Four dimensional variational assimilation of MIPAS stratospheric trace gas observations

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Outline:

- Introduction of the SACADA assimilation system
- Flow dependent background error covariance parameterisation
- Case study results (2002 vortex split)

Talk by F. Baier will present results from operational assimilation and comparison to ROSE based assimilation

SACADA:

Synoptic Analyses for Chemical Constituents with Advanced Data Assimilation

Objectives:

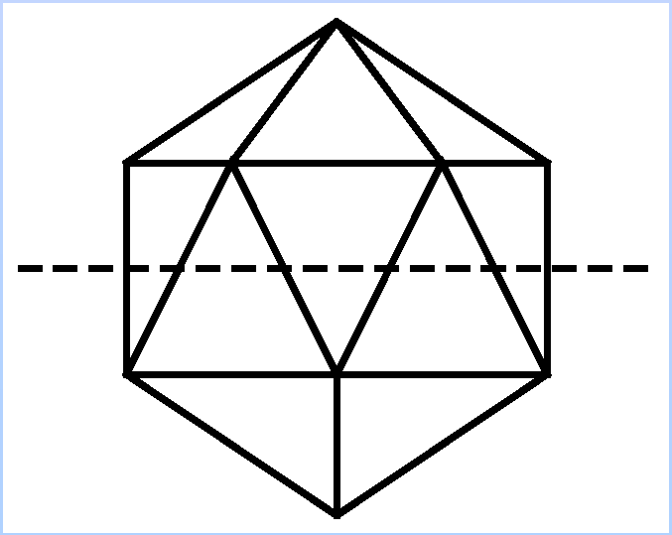
- **Develop a new stratospheric chemistry data assimilation system**
  - **-Chemical consistency of analysed fields in terms of a state of the art reaction mechanism**
  - **-Realistic background error covariances**
  - **-Consistent wind fields by avoiding space-time interpolation of meteorological data (-> online meteorological model)**
  - **-Numerical efficiency (grid design, parallelisation)**
- **System has been implemented for routine operation at the German Remote Sensing Data Centre (DLR-DFD, see presentation of F. Baier)**

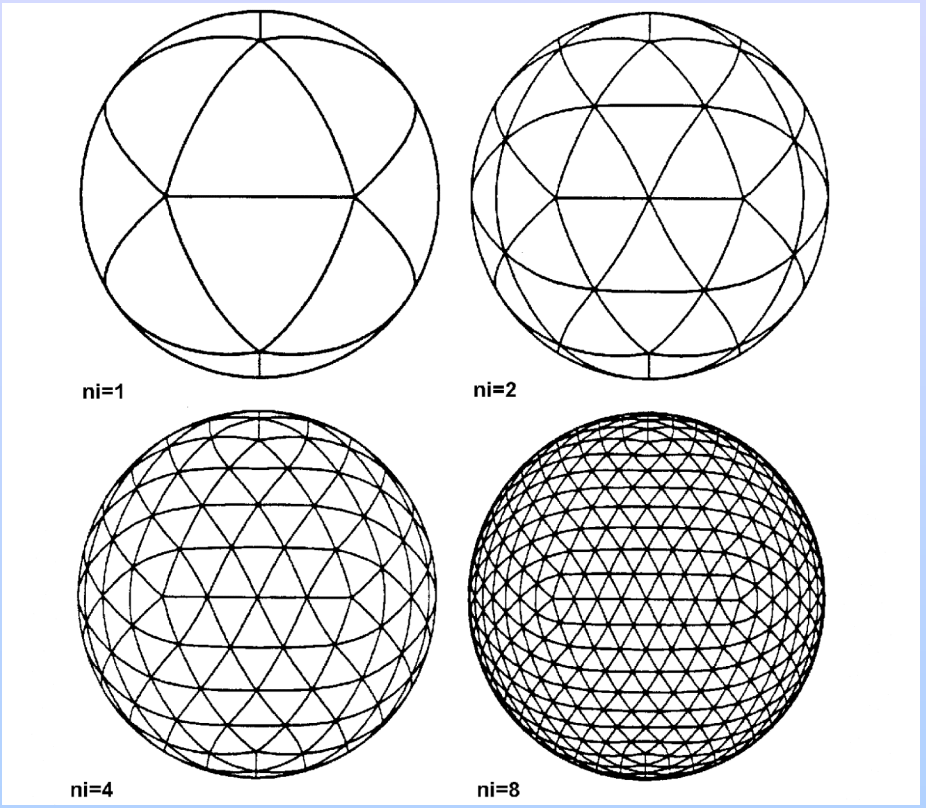
Features of the SACADA Assimilation System

- German Weather Services global forecast model (GME) serves as an online meteorological driver
- Icosahedral grid, parallelisation and semi Lagrange transport scheme are adopted from GME
- 42 level ranging from the surface to 0.1 hPa

Construction of Icosahedral Grid

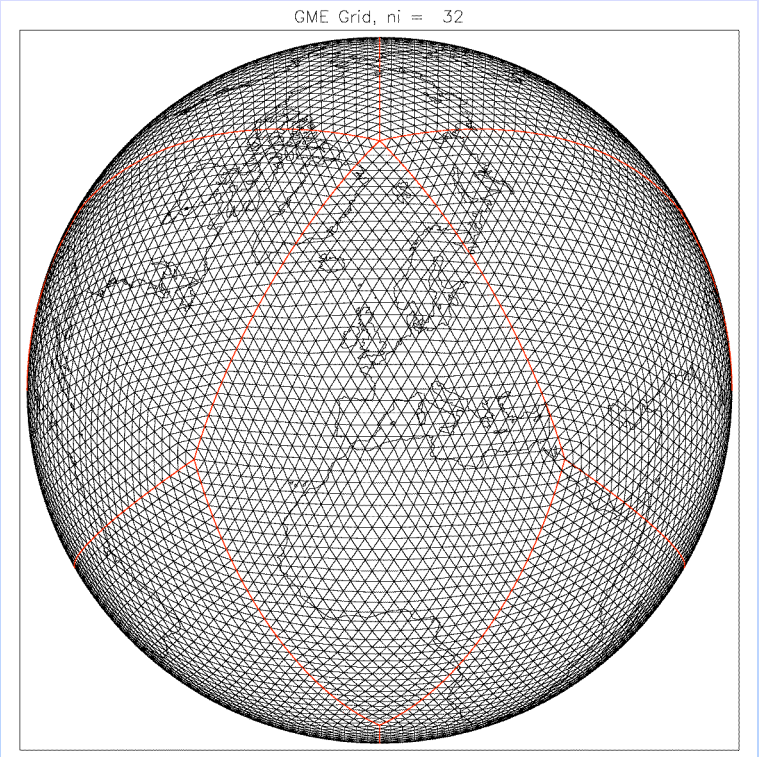
An Icosahedron (20 equi-lateral triangles) is placed in a sphere. Vertices are connected by great circles. Great circle arcs are subdivided into n_i intervals to form a regular grid.

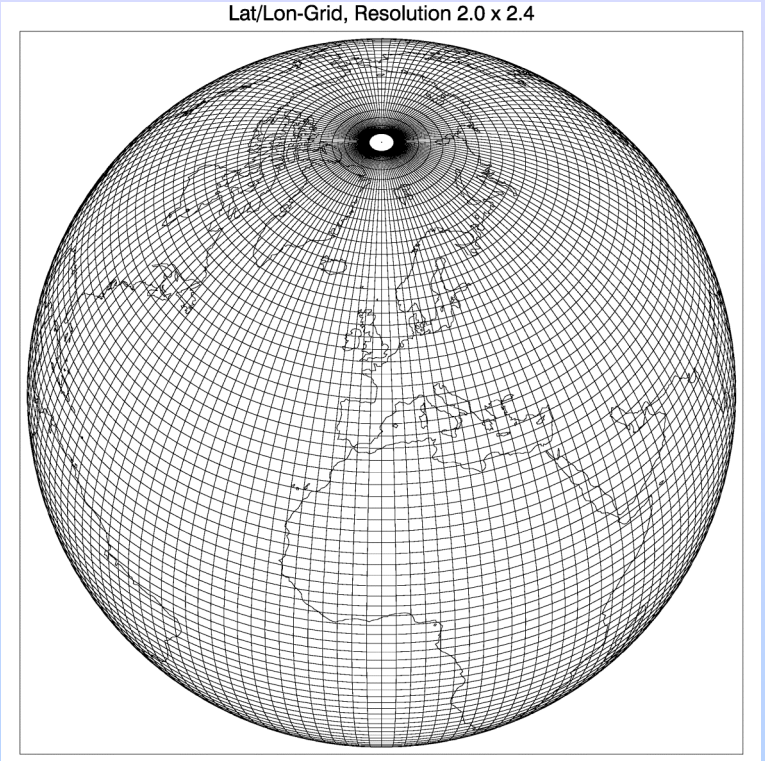




Source of Figures: DWD

Icosahedral Grid vs. Conventional lat/lon Grid

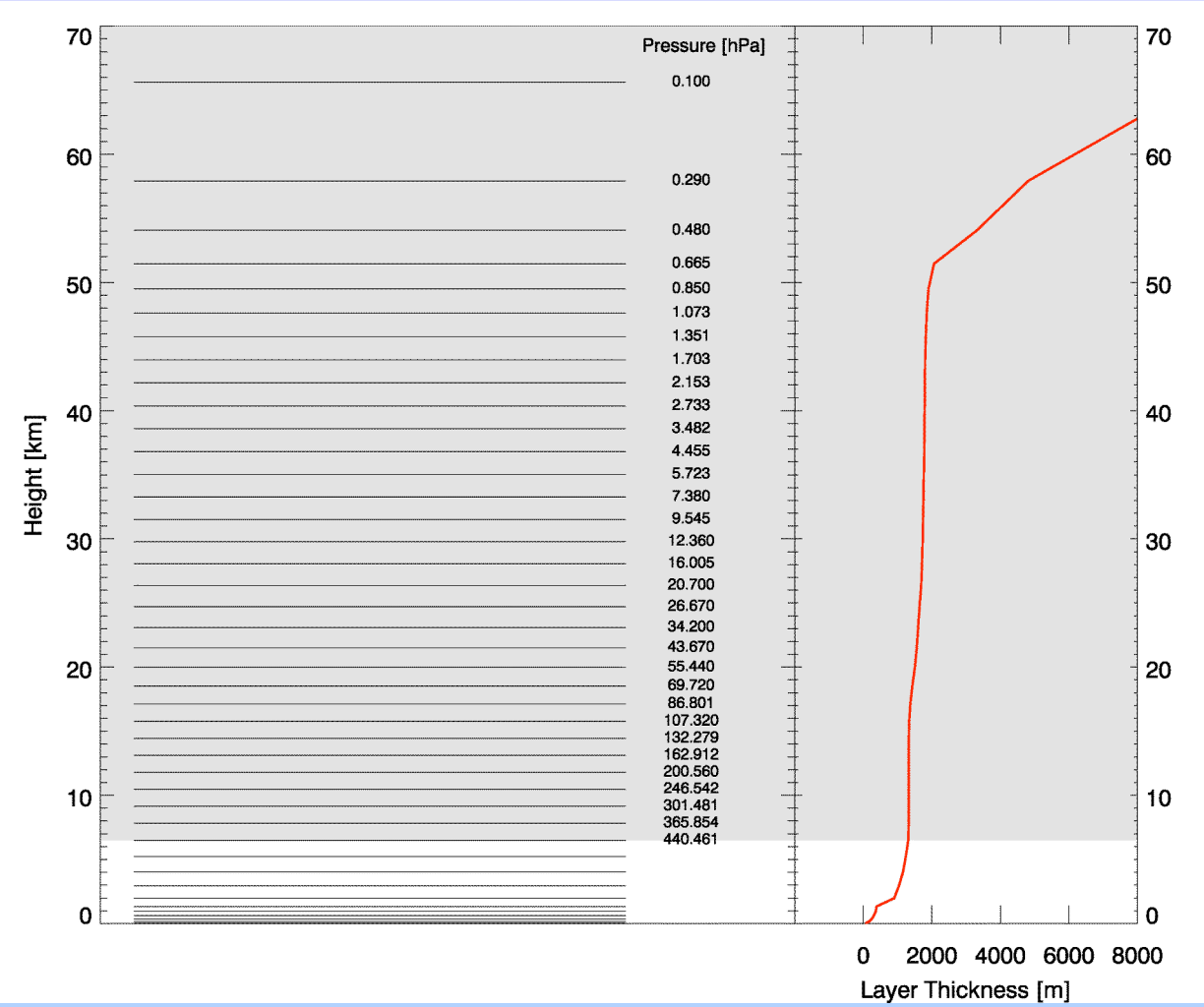




- N_i = 32 ◊ separation of grid points 220-260 km, nearly homogeneous over the globe
- 10242 grid points per level

- Equivalent resolution lat/lon grid needs 2.0° x 2.4°
- 13500 grid points per level

SACADA Vertical Model Grid



Hybrid sigma / pressure coordinate system

Assimilation currently on 32 levels from 0.1 – 440 hPa (grey shaded region)

Features of the SACADA Assimilation System (cont.)

•State of the art chemistry module

-Accounts for 148 gas phase and 7 heterogeneous reactions on aerosol and PSC surfaces

-Reaction rates taken from JPL-Recommendations (2003)

-2nd order Rosenbrock method to solve the system of stiff ODEs without any family assumption

•Adjoint modules have been build for advection, gas phase chemistry and heterogeneous chemistry

•Incremental formulation of the cost function

•Flow dependent parameterisation of the Background Error Covariance Matrix (BECM) using a diffusion approach (Weaver and Courtier, 2001)

Incremental formulation of the cost function

Define new control variable

$$\boldsymbol{v} = \mathbf{B}^{-1/2}\left[\boldsymbol{x}_0 - \boldsymbol{x}^{\mathrm{b}}\right]$$

Cost function

$$J(\boldsymbol{v}) = J^{\mathrm{b}} + J^{\mathrm{o}} = \frac{1}{2}\boldsymbol{v}^T\boldsymbol{v} + J^{\mathrm{o}}$$

Gradient of cost function

$$\nabla_{\boldsymbol{v}} J = \boldsymbol{v} + \mathbf{B}^{T/2}\nabla_{\boldsymbol{x}_0} J^{\mathrm{o}}$$

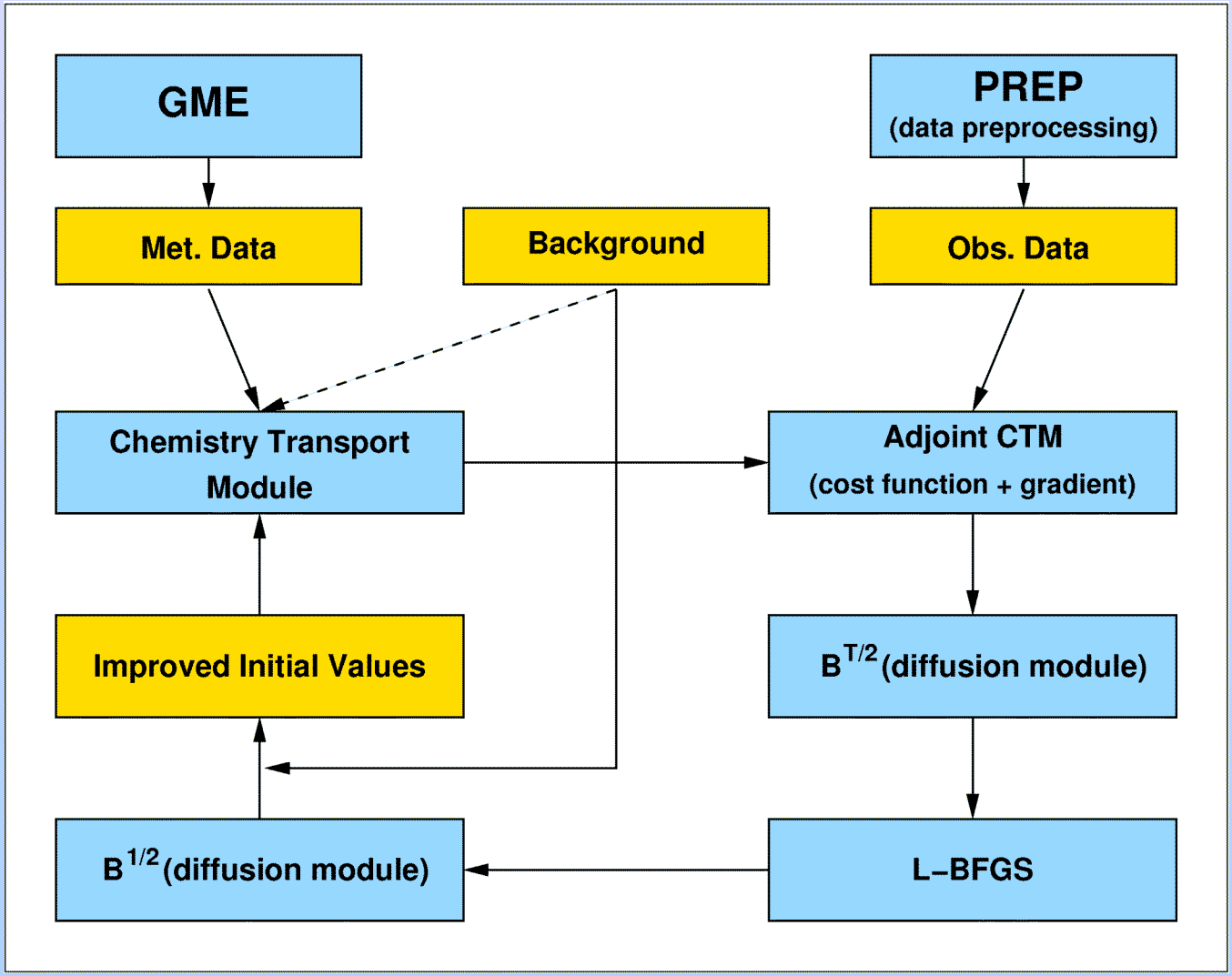
Minimasation

New initial values

$$\boldsymbol{x}_0 = \mathbf{B}^{1/2}\boldsymbol{v} + \boldsymbol{x}^{\mathrm{b}}$$

=> Inverse of **B** is never needed. $\mathbf{B}^{1/2}$ and $\mathbf{B}^{T/2}$ can be modelled using a diffusion operator

SACADA Assimilation System - Setup



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Formulation of the background error covariance matrix:

Diffusion approach (Weaver and Courtier, 2001)

$\mathbf{B}^{1/2}$ and $\mathbf{B}^{T/2}$ encoding quasi Gaussian correlations can be modelled using a diffusion operator:

$$\mathbf{B} = \mathbf{B}^{1/2}\mathbf{B}^{T/2} = \left(\mathbf{\Sigma\Lambda L}^{1/2}\mathbf{W}^{-1/2}\right)\ \left(\mathbf{W}^{-1/2}\mathbf{L}^{T/2}\mathbf{\Lambda\Sigma}\right)$$

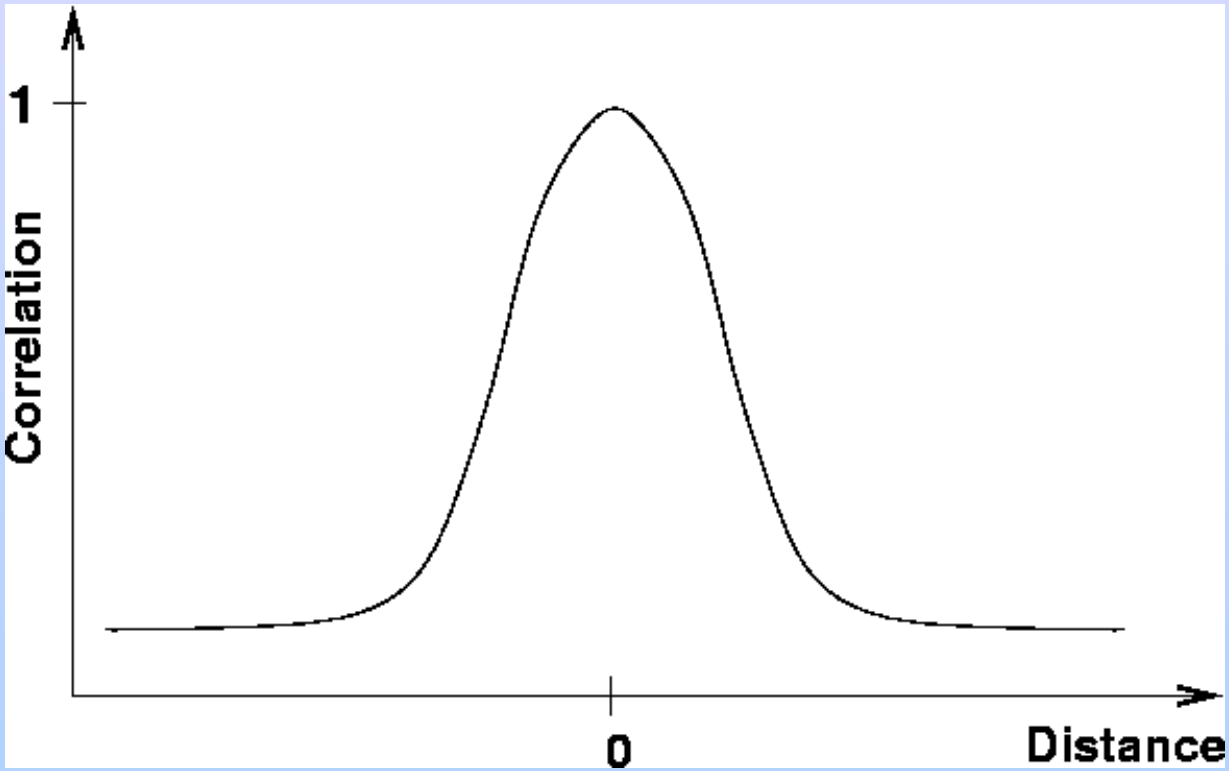
$\mathbf{\Sigma}$: Matrix of background error variances (diagonal)

$\mathbf{\Lambda}$: Matrix of normalisation factors (diagonal)

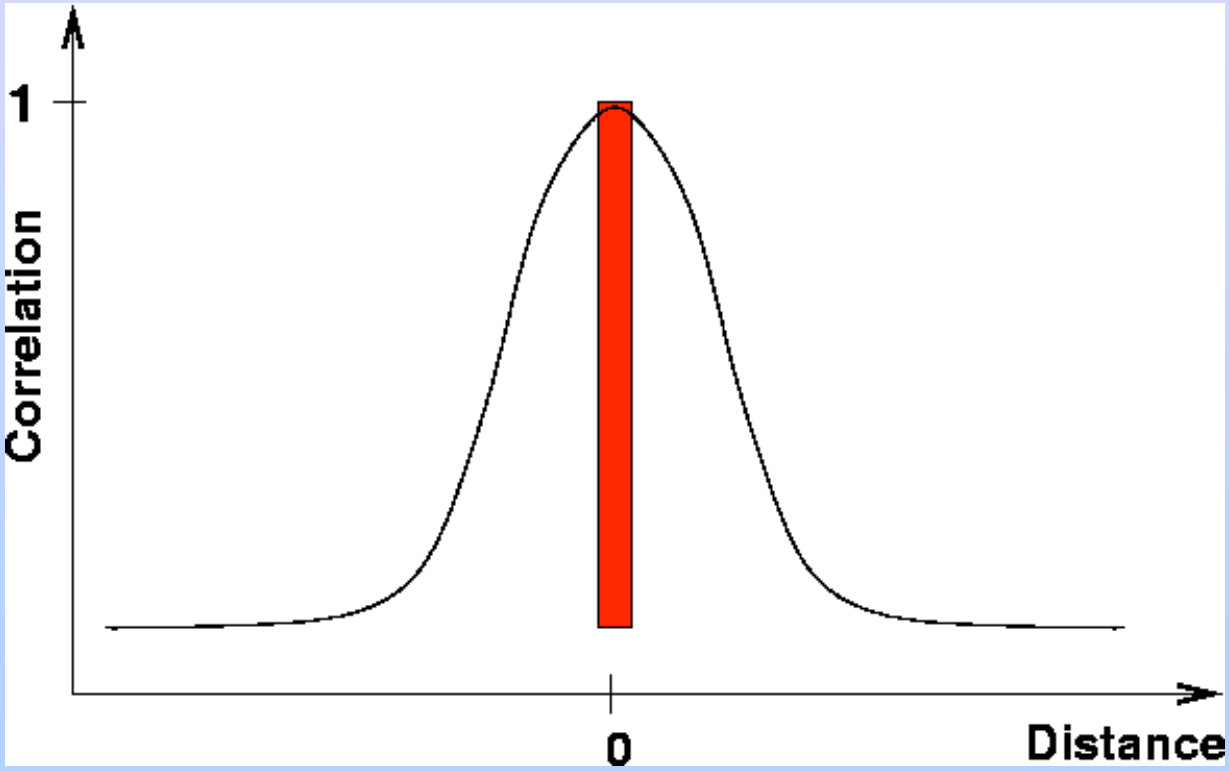
$\mathbf{L}$: Diffusion Operator

$\mathbf{W}$: Matrix of grid cell area elements (diagonal)

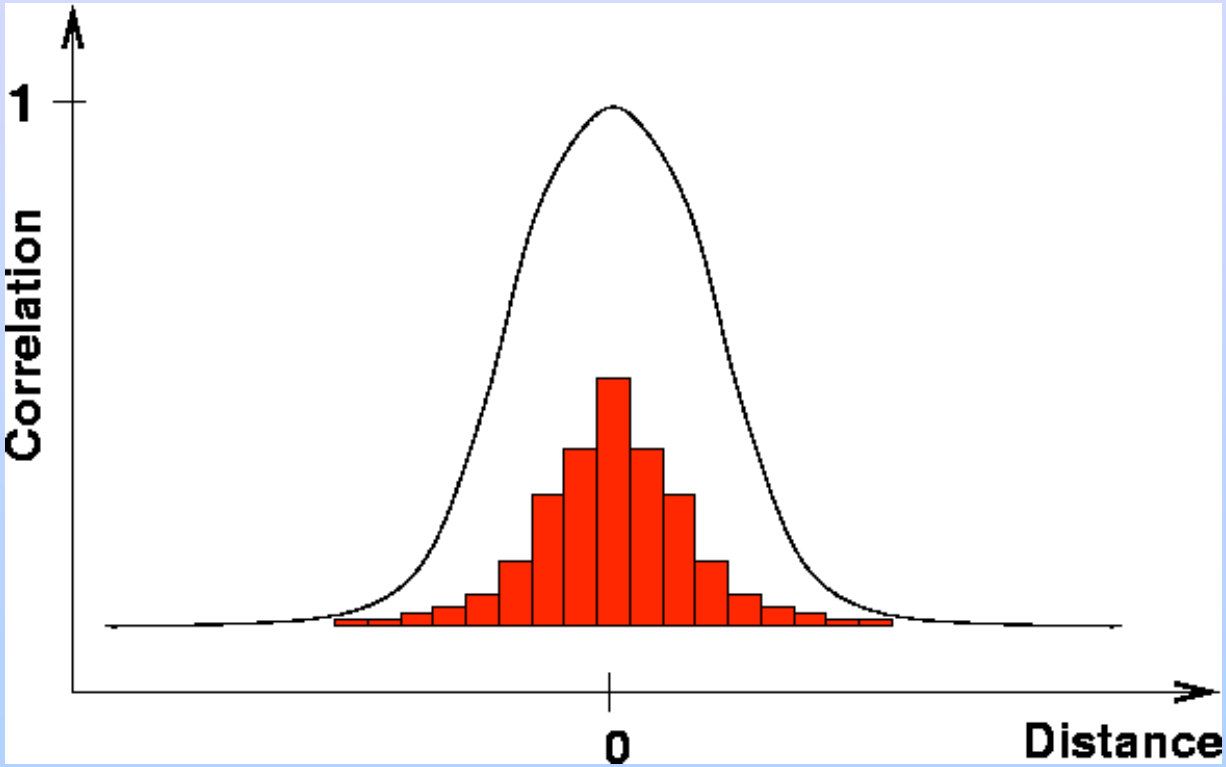
Example (1D case): Calculation of Gaussian correlation between grid cells using a diffusion operator:



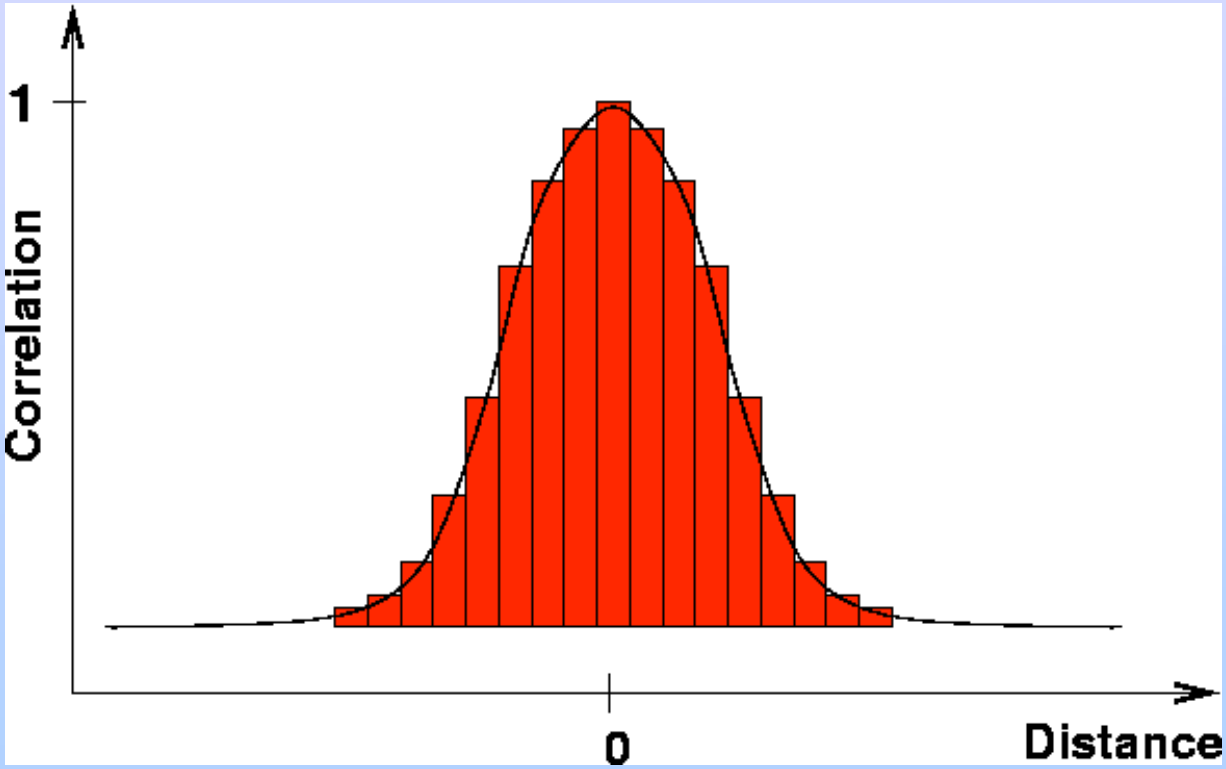
1. Place a unit value at grid cell i



2. Apply diffusion operator



3. Normalise to value 1 at the origin



Extension to allow for anisotropic and inhomogeneous background error correlations

Introduction of a local coordinate stretching tensor S into the Laplacian of the diffusion operator L:

$$\eta_{i+1} = \mathbf{L}\eta_i = \eta_i + \kappa\Delta t \,\mathrm{div}\,\mathbf{S}\,\mathrm{grad}\,\eta_i$$

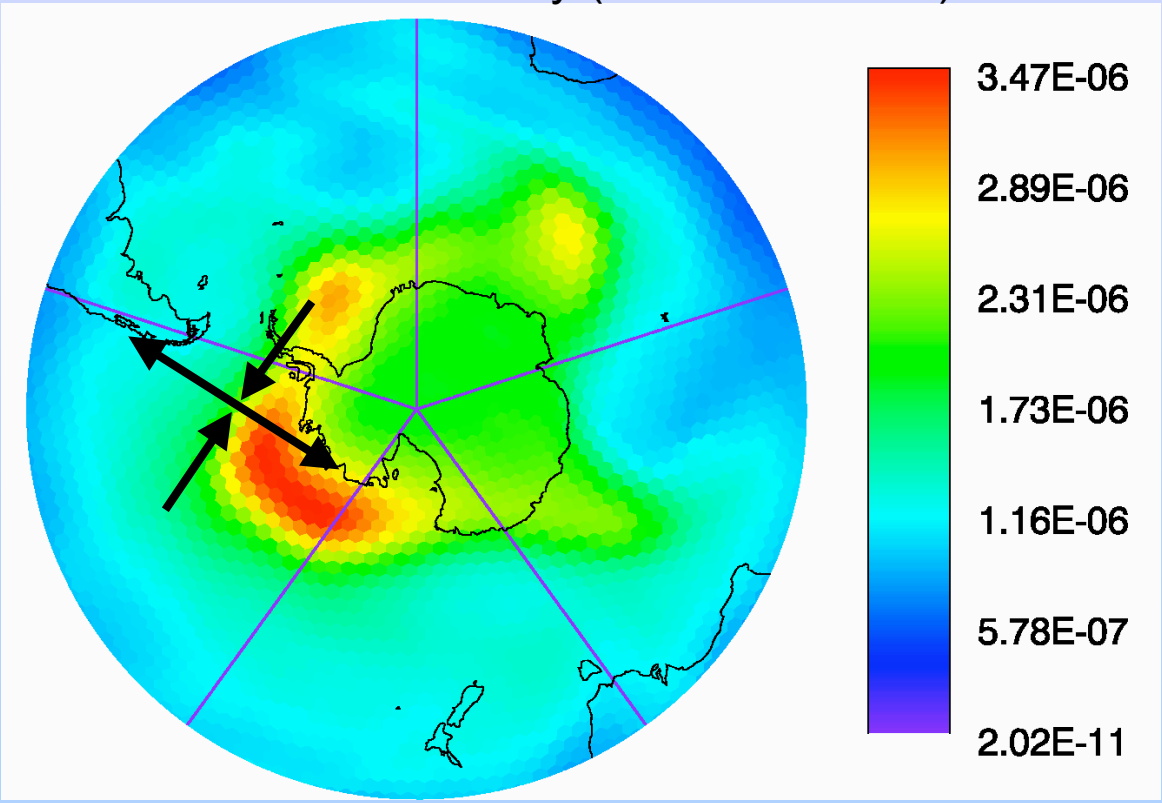
Diffusion coefficient

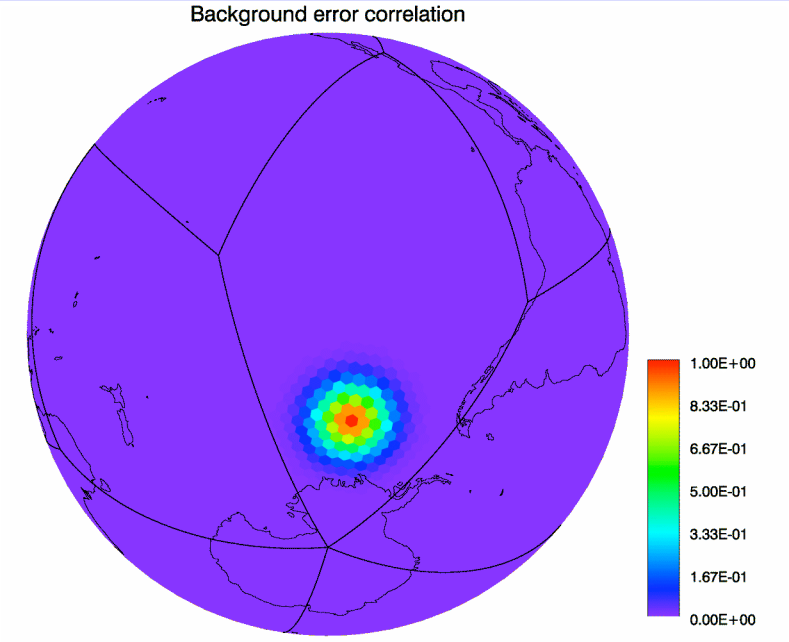
Modified Laplacian

Working hypothesis: Background errors are strongly correlated along lines of equal potential vorticity

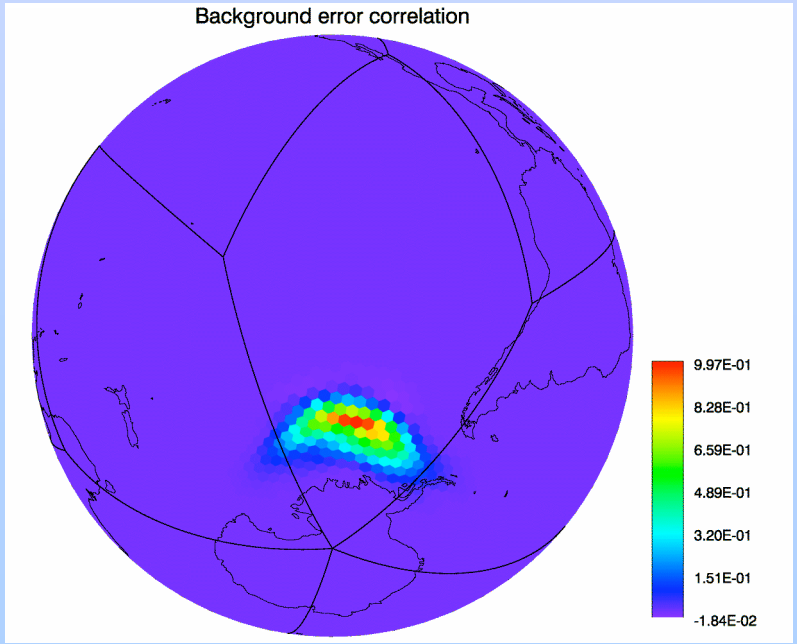
Tensor S introduces local stretching and shrinking of coordinates parallel and perpendicular to PV-gradient

Potential vorticity (absolute values)





Background error correlation, isotropic scheme, L = 500 km



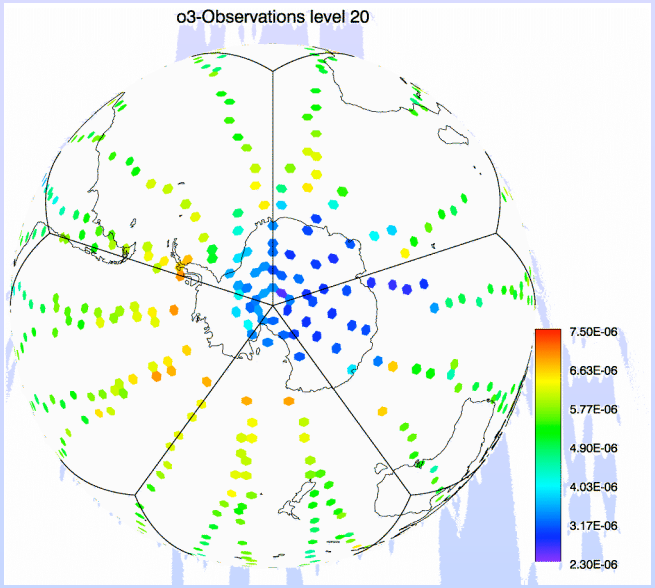
Background error correlation, anisotropic scheme, L1 = 1000 km and L2 = 250 km

RIU

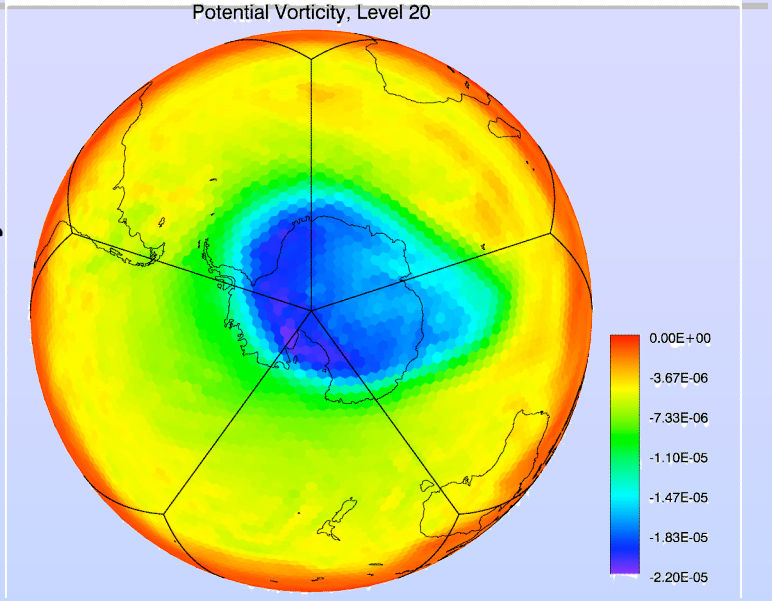
SPARC Workshop 2006, Noordwijk

SACADA

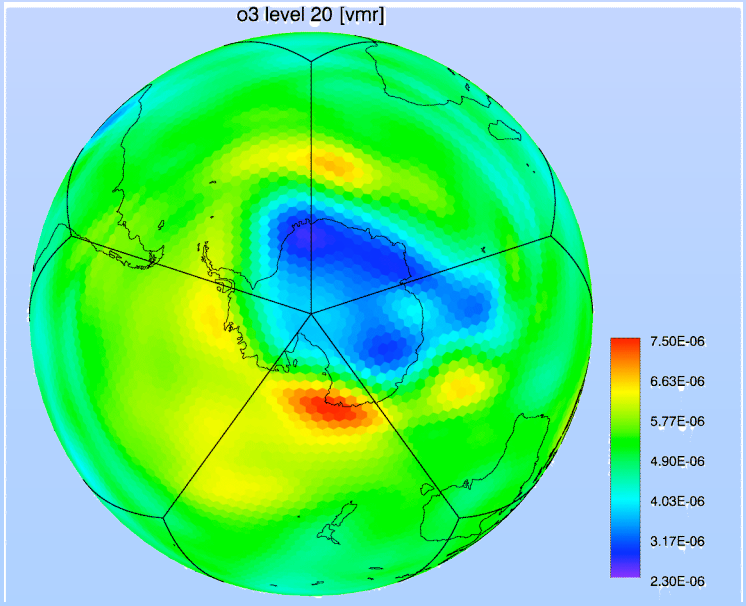
MIPAS Observations



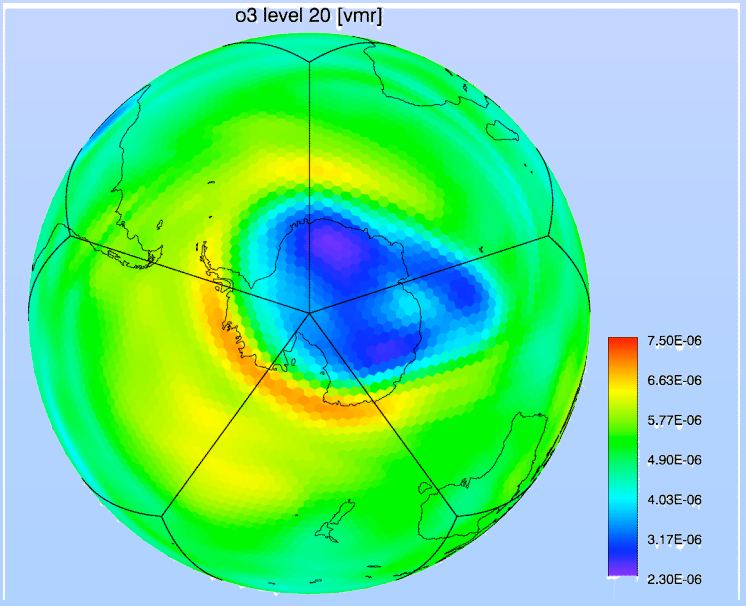
Potential vorticity



Analysis (isotropic)



Analysis (anisotropic)



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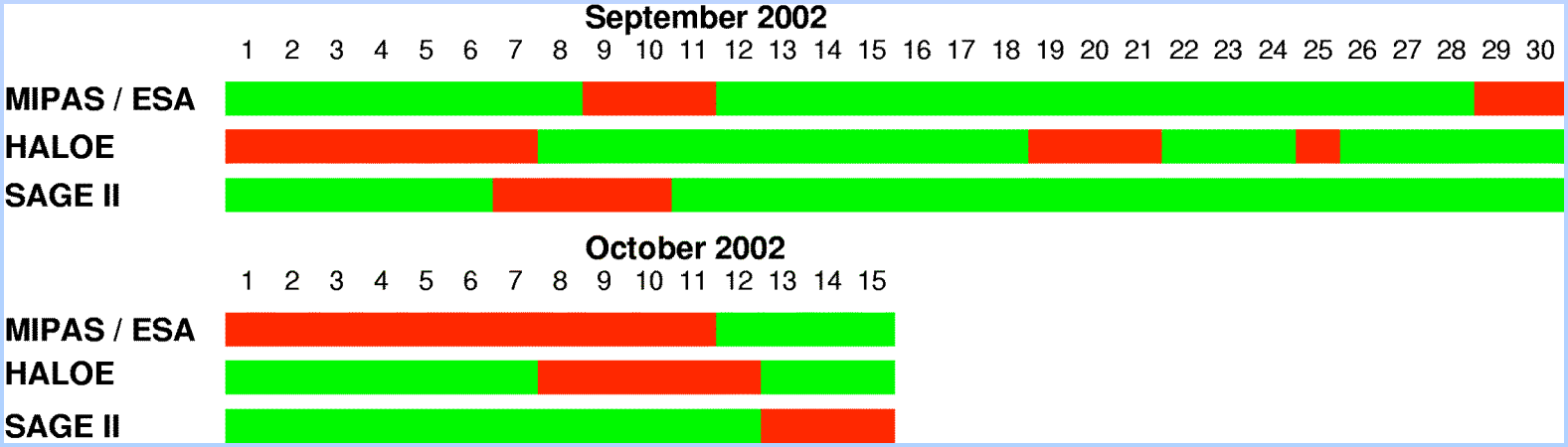
Assimilation of Sep./Oct. 2002 Vortex Split Data

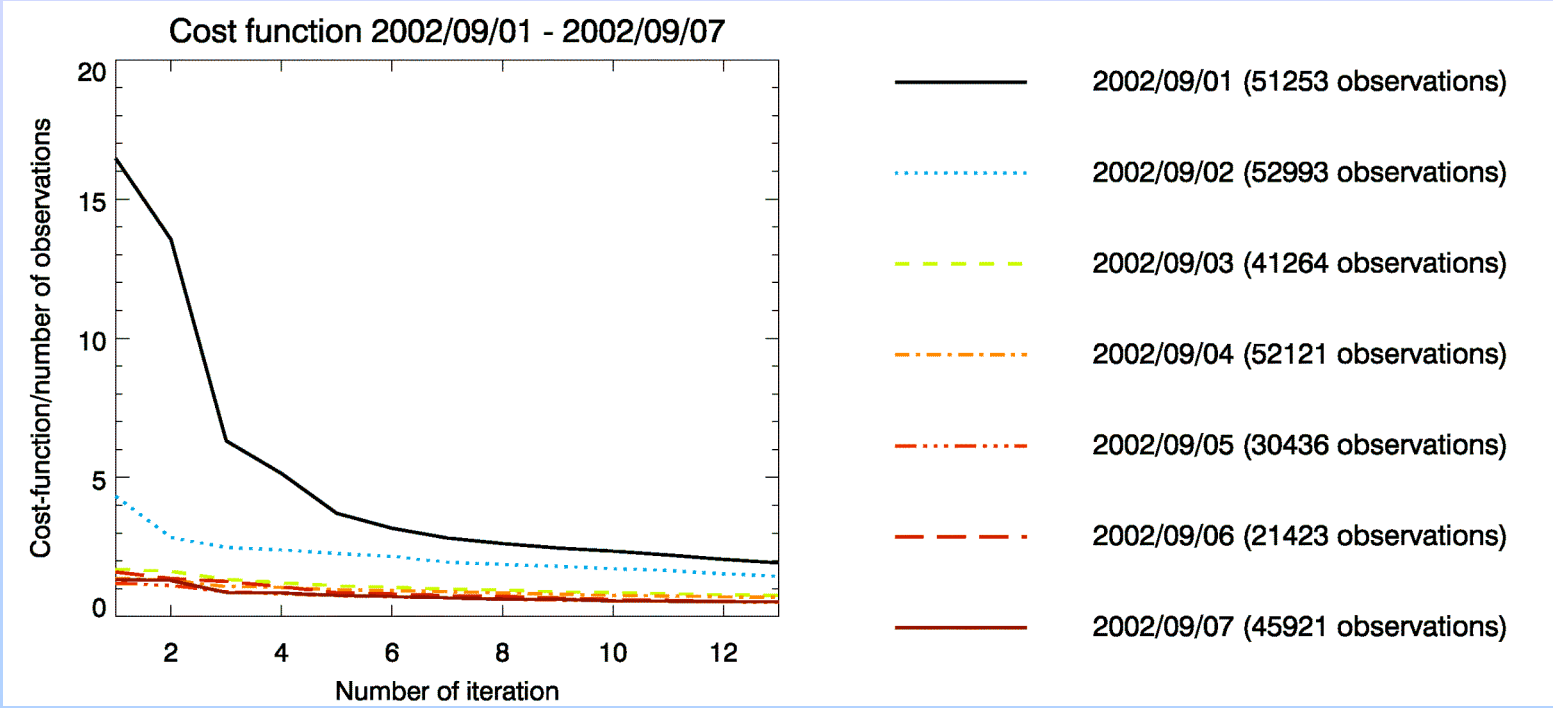
- Initial background was derived from SOCRATES model output (2D fields of chemical constituents)
- Spin-up assimilation of 6 days
- BECM parameters:
  - -Background error 80% (spin-up, first 6 days) / 40% (other days)
  - -Horizontal correlation between grid points quasi Gaussian with a correlation length of 600 km
  - -Flow dependent BECM parameters: L1=1000 km / L2 = 250 km
- Assimilation of MIPAS/ESA Profiles
- R-matrix taken to be diagonal, errors from MIPAS-ESA data
- A control model run without data assimilation was accomplished starting after the spin-up period

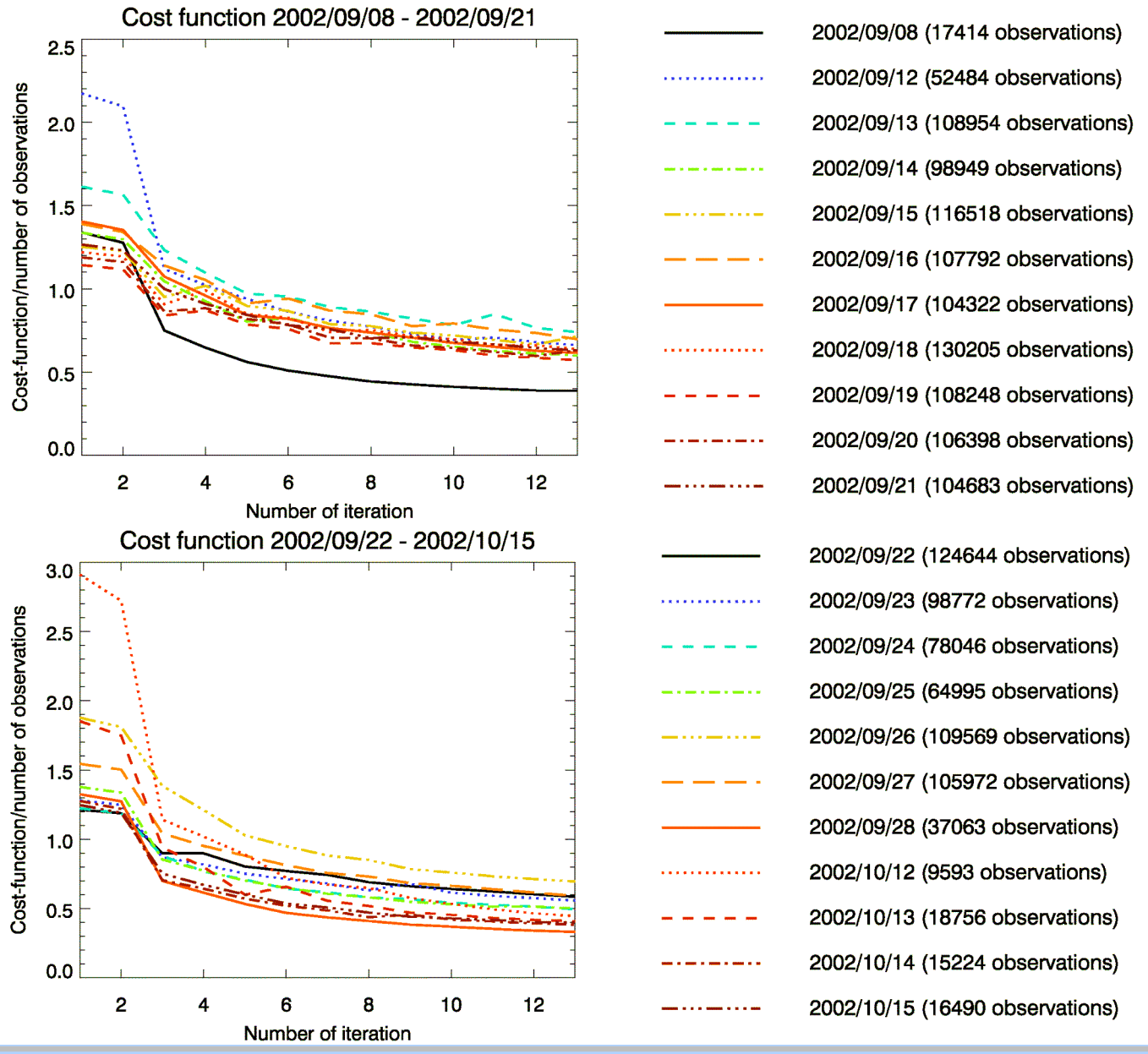
Data Availability 1 Sep. – 15 Oct. 2002

	MIPAS/ESA		Sage II		HALOE	
	Available	Assimilated	Available	Assimilated	Available	Assimilated
O3	X	X	X		X	
NO2	X	X	X		X	
N2O	X	X				
HNO3	X	X				
H2O	X	X	X		X	
CH4	X	X			X	
NO					X	
HCl					X	

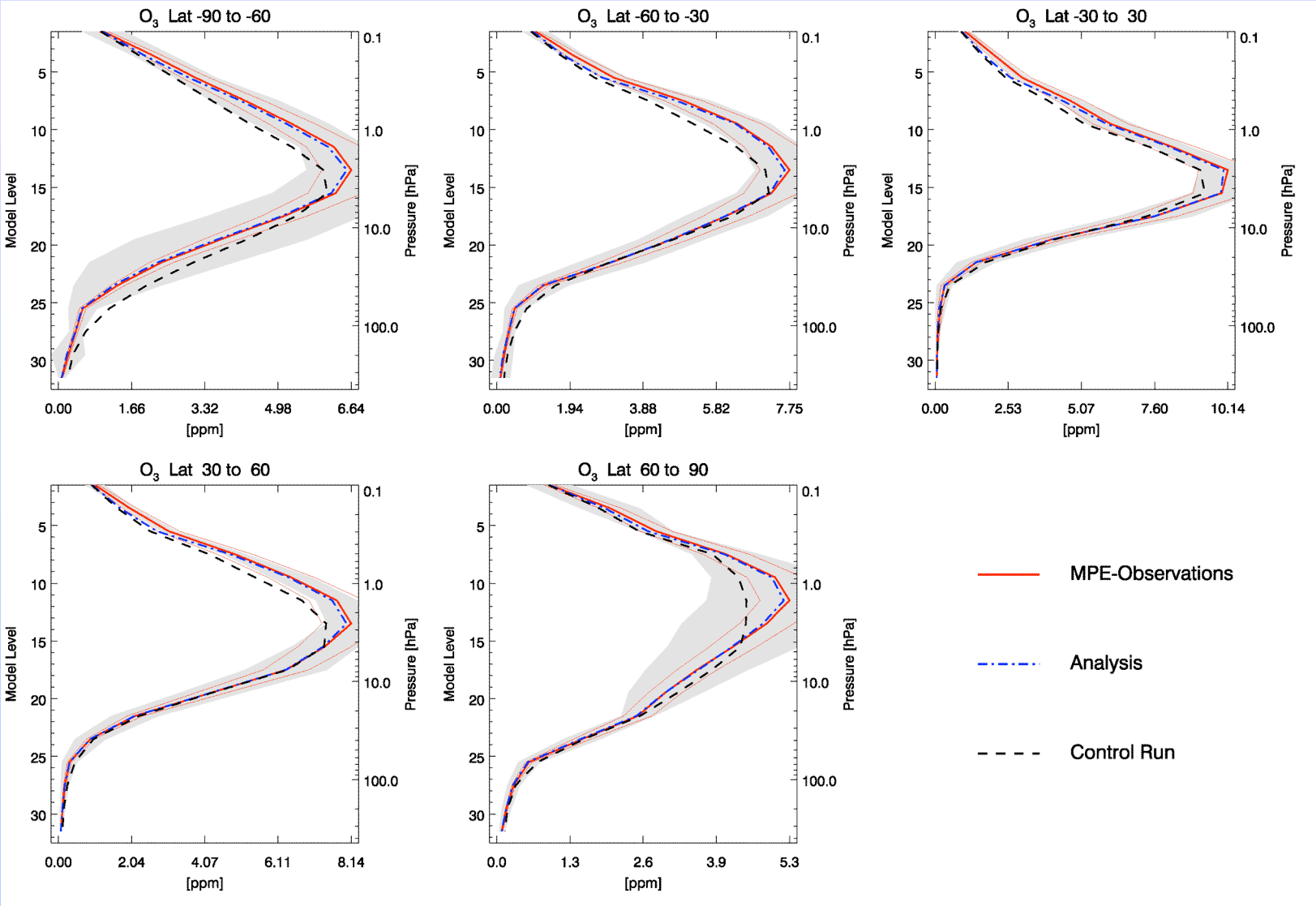


Results: Cost-functions 1 Sept. – 7. Sept. (spin-up period)

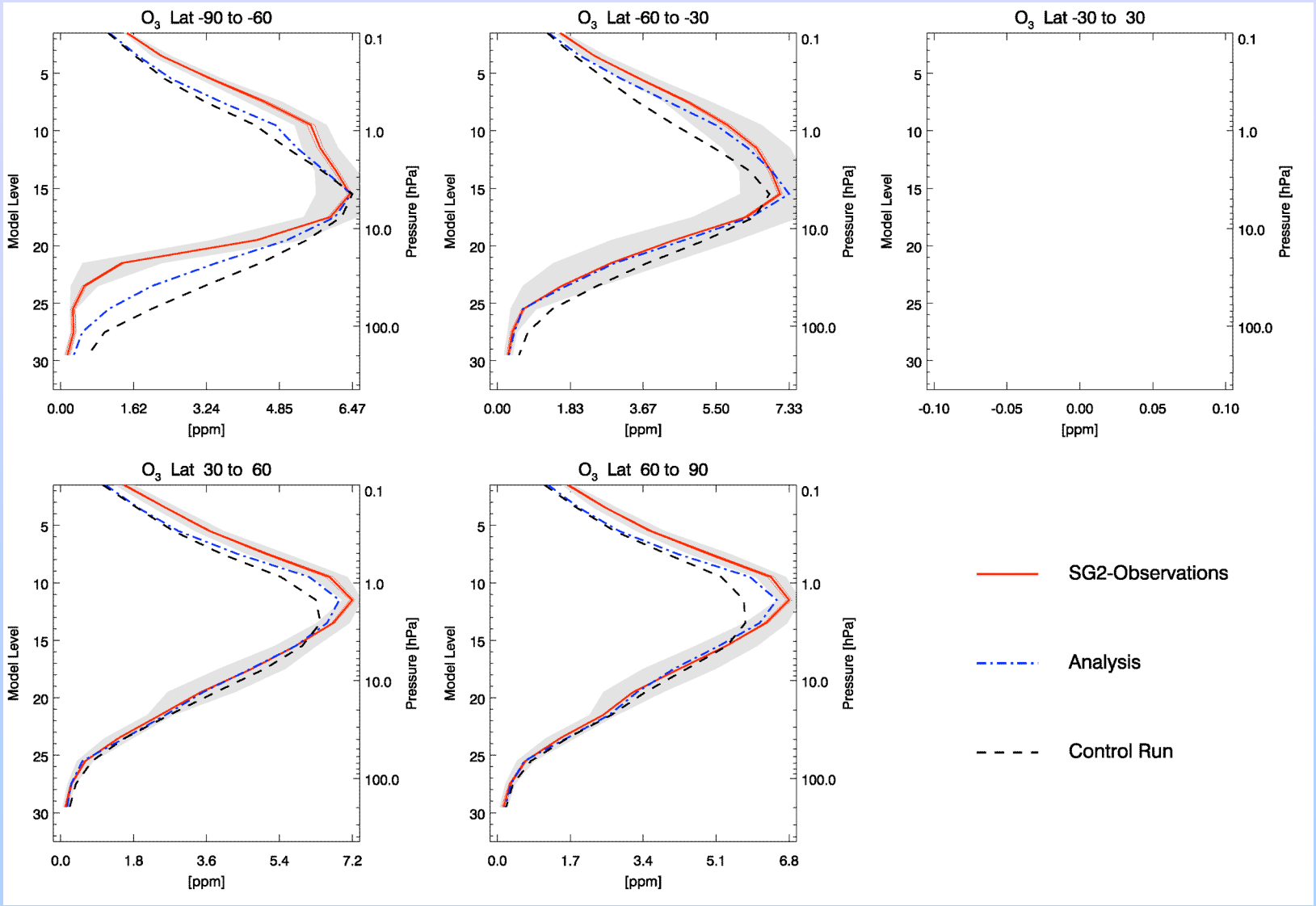



Cost function 2002/09/08 - 2002/09/21
Cost-function/number of observations
Number of iteration
2002/09/08 (17414 observations)
2002/09/12 (52484 observations)
2002/09/13 (108954 observations)
2002/09/14 (98949 observations)
2002/09/15 (116518 observations)
2002/09/16 (107792 observations)
2002/09/17 (104322 observations)
2002/09/18 (130205 observations)
2002/09/19 (108248 observations)
2002/09/20 (106398 observations)
2002/09/21 (104683 observations)
Cost function 2002/09/22 - 2002/10/15
Cost-function/number of observations
Number of iteration
2002/09/22 (124644 observations)
2002/09/23 (98772 observations)
2002/09/24 (78046 observations)
2002/09/25 (64995 observations)
2002/09/26 (109569 observations)
2002/09/27 (105972 observations)
2002/09/28 (37063 observations)
2002/10/12 (9593 observations)
2002/10/13 (18756 observations)
2002/10/14 (15224 observations)
2002/10/15 (16490 observations)

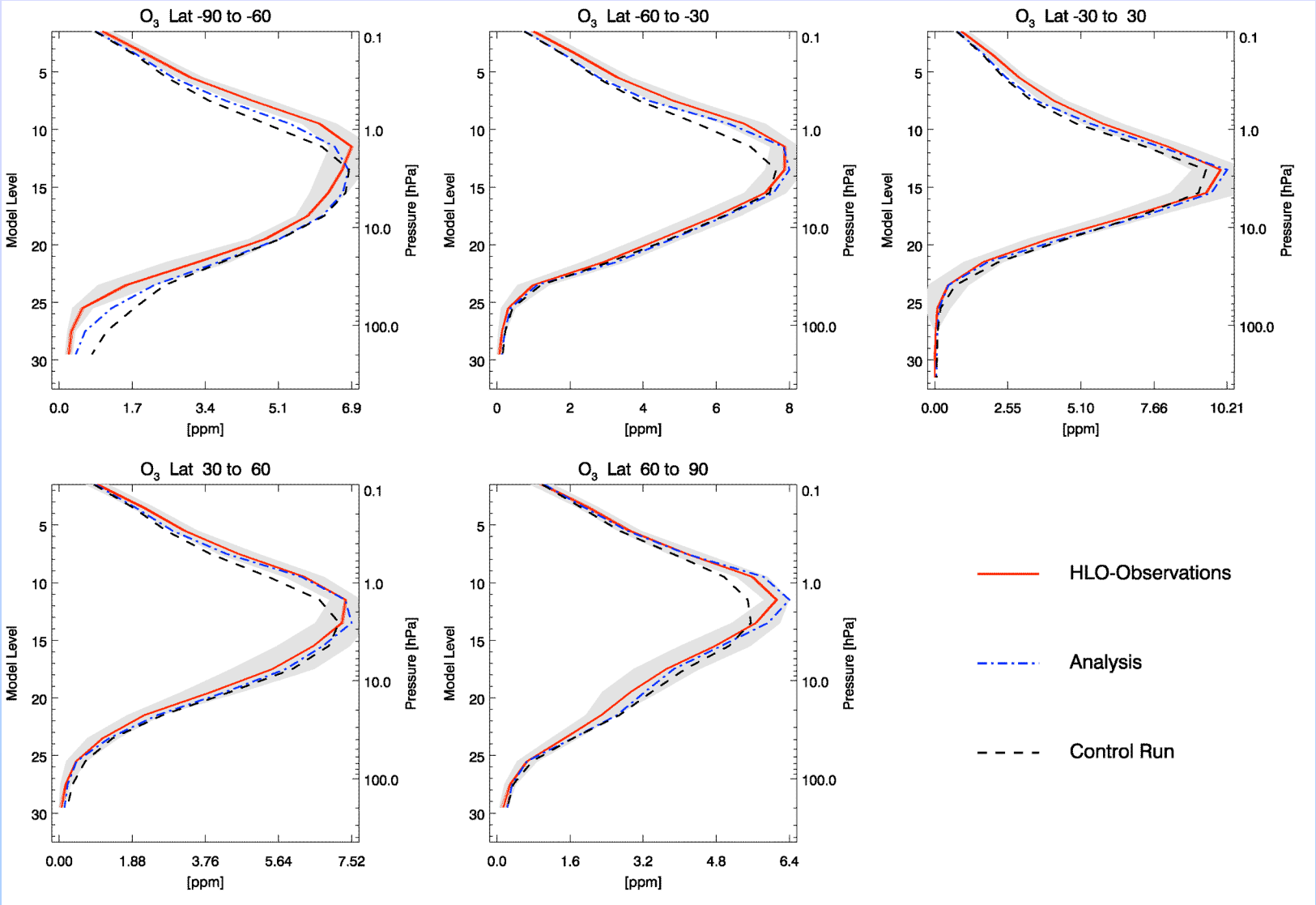
Mean MIPAS O_3 profiles (assimilated) / analysis / control run



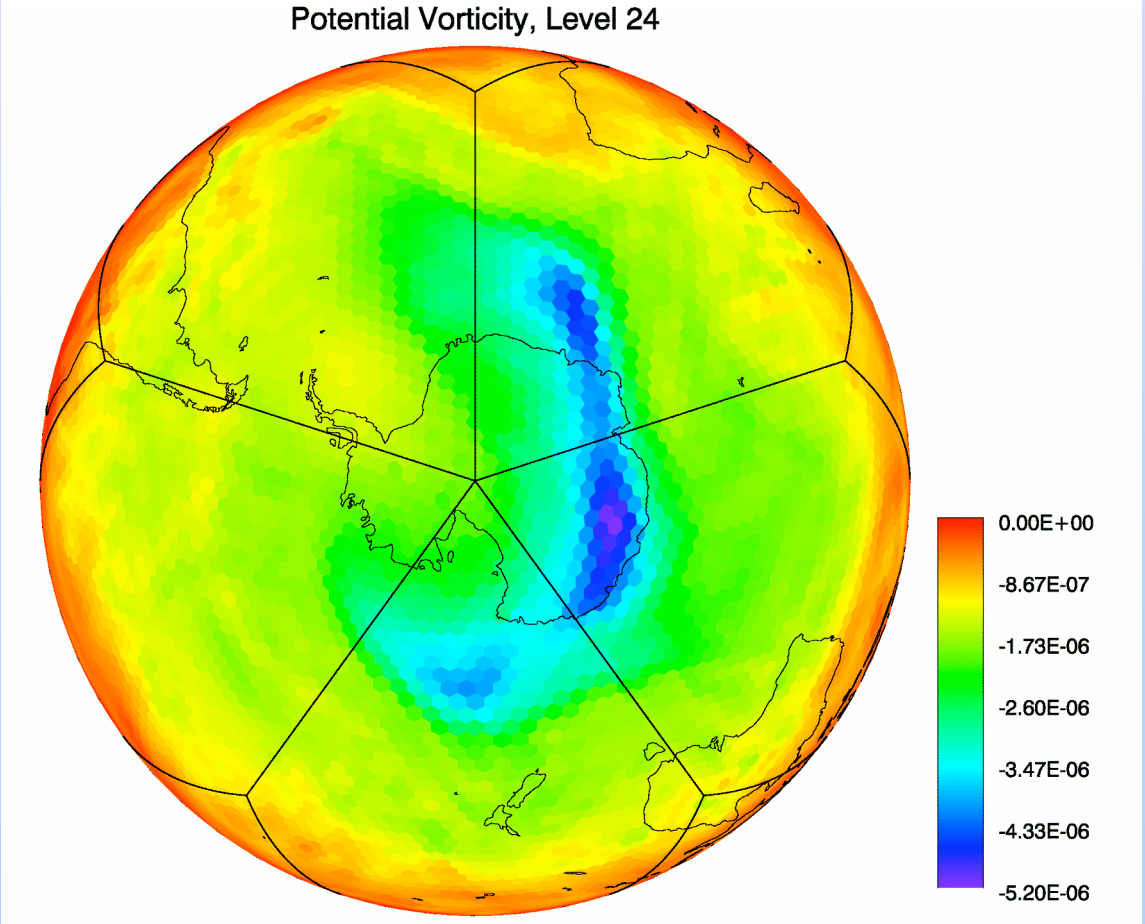
Mean SAGE II O_3 profiles (not assimilated) / analysis / control run



Mean HALOE O_3 profiles (not assimilated) / analysis / control run



Potential Vorticity 13 Sept, 78 hPa



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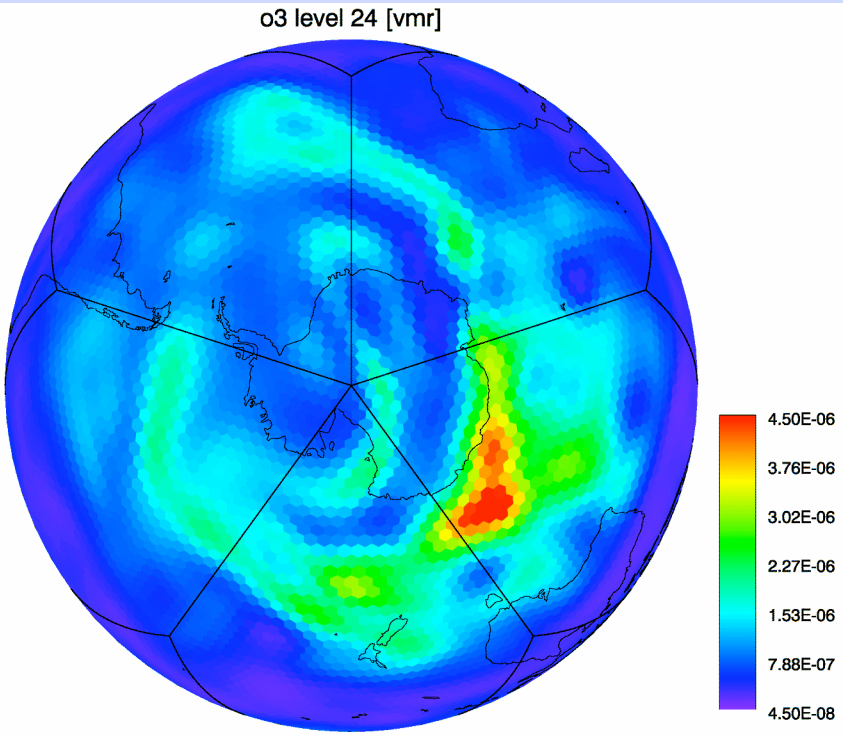
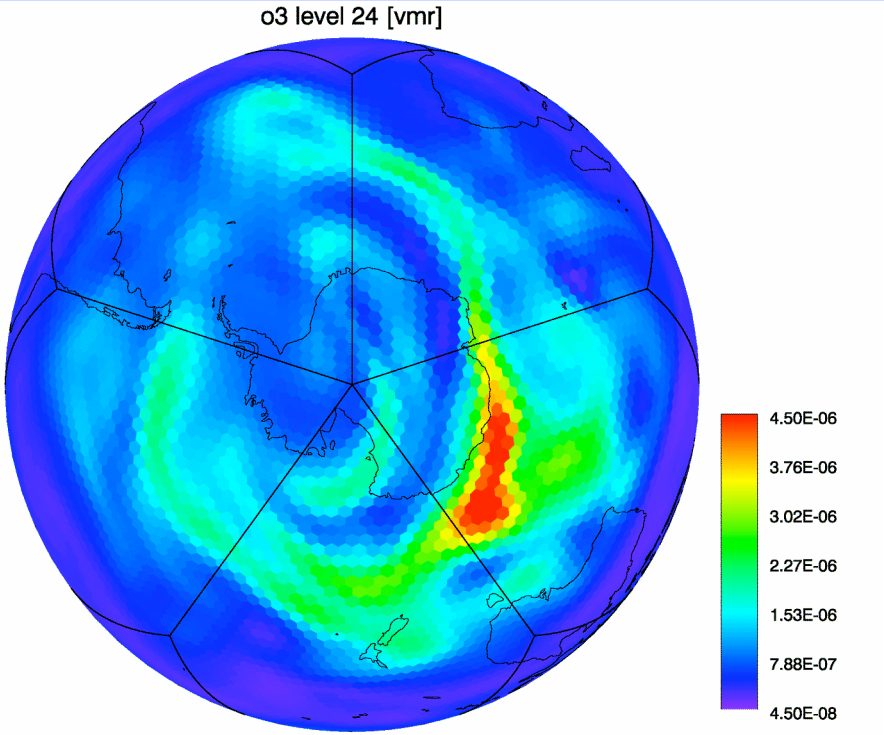
Ozone analysis 13 Sept at 78 hPa

Isotropic BECM parameterisation



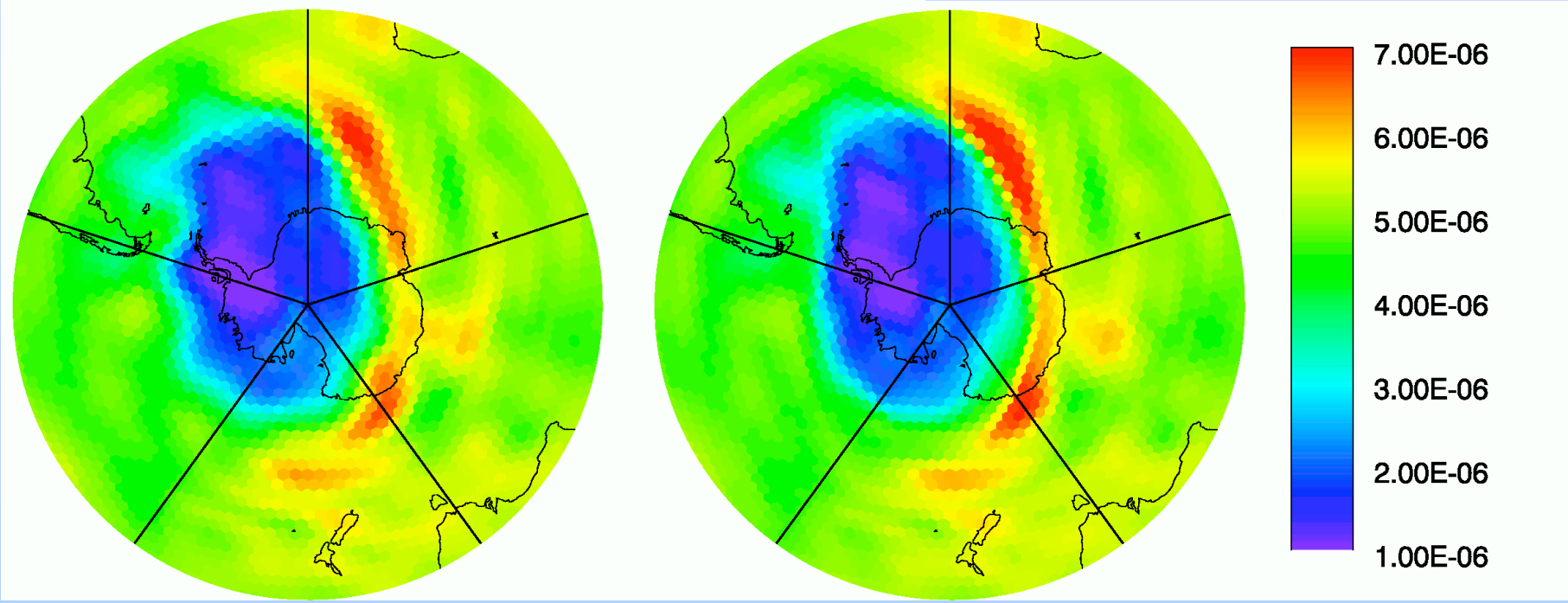
Flow dependent BECM parameterisation



Ozone analysis 13 Sept at 30 hPa

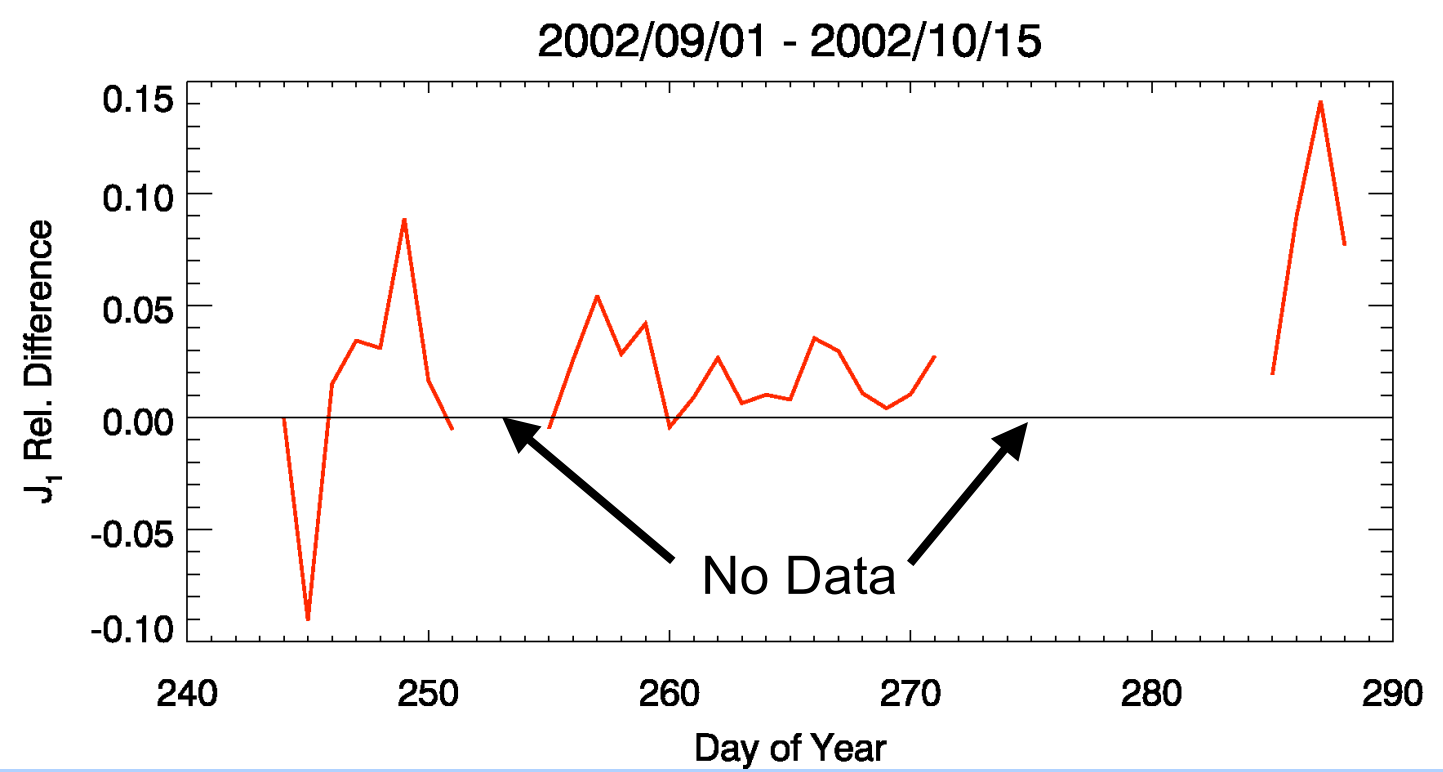
Isotropic BECM parameterisation

Flow dependent BECM parameterisation



Evaluation of flow dependent scheme in terms of forecast quality:

J_1 := Weighted mean square difference between MIPAS and one day forecast



Outlook

- System improvements:
  - -More sophisticated (location dependent) choice of BECM parameters
  - -Improovement of heterogeneous chemistry / PSC microphysics
  - -Refine resolution down to 160 km mesh size
- SACADA system has been implemented at DLR-DFD for routine operation
- Assimilation of total column data under preparation

Acknowledgements

We are especially grateful for support by the following groups, persons and institutions:

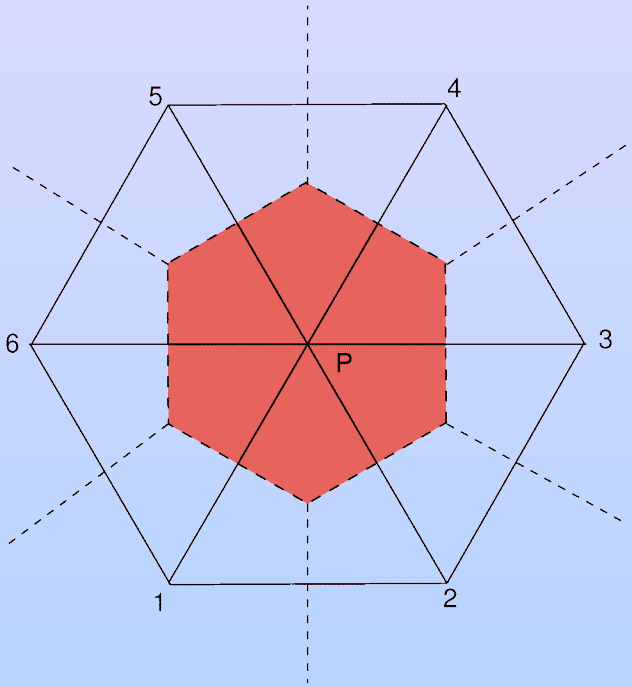
German Weather Service for provision of the GME software

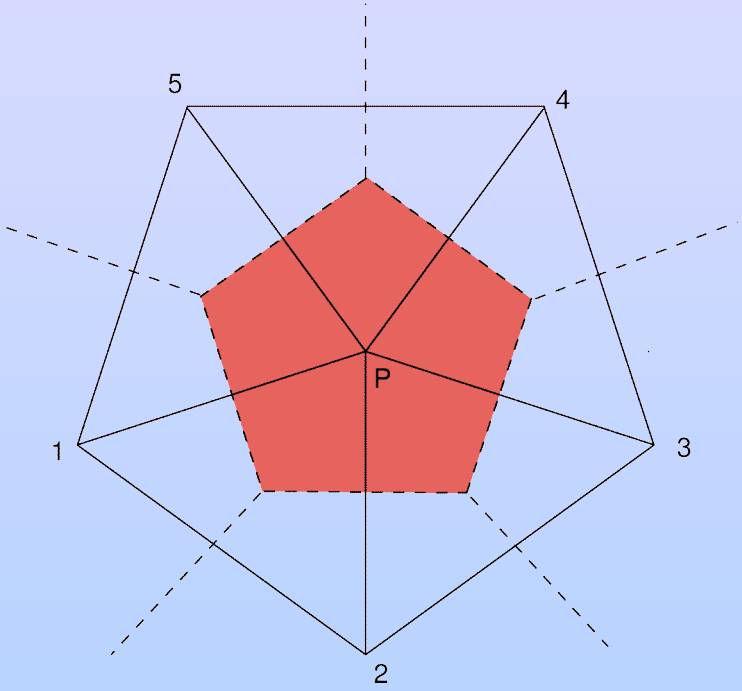
R. Botchorishvili (SCAI-FhG) who developed fast and efficient algorithms for the SACADA system

ESA for providing the MIPAS data (Thanks to T. Erbertseder for data pre-processing)

The SACADA project was funded by the German Federal Ministry of Education and Research (BMBF) in the framework of AFO-2000

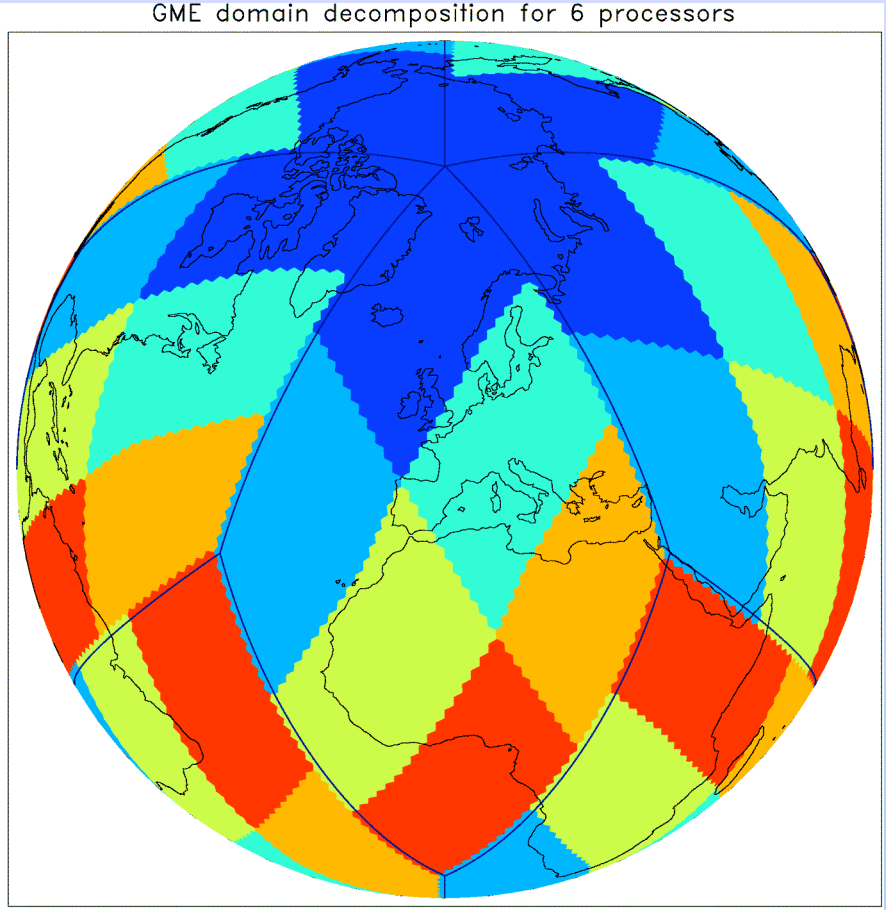
Grid Cells of Icosahedral Grid





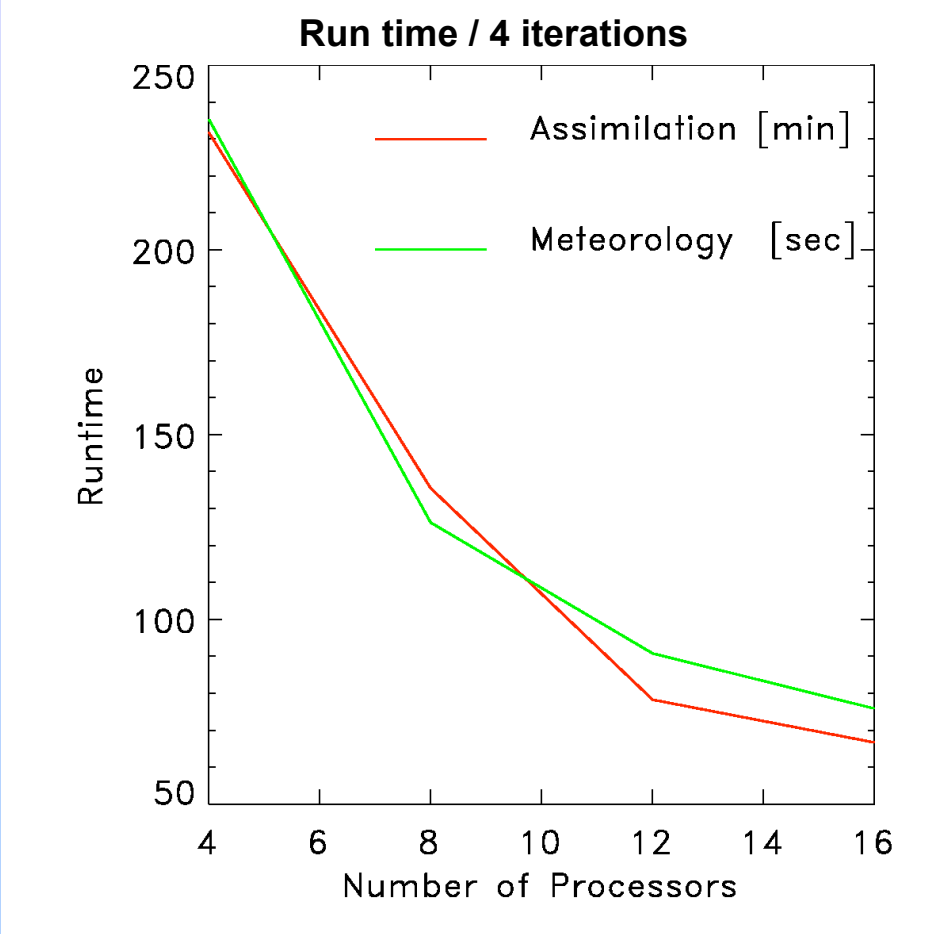
The area of representativeness belonging to one grid cell is a hexagon or (at the twelve special points) a pentagon

Computational Aspects, Parallelisation Strategy



Domain decomposition for 6 processors ◊ simple but effective strategy for load balancing

Computational Aspects



With an assimilation window of 24h and 12 using iterations, the wall clock run time is about 3 hours using 16 processors