Chemical-Dynamical Coupling in Data Assimilation

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GEM-AQ

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San Antonio, Texas, February 5-8 2006

BIRA-IASB

Environment Canada
Meteorological Service of Canada

Environnement Canada
Service Météorologique du Canada

Outline

How important is chemistry for chemical data assimilation ?

• Depends on the objective : a) prediction b) monitoring

OSSE: Vertically resolved nadir ozone measurements vs. scanning total column ozone measurements

BIAS correction

• Are tropospheric bias correction schemes appropriate for the stratosphere ?

Error statistics

• Desrosiers et al. (2005) method

Coupled chemistry-meteorology model

• comparison with a CTM

What to do with error covariances with unobserved species ?

• Rochon's method

Dynamic-chemistry cross error covariance

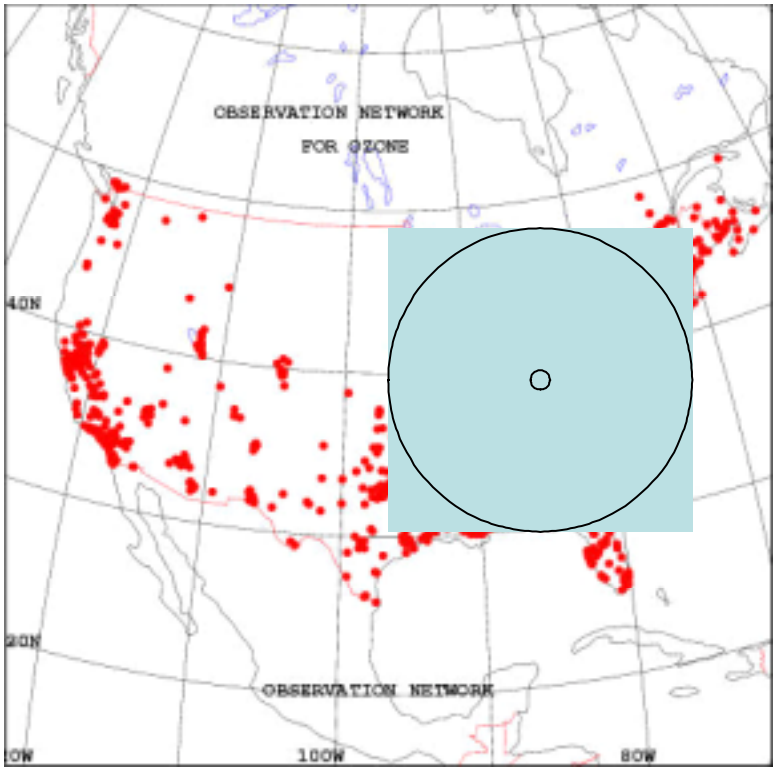
• Implementation in 3D Var-CHEM

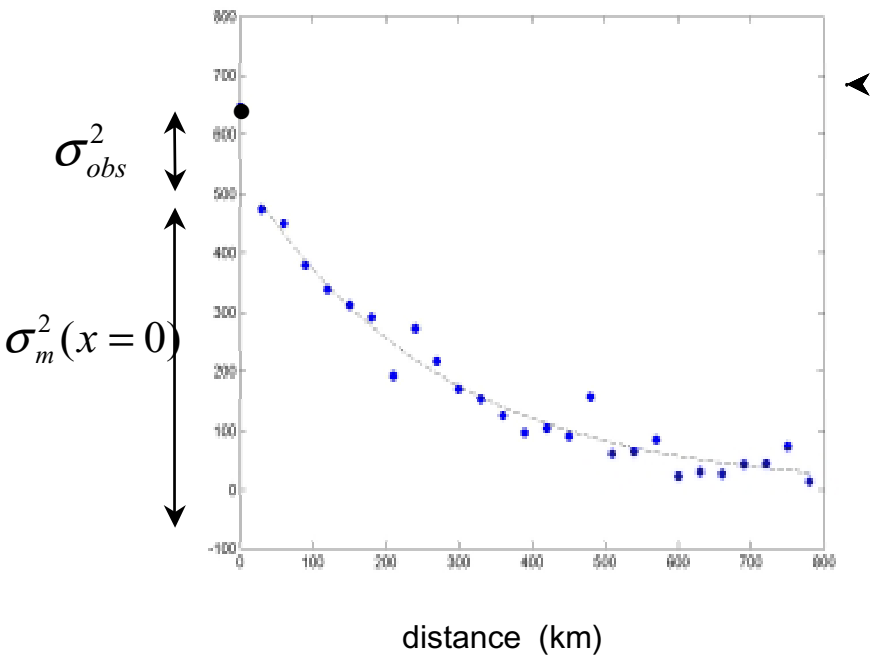
To obtain the error statistics we use innovations

obs – model (obs loc) =

(true + obs error) -
(true + model error) =

obs error – model error

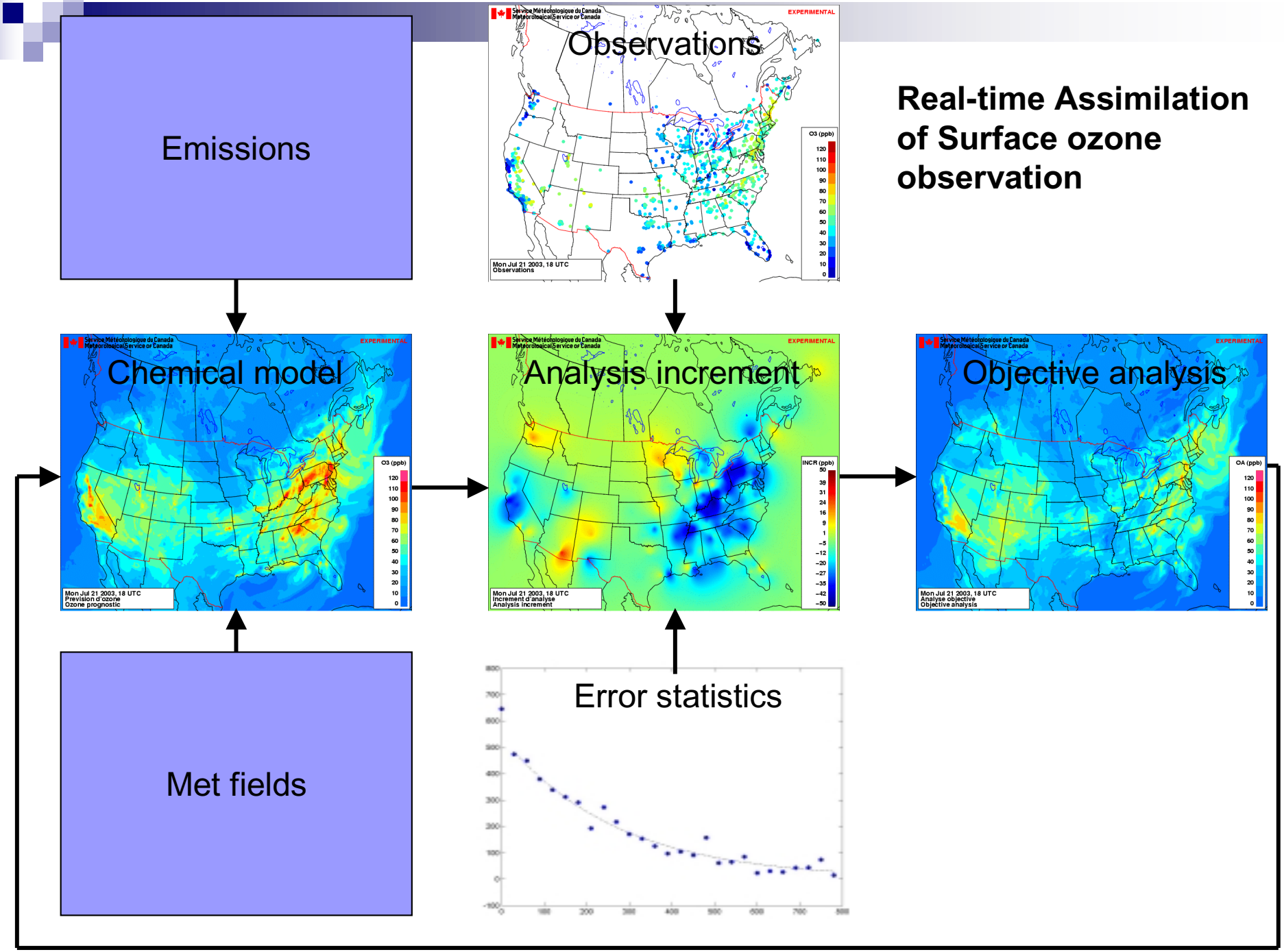




Obs. & background error variances and correlation length scale at

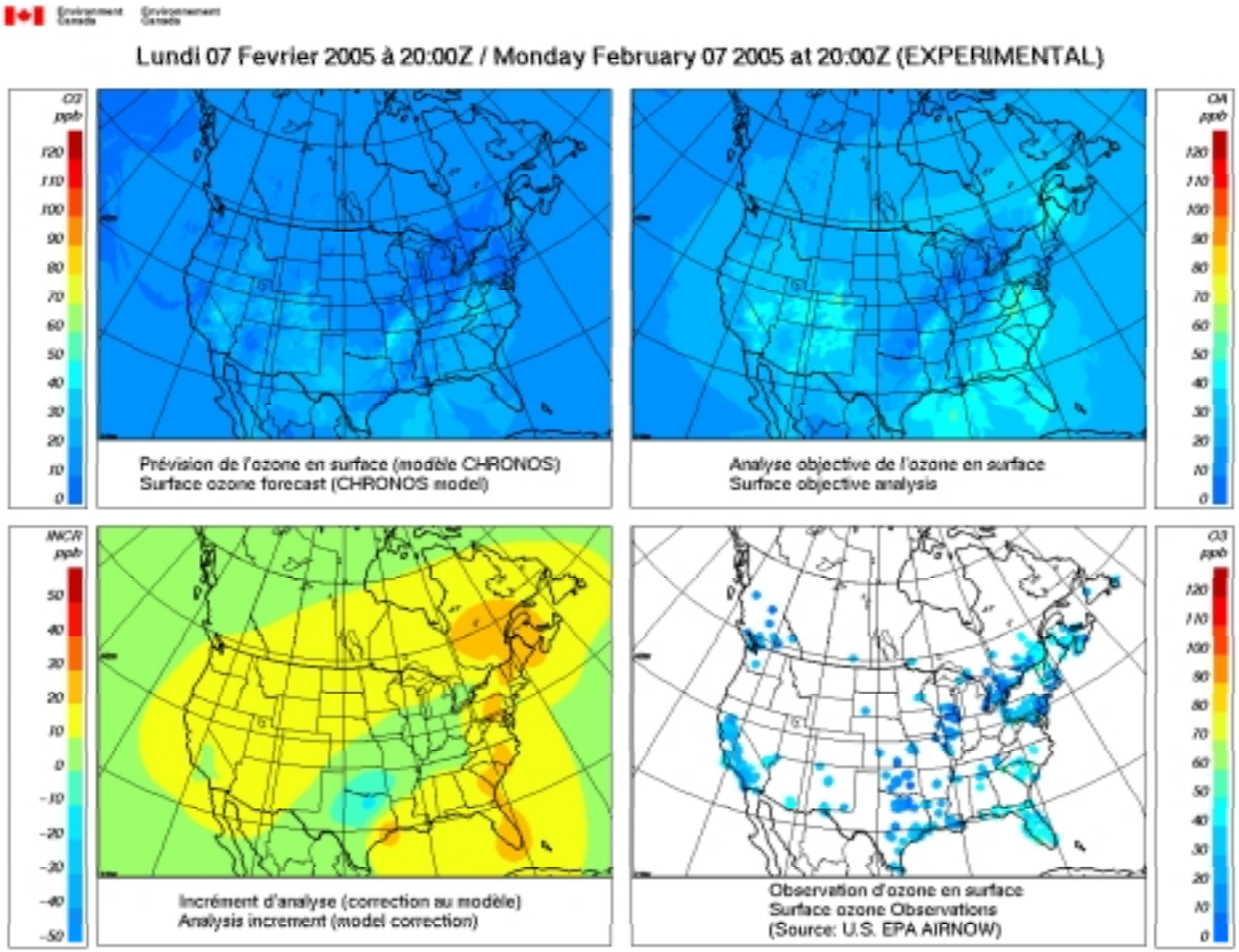
- each sites
- each hour

Real-time Assimilation of Surface ozone observation



Objective analysis of surface ozone observations

- Assimilation and objective analysis using the model CHRONOS
- Objective analysis each hour, 24/7, year round
- Near-time since June 2004
- Multiyear analyses since the summer 2002

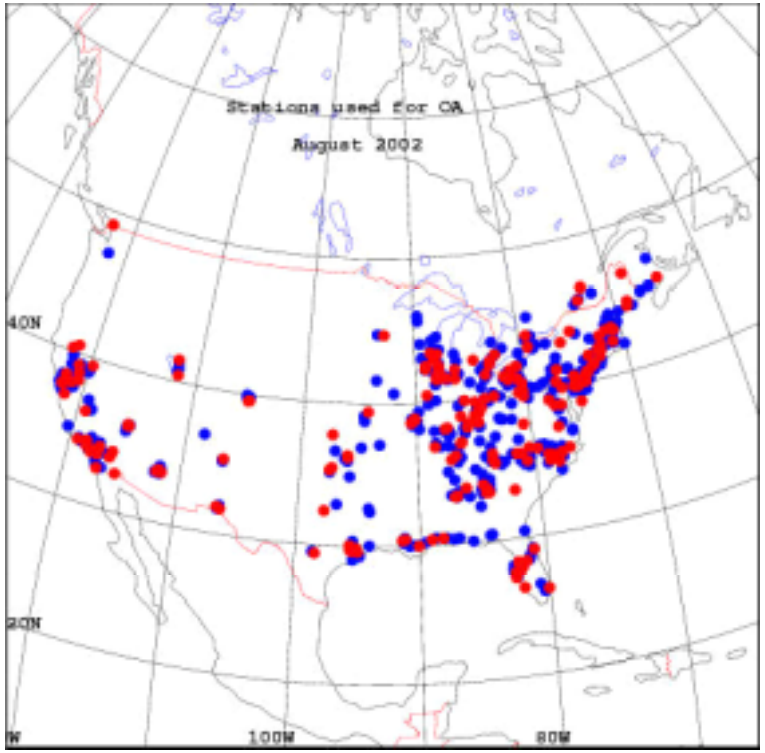


http://www.msc.ec.gc.ca/aq_smog/analysis_e.html

Verification

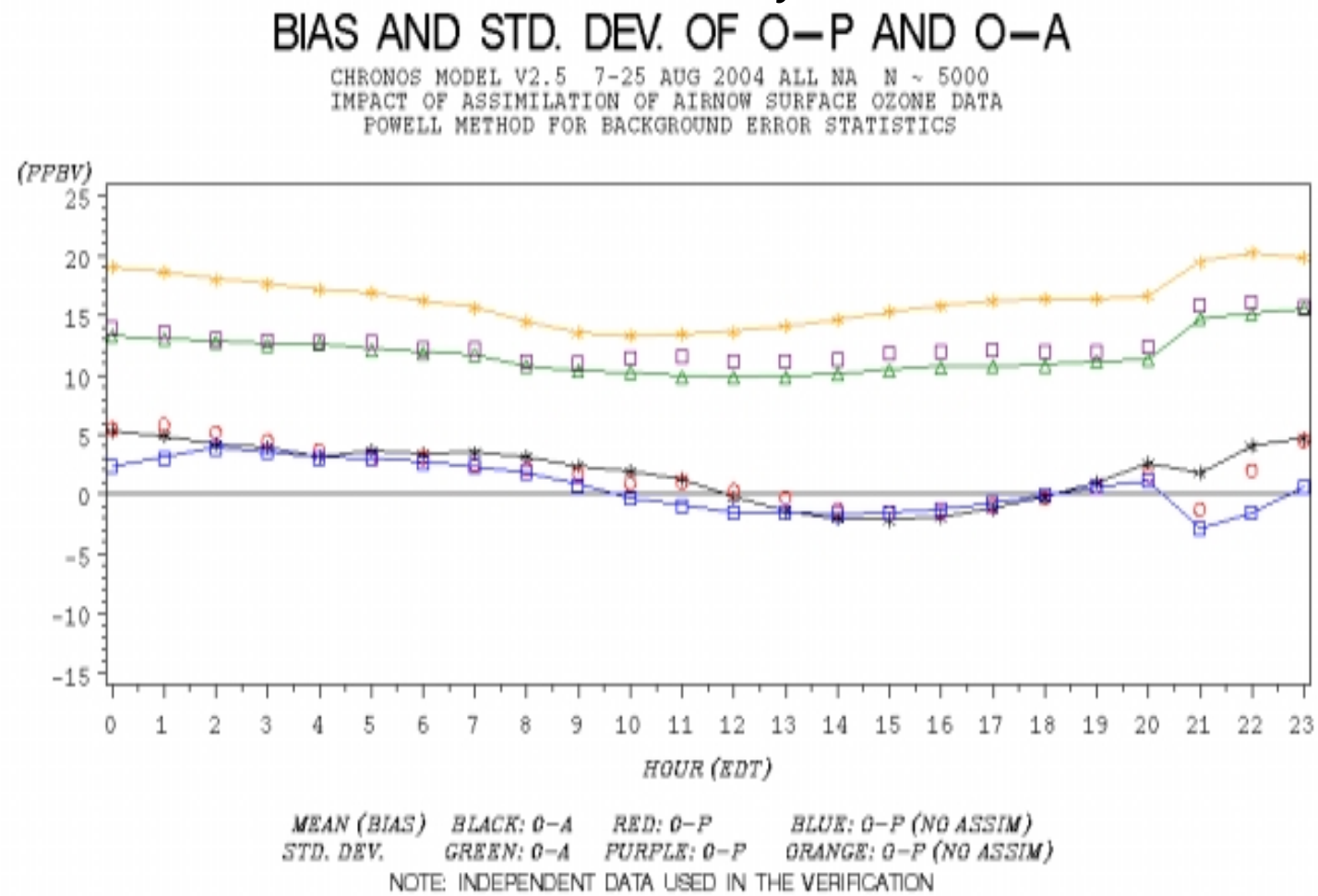
To verify against independent observations we use

- 1/3 of observations for the verification (red)
- 2/3 of observation used to produce the analysis (blue)
- rederive the error statistics (because the background error may have changed)

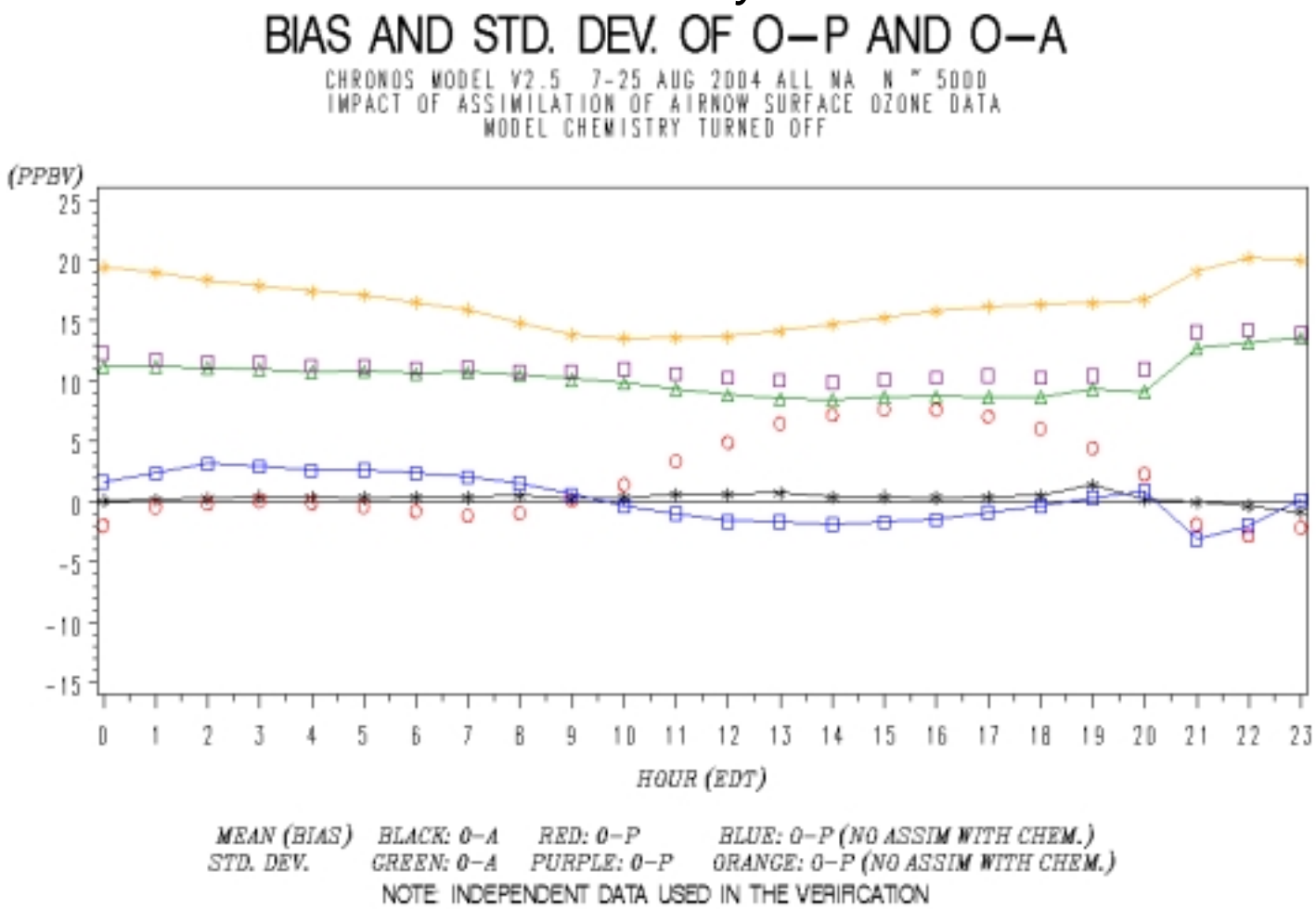


How important is chemistry in assimilation and monitoring

With chemistry



No chemistry



In summary

- chemistry + free mode (no assimilation)
  - std 20 ppb
  - bias 2 ppb

- no chemistry + assimilation
  - std ~ 12 ppb
  - bias a) ~ 1 ppb in analyses
    b) large daytime (~10 ppb) in 1hr forecast

- chemistry + assimilation
  - std ~ 14 ppb
  - bias ~ 3 ppb (both analysis and forecast)

Conclusion

The reduction of error variance is largest when there is no chemistry. The bias is nearly zero in monitoring mode. The addition of chemistry reduces the effect of observations i.e. more resilient in reducing the error variance and in adapting the bias.

Online chemistry with NWP model

Chemistry ⟶ Meteorology

- Radiation: GHG, Aerosols
- Better representation of boundary layer processes, convective effects and wet removal
- Trace gas prior for meteorological satellite assimilation (e.g. channels contaminated ozone, aerosols, …)
- Towards the integration of a one atmosphere model

Technically

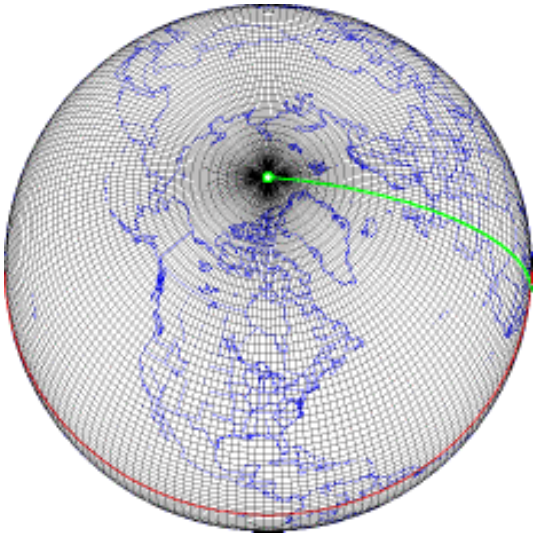
(+)

- Avoids large data transfer
- Streamline the development of models
  (e.g. MPI development)
- Relatively small computational time and memory overhead (+ 20%)
  over that of CTM at the same resolution

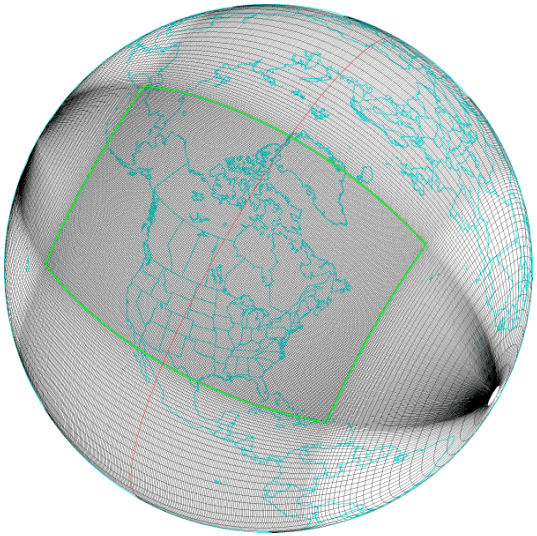
(-)

- Development of chemical interface (modest development)
- Modification of the physics (routines and buses) to include
  chemical variables (large undertaking)
- Two-way coupling needed for emission model (large undertaking)
  (e.g. OASIS-3 coupler is used for Ocean coupling)

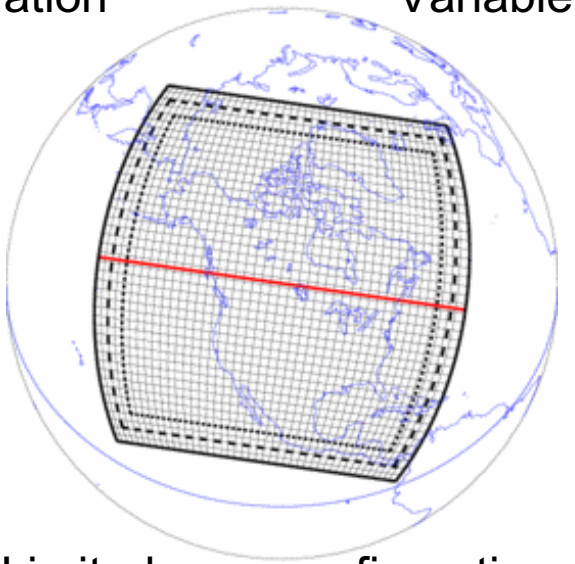
Global Environmental Multiscale model (GEM)



Global configuration



Variable resolution configuration

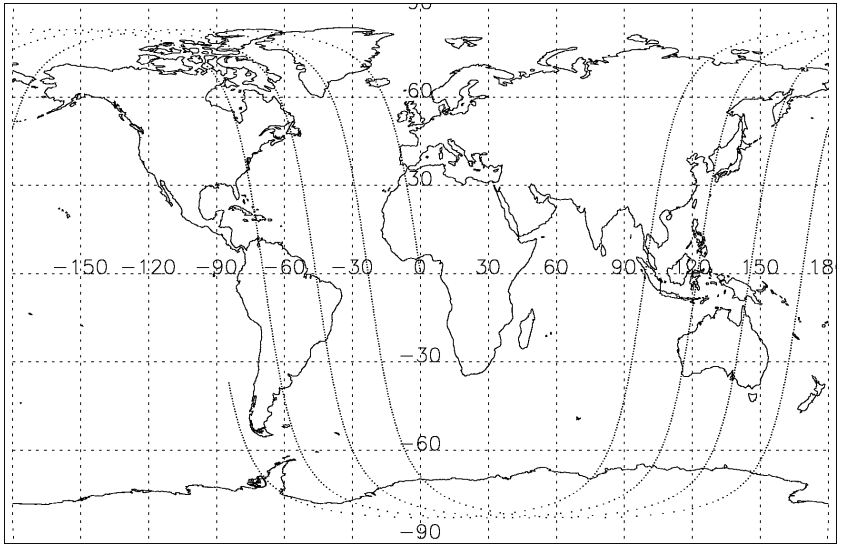


Limited area configuration

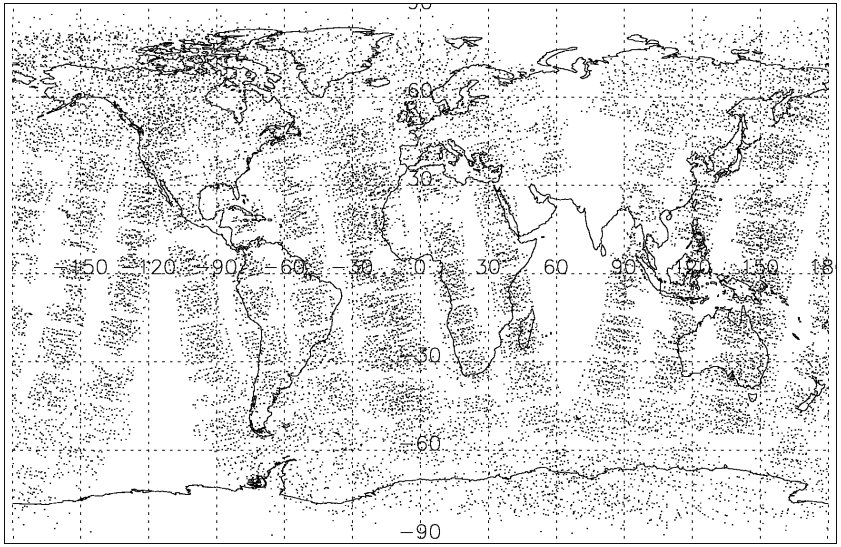
OSSE: Vertically resolved nadir ozone measurements vs. scanning total column ozone measurements

- Simulate an observation system (e.g. a new instrument) in a data assimilation environment to assess the impact of the observation system
  - Simulated truth, i.e. *nature run*, is created by a different model: SEF with CMAM chemistry
  - The "observations" are drawn from the nature run
  - 3D Var + GEM_Tracer is used as the assimilation system
- ORACLE space-based Differential Absorption Lidar (DIAL)
  - Ozone ; 1 km vertical resolution from 500 hPa to 1 hPa
- TOVS total column ozone

6h ORACLE track



6h TOSI track

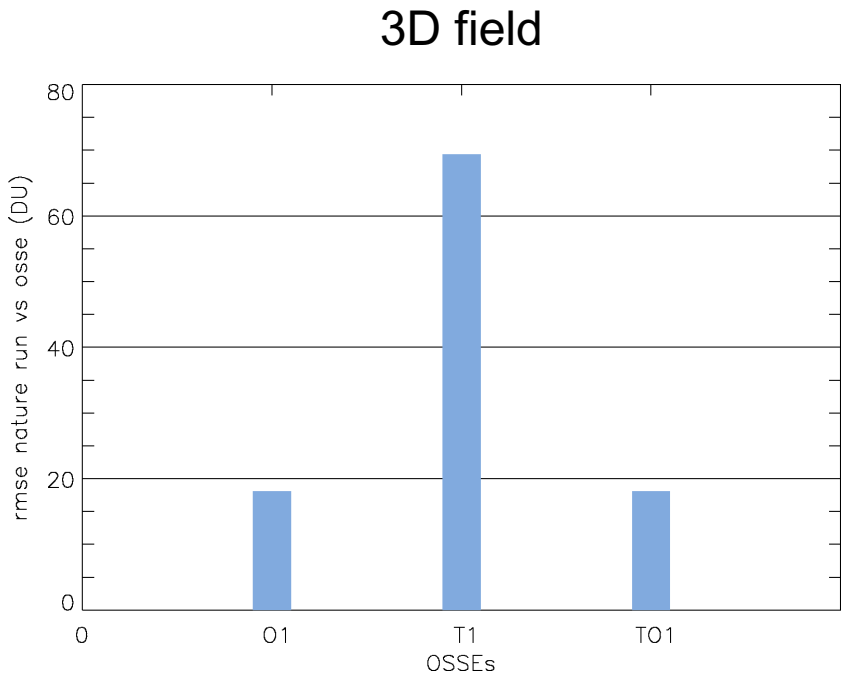


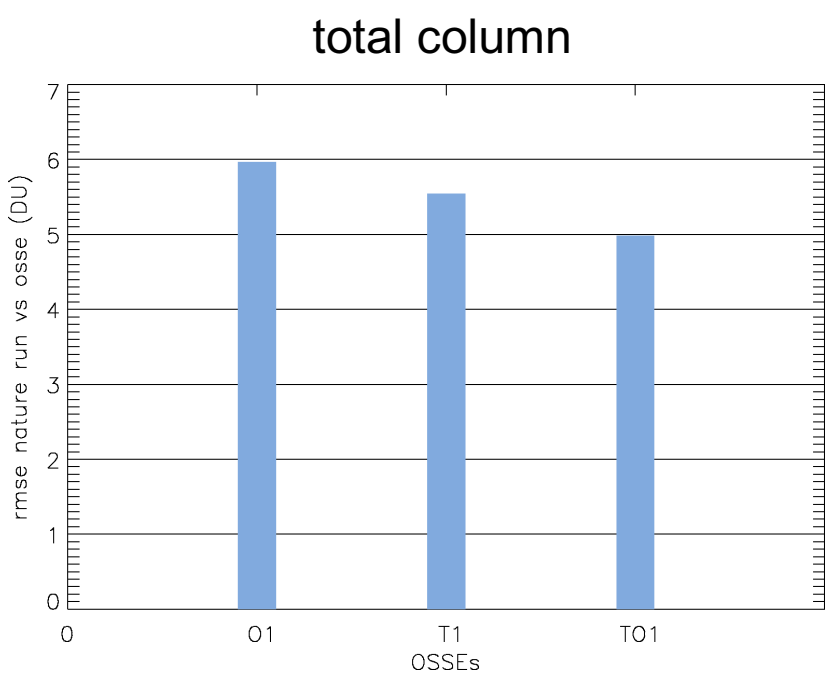
Forecast error variance

ORACLE

TOVS

ORACLE + TOVS


3D field
80
60
40
20
0
rmse nature run vs osse (DU)
0
O1
T1
TO1
OSSEs


total column
7
6
5
4
3
2
1
0
rmse nature run vs osse (DU)
0
O1
T1
TO1
OSSEs

Two main projects

- GEM – Air Quality
  - Focus on troposphere and emission model interface
  - Online integration of CHRONOS in GEM
  - Timelines: 09/05 start – 2007 End (Technical integration phase)
  - People: ARQI (3) Modelling and integration section
    - AQMAG (3) CMC/Air Quality Modelling and Application Group

- GEM – Stratosphere
  - Focus on stratospheric chemistry and data assimilation issues
  - Timelines: 01/05 start – July 2007 end
  - People: ARQI (5) Modelling and Integration section
    - ARQX (1) Ozone
    - ARMA (1) Satellite observations and data assimilation
    - ARMN (1) Meteorological modelling
    - CMC (3) Operations
    - BIRA (1) Belgium Institute for Space Aeronomy
    - MAQNet (1) York University

Main development tasks

Model

- chemical interface;
  chemical bus, no change to phys_exe
- coupled chemistry-meteorology validation
- GHG radiation interaction;
  chemical variables passed to phys_exe

Assimilation

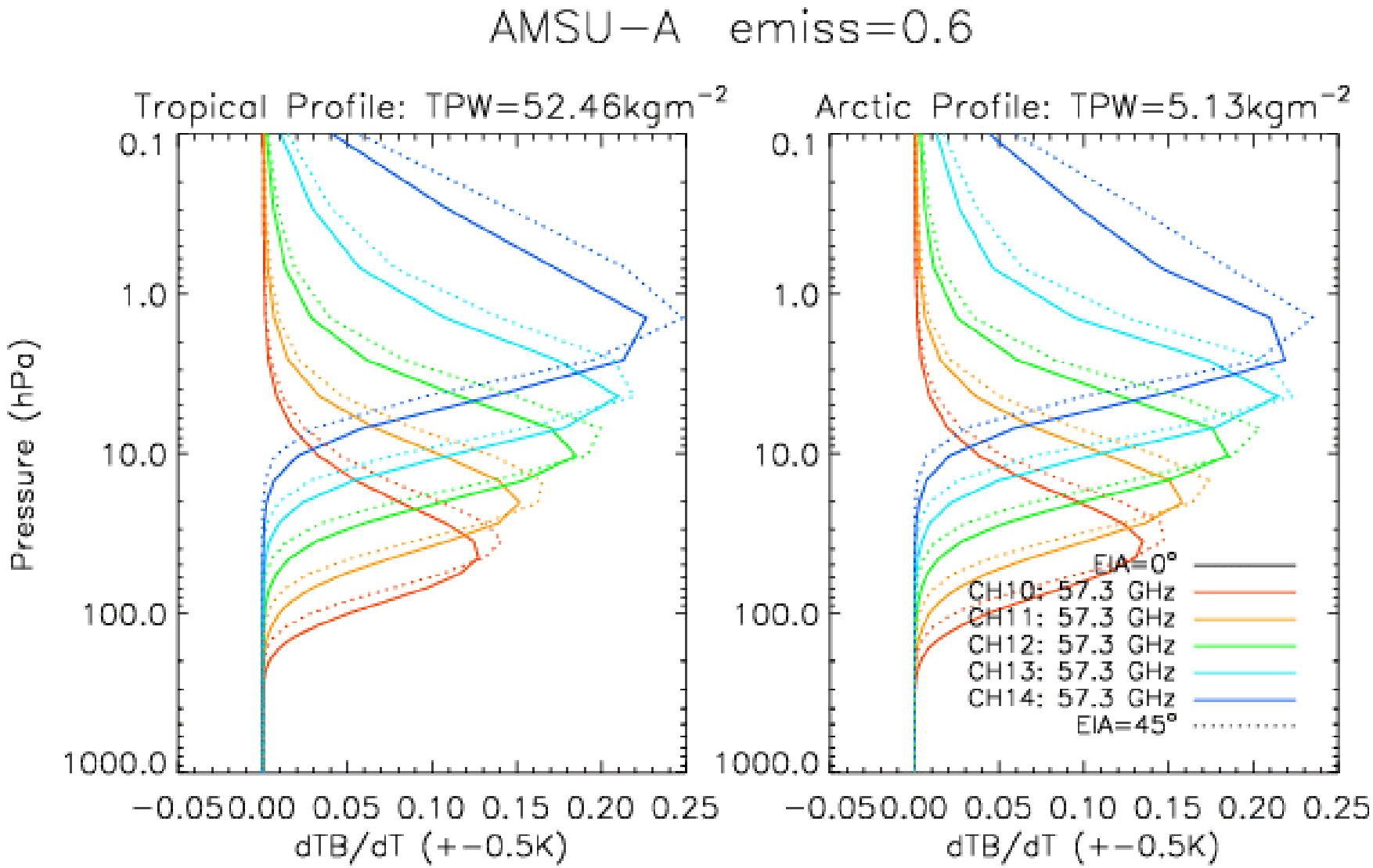
- extension of 3D Var for chemical species
- BUFR (BURP) format for chemical species. Proposition to WMO
- construction of error statistics;
  extension of meteorological tools for chemical species, cross error chemistry-meteorology statistics
- changes in assimilation launching scripts

Stratospheric Meteorological Assimilation

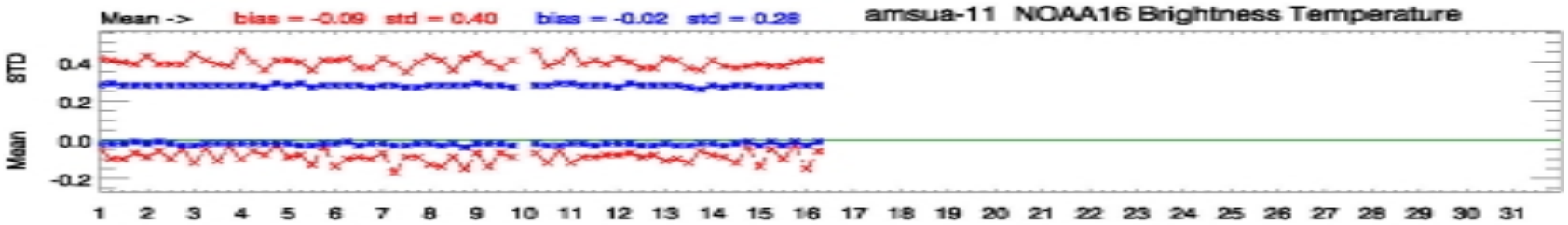
RTTOV Bias Correction

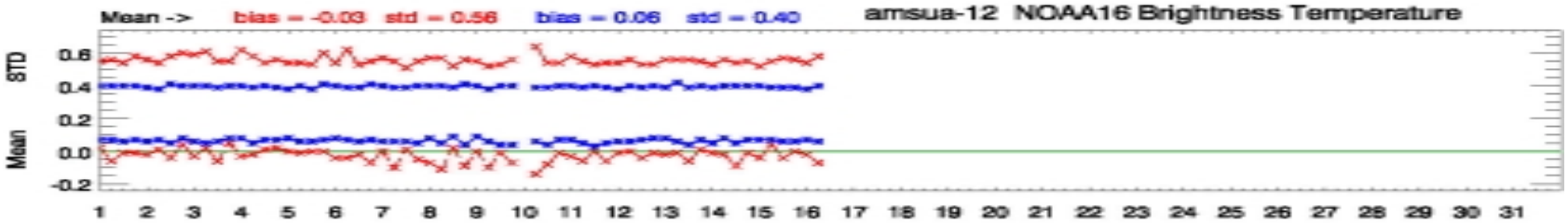
- Observed radiances compared with model simulated radiances
- Scan angle bias correction
- Air-mass dependence (regression)
- *In the troposphere the model is assumed to be unbiased! Is this a valid assumption for the stratosphere*

Jacobians with respect to temperature for channels 10-14 of AMSU-A

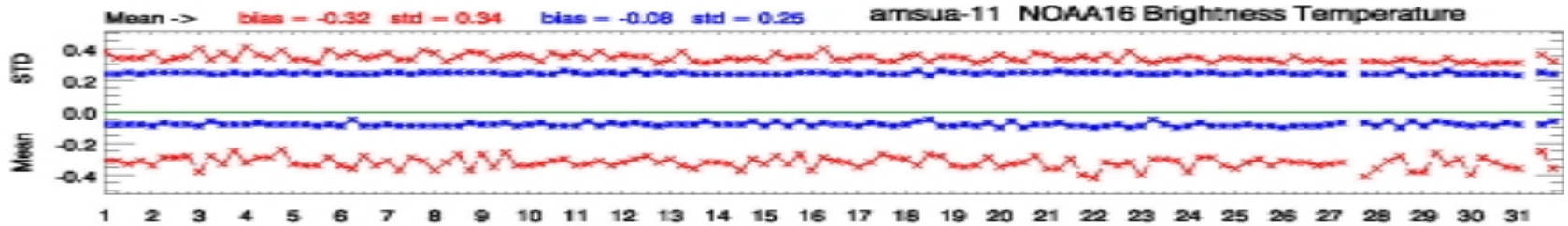


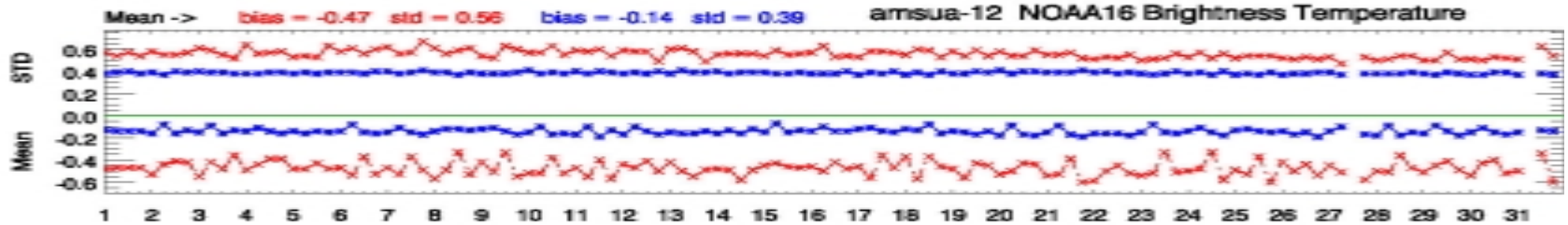
No bias correction



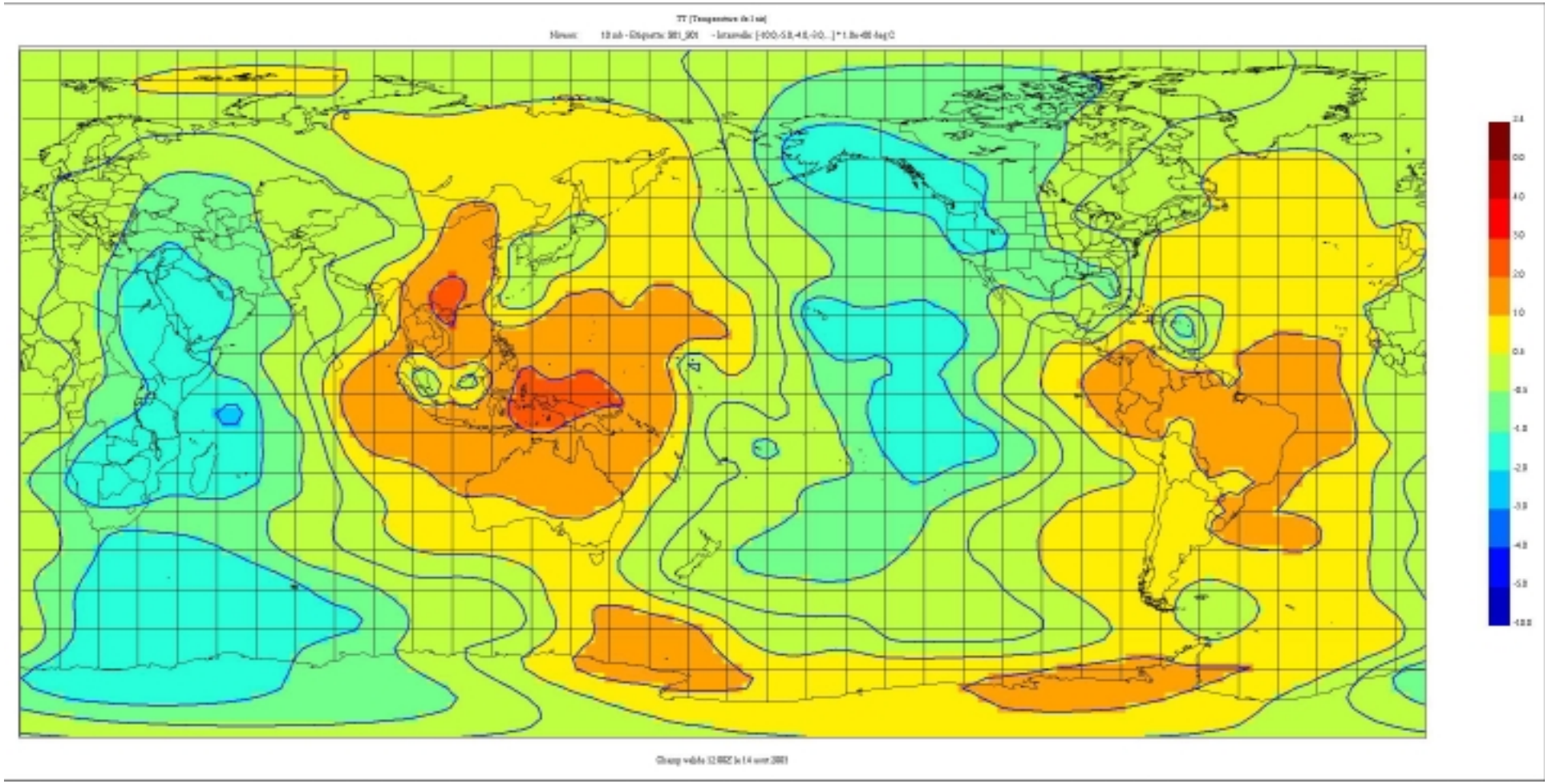


bias correction

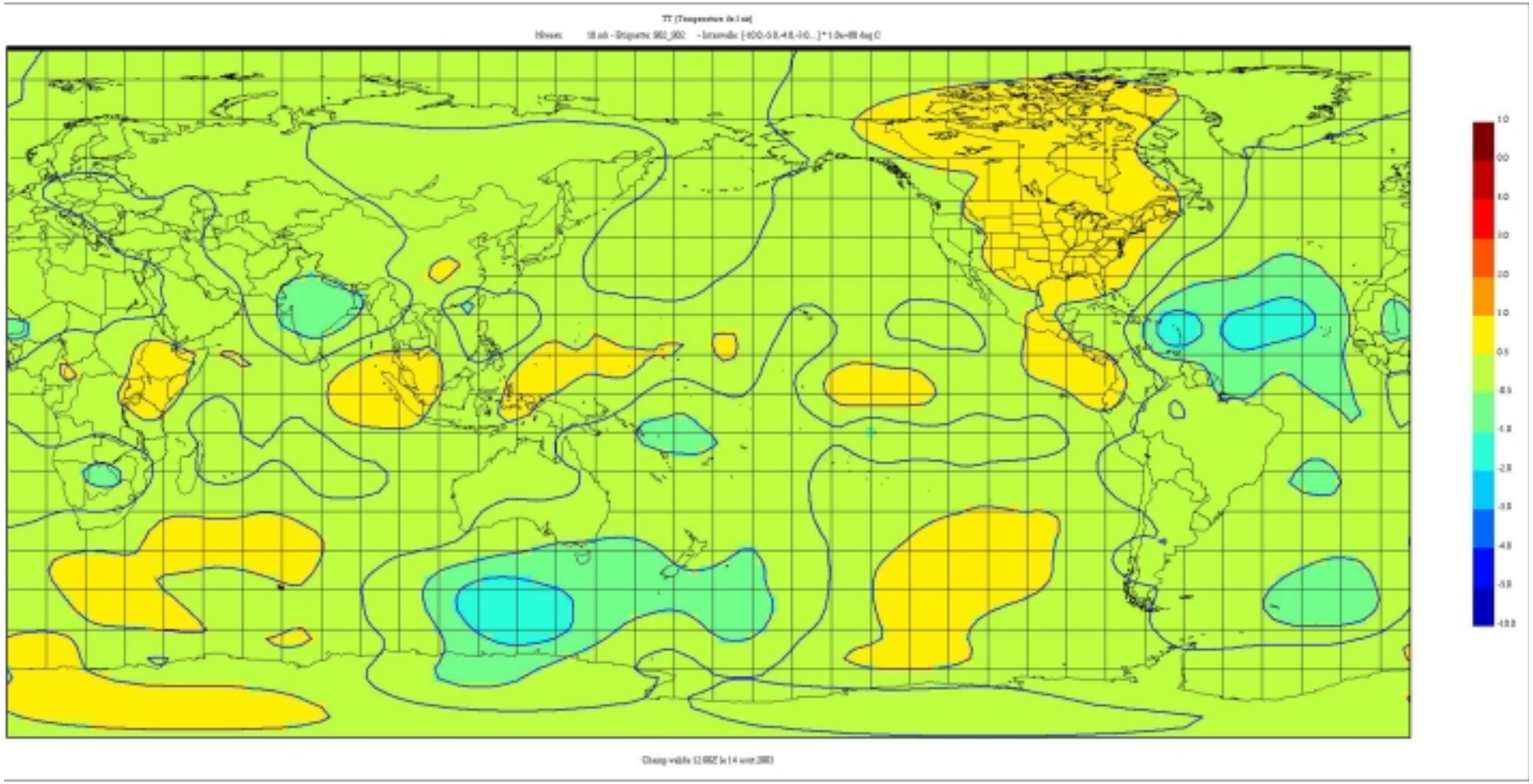




Mean temperature analysis increments at 10 hPa
(with bias correction applied to AMSU-A channels 11-14)

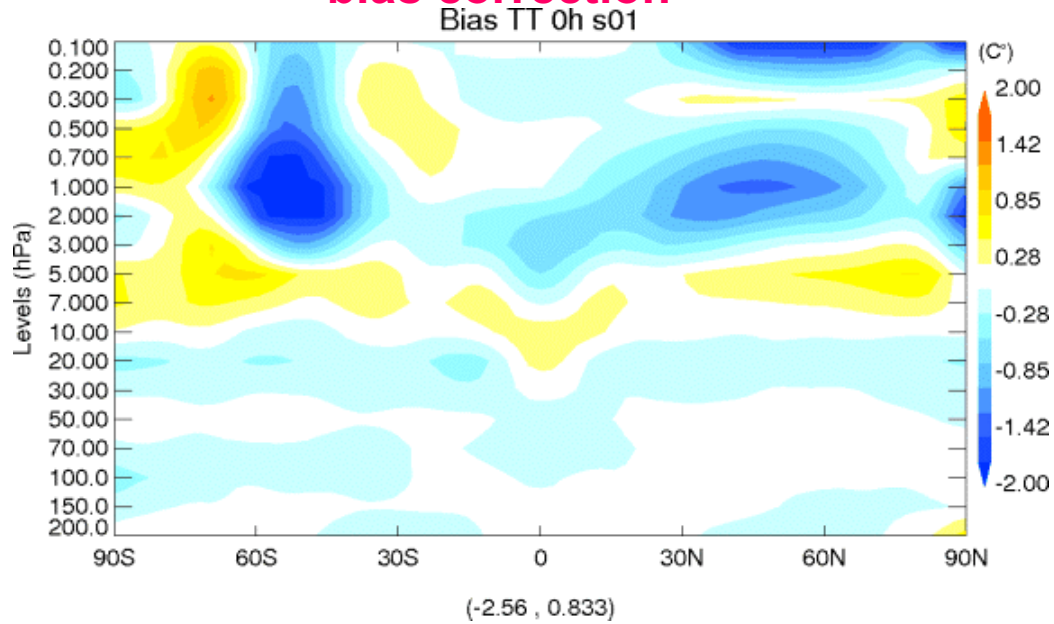


Mean temperature analysis increments at 10 hPa
(no bias correction applied to AMSU-A channels 11-14)

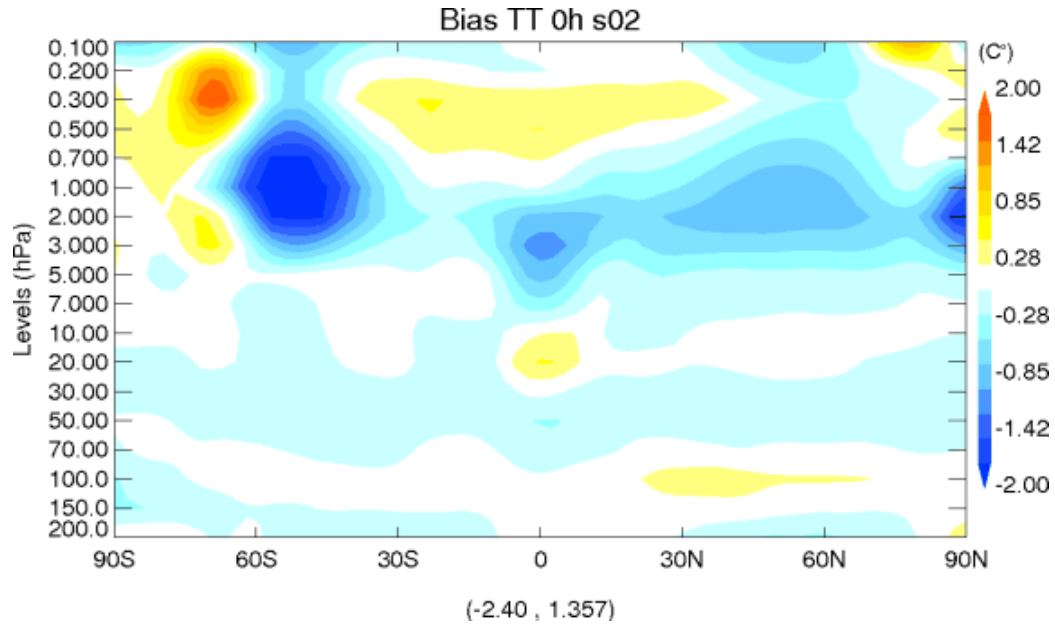


Zonal mean of temperature increments

bias correction



no bias correction



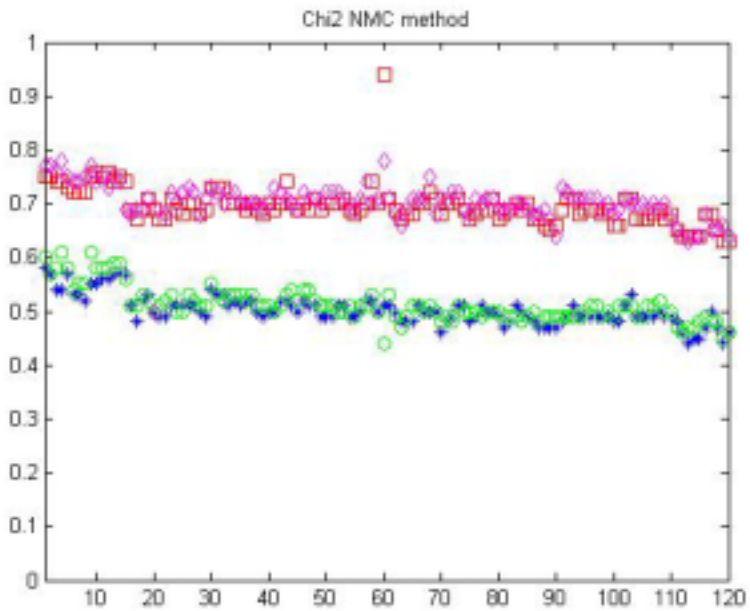
Error Statistics

A- Standard method

- Lagged forecast differences (i.e. NMC method) are used to construct error correlations and spatial variation of background error statistics.

- Prior knowledge of observation error variance, and zonal monthly averages of innovations are used to derive a scaling factor to the NMC derived error variances

$$\langle \chi^2 \rangle = \left\langle \mathbf{v}^T \left(\mathbf{HBH}^T + \mathbf{R} \right)^{-1} \mathbf{v} \right\rangle = p$$



B – Desrosiers et al. (2005) method

$$\langle OmF, OmF \rangle = \langle \mathbf{d}, \mathbf{d}^T \rangle = \mathbf{HBH}^T + \mathbf{R} \quad \text{.....(1)}$$

$$\langle OmA, OmF \rangle = \langle \mathbf{d} - \mathbf{HKd}, \mathbf{d}^T \rangle = (\mathbf{I} - \mathbf{HK}) \langle \mathbf{d}, \mathbf{d}^T \rangle$$

$$\underset{1}{\approx} \langle \mathbf{d}, \mathbf{d}^T \rangle - \mathbf{HBH}^T \approx \mathbf{R} \quad \text{.....(2)}$$

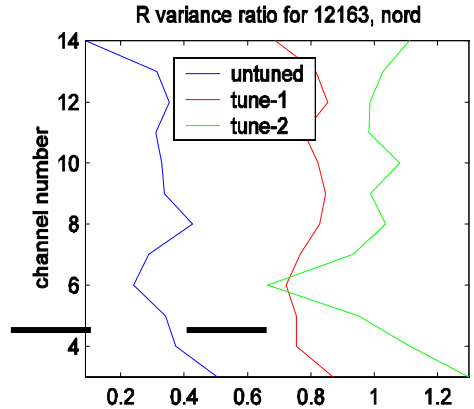
$$\langle AmF, OmF \rangle = \langle \mathbf{HKd}, \mathbf{d}^T \rangle \underset{1}{\approx} \mathbf{HBH}^T \quad \text{.....(3)}$$

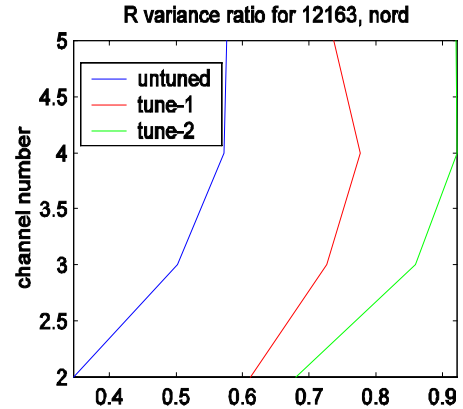
Remark: In the case the prescribed error statistics is incorrect, an iterative method has been proposed

$\langle OmA, OmP \rangle_n / \langle OmA, OmP \rangle_{n-1}$

Northern Hemisphere

AMSUA, B

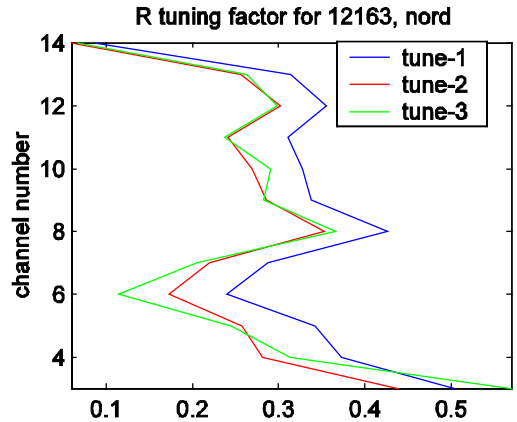


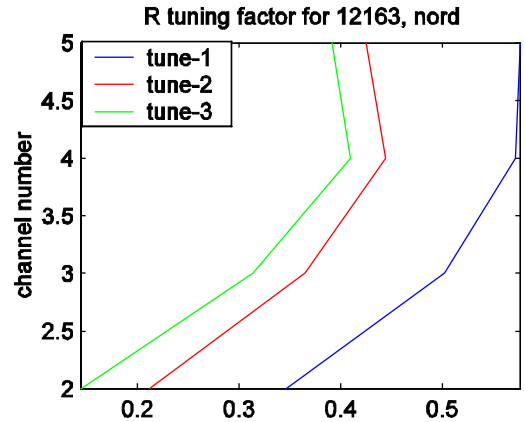


R_n / R_0

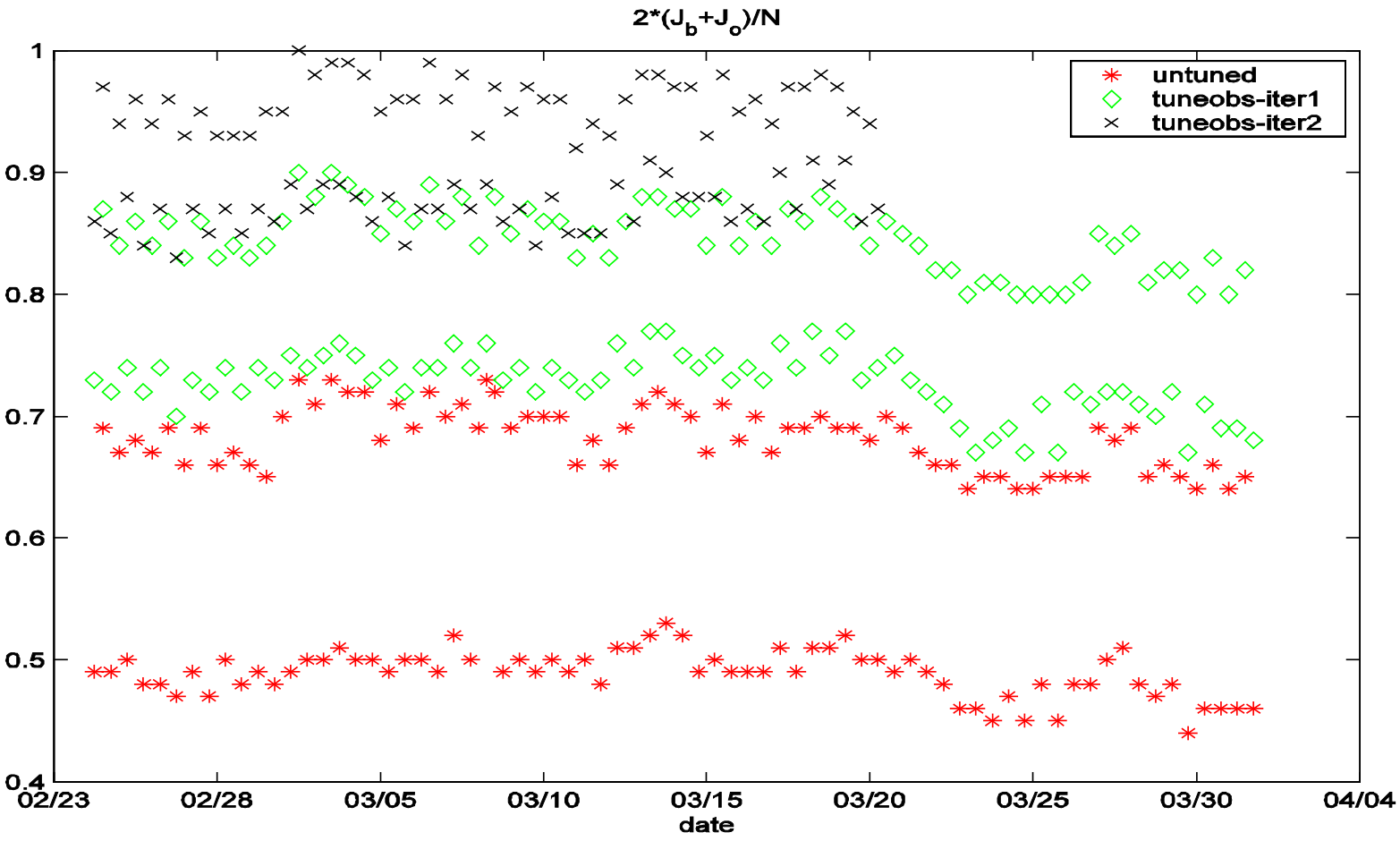
Northern Hemisphere

AMSUA, B





Conclusion: the operational AMSU radiance observation error variance is *underestimated*


2*(J_b+J_o)/N
untuned
tuneobs-iter1
tuneobs-iter2
1
0.9
0.8
0.7
0.6
0.5
0.4
02/23
02/28
03/05
03/10
03/15
03/20
03/25
03/30
04/04
date

Coupled chemistry-meteorology validation

Stratospheric chemistry developed by BIRA (Belgium Institute for Space Aeronomy)

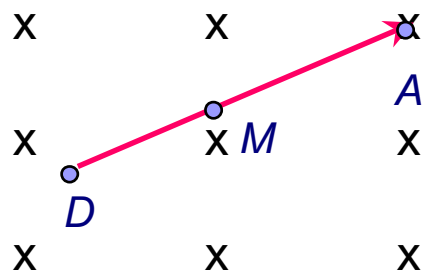
- Solver generated by KPP and manually modified
- Numerical method: 3rd – order Rosenbrock
- 57 chemical species, all advected
- 142 gas-phase reactions
- 7 heterogeneous reactions
- 52 photodissociation (*J*) reactions
- *J* values interpolated in tables
- Heterogeneous chemistry with simplified parameterizations for surface area densities

Computational Issues

§ Transport

Can save computation in semi-Lagrangian advection transport

- upstream point (*D* or *M*) is the same for all advected species



- interpolation weights $C_i(x)$ are the same for all advected species

e.g. cubic Lagrange interpolation

$$\varphi(x) = \sum_{i=1}^{4} C_i(x)\varphi_i \quad \text{with weights} \quad C_i(x) = \frac{\prod_{k\neq i}^{4}(x - x_k)}{\prod_{k\neq i}^{4}(x_i - x_k)}$$

- *Approximation* of computing costs :
  - for 240*120 horiz points (1.5°×1.5°) and 80 levels
  - on 16 CPUs of IBM p690s 64 bit Power 4

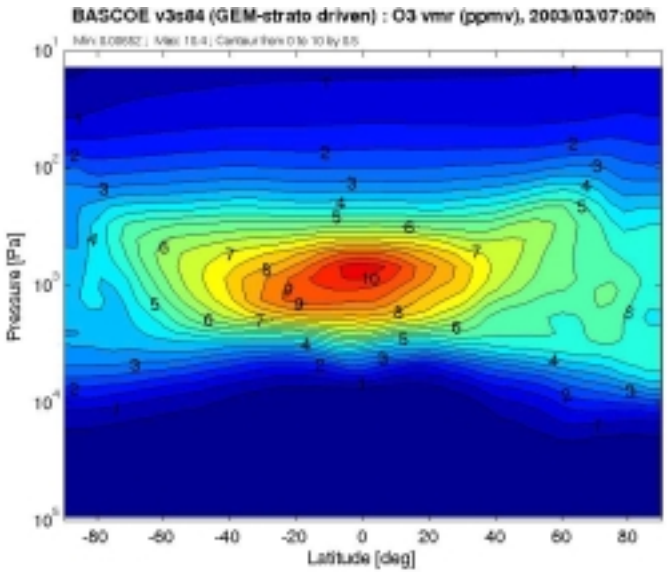
  1 simulation day takes ~ 30 minutes wallclock time

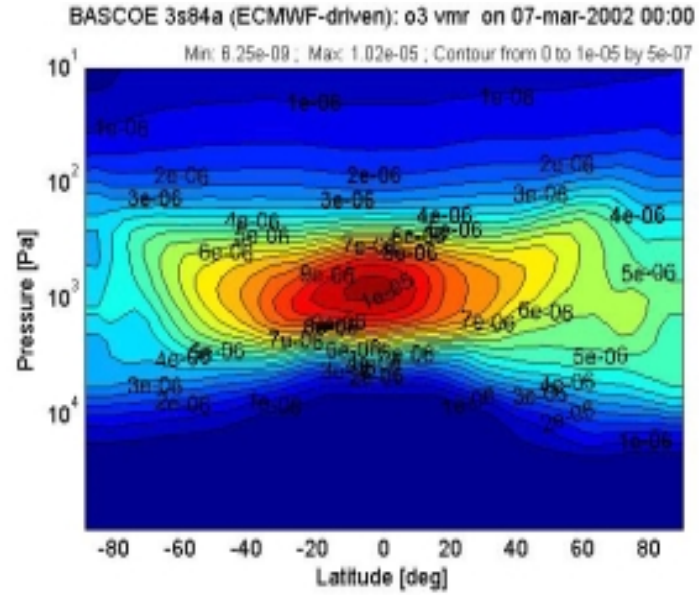
  → **GEM-strato + BIRA-chem is 4-5 times slower than GEM-strato alone**

- *Rough estimate* :GEM and transport → 1/4 CPU time
  J interpolation → 1/4 CPU time
  BIRA-chem solver → 1/2 CPU time

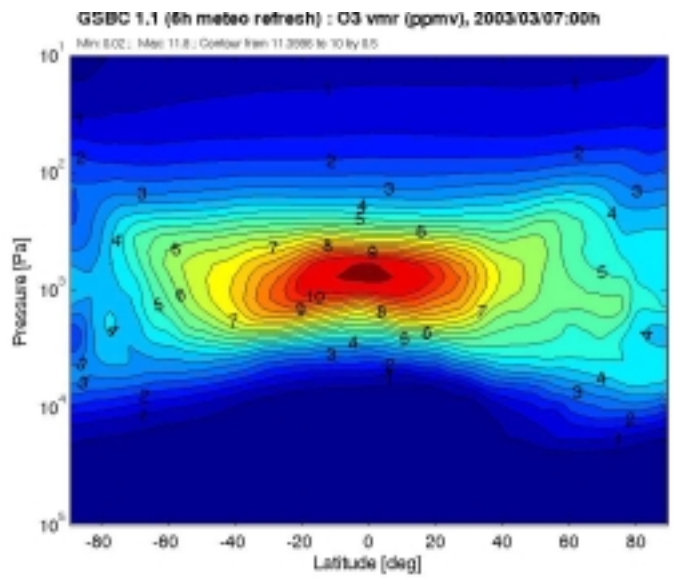
Ozone

CTM (off-line)
Low resolution
3.75° x 2.75°



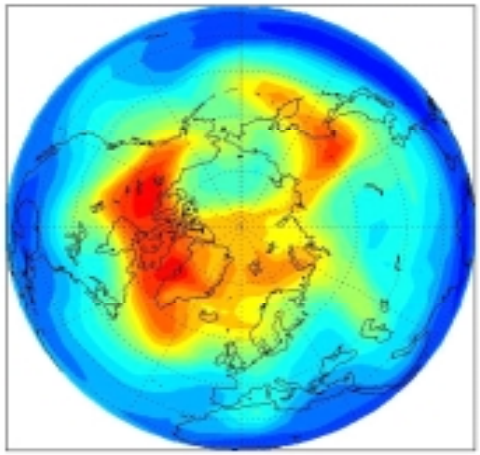


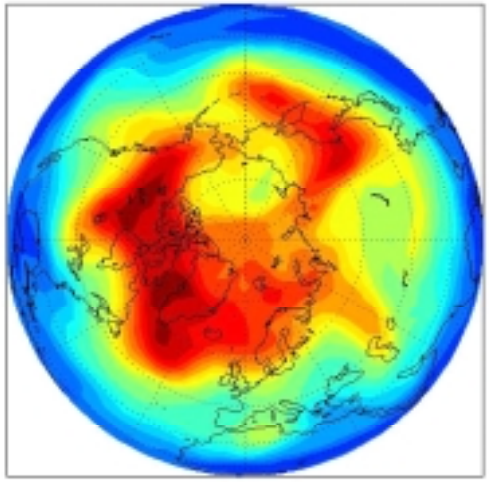
GEM-Strato-BIRA (online)
1.5° x 1.5°

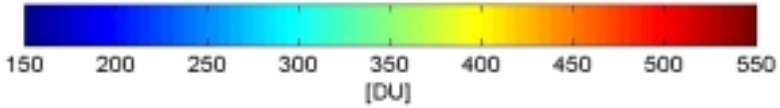


Ozone

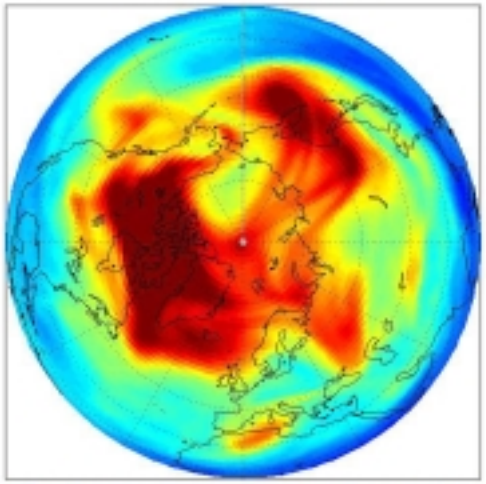
CTM (off-line)
Low resolution
3.75° x 2.75°

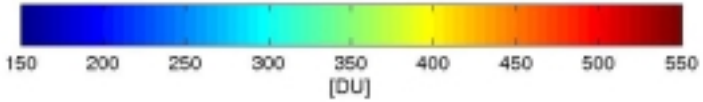






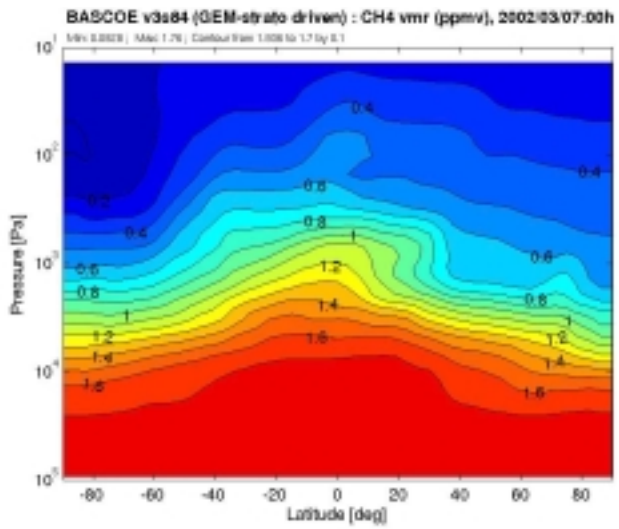
GEM-Strato-BIRA (online)
1.5° x 1.5°

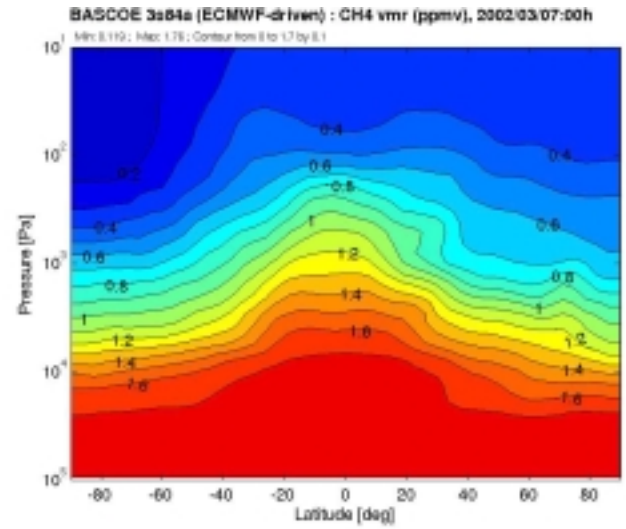




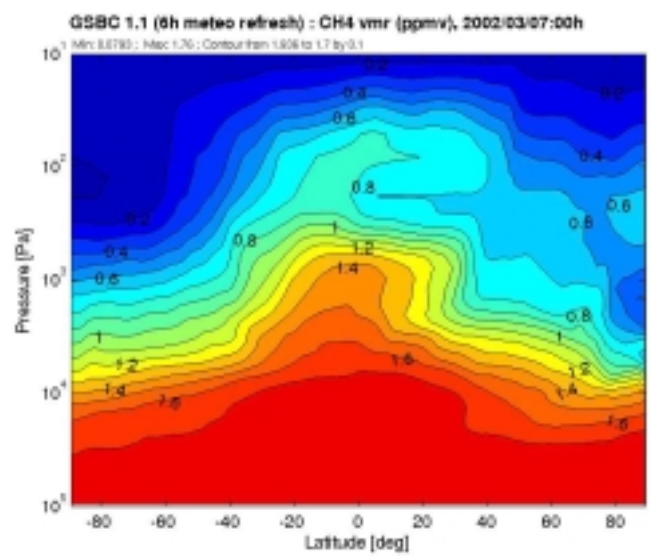
Methane

CTM (off-line)
Low resolution
3.75° x 2.75°





GEM-Strato-BIRA (online)
1.5° x 1.5°



Science question: How can we develop error covariances for unobserved variables (such as in chemical data assimilation) ?

Solutions:

A- Produce no analysis increments on unobserved variables

In 3D Var it suffices to have $\mathbf{P}_{ux} = 0$ (zero cross error covariance) which arises when either

1- $\mathbf{C}_{ux} = 0$
2- var(u) = 0 Perfect modelling of unobserved variable

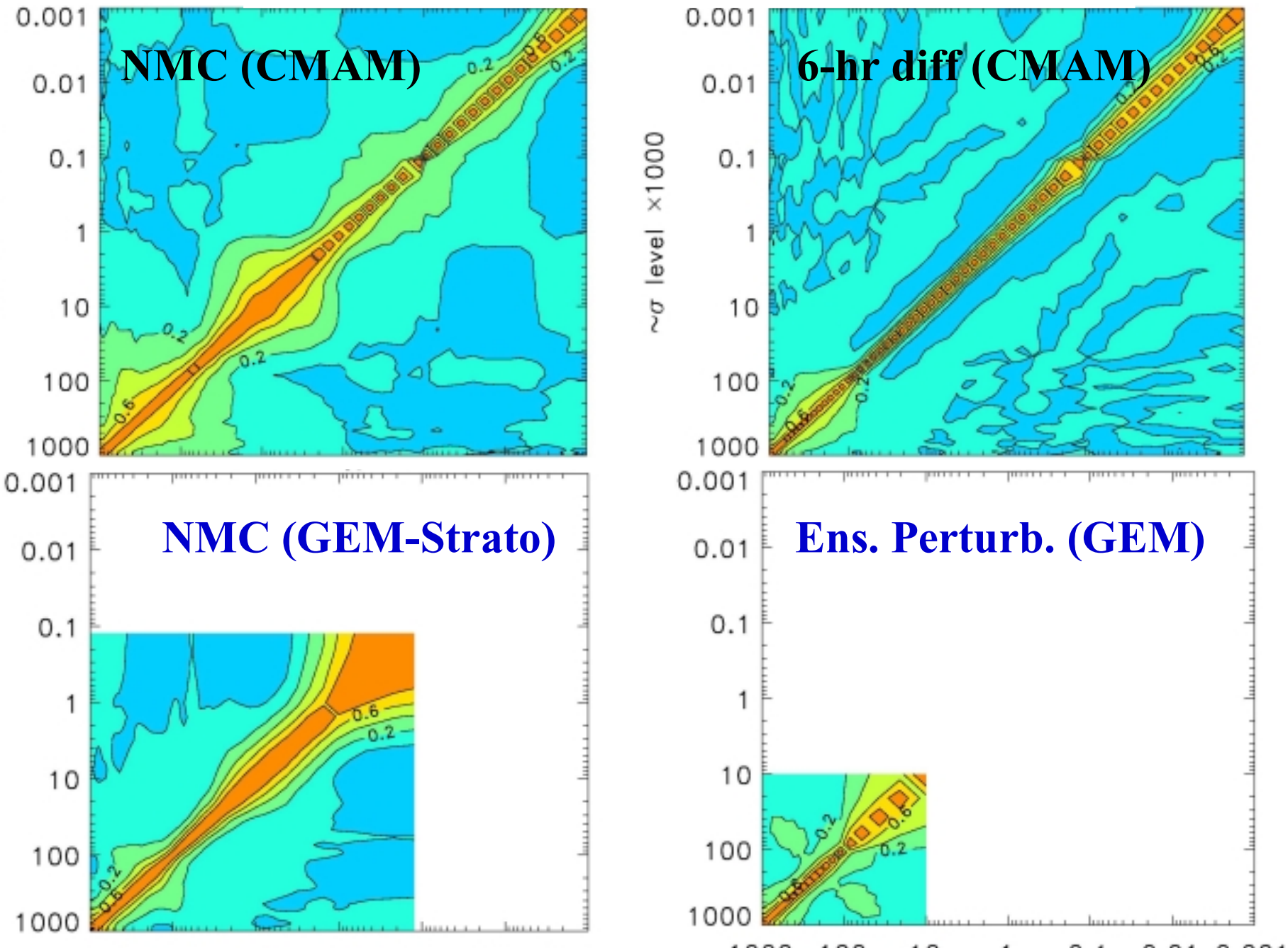
B – Use difference of forecast method (Rochon's method)

$$x_{t+6}^{m} - x_{t}^{m} - \left\langle x_{t+6}^{m} - x_{t}^{m} \right\rangle \qquad t = 0, 6, 12, 18 \text{ hrs}$$

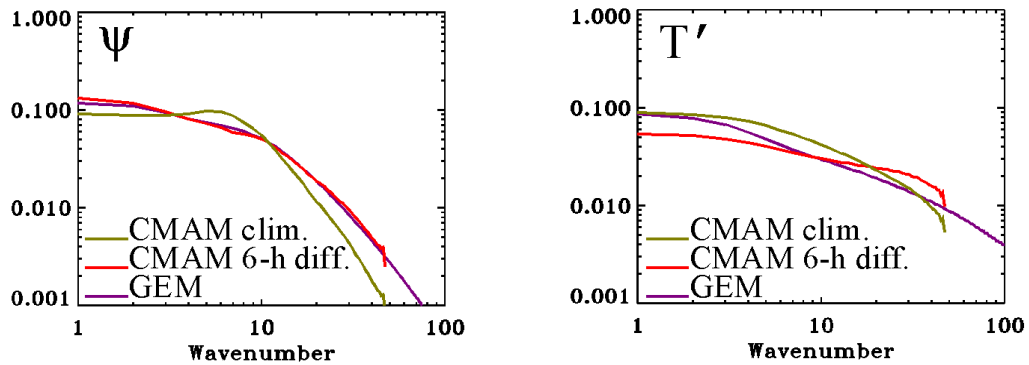
The relative error of observed variables will tend to be in general smaller than the relative error of unobserved variables, thus condition ***A2*** above is not realistic.

The error statistics of unobserved variables can be assumed to be nearly independent of the analysis scheme – thus Rochon's method seems to be the right answer

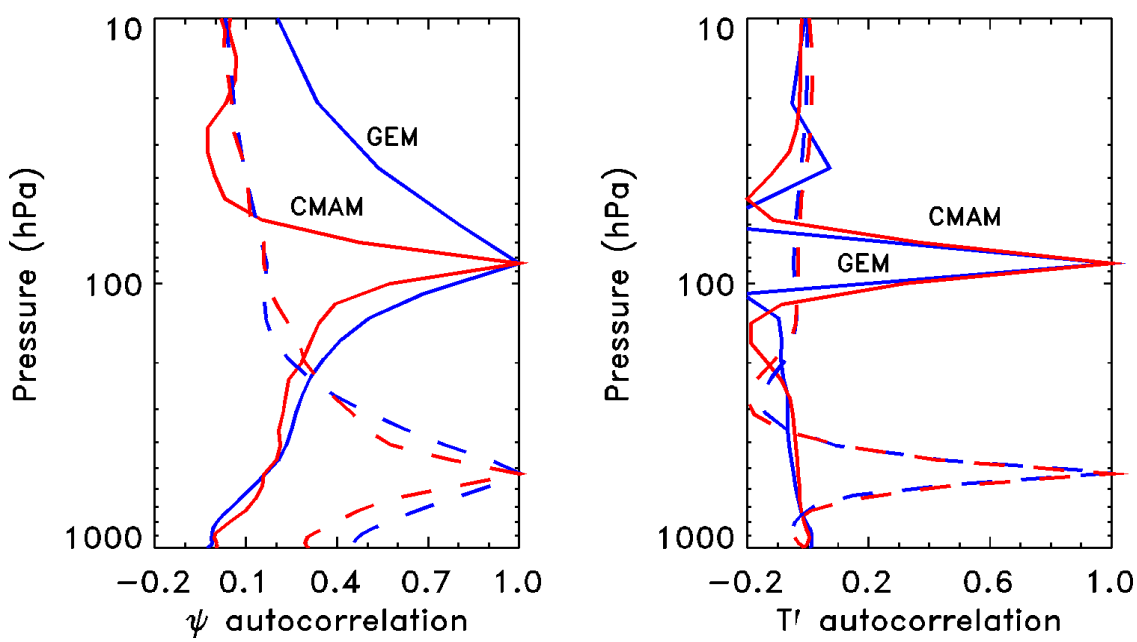
Vertical correlation matrices for ψ



Spectra of hor. autocorrelation functions near 500 hPa

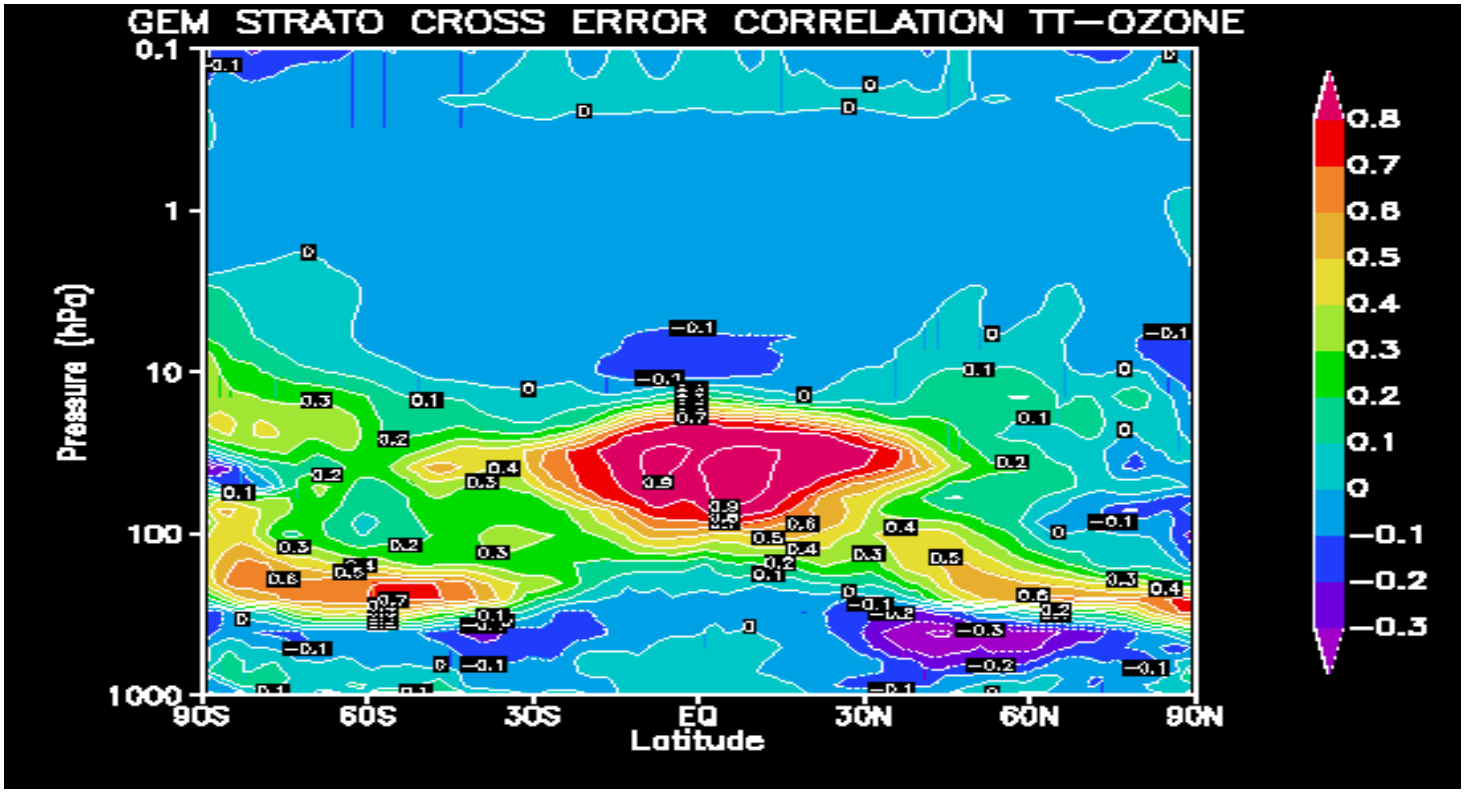


Vertical correlations at 84 and 520 hPa



Dynamic-chemistry cross error covariance

Using the method of difference's of forecast (Rochon's)



Implementation of cross error dynamical-chemical covariance

- **3D Var-CHEM**

  Addition to an abritrary number of chemical tracer in the operational 3D Var

  Can accommodate cross-error covariance either operator form or explicit form

$$\begin{pmatrix} \psi \\ \chi \\ (T, p_s) \\ \ln q \\ \ln[O_3] \end{pmatrix} = \begin{pmatrix} I & 0 & 0 & 0 & 0 \\ E & I & 0 & 0 & 0 \\ N & 0 & I & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ M & 0 & F & 0 & I \end{pmatrix} \begin{pmatrix} \psi \\ \chi_u \\ (T_u, p_{su}) \\ \ln q \\ \ln[O_3]_u \end{pmatrix}$$

Not all chemical species are observed

Analysis splitting ? only observed variables in control vector

The problem of minimizing

$$J(\mathbf{x},\mathbf{u}) = \frac{1}{2}\begin{pmatrix}\mathbf{x}-\mathbf{x}^f \\ \mathbf{u}-\mathbf{u}^f\end{pmatrix}^T \begin{pmatrix}\mathbf{P}^f_{xx} & \mathbf{P}^f_{xu} \\ \mathbf{P}^f_{ux} & \mathbf{P}^f_{uu}\end{pmatrix}^{-1} \begin{pmatrix}\mathbf{x}-\mathbf{x}^f & \mathbf{u}-\mathbf{u}^f\end{pmatrix} + \frac{1}{2}\left(\mathbf{y}-H(\mathbf{x})\right)^T \mathbf{R}^{-1}\left(\mathbf{y}-H(\mathbf{x})\right)$$

*with respect to **x** and **u** is mathematically equivalent to minimizing*

$$J(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^f\right)^T \mathbf{P}^{-1}_{xx}\left(\mathbf{x}-\mathbf{x}^f\right) + \frac{1}{2}\left(\mathbf{y}-\mathbf{H}(\mathbf{x})\right)^T \mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{H}(\mathbf{x})\right)$$

followed by the update (Ménard et al. 2004)

$$\mathbf{u}^a = \mathbf{u}^f + \mathbf{P}_{ux}\left(\mathbf{P}_{xx}\right)^{-1}\left(\mathbf{x}^a-\mathbf{x}^f\right)$$

- **4D Var extension**

Uses same solver as in 3D Var

tangent linear integration

$$J(\xi) = \frac{1}{2}\left(\xi-\xi^f\right)^T\left(\xi-\xi^f\right) + \frac{1}{2}\left(\mathbf{y}-\mathbf{H}(\mathbf{L}(\xi))\right)^T \mathbf{R}^{-1}\left(\mathbf{y}-\mathbf{H}(\mathbf{L}(\xi))\right)$$