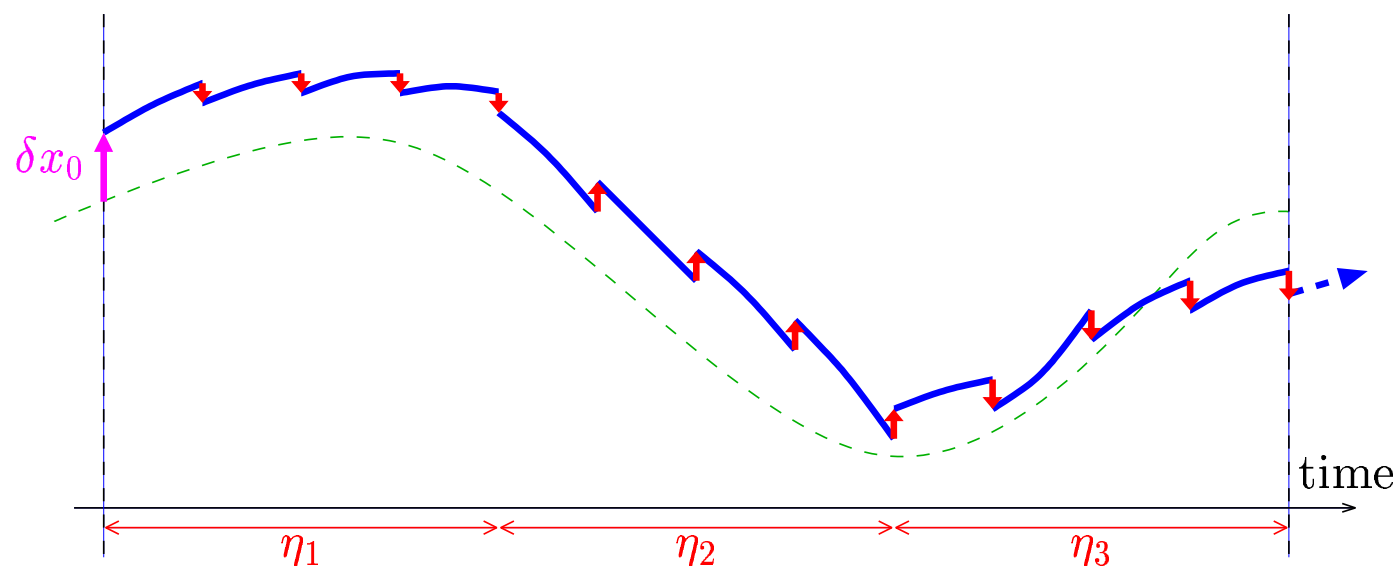
4D-Var with Model Error Forcing

$$J(x_0, \eta) = \frac{1}{2} \sum_{i=0}^n [\mathcal{H}(x_i) - y_i]^T R_i^{-1} [\mathcal{H}(x_i) - y_i] \\ + \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \eta^T Q^{-1} \eta$$

with $x_i = \mathcal{M}_i(x_{i-1}) + \eta_i$.

- The *usual* model error term in 4D-Var.
- η_i is a 3D atmospheric state,
- η_i represents the instantaneous model error,
- η is constrained by the fact that it is propagated by the model.

4D-Var with Model Error Forcing



- TL and AD models can be used with little modification,
- Information is propagated between observations and IC control variable by TL and AD models.

Model Error Forcing: Properties

$$J'' = \begin{pmatrix} B^{-1} & & & 0 \\ & Q_1^{-1} & & \\ & & \ddots & \\ 0 & & & Q_n^{-1} \end{pmatrix} + \begin{pmatrix} H_{0,n}^T R_0^{-1} H_{0,n} & & & 0 \\ & H_{1,n}^T R_1^{-1} H_{1,n} & & \\ & & \ddots & \\ 0 & & & H_n^T R_n^{-1} H_n \end{pmatrix}$$

- Hessian of the preconditioned problem:

$$I + B^{T/2} H_{0,n}^T R_0^{-1} H_{0,n} B^{1/2}$$

$$I + Q_i^{T/2} H_{i,n}^T R_i^{-1} H_{i,n} Q_i^{1/2}$$

- Largest eigenvalue:

$$\lambda_{max} \approx 1 + 2n_{obs} \max [(\sigma_b/\sigma_o)^2, (\sigma_q/\sigma_o)^2]$$

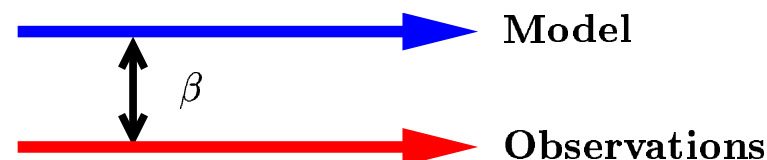
- This is similar to strong constraint 4D-Var.

Model Bias Control Variable

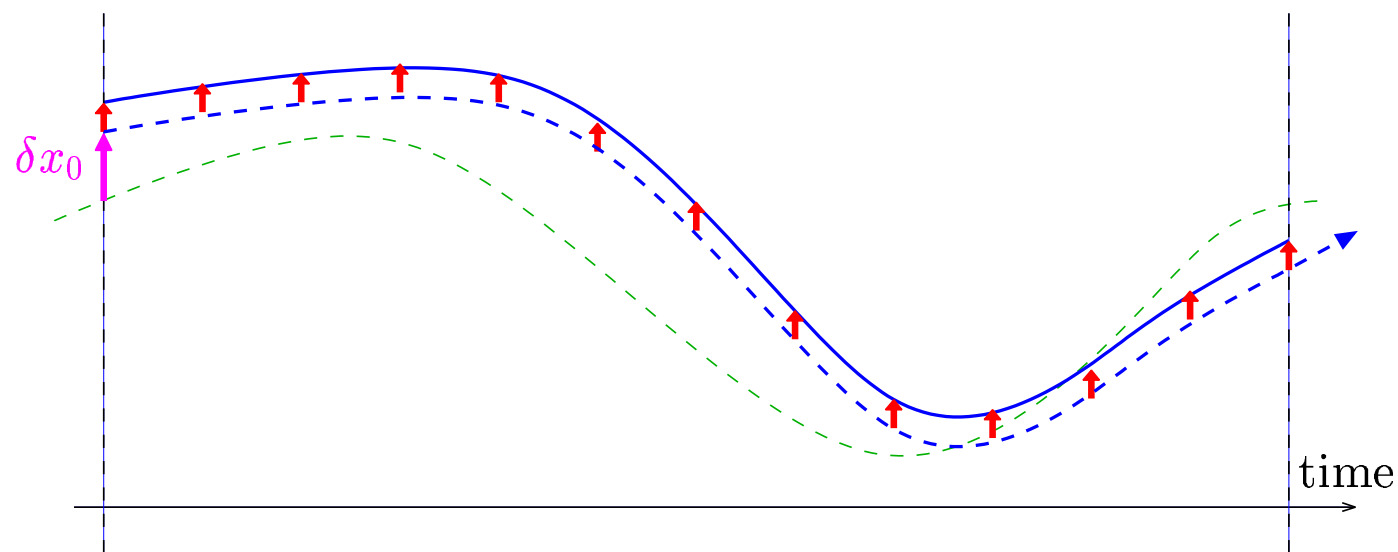
4D-Var with Model Bias

$$\begin{aligned}
 J(x_0, \beta) &= \frac{1}{2} \sum_{i=0}^n [\mathcal{H}(x_i^m + \beta_i) - y_i]^T R_i^{-1} [\mathcal{H}(x_i^m + \beta_i) - y_i] \\
 &+ \frac{1}{2} (x_0 - x_b)^T B^{-1} (x_0 - x_b) + \beta^T Q_\beta^{-1} \beta \\
 &\text{with } x_i^m = \mathcal{M}_{i,0}(x_0).
 \end{aligned}$$

- β_i is a 3D atmospheric state,
- The model is not perturbed,
- β sees global (model – all observations) bias,
- Does not correct for bias of one subset of observations against another subset of observations.



4D-Var with Model Bias



- Bias added to forecast at post-processing stage,
- Makes sense if β is slowly varying or constant ($\beta_i = \beta$),
- Information is propagated between observations and IC control variable by TL and AD models (not modified).

Model Bias: Properties

$$J'' = \begin{pmatrix} B^{-1} & 0 \\ 0 & Q_{\beta}^{-1} \end{pmatrix} + \begin{pmatrix} H^T R^{-1} H & 0 \\ 0 & H^T R^{-1} H \end{pmatrix}$$

- Change of variable: $\chi_0 = B^{-1/2}x_0$ and $\chi_1 = Q_{\beta}^{-1/2}\beta$,

$$\hat{J}'' = \begin{pmatrix} I + B^{T/2}H^T R^{-1}HB^{1/2} & 0 \\ 0 & I + Q_{\beta}^{T/2}H^T R^{-1}HQ_{\beta}^{1/2} \end{pmatrix}$$

- Largest eigenvalue: $\lambda_{max} \approx 1 + 2n_{obs} \max [(\sigma_b/\sigma_o)^2, (\sigma_{\beta}/\sigma_o)^2]$,
- Model bias is represented by additional parameters, without entering the model equations,
- Optimisation problem is very similar to strong constraint 4D-Var.

Model State Control Variable

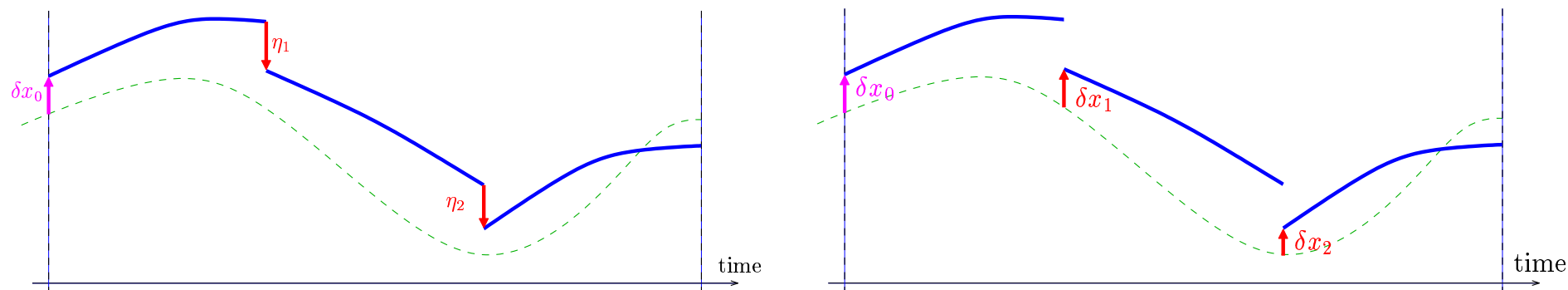
Model State Control Variable

- Use $\{x_i\}_{i=0,\dots,n}$ as the control variable.
- Incremental cost function:

$$\begin{aligned}
 J(\delta x) &= \frac{1}{2}(\delta x_0 - b)^T B^{-1}(\delta x_0 - b) + \frac{1}{2} \sum_{i=0}^n (H\delta x_i - d_i)^T R_i^{-1}(H\delta x_i - d_i) \\
 &+ \frac{1}{2} \sum_{i=1}^n (q_i + M_{i-1}\delta x_{i-1} - \delta x_i)^T Q_i^{-1}(q_i + M_{i-1}\delta x_{i-1} - \delta x_i)
 \end{aligned}$$

where $b = x^g - x_b$, $d_i = \mathcal{H}(x_i^g) - y_i$ and $q_i = \mathcal{M}_{i-1}(x_{i-1}^g) - x_i^g$.

Model State Control Variable



Forcing Control Variable

Model State Control Variable

- Model integrations within each time-step (or sub-window) are independent:
 - Information is not propagated across sub-windows by TL/AD models,
 - Natural parallel implementation (in theory...).
- Tangent linear and adjoint models:
 - can be used without modification,
 - propagate information between observations and control variable within each sub-window.

Model State Control Variable: Properties

- Preconditioning with $B^{-1/2}, Q_1^{-1/2}, \dots, Q_n^{-1/2}$
- The Hessian of the preconditioned cost function is:

$$\hat{J}'' = \begin{pmatrix} I + M_1^T M_1 & -M_1^T & & 0 \\ -M_1 & I + M_2^T M_2 & -M_2^T & \\ & -M_2 & I + M_3^T M_3 & \\ & & & I + M_n^T M_n & -M_n^T \\ 0 & & & -M_n & I \end{pmatrix} + \hat{J}_o''$$

- The off-diagonal terms propagate the information between the sub-windows.

Model State Control Variable: Properties

- Over one time step, $M_i \approx I$:

$$\hat{J}'' \approx \begin{pmatrix} 2I & -I & & & 0 \\ -I & 2I & -I & & \\ & -I & \ddots & \ddots & \\ & & \ddots & 2I & -I \\ 0 & & & -I & I \end{pmatrix} + \hat{J}_o''$$

- The largest eigenvalue is:

$$\lambda_{max} \approx 4 + 2n_{obs}/n \max [(\sigma_b/\sigma_o)^2, (\sigma_q/\sigma_o)^2]$$

- Approximately the same as the maximum eigenvalue of strong constraint 4D-Var for the sub-windows.
- But...

Model State Control Variable: Properties

- Smallest eigenvalue:

$$\lambda_{min} \propto 1/n^2$$

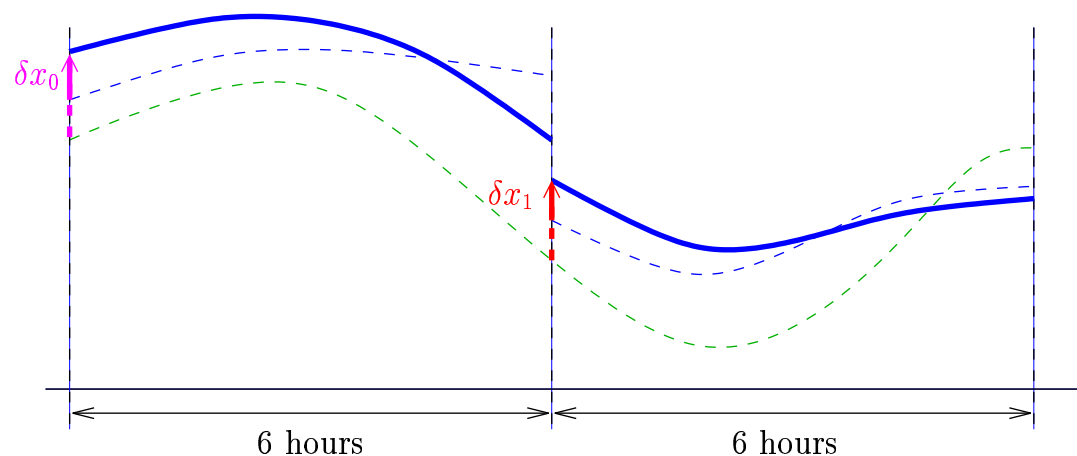
- Condition number:

$$\kappa \approx 2 n n_{obs} (\sigma_q/\sigma_o)^2$$

- Larger than for strong constraint 4D-Var,
 - Increases with the number of sub-windows (it takes n iterations to propagate information).
- Simplified Hessian of the cost function
 - can be used as preconditioner,
 - \approx Laplacian operator: small eigenvalues are obtained for constant perturbations which might be well observed and project onto eigenvectors of J_o ” associated with large eigenvalues.

Weak Constraint 4D-Var: Examples

- 6-hour sub-windows:

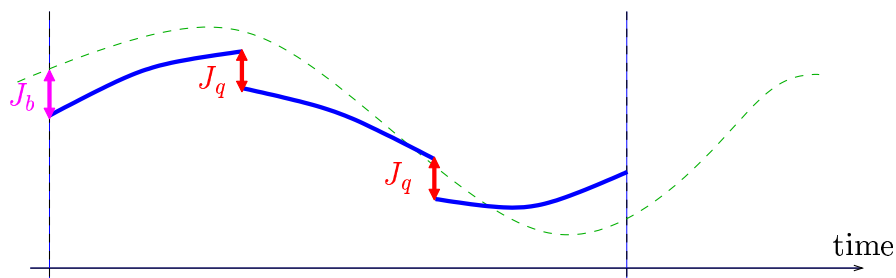


- Better than 6-hour 4D-Var: two cycles are coupled through J_q ,
- Better than 12-hour 4D-Var: more information (imperfect model), more control,
- It makes more sense to use $Q = \alpha B$ in that case.

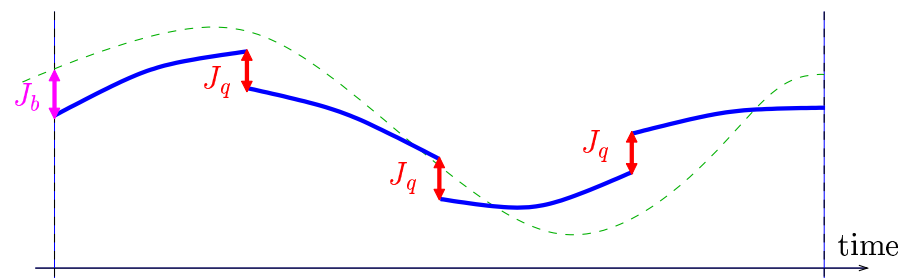
- One time step sub-windows:

- Each assimilation problem is instantaneous = 3D-Var,
- Equivalent to a string of 3D-Var problems coupled together and solved as a single minimisation problem,
- Approximation can be extended to non instantaneous sub-windows.

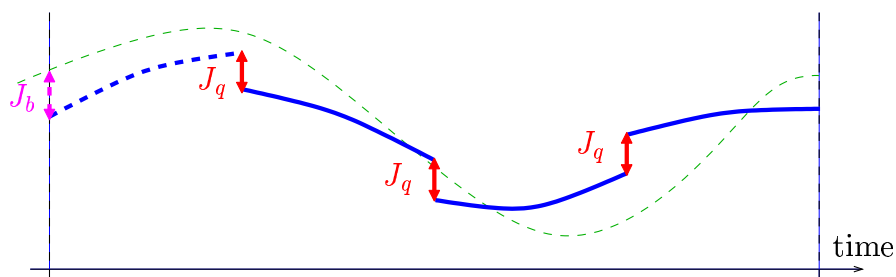
Weak Constraint 4D-Var: Sliding Window



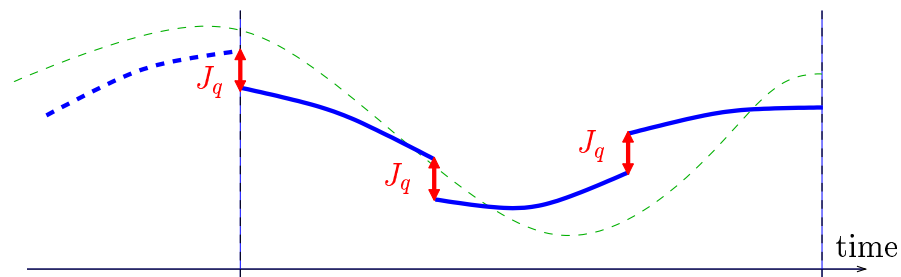
(1) Weak constraint 4D-Var



(2) Extended window



(3) Initial term has converged



(4) Assimilation window is moved forward

- This implementation is an approximation of weak constraint 4D-Var with an assimilation window that extends indefinitely in the past...
- ...which is equivalent to a Kalman filter that has been running indefinitely.

Model Error Covariance Matrix

Model error covariance matrix

- The usual choice is $Q = \alpha B$.
- Linearisation in incremental formulation gives:

$$\delta x_n = M_n \dots M_1 \delta x_0 + \sum_{i=1}^n M_n \dots M_{i+1} \eta_i$$

- δx_0 can be identified with η_0 .
- The solution of the analysis equation satisfies:

$$\delta x_0 = BH^T (R + HBH^T)^{-1} (y - \mathcal{H}(x_b))$$

$$\eta = QH^T (R + HQH^T)^{-1} (y - \mathcal{H}(x_b))$$

- If Q and B are proportional, δx_0 and η are constrained in the same directions, may be with different relative amplitudes.
- They both predominantly retrieve the same information: $Q = \alpha B$ is too limiting.

Generating a Model Error Covariance Matrix

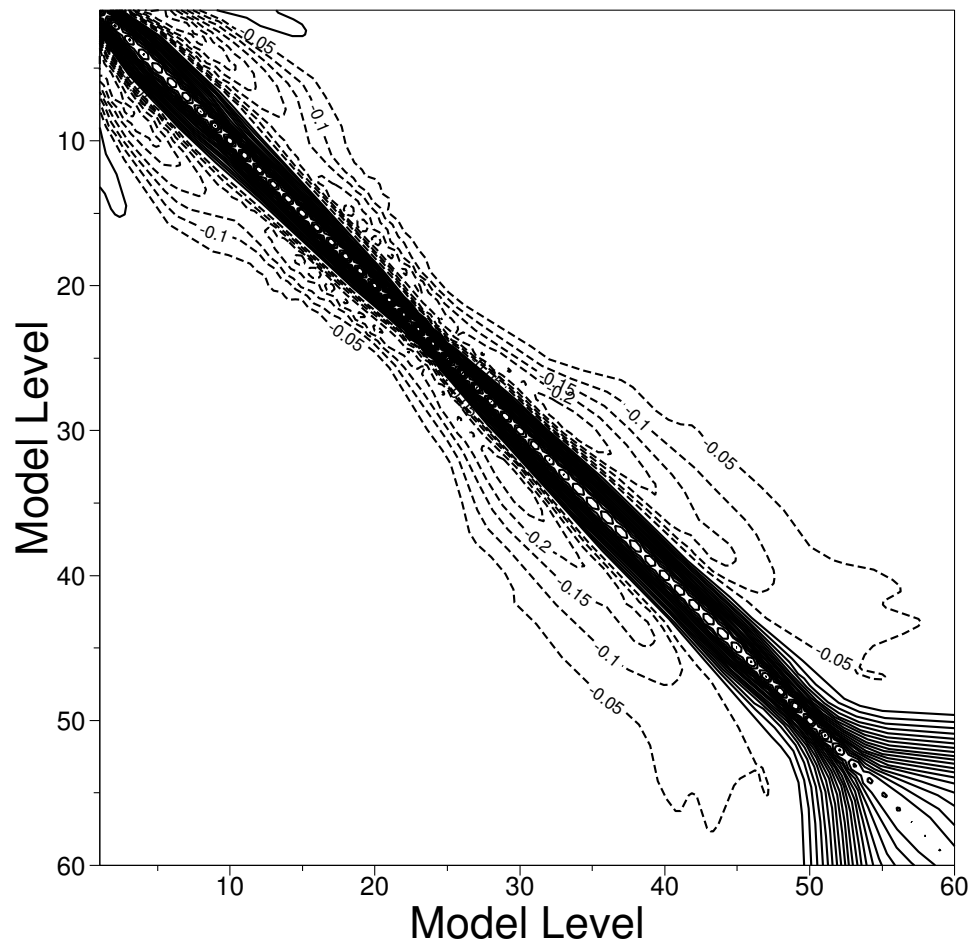
- B is estimated from an ensemble of 4D-Var assimilations.
- Considering the forecasts run from the 4D-Var members:
 - At a given step, each model state is supposed to represent the same *true* atmospheric state,
 - The tendencies from each of these model states should represent possible evolutions of the atmosphere from that same *true* atmospheric state,
 - The differences between these tendencies can be interpreted as possible uncertainties in the model or realisations of *model error*.
- Q can be estimated by applying the statistical model used for B to tendencies instead of analysis increments.

Model Error Covariance Matrix

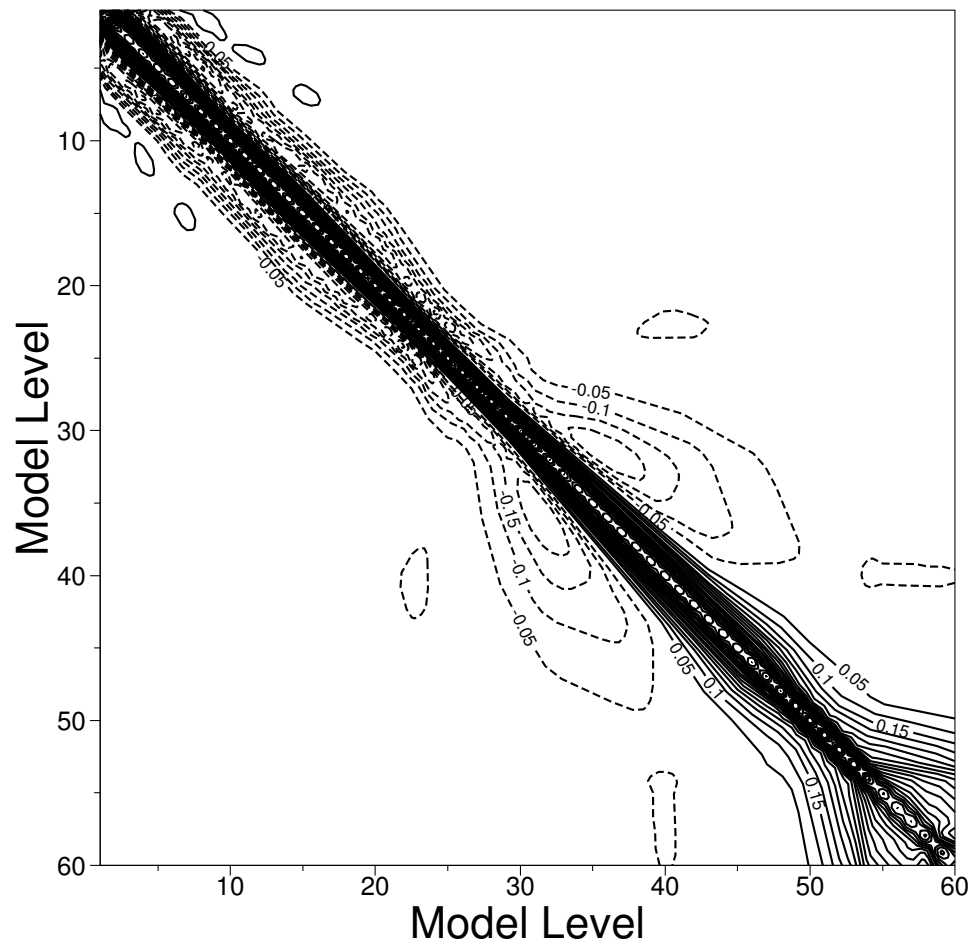
- Run forecasts from 4D-Var ensemble (T319),
- Save tendencies after 12h, 18h, 24h, 30h,
- Normalise tendencies to 1 hour time-steps,
- 10 members, one month (26 days),
- 936 realisations of *model errors*,
- Run statistical model.

Average Temperature Vertical Correlations

Background Error

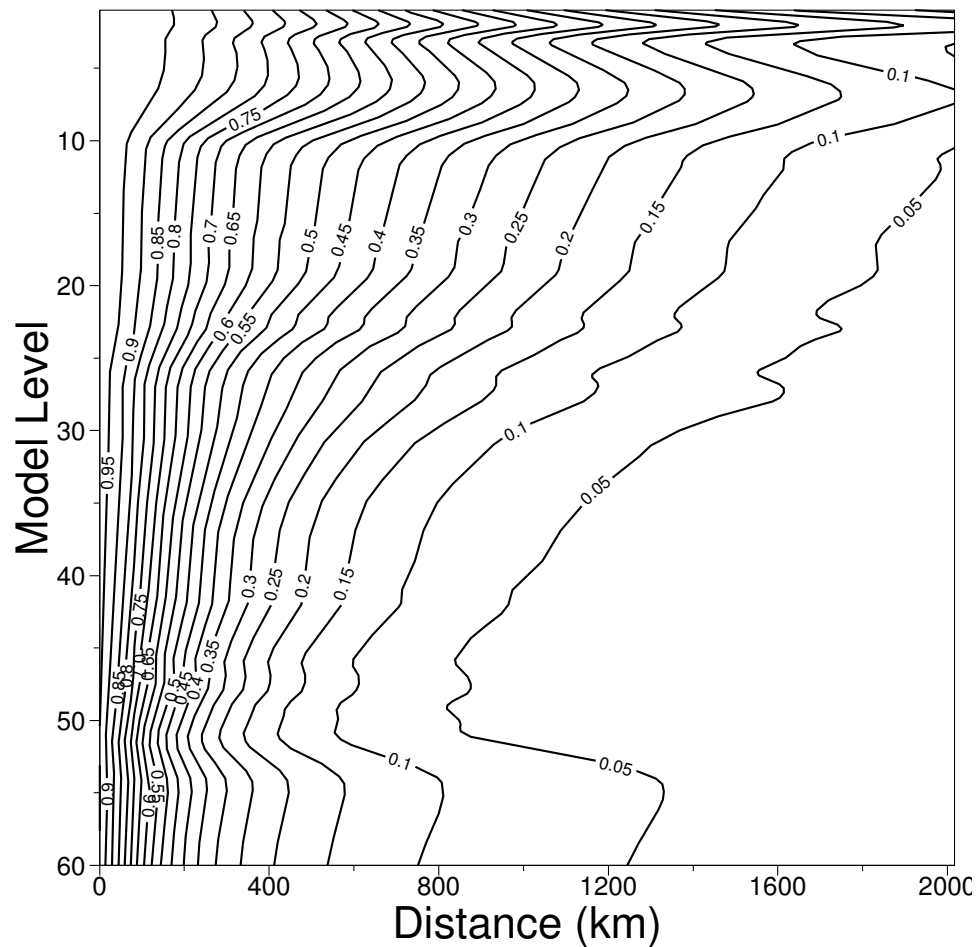


Model Error

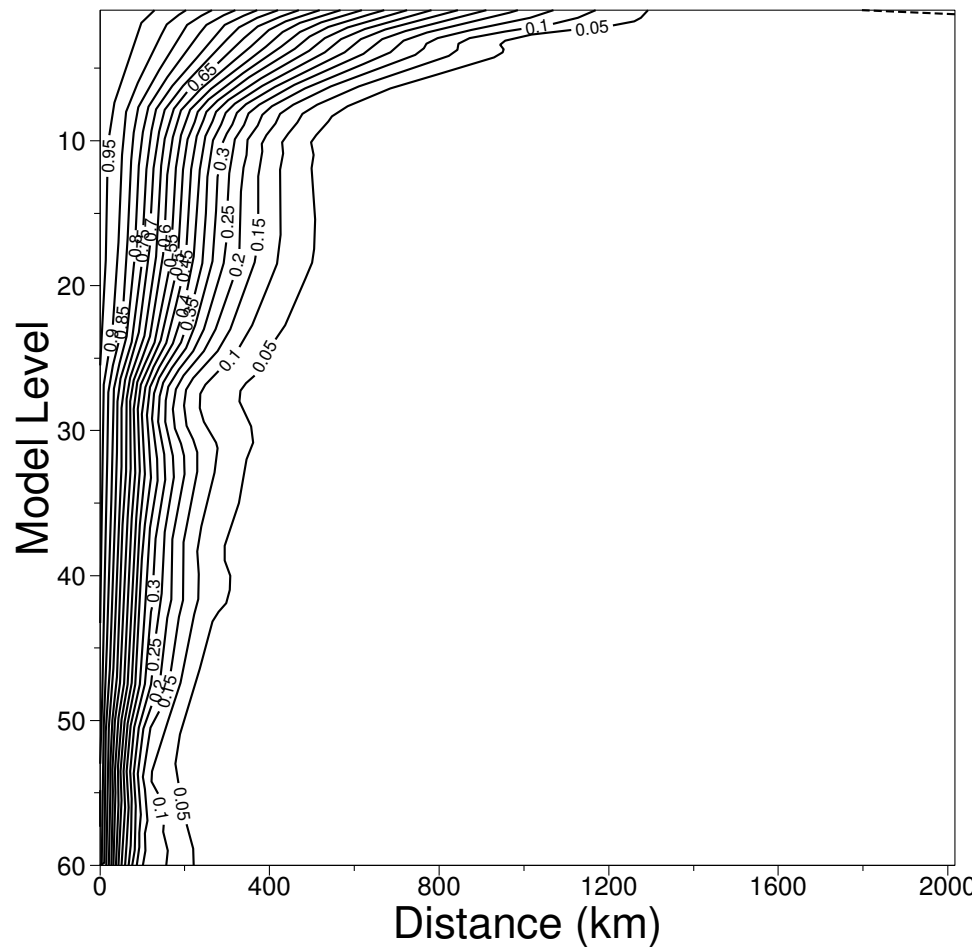


Temperature Horizontal Correlations

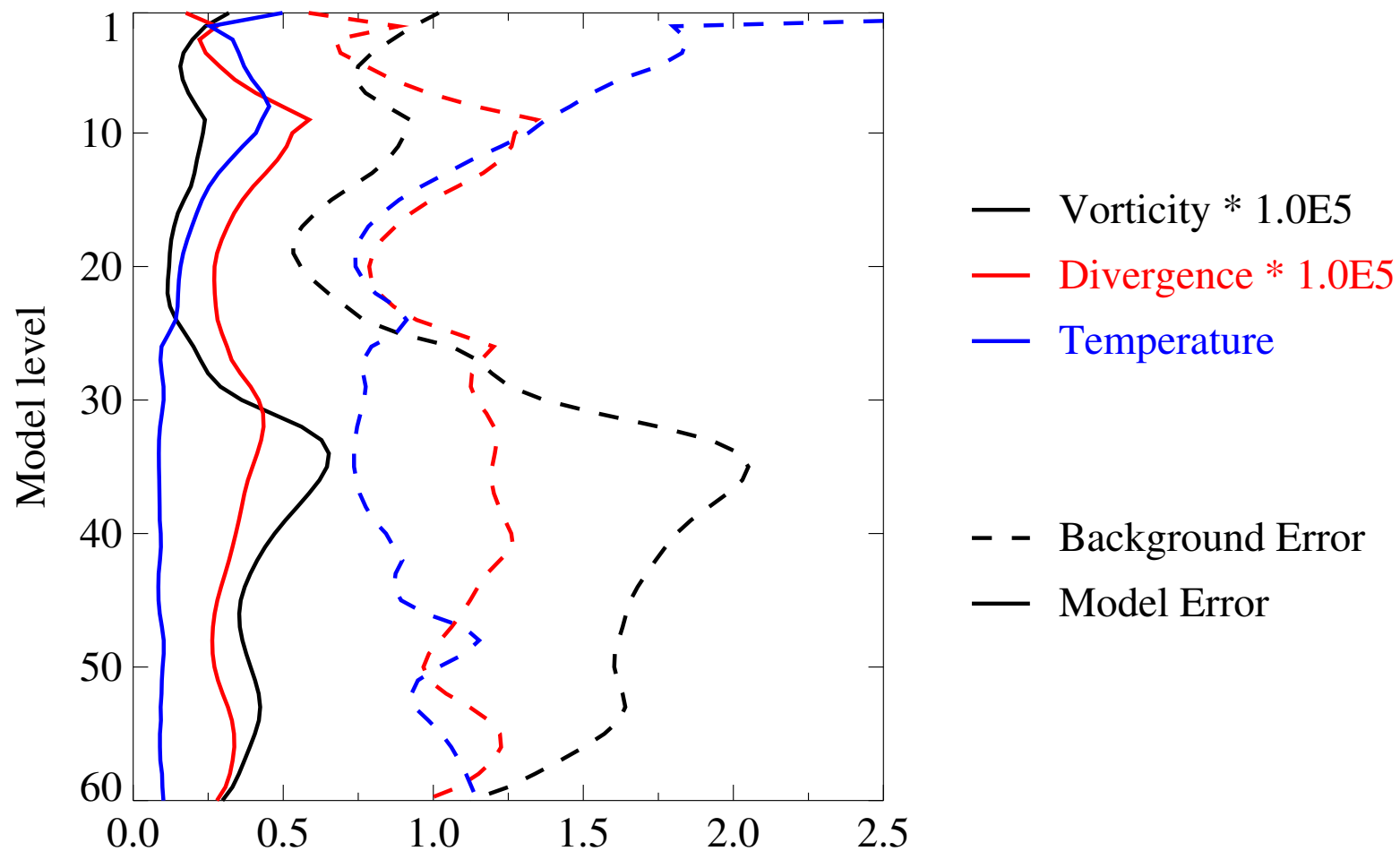
Background Error



Model Error



Average Standard Deviation Profiles



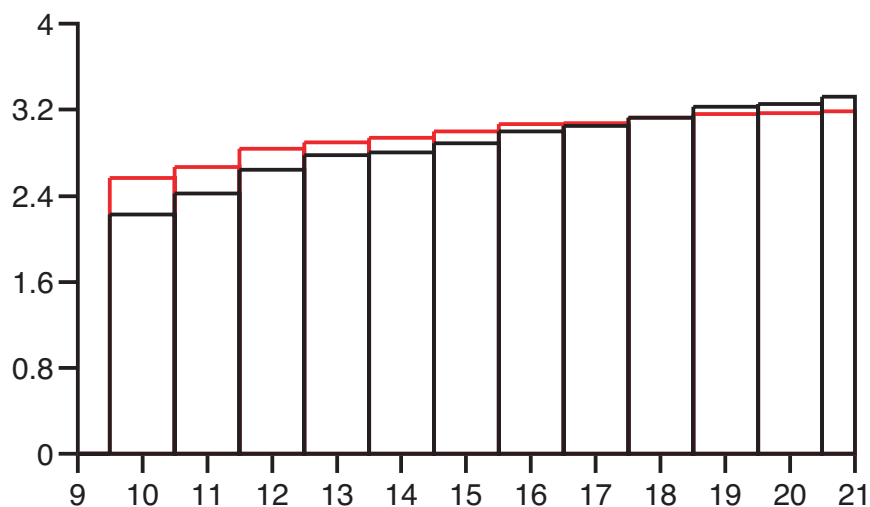
Q has narrower correlations and smaller amplitudes than B

Results: Constant Model Error Forcing

Results: Fit to observations

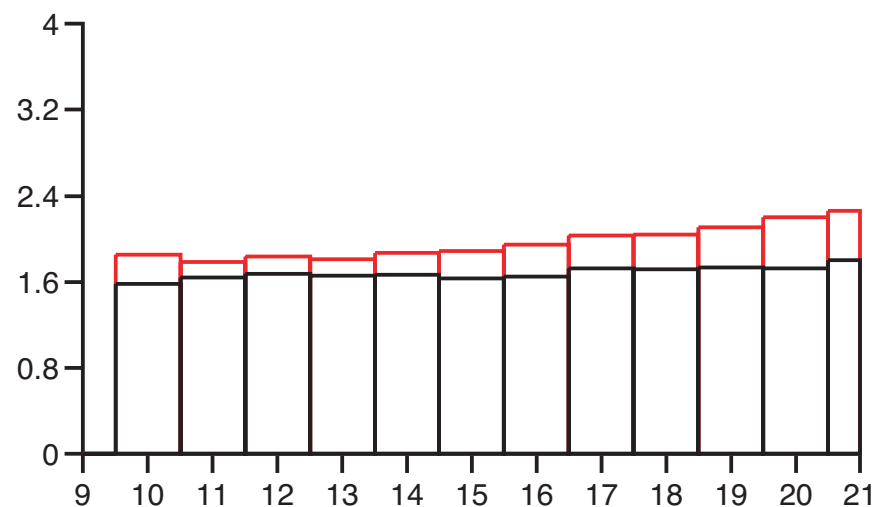
AMprofiler-windspeed Std Dev N.Amer

Background Departure



— Model Error

Analysis Departure



— Control

- Fit to observations is more uniform over the assimilation window.
- Background fit improved only at the start: error varies in time ?

Model Error Forcing

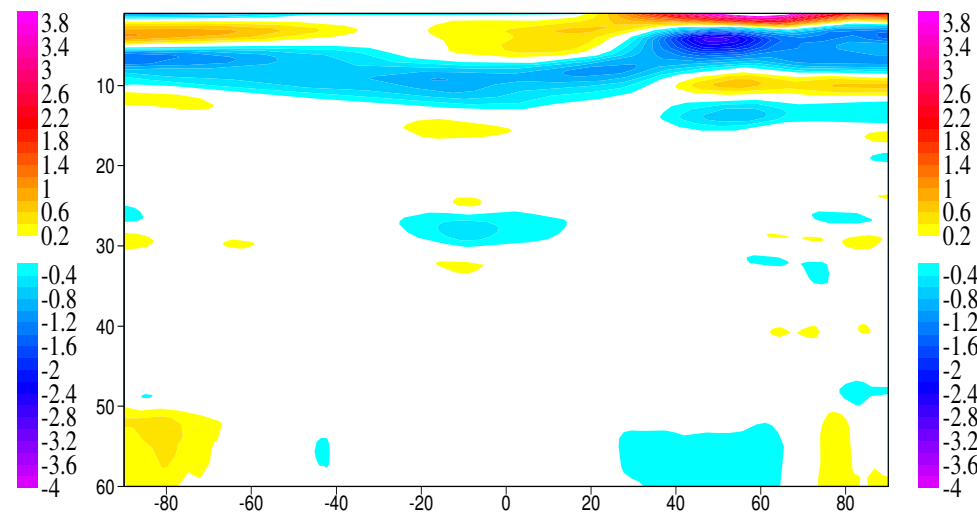
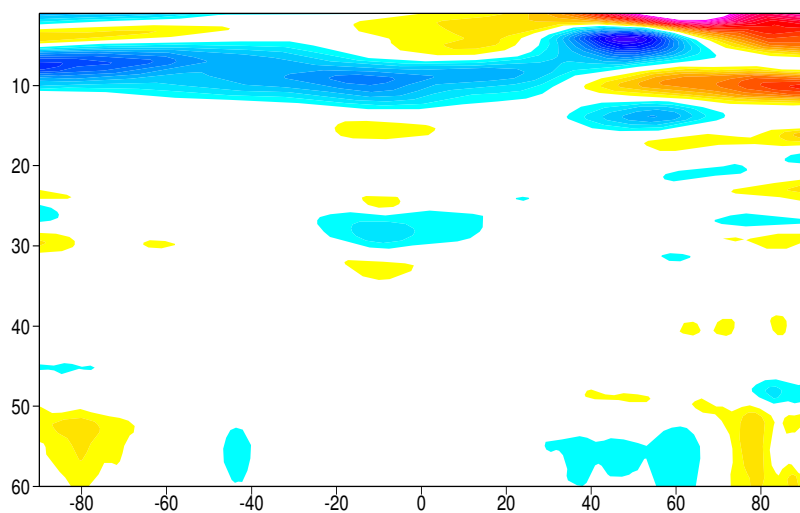
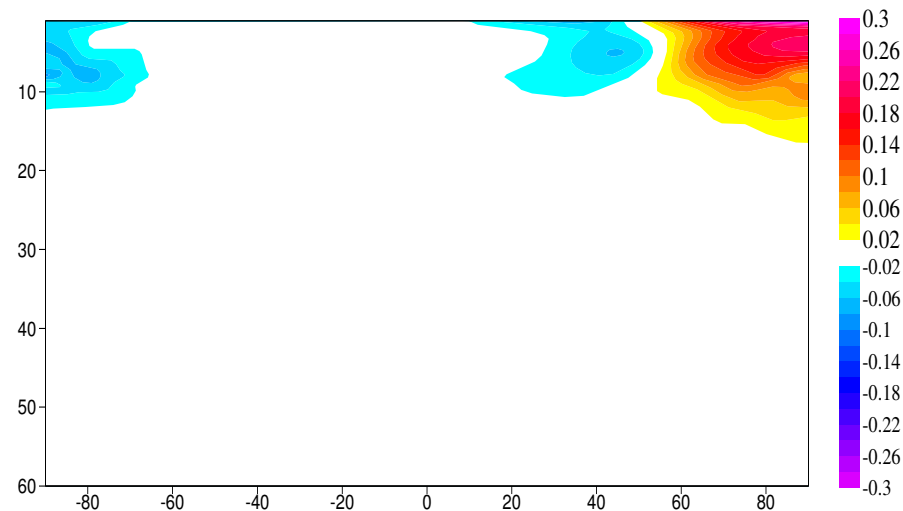
Zonal Mean Temperature

July 2004

M.E. Forcing →

M.E. Mean Increment ↘

Control Mean Increment ↓



Mean Model Error Forcing

Temperature

Model level 11 ($\approx 5\text{hPa}$)

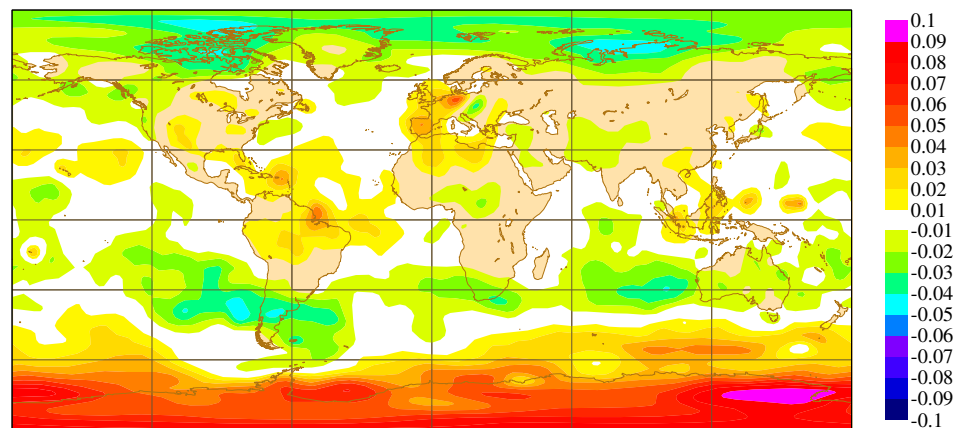
Mean M.E. Forcing \rightarrow

M.E. Mean Increment \searrow

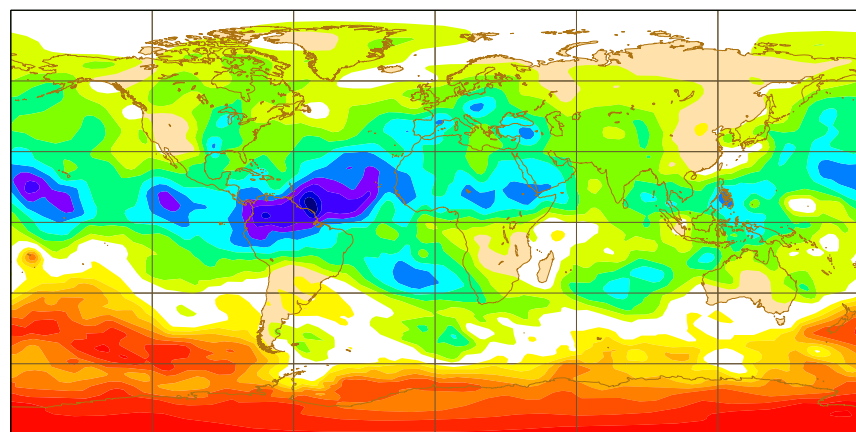
Control Mean Increment



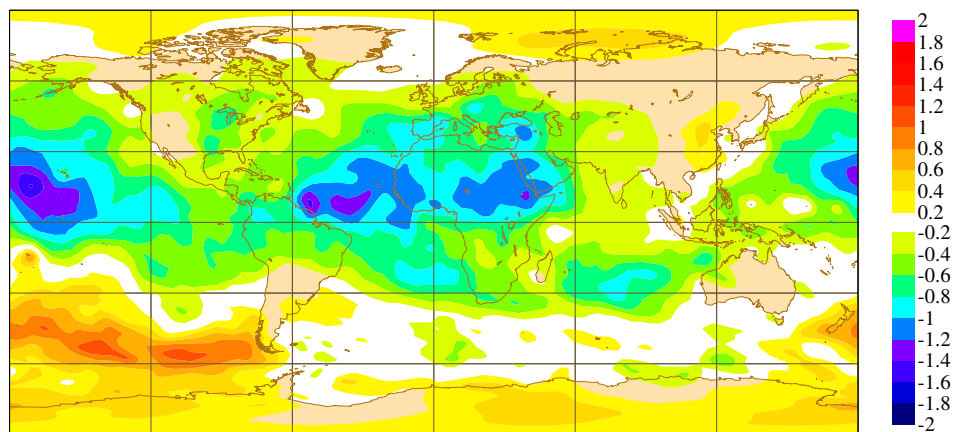
Wednesday 30 June 2004 21UTC ©ECMWF Mean Model Error Forcing (eptg)
Temperature, Model Level 11
Min = -0.05, Max = 0.10, RMS Global=0.02, N.hem=0.01, S.hem=0.03, Tropics=0.01



Monday 5 July 2004 00UTC ©ECMWF Mean Increment (enrc)
Temperature, Model Level 11
Min = -1.97, Max = 1.61, RMS Global=0.66, N.hem=0.54, S.hem=0.65, Tropics=0.77



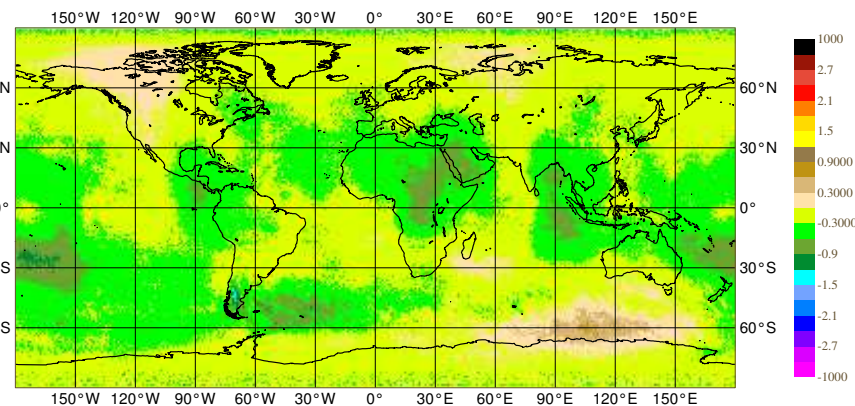
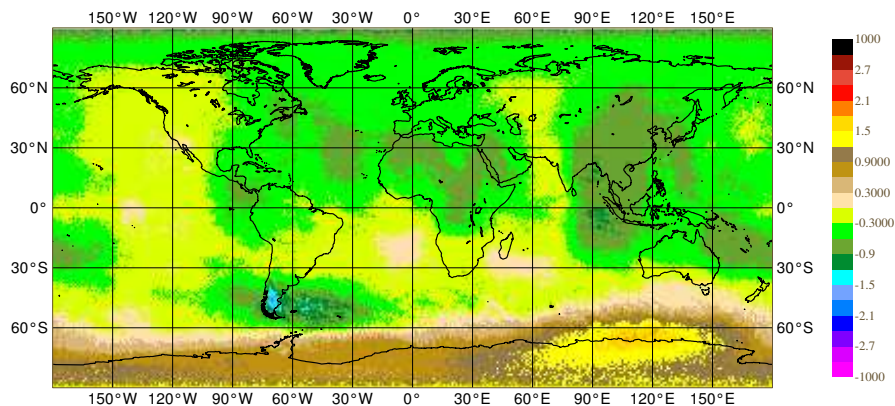
Monday 5 July 2004 00UTC ©ECMWF Mean Increment (eptg)
Temperature, Model Level 11
Min = -1.60, Max = 1.15, RMS Global=0.55, N.hem=0.51, S.hem=0.41, Tropics=0.69



AMSU-A Departures

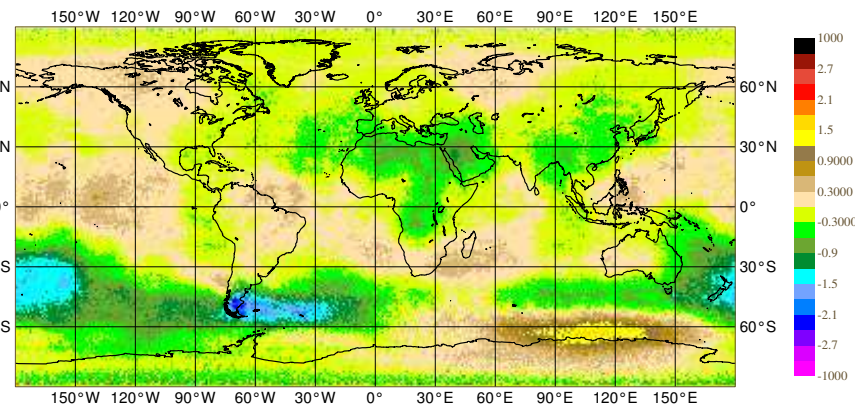
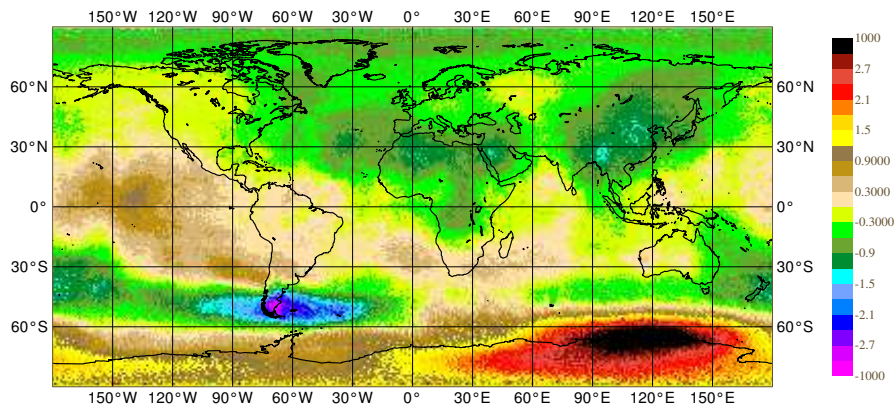
STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 13
 MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
 DATA PERIOD = 2004070200 - 2004073118 , HOUR = ALL
 EXP = ENRC
 Min: -1.9618 Max: 2.7 Mean: -0.169506

STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 13
 MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
 DATA PERIOD = 2004070100 - 2004073118 , HOUR = ALL
 EXP = EPTG
 Min: -1.6688 Max: 0.8 Mean: -0.231773



STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 14
 MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
 DATA PERIOD = 2004070200 - 2004073118 , HOUR = ALL
 EXP = ENRC
 Min: -3.3564 Max: 5.46 Mean: 0.006309

STATISTICS FOR RADIANCES FROM NOAA-16 / AMSU-A - 14
 MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
 DATA PERIOD = 2004070100 - 2004073118 , HOUR = ALL
 EXP = EPTG
 Min: -2.6 Max: 2.16 Mean: -0.111883



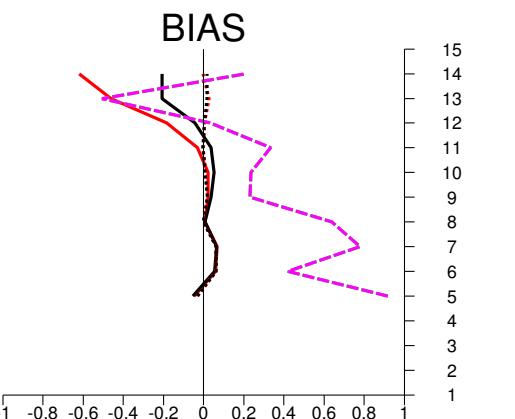
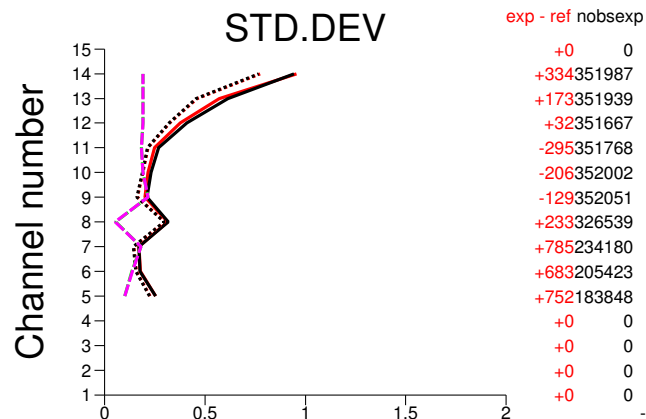
Control

Model Error

AMSU-A Statistics

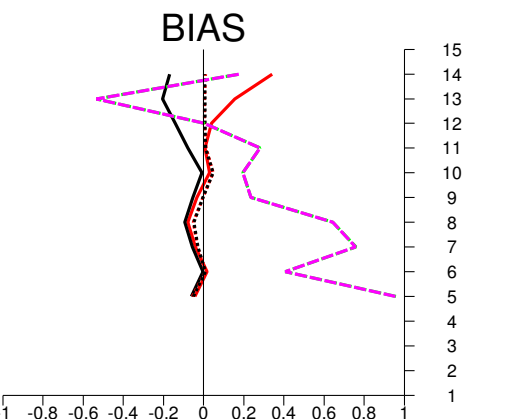
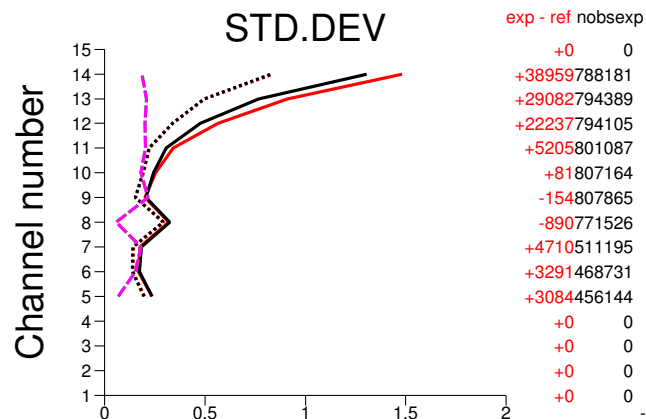
exp:eptg /DA (black) v. enrc/DA 2004070700-2004081512(12)
 NESDIS TOVS-1C noaa-16 AMSU-A Tb N.Hemis
 used Tb noaa-16 amsu-a

— background departure o-b(ref) analysis departure o-a
 — background departure o-b - - - bias correction of obs(ref)
 analysis departure o-a(ref) - - - bias correction of obs



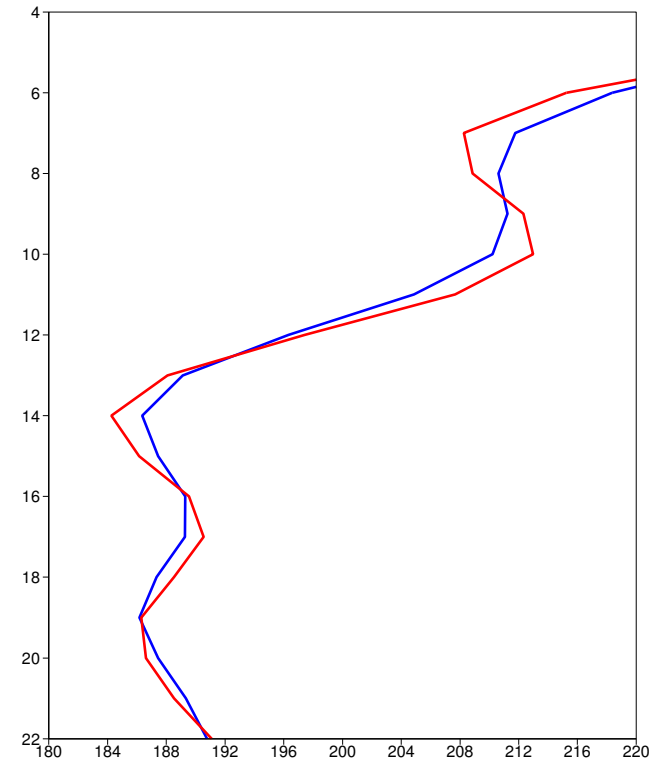
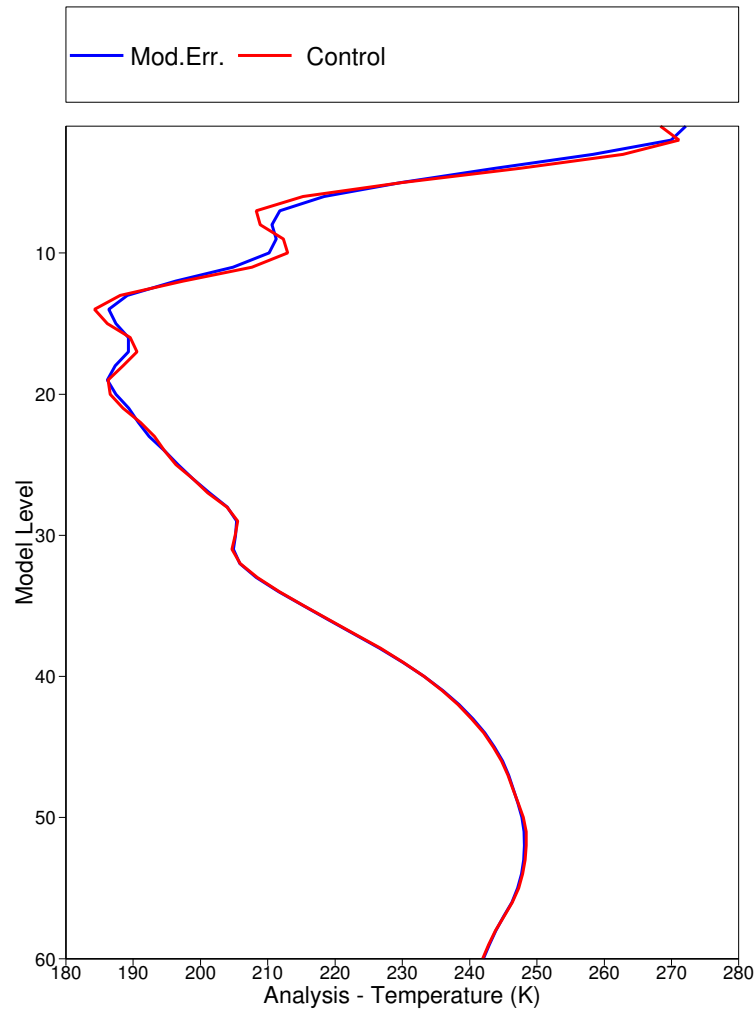
exp:eptg /DA (black) v. enrc/DA 2004070700-2004081512(12)
 NESDIS TOVS-1C noaa-16 AMSU-A Tb S.Hemis
 used Tb noaa-16 amsu-a

— background departure o-b(ref) analysis departure o-a
 — background departure o-b - - - bias correction of obs(ref)
 analysis departure o-a(ref) - - - bias correction of obs

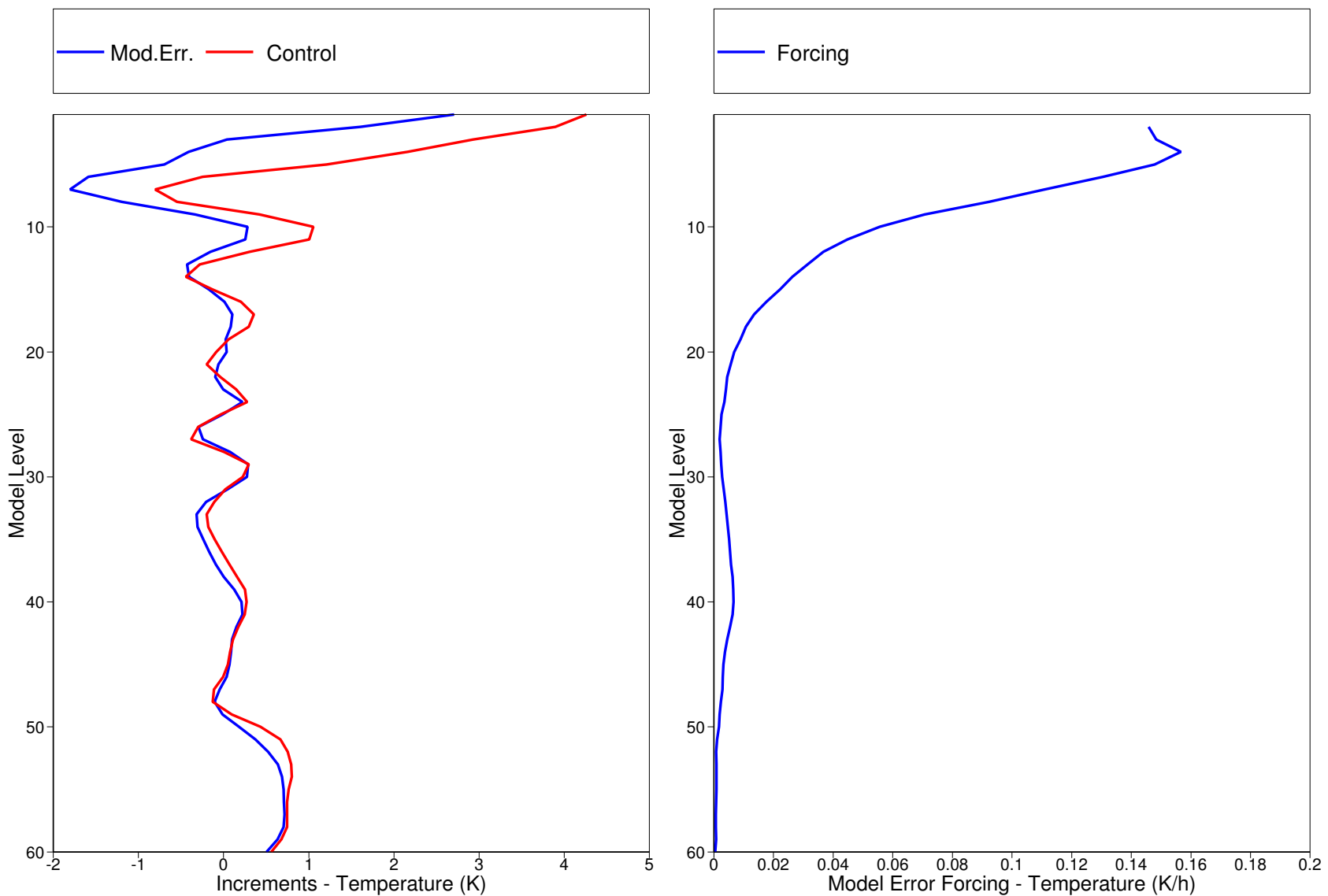


- Bias is more uniform,
- BG std. dev. is reduced in SH,
- More data is used.

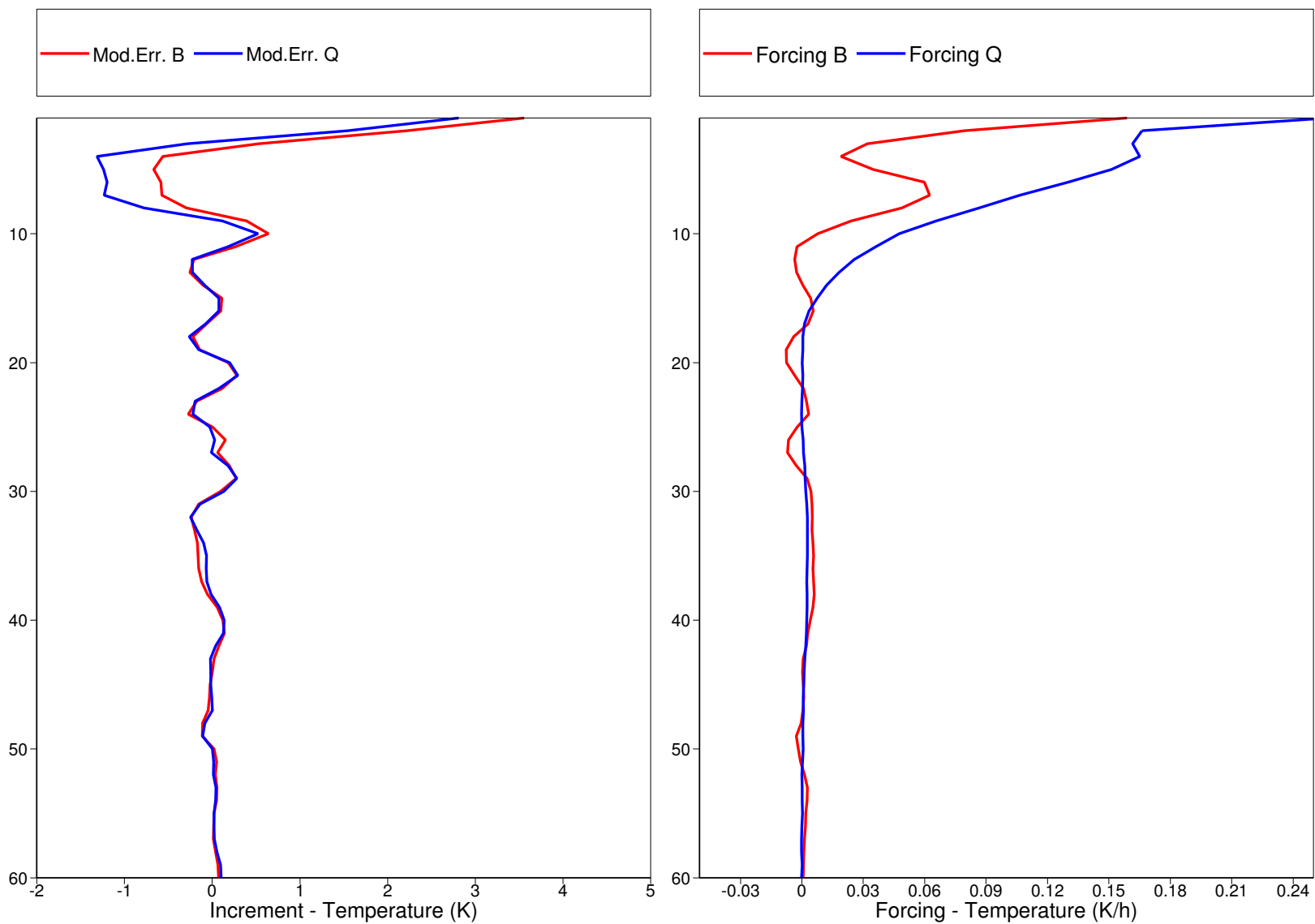
Temperature Analysis Profile



Temperature Increments Profile

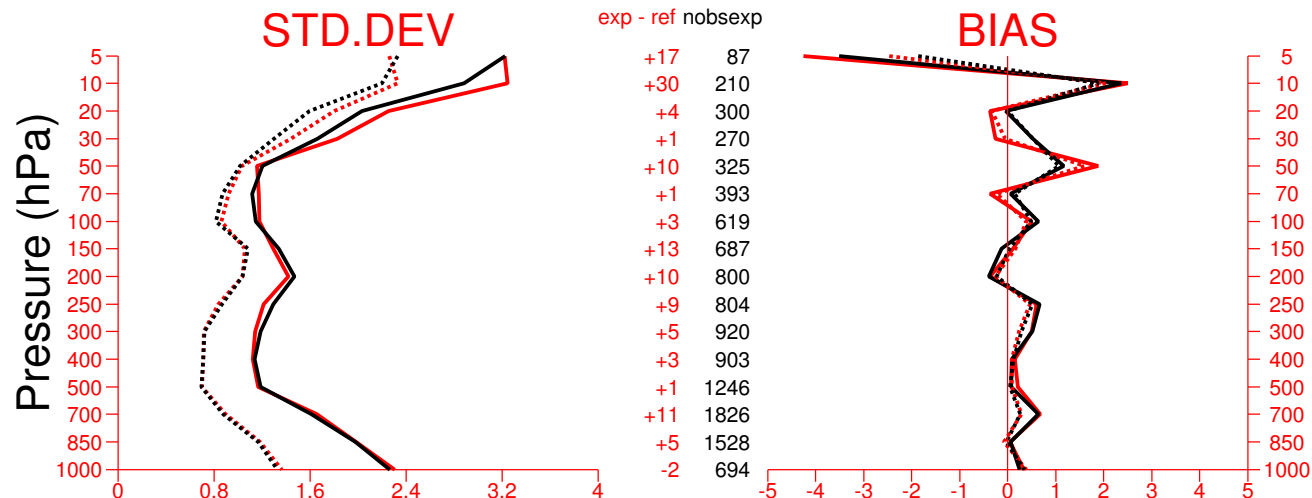


Temperature Increments Profile



Fit to radiosonde data

exp:eptg /DA (black) v. enrc/DA 2004070700-2004081512(12)
 TEMP-T S.PolarC
 used T



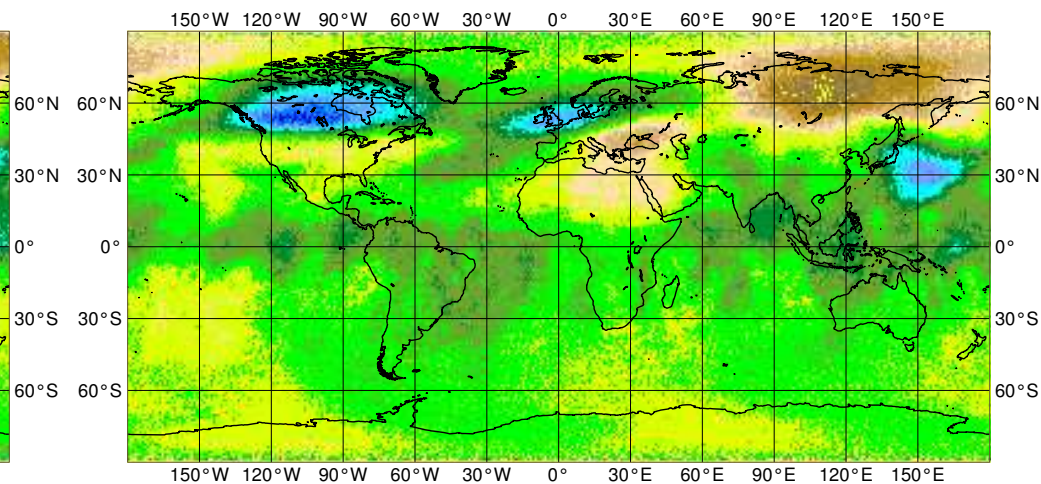
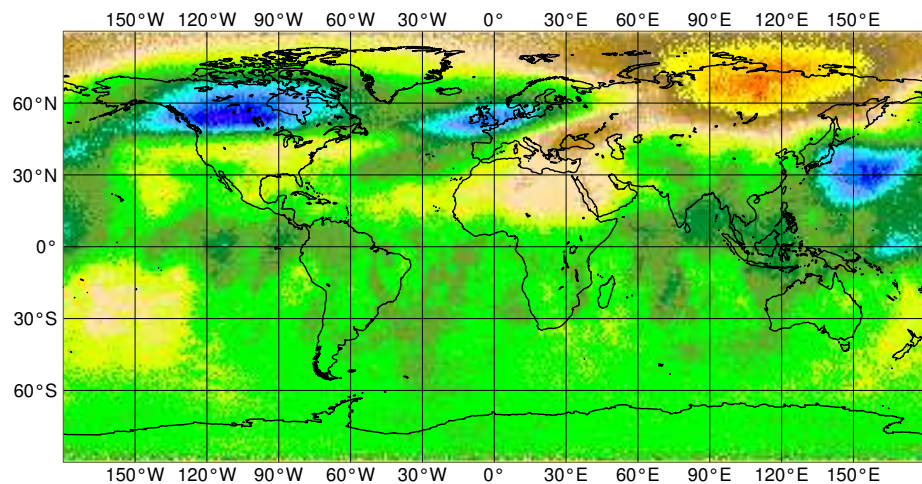
- Oscillations in bias are reduced,
- Std. deviation is reduced above 50 hPa (bg and an).

One source of model error was corrected by the forcing term.

Model Error Forcing

STATISTICS FOR RADIANCES FROM NOAA-15 / AMSU-A - 13
MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
DATA PERIOD = 2004013118 - 2004021512 , HOUR = ALL
EXP = EJ5H
Min: -2.1916 Max: 1.8620 Mean: -0.309585

STATISTICS FOR RADIANCES FROM NOAA-15 / AMSU-A - 13
MEAN FIRST GUESS DEPARTURE (OBS-FG) (BCORR.) (CLEAR)
DATA PERIOD = 2004013118 - 2004021512 , HOUR = ALL
EXP = EJ5J
Min: -1.9278 Max: 1.2571 Mean: -0.333228



Northern hemisphere winter case (February 2004)

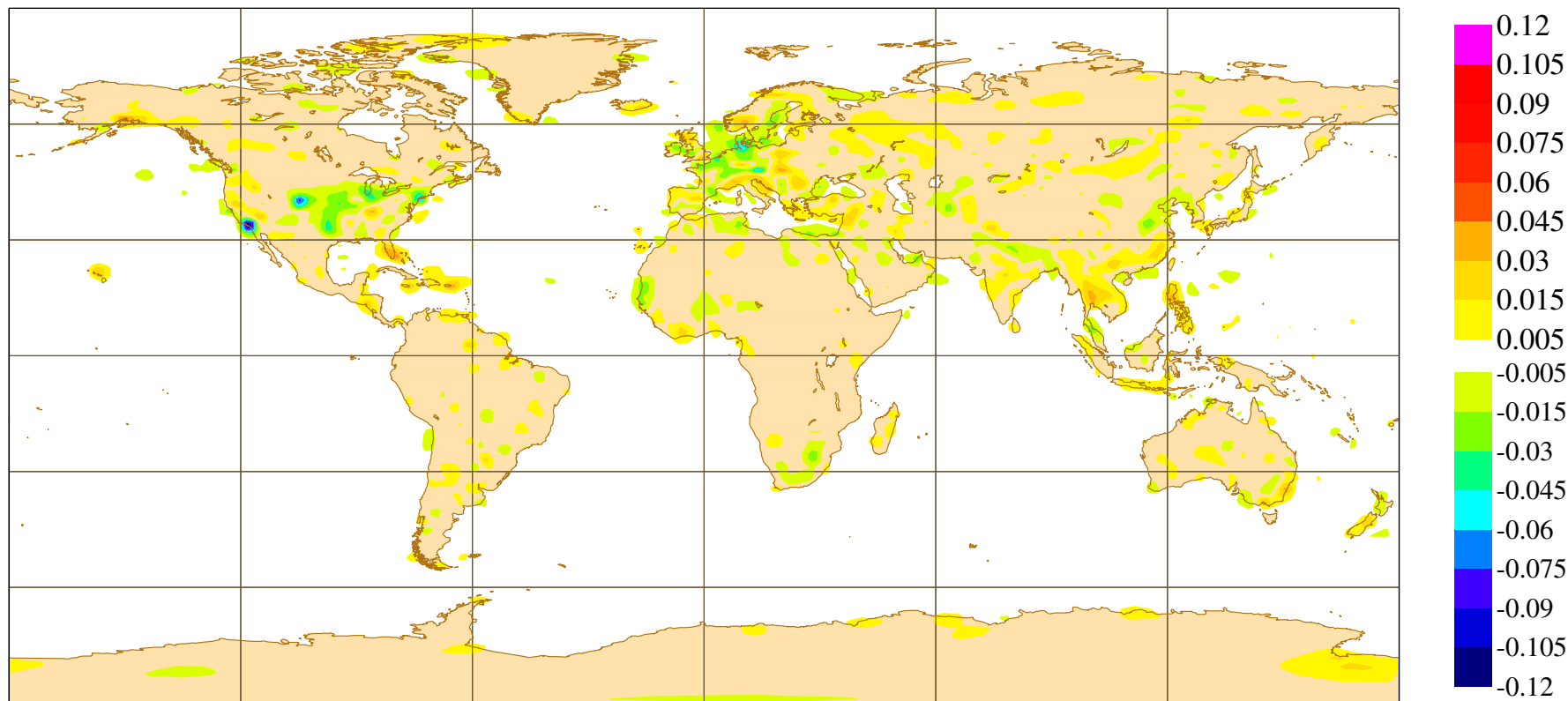
Model bias in the stratosphere is reduced.

Low Level Mean Model Error Forcing

Friday 30 April 2004 21UTC ©ECMWF Mean Model Error (ej6a)

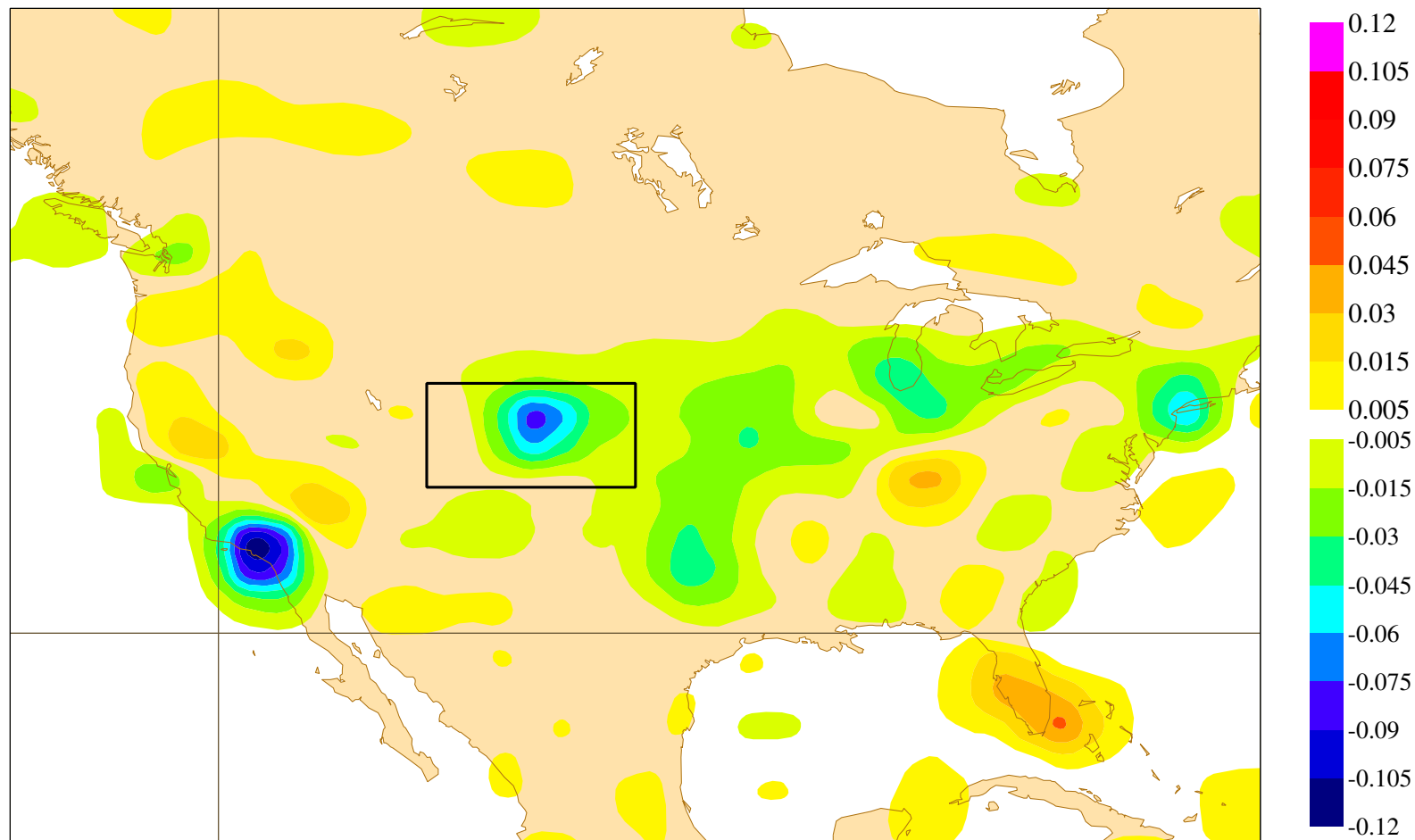
Temperature, Model Level 60

Min = -0.10, Max = 0.05, RMS Global=0.00, N.hem=0.01, S.hem=0.00, Tropics=0.00



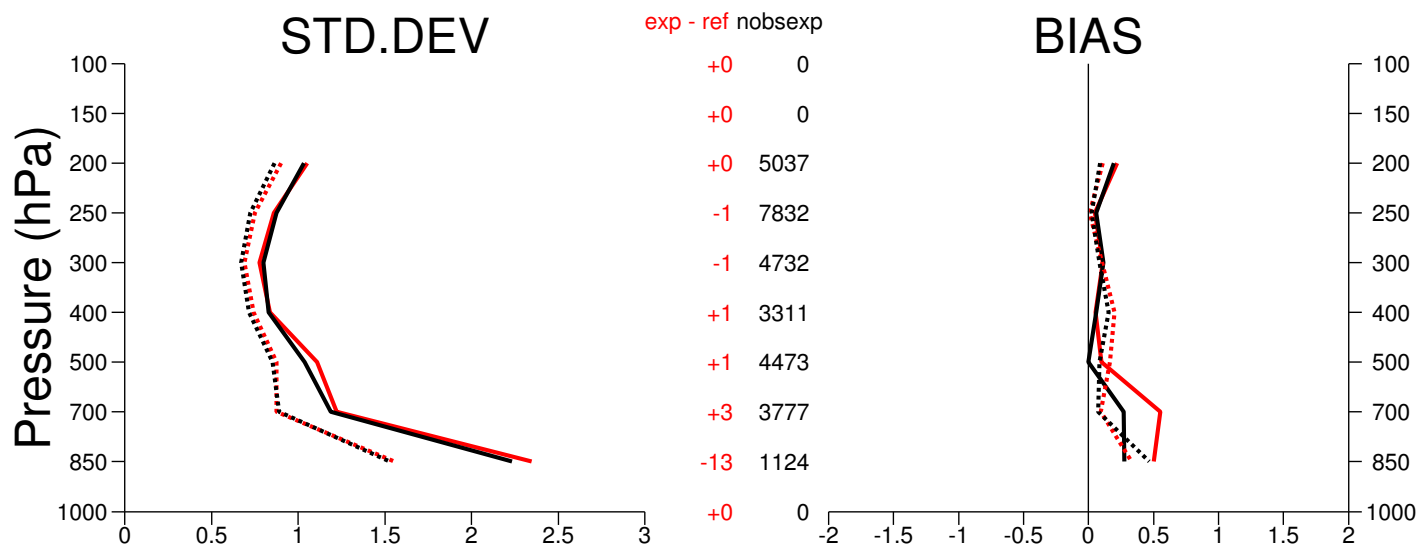
Low Level Mean Model Error Forcing

Friday 30 April 2004 21UTC ©ECMWF Mean Model Error (ej6a)
Temperature, Model Level 60
Min = -0.10, Max = 0.05, RMS Global=0.00, N.hem=0.01, S.hem=0.00, Tropics=0.00



Fit to Observation with Model Error

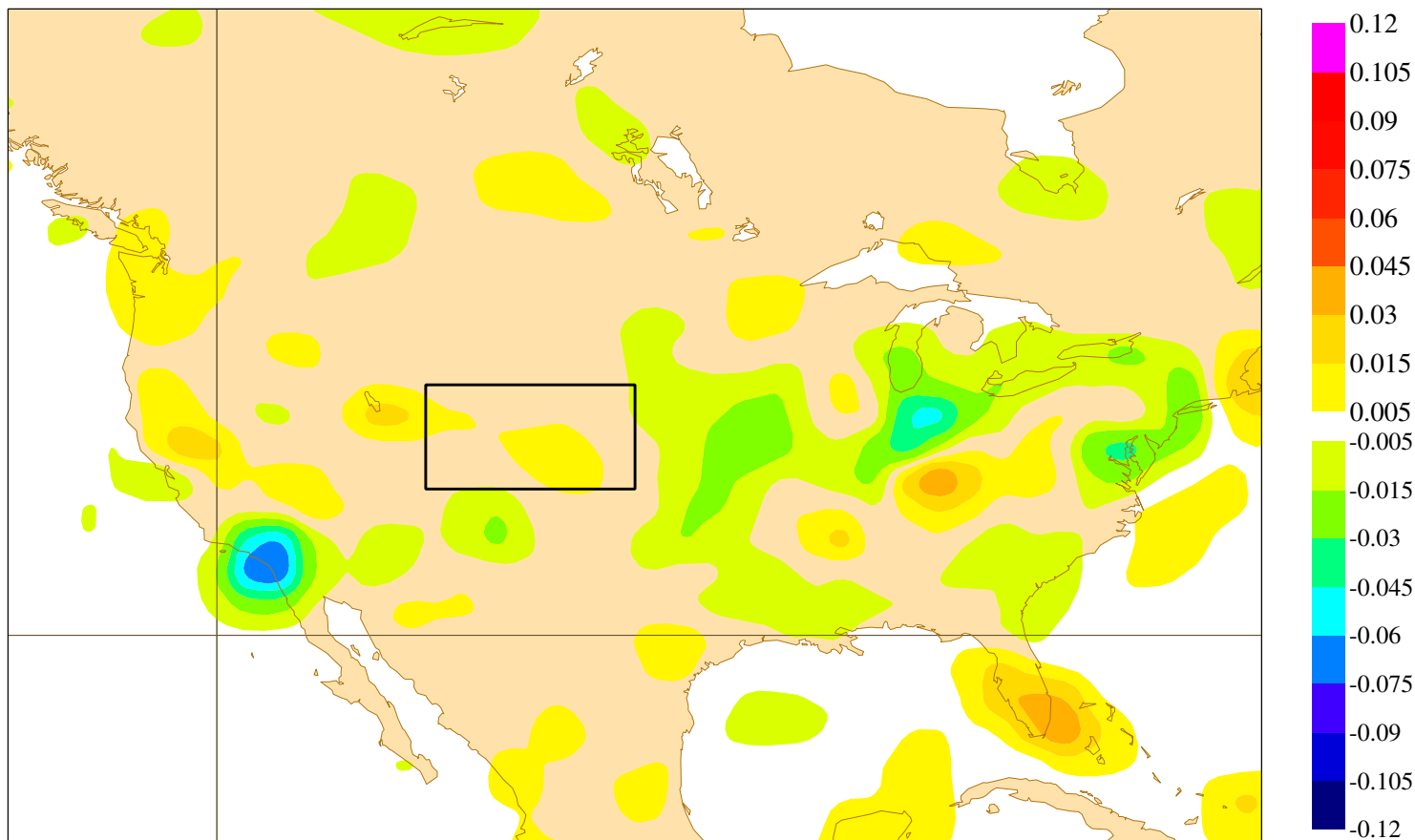
exp:ej6a Model Error 2004050100-2004050712(6)
 AIREP-T MyBox
 used T



- The only significant source of data in the box is aircraft data (Denver airport).
- The bias for aircraft low level temperature observations was reduced.

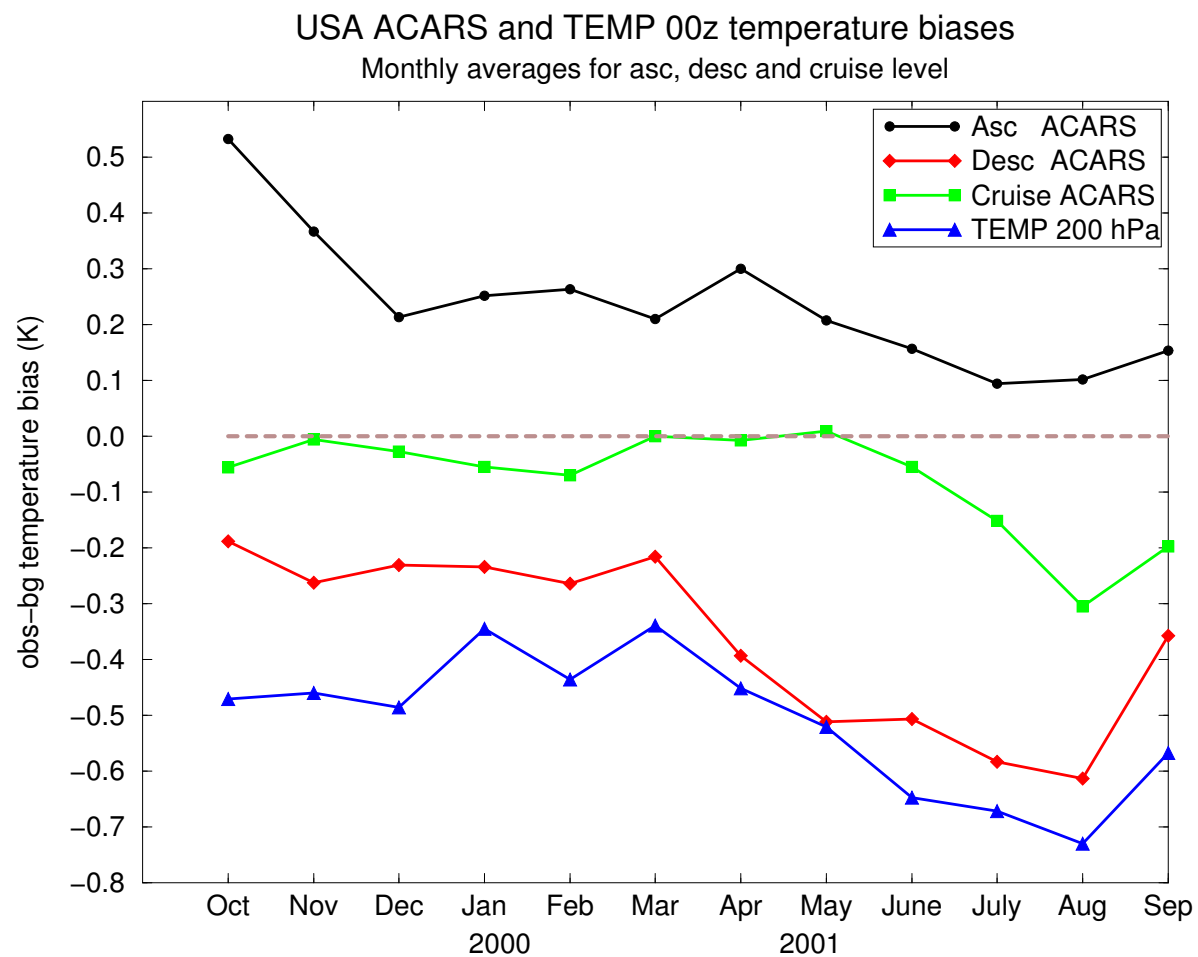
Low Level Mean Model Error Forcing

Friday 30 April 2004 21UTC ©ECMWF Mean Model Error (ej8k)
Temperature, Model Level 60
Min = -0.07, Max = 0.06, RMS Global=0.00, N.hem=0.01, S.hem=0.00, Tropics=0.00



Removing aircraft data in the box eliminates the spurious forcing.

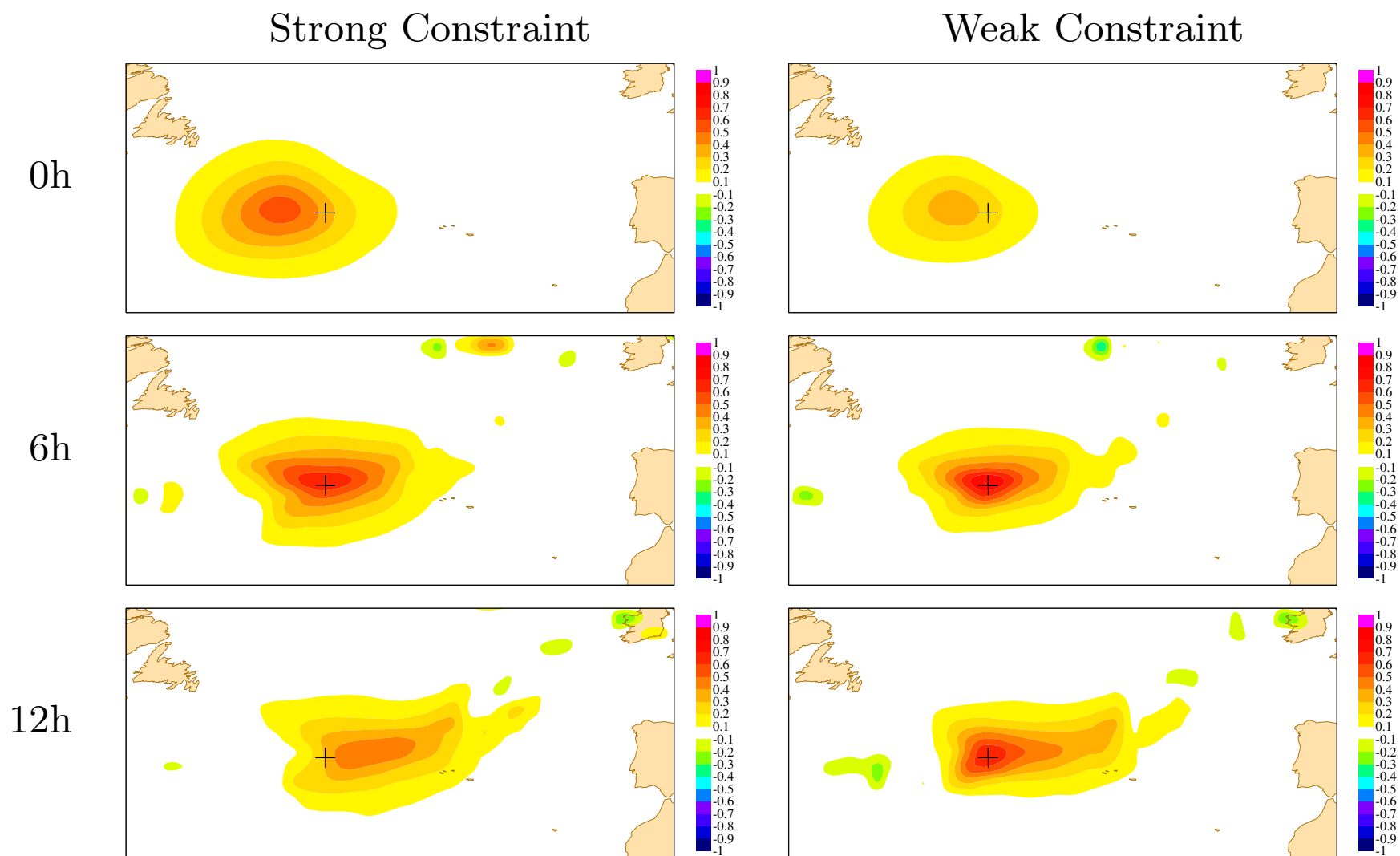
Aircraft Temperature Bias



Observations are biased.

Figure from Lars Isaksen

12 Observations Experiment



Systematic model error captures stationary errors (model or observations).

Model Bias Experiments

Final Cost Function
Model Bias (enxh) Control (enrc)



Model Bias Experiments

- Fits observations and background better,
- Observation statistics show some improvements and some degradations,
- Might absorb some of the signal,
- Scores slightly negative,
- Add bias to forecast at post-processing stage,
- Q should have large scale correlations?

Conclusions

Weak Constraint 4D-Var

- *Weak constraint 4D-Var* with model bias or forcing model error is essentially an initial value problem with parameter estimation (parameters happen to represent model error).
- *Weak constraint 4D-Var* with model state control variable is a 4D problem.
- J_q acts as coupling between sub-windows:
 - propagates information across sub-windows,
 - forgetting factor because model equations are not strictly verified.
- Takes into account the fact that the model is imperfect without directly estimating model error.
- *Long window weak constraint 4D-Var* is equivalent to a full rank Kalman smoother: the sliding window is an efficient algorithm to implement it.

Results

- Weak constraint 4D-Var is technically implemented in the IFS (x coming...),
- With constant model error forcing:
 - Fits the data more uniformly over the assimilation window,
 - Capture some model errors (winter stratosphere),
 - Captures some observation bias (ascending/descending aircrafts),
- Systematic differences between model and observations:
 - Distinction between model bias and observation bias?
 - Interactions with variational observation bias correction?
- Two tools to define the errors we wish to capture:
 - Model error covariance matrix (scales, ...),
 - Model for model error in η and β formulations (constant 3D state).

Future Work

- Compare various formulations of weak constraint 4D-Var (η , β , x),
- What type of model error (random vs. systematic vs. bias)?
- Determine appropriate model error covariance matrix,
- Interactions between model error and observation bias,
- Long window 4D-Var,
- Operational analysis and Reanalysis.