Spectral Representation of Spatial Correlations in Variational Assimilation Systems with Grid Point Models: Application to the Belgian Assimilation System of Chemical ObsErvations (BASCOE)

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Outline

1. Formulation of the **B** matrix on a spherical harmonic basis
2. Real experiments with MIPAS (SH Winter 2003) and Eos/MLS (SH Winter 2007) observations
3. Conclusions

Formulation: Variational Data Assimilation

The classical (i.e. non-incremental) formulation of variational assimilation:

$$J(\mathbf{x}) = \underbrace{\frac{1}{2}[\mathbf{x}-\mathbf{x}^{\mathrm{b}}]^T\mathbf{B}^{-1}[\mathbf{x}-\mathbf{x}^{\mathrm{b}}]}_{J^{\mathrm{b}} \equiv \text{background term}} + \underbrace{\frac{1}{2}[\mathbf{y}-H(\mathbf{x})]^T\mathbf{R}^{-1}[\mathbf{y}-H(\mathbf{x})]}_{J^{\mathrm{o}} \equiv \text{observation term}}$$

- As the typical dimension of **x** is around 10^6, a full **B** matrix is of size 10^{12}. This is far too large to deal by current computers.
- Prop: On a spherical harmonic (SH) basis, homogeneous and isotropic horizontal correlations are represented by a diagonal matrix (Boer, 1983, JAS).
- Assuming homogeneous and isotropic horizontal correlations, the spherical harmonic representation of **B** is block diagonal

Formulation: Control Variable Transform (CVT, see Courtier et al., 1998, QJRMS)

$$\mathbf{L}\chi = \mathbf{x} - \mathbf{x}^{\mathrm{b}}$$

$$\mathbf{B} = \mathbf{L}\mathbf{L}^{T} \Leftrightarrow \mathbf{L} = \mathbf{B}^{1/2}$$

χ is defined in the spectral space and **L** is defined by

$$\mathbf{L} = \mathbf{\Sigma}\mathbf{S}\mathbf{\Lambda}^{1/2}$$

where

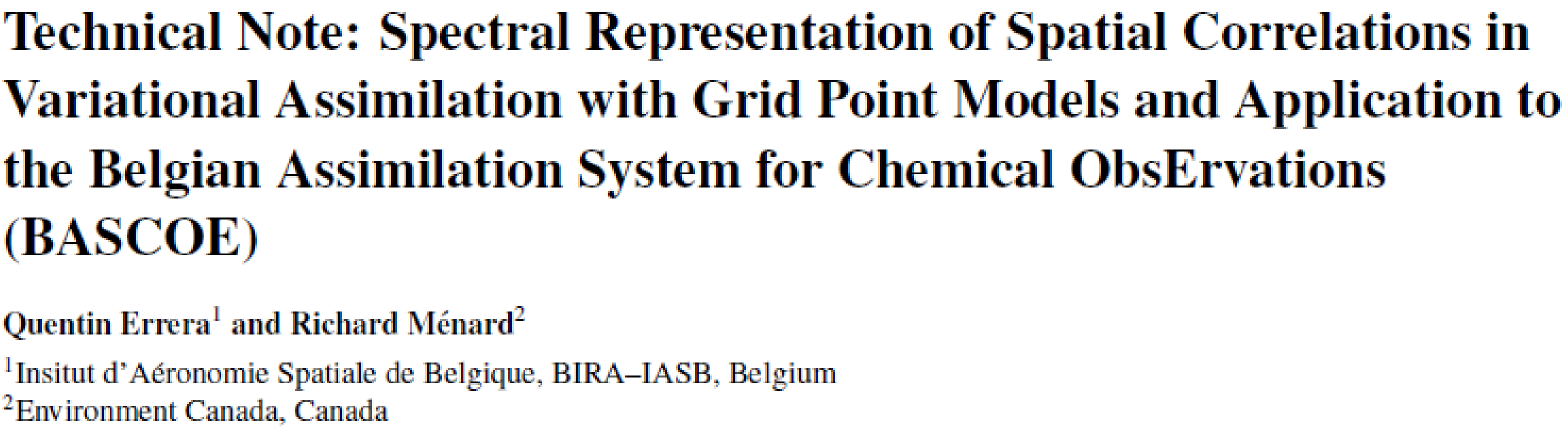
- **Λ** is the spatial correlation matrix (block diagonal) defined in the spectral space
- **S** is the direct spectral transform operator from the SH basis to the model grid
- **Σ** is the background error standard deviation matrix (diagonal)

As usual in variational assimilation, **L*** must also be provided

$$\mathbf{L}^{*} = \mathbf{\Lambda}^{1/2}\mathbf{S}^{*}\mathbf{\Sigma}$$

Formulation

This formulation and the F90 code of the different operators are described/reviewed in



Technical Note: Spectral Representation of Spatial Correlations in Variational Assimilation with Grid Point Models and Application to the Belgian Assimilation System for Chemical ObsErvations (BASCOE)

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Formulation: Comment about the Gaussian grid

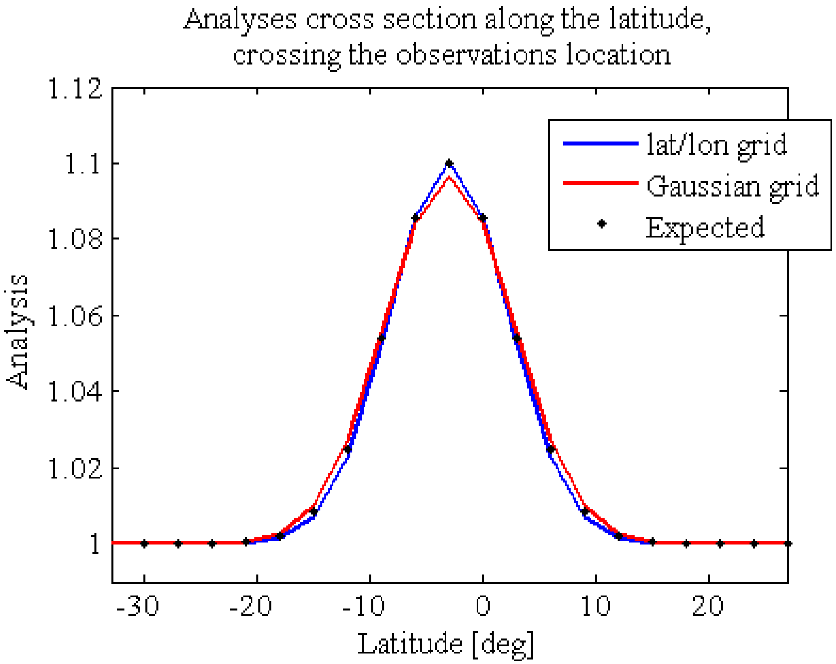
This formulation does not need the Gaussian grid

- The Gaussian grid is necessary for spectral model where some operations are done on the model grid and others in the spectral space
- **S*** can be built to work directly from the (lat/lon) model grid to the SH basis

→The SH spectral method can thus be applied to any grid point model without any mapping transformation form the spectral grid to the model grid

Example: Assimilation of a single obs

- $\mathbf{y}^o = 1.2$; $\boldsymbol{\sigma}^o = 0.1$
- $\mathbf{x}^b = 1$; $\boldsymbol{\sigma}^b = 0.1$
- **B**: Gaussian correlations; L_h=600 km; L_v=3 levels
- Expected results: Gaussian shape analysis with L_h=600 km and L_v=3 levels levels, and the value of 1.1 at the obs location



Formulation: Comment about the Aliasing

Aliasing in *spectral assimilation* less strict than in spectral modeling

- N is the truncation degree
- K is the number of latitudes
- M is the number of longitudes

- Preventing for aliasing in spectral modeling:

$$N=K-1$$

$$N=M/2 - 1$$

$$\text{i.e. } K=M/2$$

- Preventing for aliasing in *spectral assimilation:*

$$N=\max(K,M/2)$$

→ Lat and lon resolution of our model can be different

Assimilation of real data: General setup of the experiments

BASCOE

- 4D-Var system dedicated to stratospheric chemical observations
- CTM including 57 species, 200 chemical reactions
- PSC parameterization
- Chemistry (and PSC param.) can be turned off
- Source of Mesospheric NOx NOT modeled
- Assimilation window is 24h

Dynamic

- ECMWF Era-Interim

Resolution

- Chemistry off: 2° long x 2° lat x 37 levels x 15 minutes
- Chemistry on: 3.75° long x 2.5° lat x 37 levels x 30 minutes

Data

- MIPAS v4.61 ; Antarctic spring-winter 2003
- MLS v3.3 ; Antarctic spring-winter 2007

Assimilation of real data

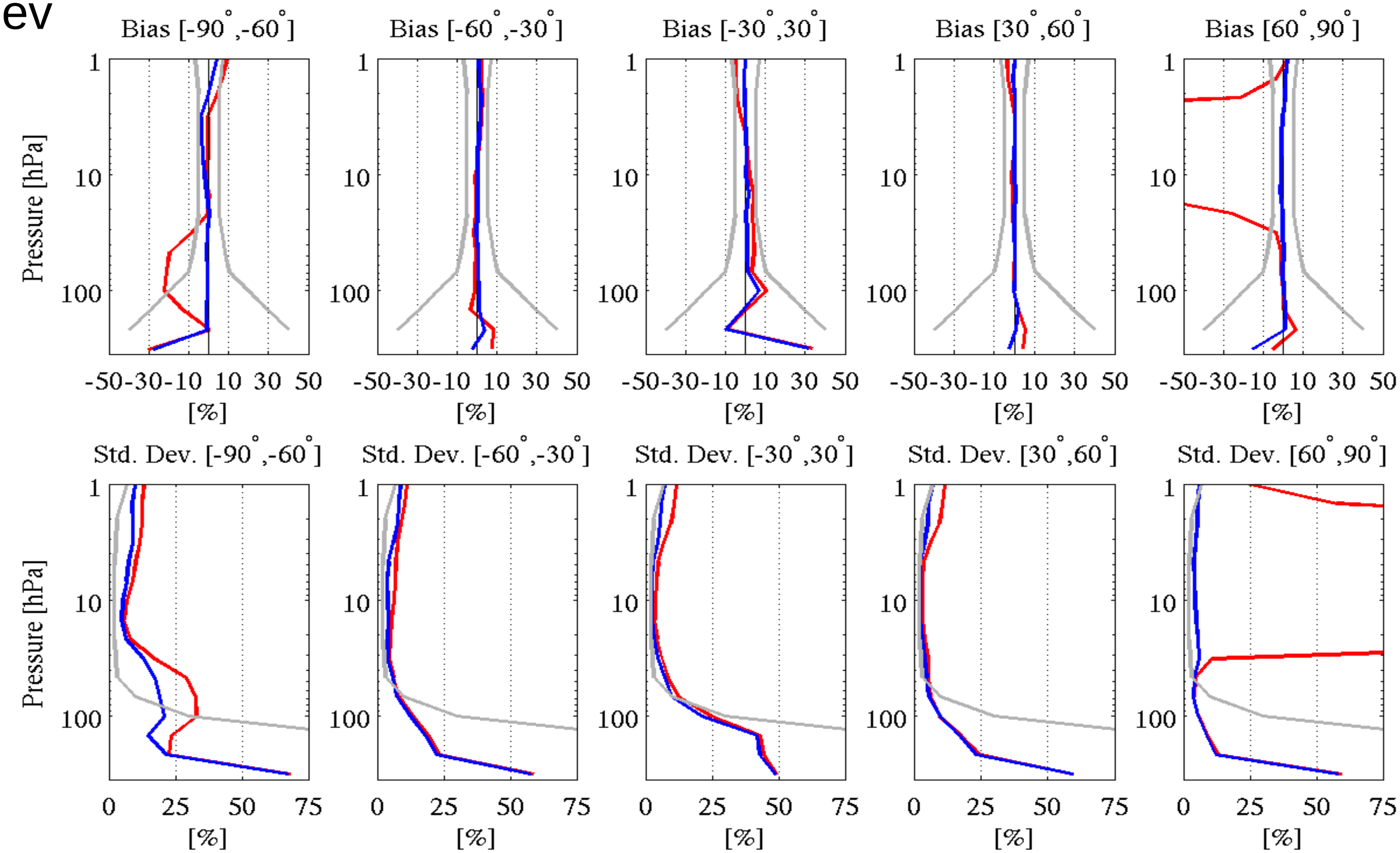
Assimilation with chemistry turned off

Ozone is assimilated as a passive tracer

Assimilation of MLS O3: Chemistri is off

Bias and Std Dev of OmF for Sep-Oct 2007 from MLS assimilation

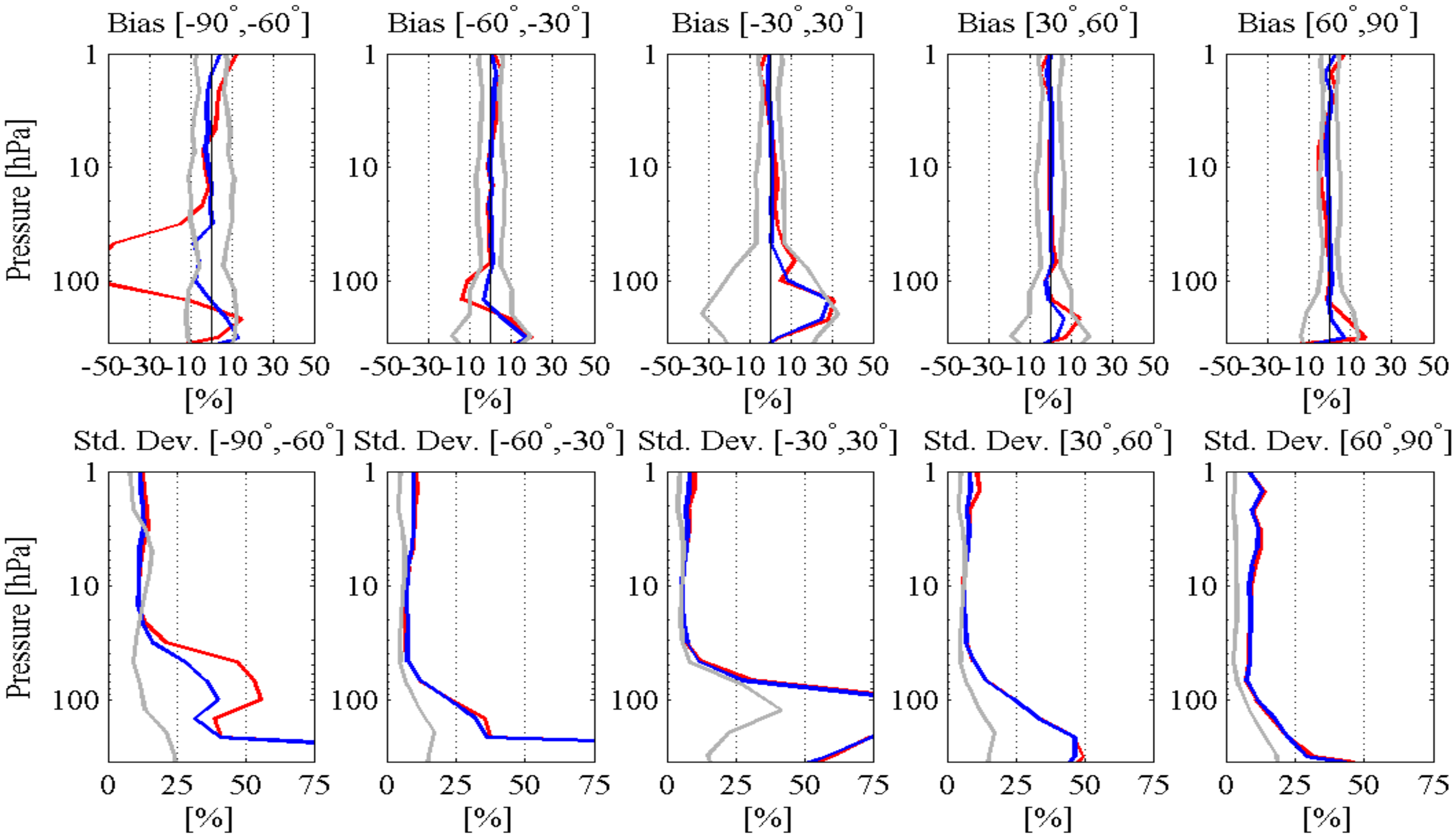
- Diagonal **B** : **Σ** = 0.3 $\mathbf{x}^b$
- Correlations : **Σ** = 0.3 $\mathbf{x}^b$, Correlation model: Gaussian, L_h=600 km, L_v=1.5 lev



Assimilation of MIPAS O3: Chemistry is off

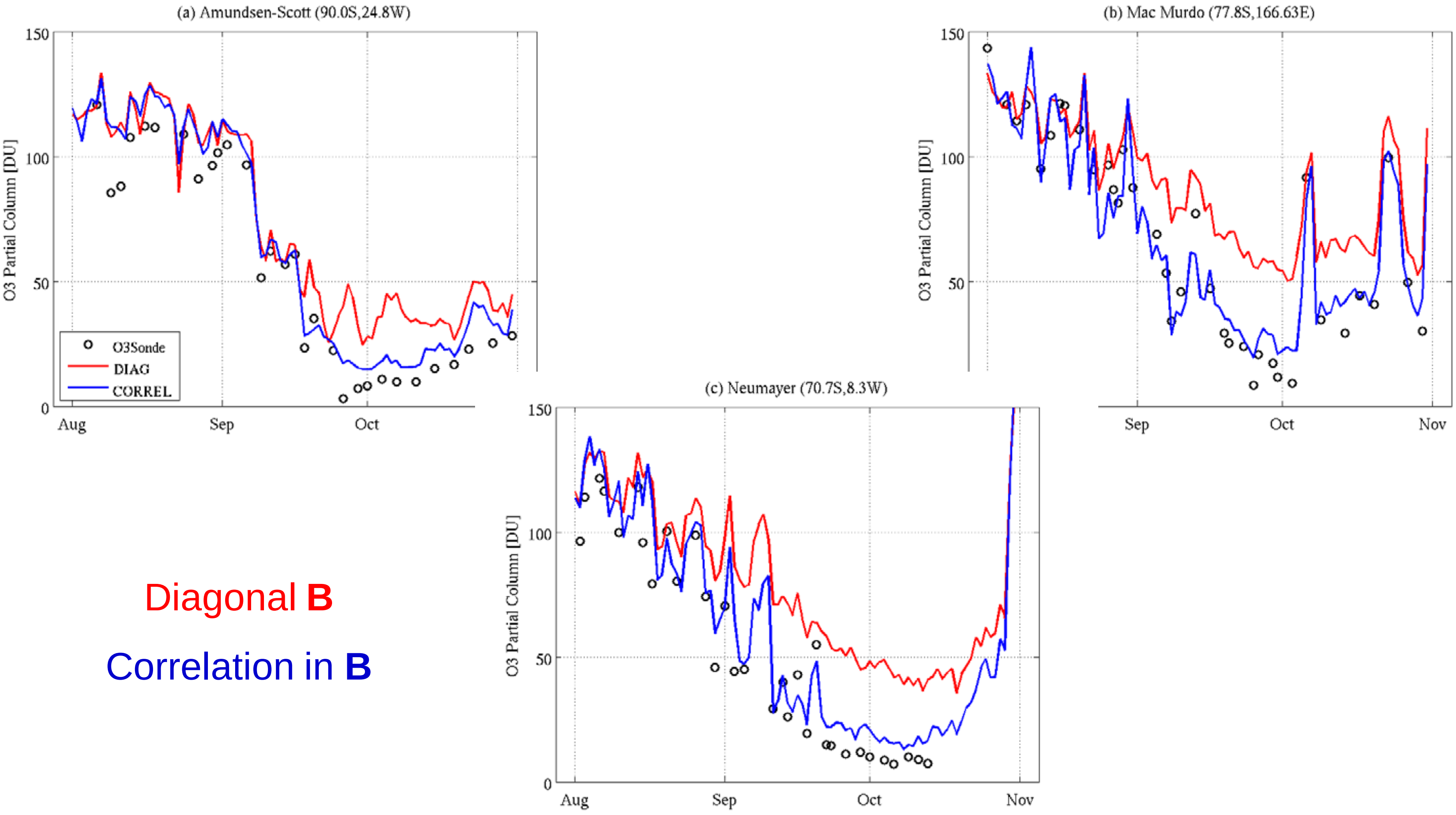
Bias and Std Dev of OmF for Sep-Oct 2003 from MIPAS assimilation

- Diagonal **B** : **Σ** = 0.3 $\mathbf{x}^b$
- Correlations : **Σ** = 0.3 $\mathbf{x}^b$, Correlation model: Gaussian, L_h=600 km, L_v=1.5



Assimilation of MIPAS O3: Chemistry is off

Time series of O3 partial column [10-100 hPa] above three NDACC groundbased stations in Antarctica

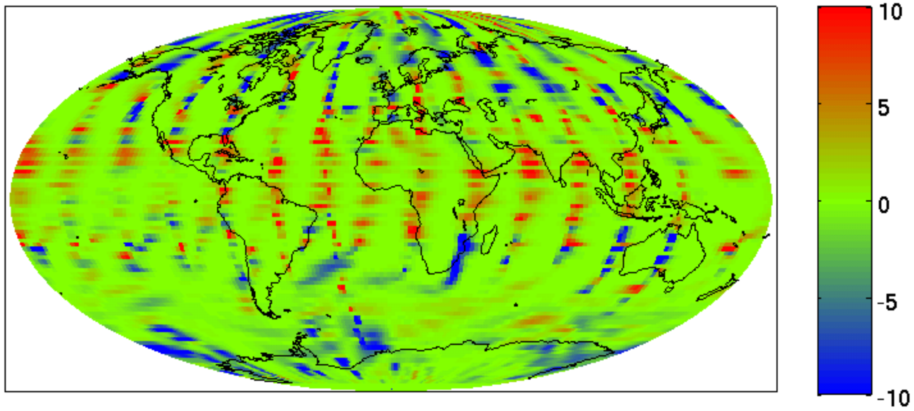


Diagonal **B**

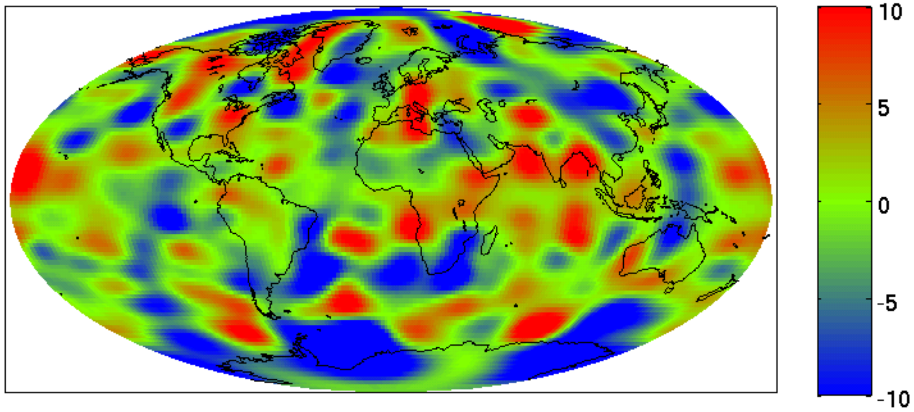
Correlation in **B**

Assimilation of MIPAS O3: Chemistry off

(a) Analysis Increments [%] for run DIAG at 44.335 hPa



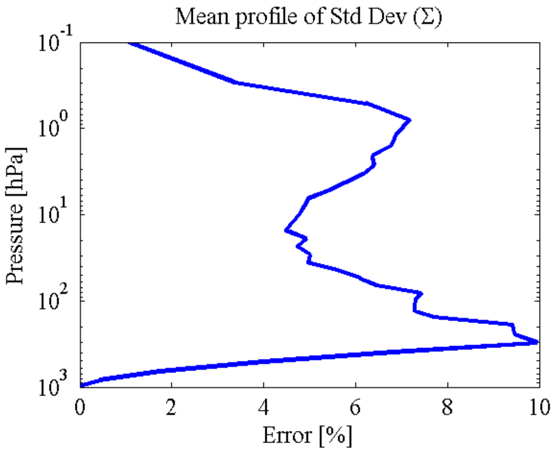
(b) Analysis Increments [%] for run CORREL at 44.335 hPa

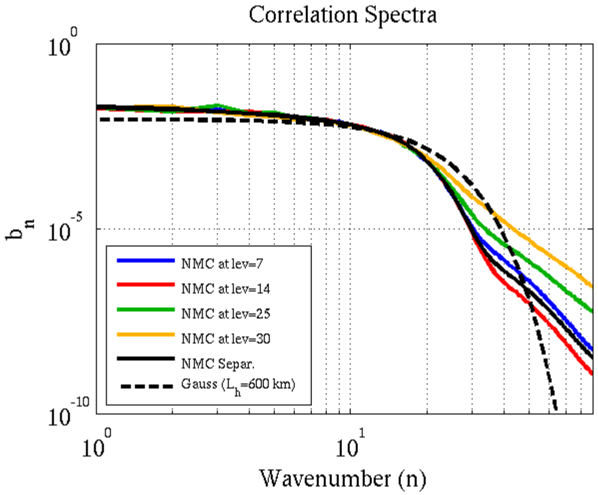


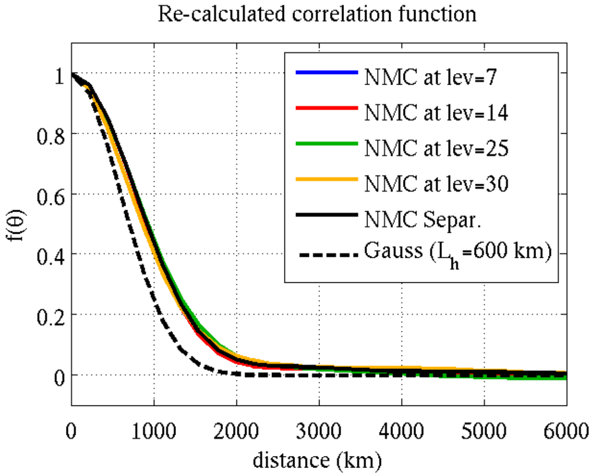
→ Correlations increase the size of the analysis increments

Calibration of **B** (1/2): NMC method (Rabier et al., 1998, QJRMS)

1. By making an ensemble of error fields ζ, one can calibrate **Σ** and **Λ**
2. ζ are defined as $\mathbf{x}^{48h}$-$\mathbf{x}^{24h}$ (as in NWP) or $\mathbf{x}^{24h}$-$\mathbf{x}^{0h}$ (this work)
3. From that, you can estimates (here based on MIPAS O3 assimilation):

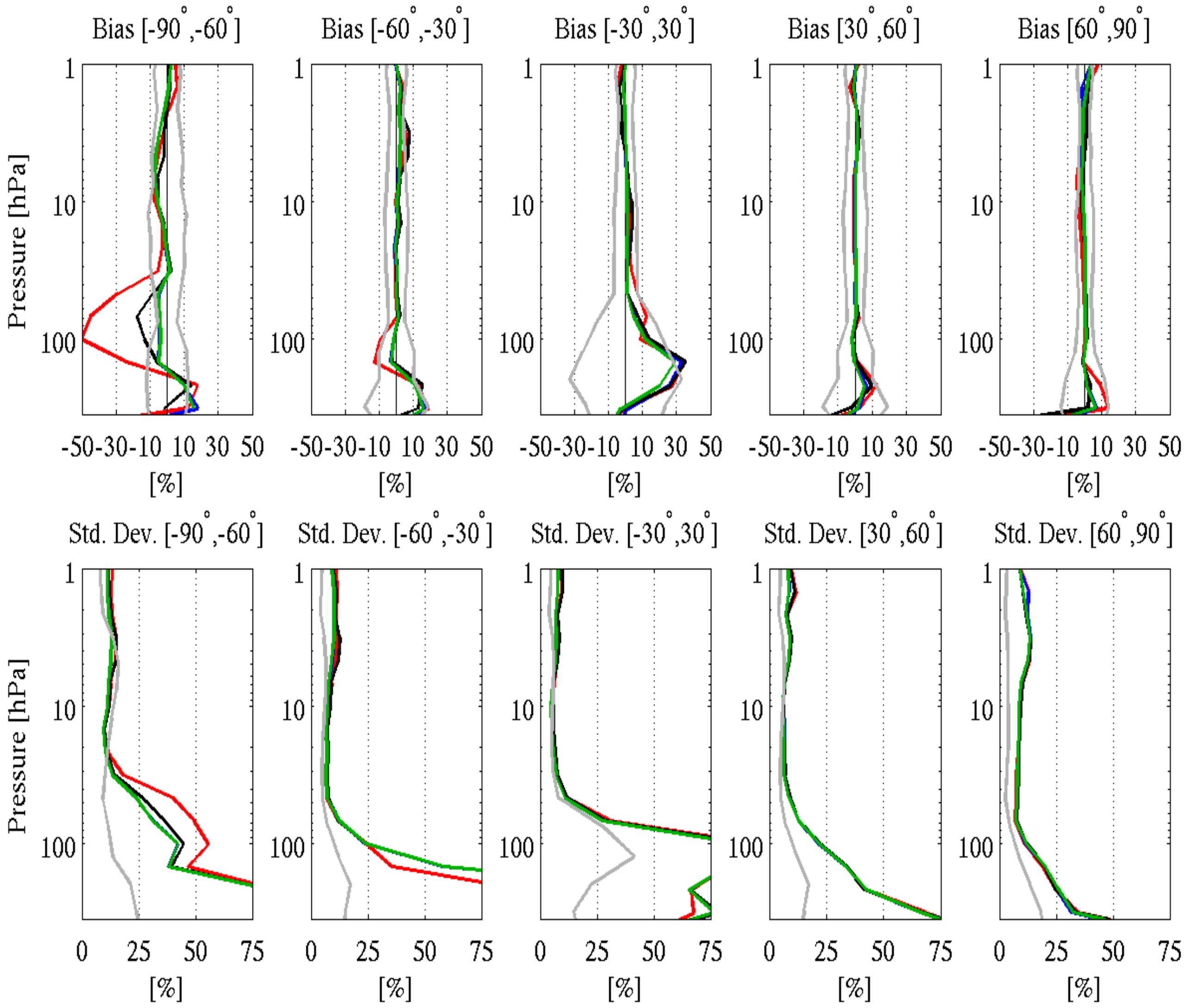






Assimilation of MIPAS with calibrated **B** (NMC method)

Bias and Std Dev of OmF for Sep-Oct 2003 from MIPAS assimilation



DIAG

Correlation Default

b_n: NMC; C^v: NMC; Σ: 0.3 x^b

b_n & C^v : Default, Σ: 5*NMC

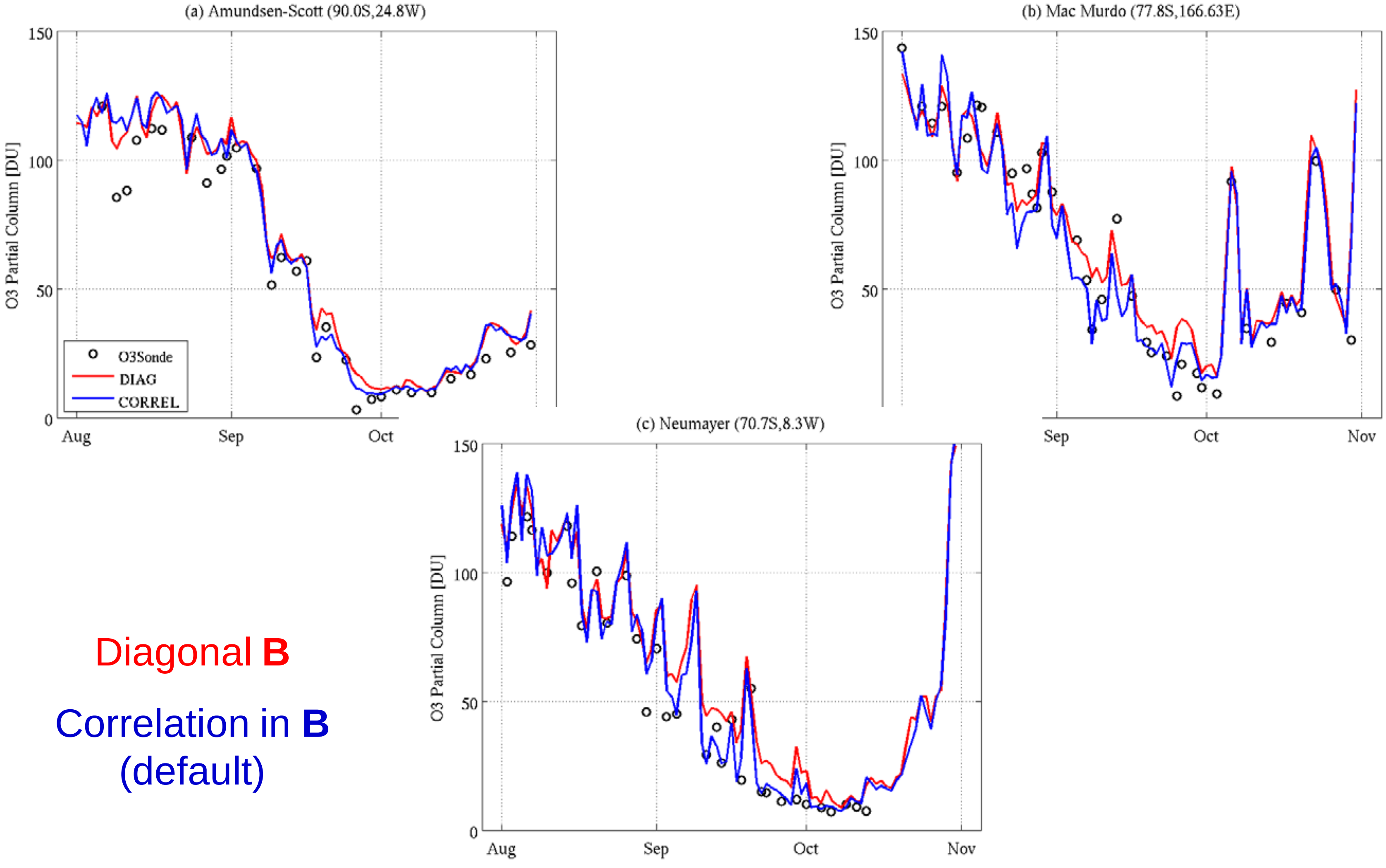
Assimilation of real data

Assimilation with chemistry turned on

All available species assimilated

Assimilation of MIPAS O3: Chemistry on

Time series of O3 partial column [10-100 hPa] above three NDACC groundbased stations in Antarctica



Diagonal **B**

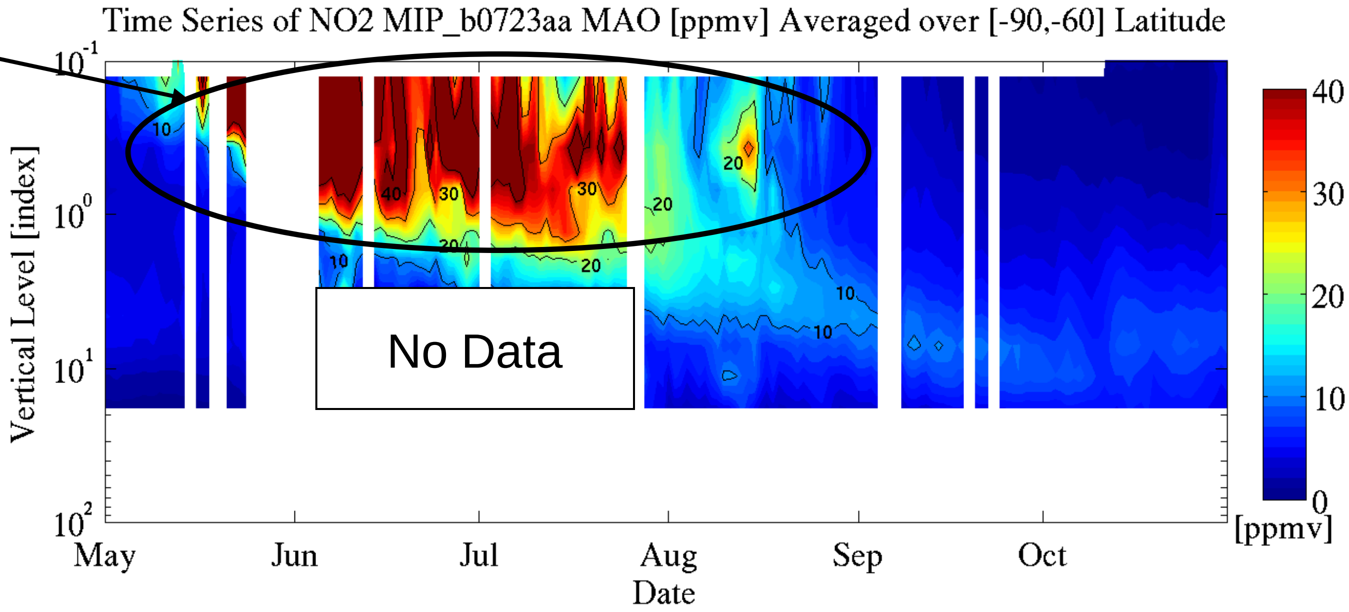
Correlation in **B** (default)

Assimilation of MIPAS NO2 and HNO3 (May-Nov 2003): Chemistry on

Downward transport of Mesopheric NOx produced by EPP.

Funke et al., JGR, 2005

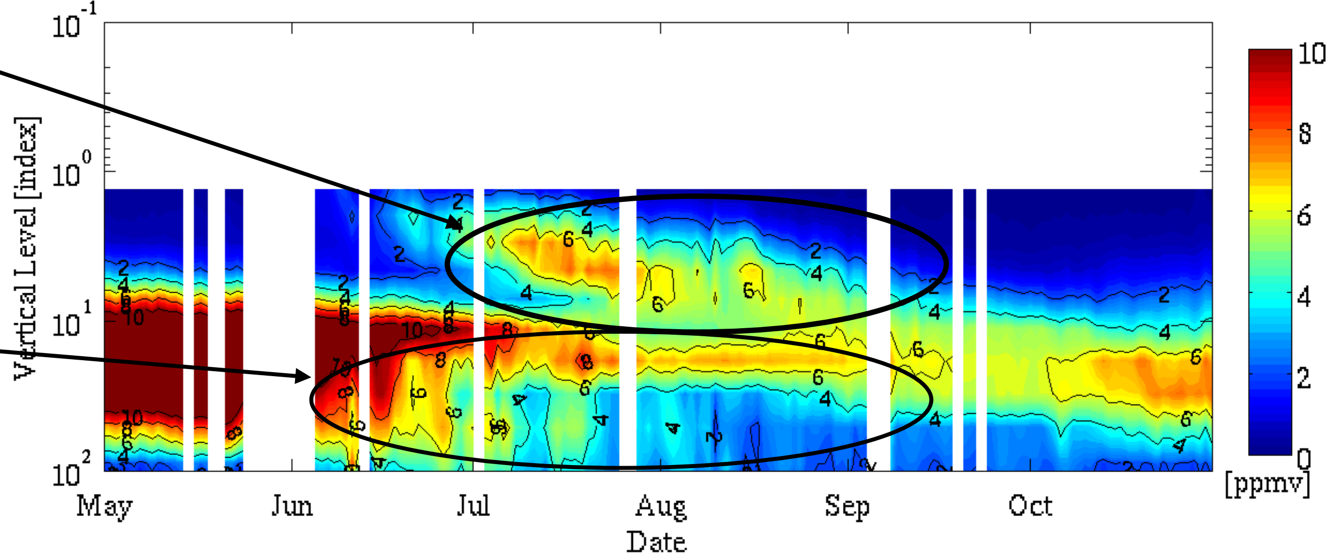
Time Series of NO2 MIP_b0723aa MAO [ppmv] Averaged over [-90,-60] Latitude



Local production of HNO3 due to NOx enhancement

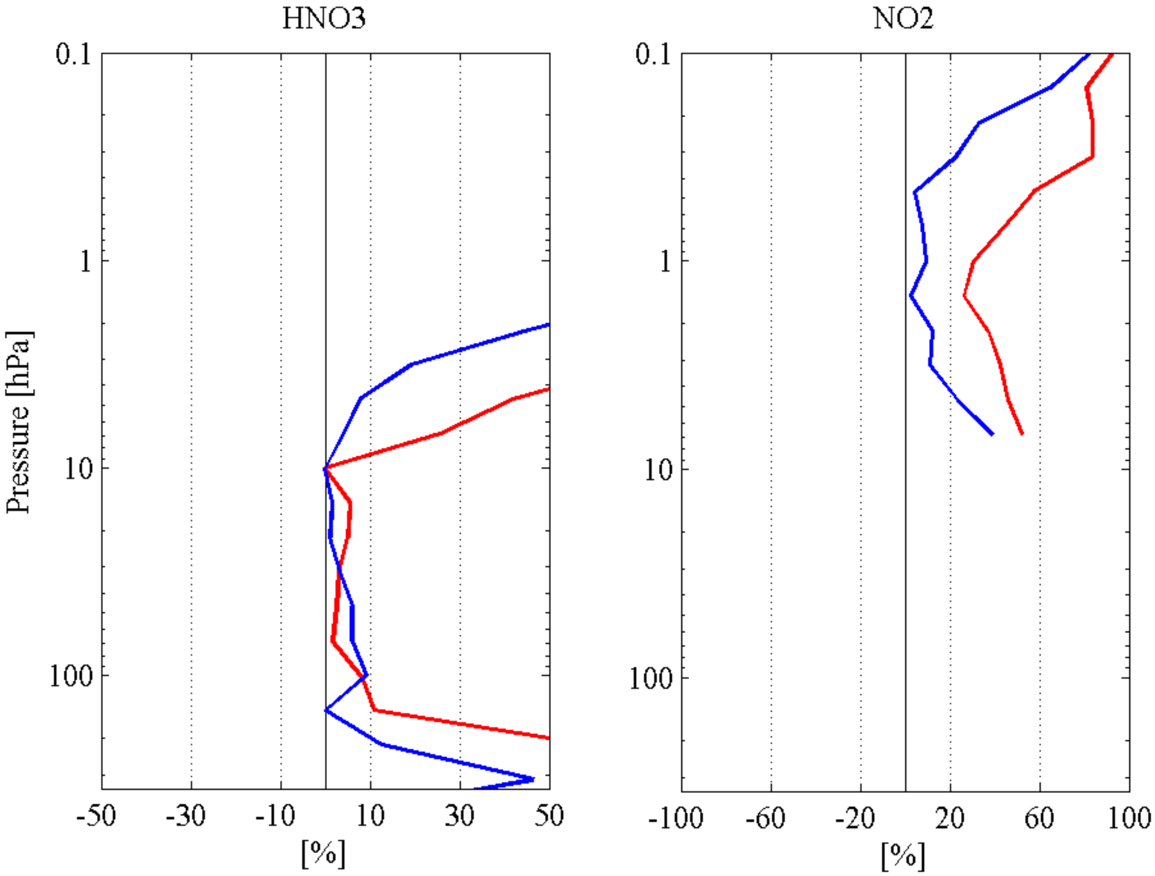
Denitrification

Time Series of HNO3 MIPAS_505 [ppmv] Averaged over [-90,-60] Latitude

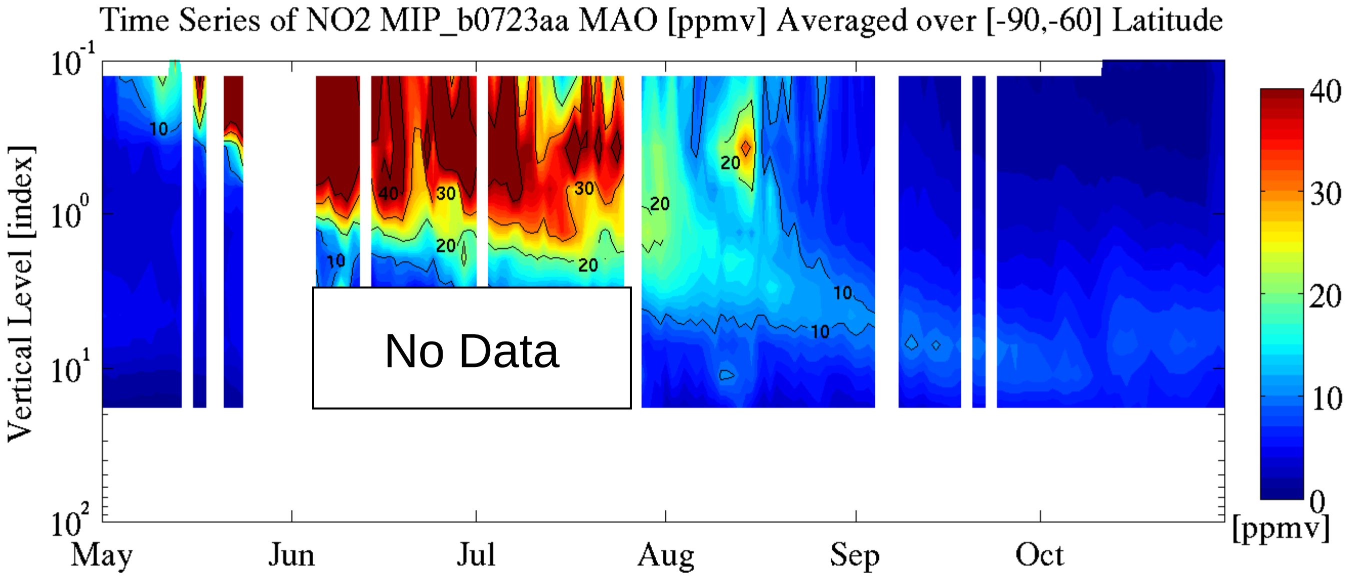


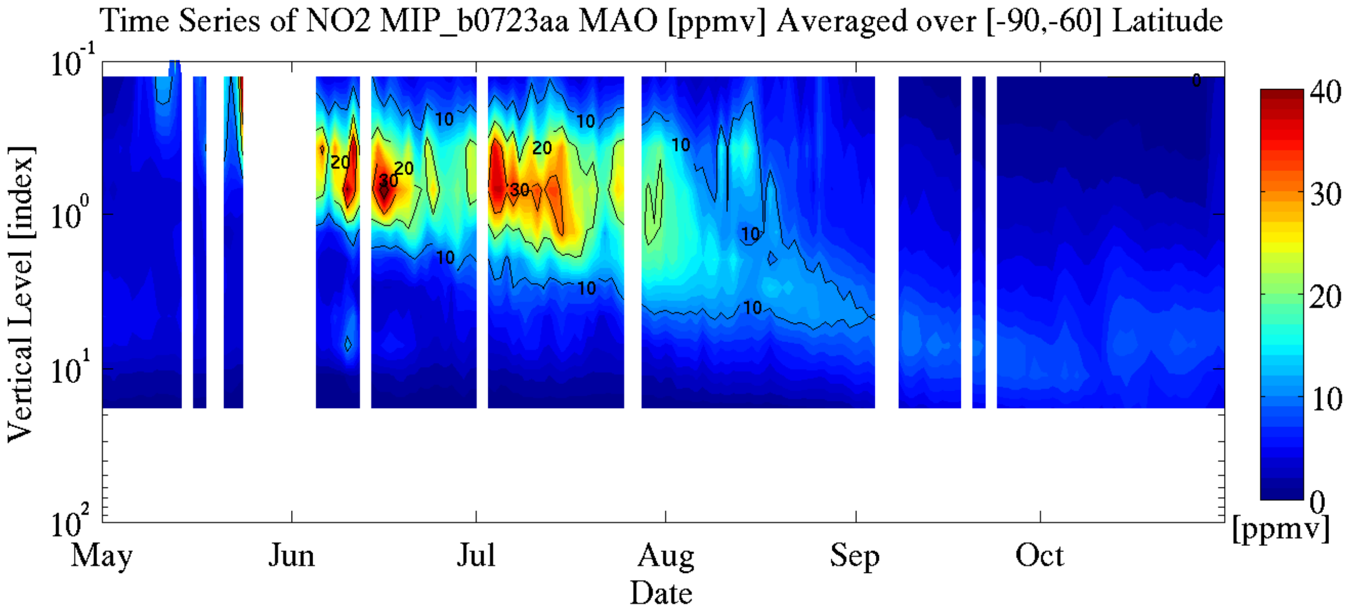
Assimilation of MIPAS NO2 and HNO3 (May-Nov 2003): Chemistry on

- OmF Bias for HNO3 and NO2 during 15Jul-15Aug 2003

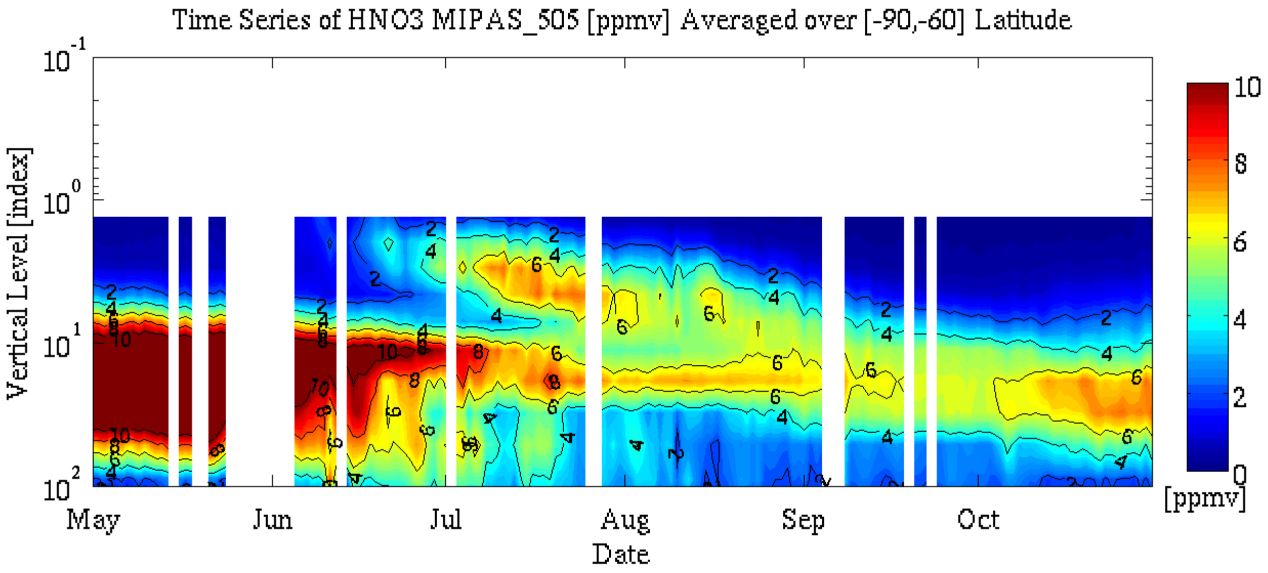


Assimilation of MIPAS NO2 and HNO3 (May-Nov 2003): Chemistry on

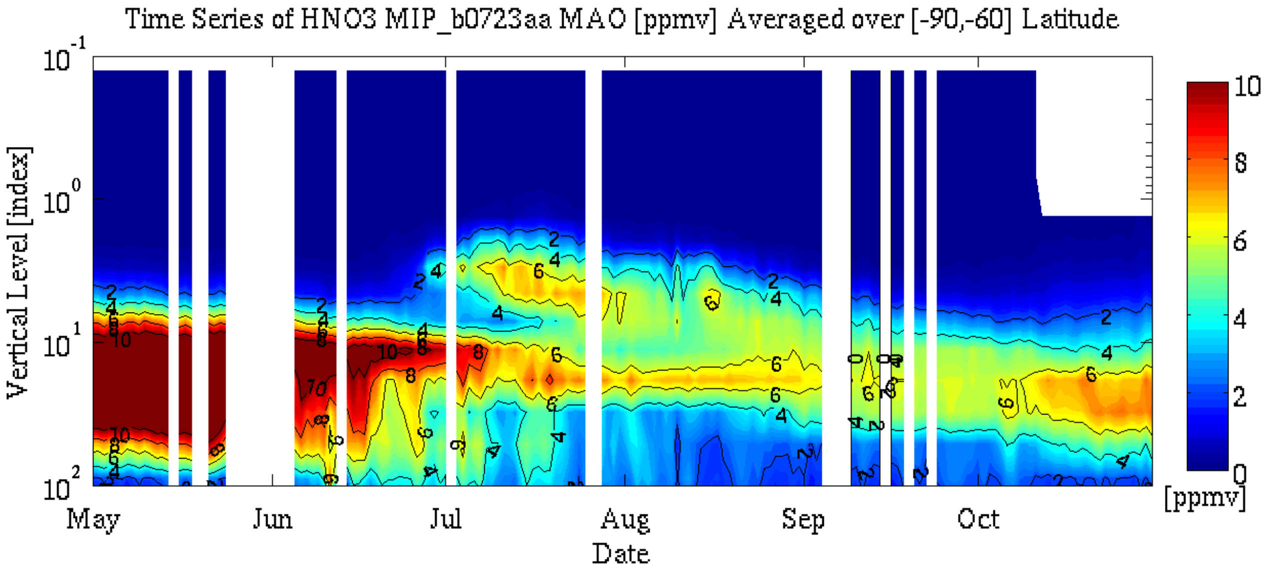




Assimilation of MIPAS NO2 and HNO3 (May-Nov 2003): Chemistry on



Time Series of HNO3 MIPAS_505 [ppmv] Averaged over [-90,-60] Latitude



Time Series of HNO3 MIP_b0723aa MAO [ppmv] Averaged over [-90,-60] Latitude

Conclusions

Summary

1. New **B** matrix in BASCOE using homogeneous and isotropic horizontal correlations represented on a spherical harmonic basis
2. This implementation improves all constituent's analyses (O3, NO2 and HNO3)
3. Error statistics calculated by the NMC method and implemented in BASCOE does not seems to improve the analyses

Perspective

- Reanalysis of Envisat stratospheric data using BASCOE
- List of available species:
  - MIPAS v6.00 : O3, HNO3, NO2, N2O5, ClONO2, N2O, CH4, H2O, CFC11, CFC12
  - GOMOS : O3, NO2
  - SCIAMACHY : O3, BrO

Calibration of **B** (1/2): innovation method (Hollingsworth and Lonnberg, 1986, Tellus)

$$\mathbf{x}^{\mathrm{b}} = \mathbf{x}^{\mathrm{truth}} + \epsilon^{\mathrm{b}}$$

$$\mathbf{y}^{\mathrm{o}} = \mathbf{H}\mathbf{x}^{\mathrm{truth}} + \epsilon^{\mathrm{o}}$$

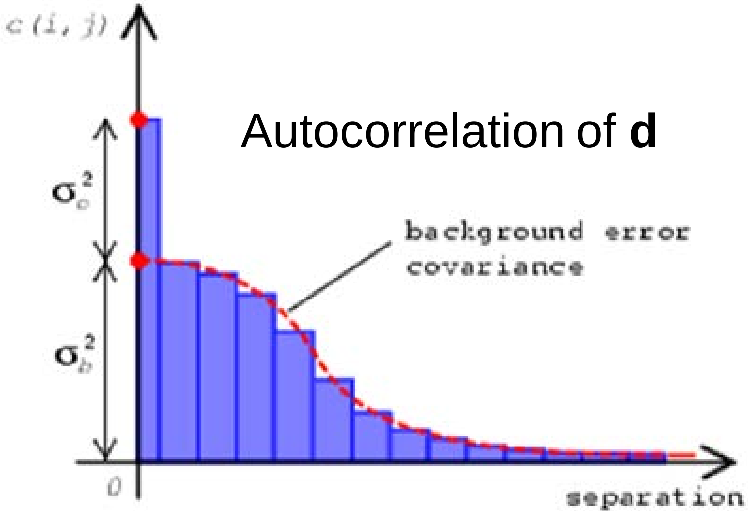
then:

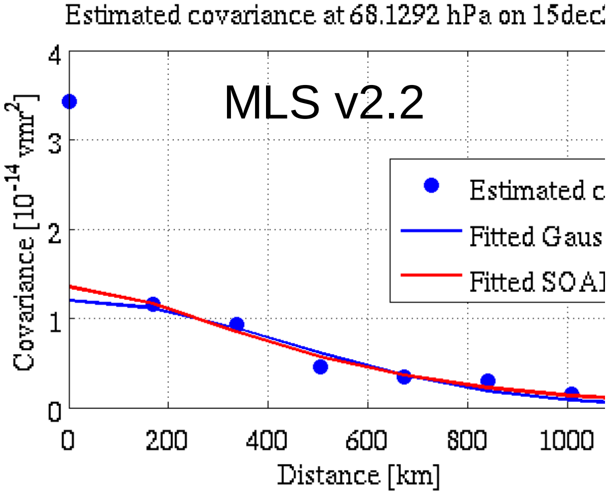
$$\mathbf{d} \equiv \mathbf{y}^{\mathrm{o}} - \mathbf{H}\mathbf{x}^{\mathrm{b}} = \epsilon^{\mathrm{o}} - \mathbf{H}\epsilon^{\mathrm{b}}$$

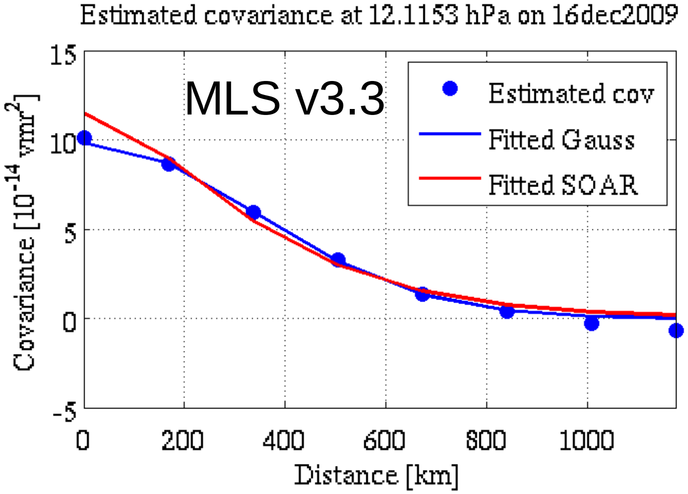
Thus: $\langle \mathbf{d}(i,i), \mathbf{d}(i,i) \rangle = (\sigma^{\mathrm{b}})^2 + (\sigma^{\mathrm{o}})^2$

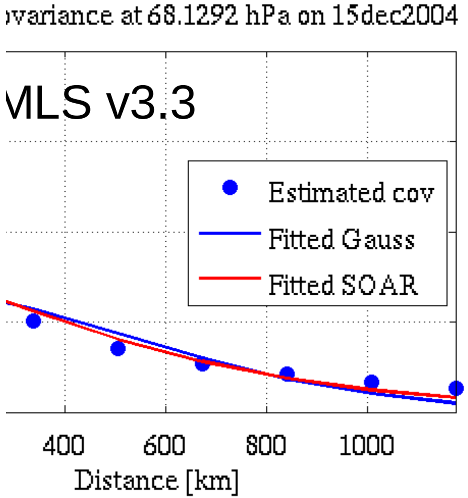
$$\langle \mathbf{d}(i,j), \mathbf{d}(i,j) \rangle = (\sigma^{\mathrm{b}})^2 \rho(r_{ij})$$

- Assuming that observation errors are **horizontally uncorrelated** and that background errors are spatially correlated, auto-covariance of **d** can be used to estimates the errors


Autocorrelation of **d**

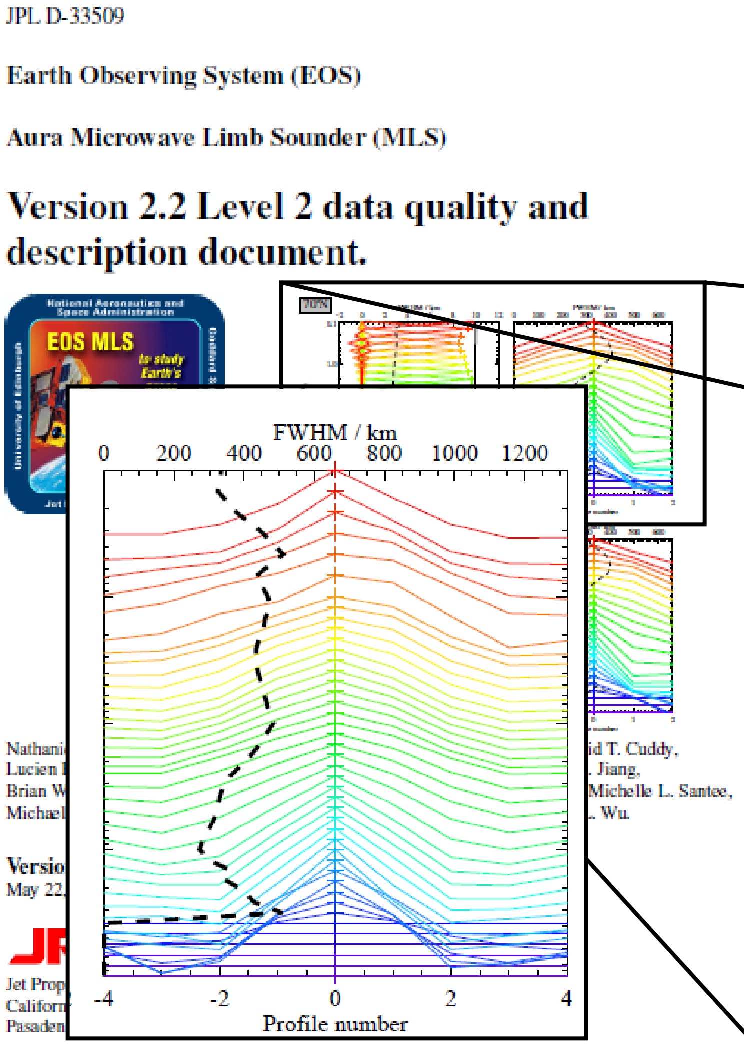






Calibration of **B** (2/3): innovation method

- Inefficiency of innovation method due to MLS retrieval



JPL D-33509

Earth Observing System (EOS)

Aura Microwave Limb Sounder (MLS)

Version 2.2 Level 2 data quality and description document.

Nathani
Lucien I
Brian W
Michael

id T. Cuddy,
. Jiang,
Michelle L. Santee,
. Wu.

Versio
May 22

Jet Prop
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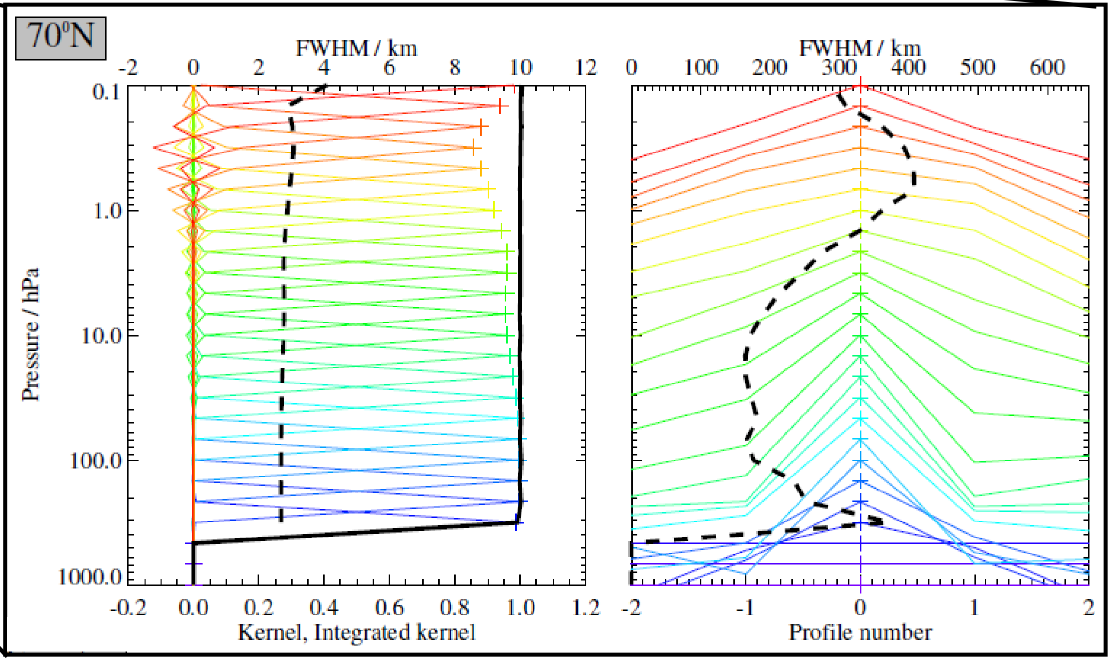
MLS O3 v3.3 AKs

In the v2.2 *(and v3.3)* Level 2 algorithms, the state vector consists of “chunks” of several profiles […] which are then simultaneously retrieved from radiances.

see Section 2.2



MLS O3 v2.2 AKs