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Variational Assimilation of ENVISAT Data and the new Icosahedral 4D-var Assimilation System

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RIU EURAD

SACADA

Project objectives:

Given the expected wealth of geolocated trace gas retrievals from MIPAS, SCIAMACHY, and GOMOS, as well as forthcomming satellite sensors, all offering an unprecedented surveillance capacity of a changing atmosphere, SACADA aims to devise an operational assimilation system to estimate synoptic fields of constituents. Respecting the general objective to upgrade data to information, in this 5 years project the following items are aspired (among others):

(i) optimal exploitation of satellite retrievals of various trace gases scattered in space and time and obtained from different sensors,
(ii) extension to the estimation of not observed species, which are chemically coupled to observed species,
(iii) portability of the system to future computational platforms, namely parallelisation.

Project methodology:

To comply with these and other requirements, an approach with the following features is selected:

1. four dimensional varaiational method as a feasible spatio-temporal data assimilation algorithm with the BLUE property (Best Linear Unbiased Estimator)
2. GCCM: fully coupled Global Chemistry Circulation Model set-up
3. icosahedral grid structure and meteorological driver adopted from GME, after extension to 0.1 hPa.

The basic idea of 4D-var is to minimise a scalar cost function that measures the distance between a GCCM model run and the observations on the one hand and an appropriate background field on the other hand. For a proper weighting of the information that is contained in the observations and in the background, covariances of all quantities have to be specified as accurate as possible. A simple method to model off-diagonal elements of the background error covariance matrix is to add a curvature penalty term to the cost function J:

$$J(\mathbf{x}(t_0)) = \frac{1}{2}(\mathbf{x}^b(t_0)-\mathbf{x}(t_0))^T\mathbf{B}_0^{-1}(\mathbf{x}^b(t_0)-\mathbf{x}(t_0)) + \frac{1}{2}\int_{t_0}^{t_N}\left(\mathbf{y}^0(t)-\mathbf{H}\mathbf{M}(t,t_0)\mathbf{x}(t_0)\right)^T\mathbf{R}^{-1}(\mathbf{y}^0(t)-\mathbf{H}\mathbf{x}(t))dt + \frac{1}{2}[\Delta\mathbf{x}(t_0)]^T\mathbf{A}^{-1}[\Delta\mathbf{x}(t_0)]$$

$\mathbf{x}^b(t_0)$	background state at $t=0$
$\mathbf{x}(t)$	model state at time t
$\mathbf{y}^0(t)$	observation at time t
$\mathbf{B}_0$	background error covariance matrix
$\mathbf{A}$	smoothness weighting matrix

Advanced background error covariance modelling using a diffusion approach is currently under development (see poster of SCAI-FHG).

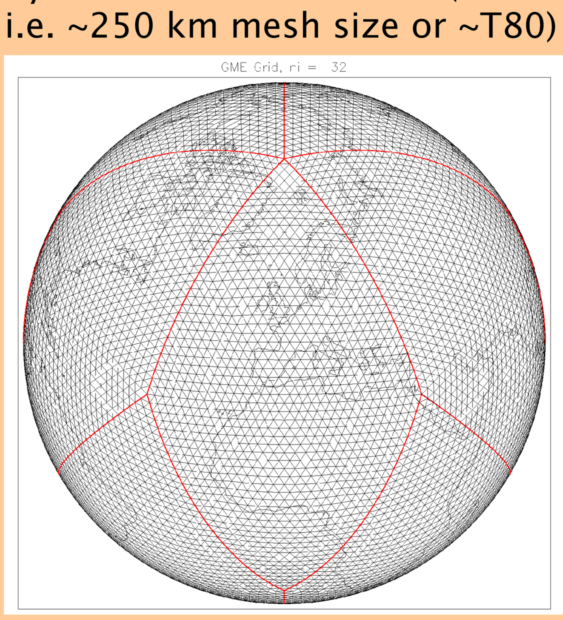


Figure 1: Icosahedral grid in the resolution that is currently used by the SACADA GCCM (ni=32, i.e. ~250 km mesh size or ~T80)

Consortium composition:

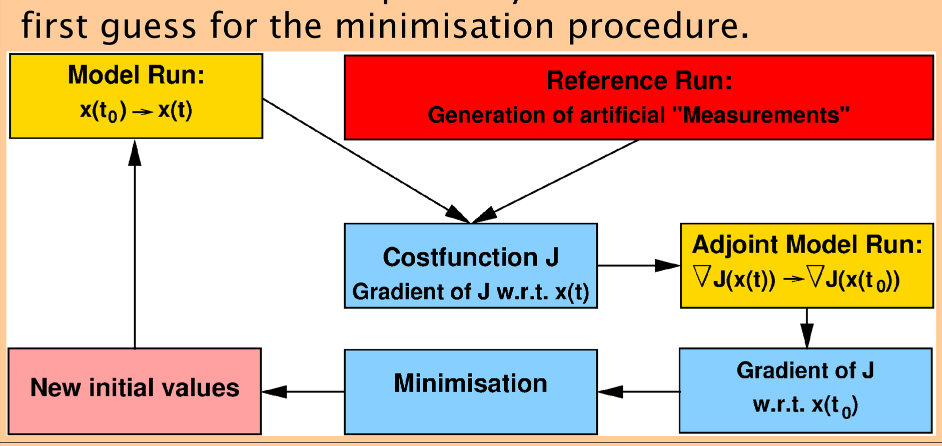
RIU at the University of Cologne: development of the adjoint model and 4D-var system;
SCAI, FhG: development of the forward GCCM and the square root covariance operator;
DLR-DFD: estimation of correlation lengths and standard ENVISAT data provision;
FZK-IMK: MIPAS extended retrieval sets;
IFE, University of Bremen: SCIAMACHY occultation data;
FZJ-ICG-I: CRISTA data expertise and Eliassen-Palm flux diagnostics.

Data status:

ESA MIPAS standard data contain profiles of N_2O, CH_4, HNO_3, O_3, H_2O and NO_2. This data is presently only usable with preceeding quality control. Different error types occur for concentration values, location and error margins. The IMK group provides an extended data set containing the standard species plus $ClONO_2$, N_2O_5, NO, CFC-11 and in the future also HNO_4 and ClO. Non-operational SCIAMACHY sun occultation measurements (O_3 and NO_2) processed by the IFE group are available for selected periods.

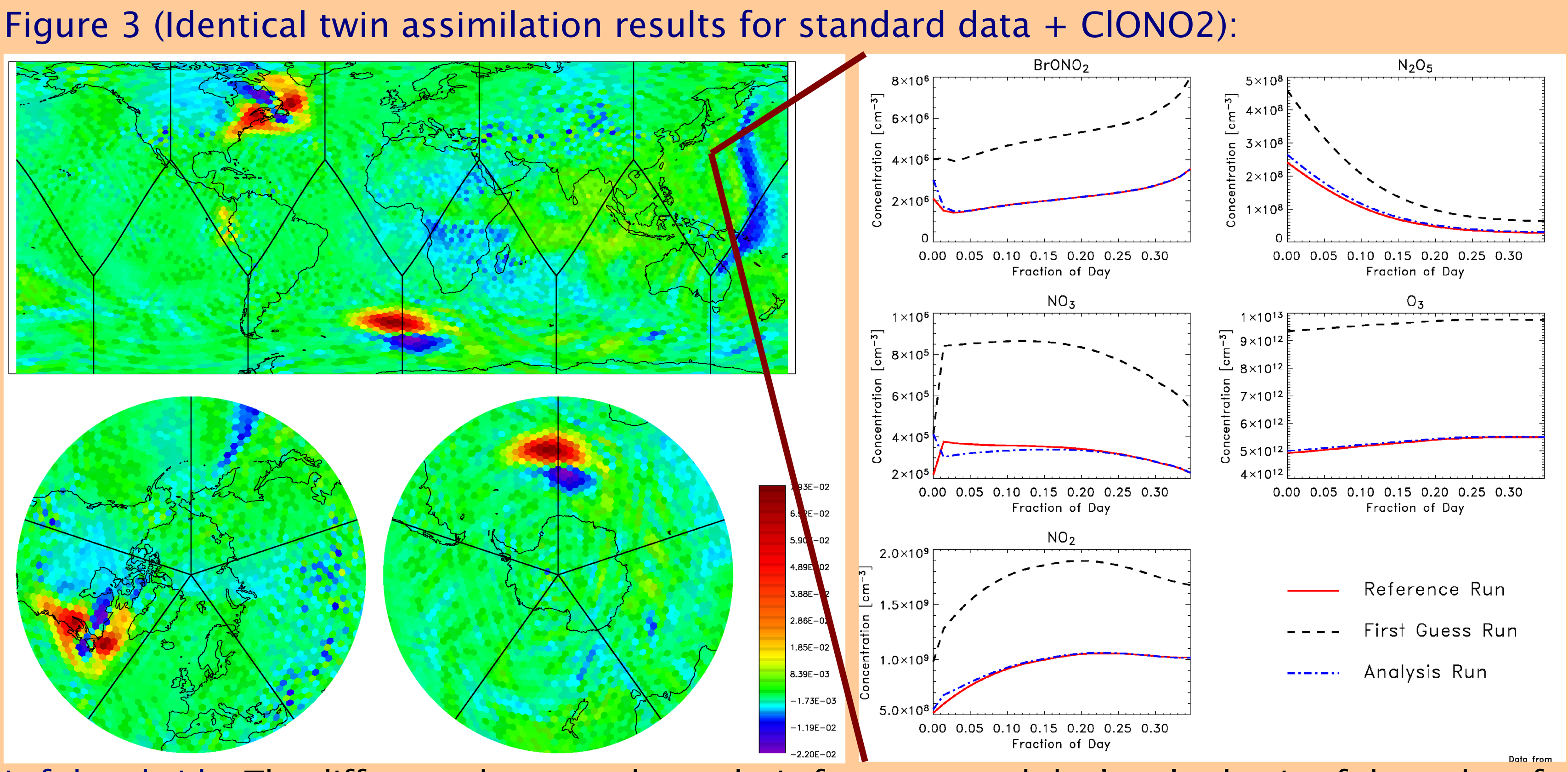
First tests of the new icosahedron-based assimilation system:

Figure 2 (Experiment Setup): A GCCM run for 01.09.2002, 00:00-08:30 UTC was conducted with meteorological start data from ECMWF initial concentrations derived from SOCRATES data. This run serves as reference and represents the 'true' chemical state of the atmosphere. The initial reference concentrations multiplied by 1.9 are then taken as first guess for the minimisation procedure.



Kernel of the new system is a novel stratospheric global chemistry circulation model (GCCM) and its adjoint version, with the grid design adopted from the global weather forcast model (GME) of German Weather Service (see figure 1). The GME serves as an online meteorological driver for the GCCM while the icosahedral grid structure (see figure 1), the horizontal transport and the parallelisation strategy are adopted from GME. The stratospheric chemistry module accounts for 148 gas phase and 7 heterogenous reactions between 43 stratospheric constituents. To verify the numerical correctness and robustness of the program code, a comprehensive suite of so called observability and identical twin tests was conducted. Moreover, these tests were used to explore the potential and limits of 4D-var data assimilation applied to the particular problem of assimilating artificial ENVISAT MIPAS and SCIAMACHY observations. The experimental setup is described in figure 2 and selected results are shown in figures 3 and 4.

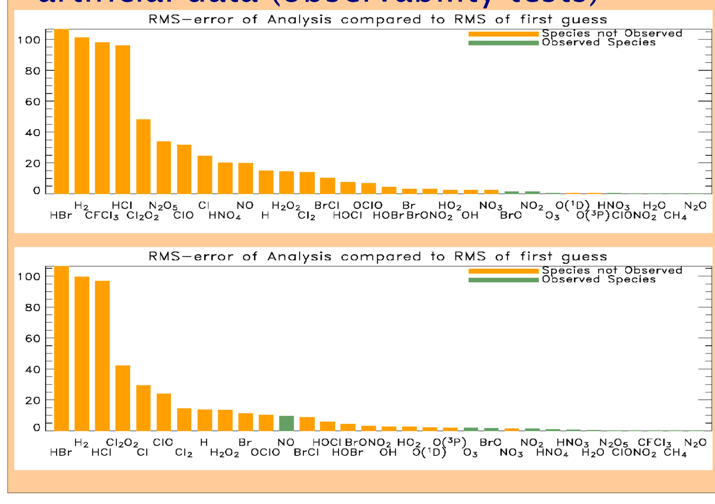
Figure 3 (Identical twin assimilation results for standard data + ClONO2):



Left hand side: The difference between the analysis for ozone and the 'true' value is of the order of a few percent after 20 iterations of the minimisation procedure.

Right hand side: Time series for selected species for the same configuration. Note that $BrONO_2$, N_2O_5 and NO_3 are not observed in this experiment.

Figure 4: Improvement of chemical state of the stratosphere derived from experiments with artificial data (observability tests)



RMS error of analysis compared with RMS of first guess for different data sets. The RMS is taken at the time of measurements for all gridpoints with daylight-observations. The first panel shows results for MIPAS and SCIAMACHY standard data set + $ClONO_2$, while the second panel shows the results for the extended data set. There is considerable improvement for many species that are not directly observed in both cases. It is remarkable, that the standard data set enriched by $ClONO_2$ works almost as well as the extended data set. See text for a detailed description of the experimental setup.

Operational efficiency estimate:

The SACADA icosahedral system is fully parallelised (MPI) and running on a local PC cluster in readiness for operational application. With 6 processors a near real time efficiency is closely attained with targeted ni=32 (=250 km) resolution. Parallel scaling performance clearly indicates a fully sufficient performance with 8 processors or next generation PCs.

Assimilation of ENVISAT data into the AMMOC-CTM:

The global COMMA-CTM (Cologne Model of the Middle Atmosphere in its CTM version) calculates the transport of chemical constituents using the Bott algorithm and chemical conversions using the aforementioned chemistry scheme. Together with its adjoint, it constitutes the AMMOC-CTM and has been successfully tested with CRISTA data during the first phase of the SACADA project.

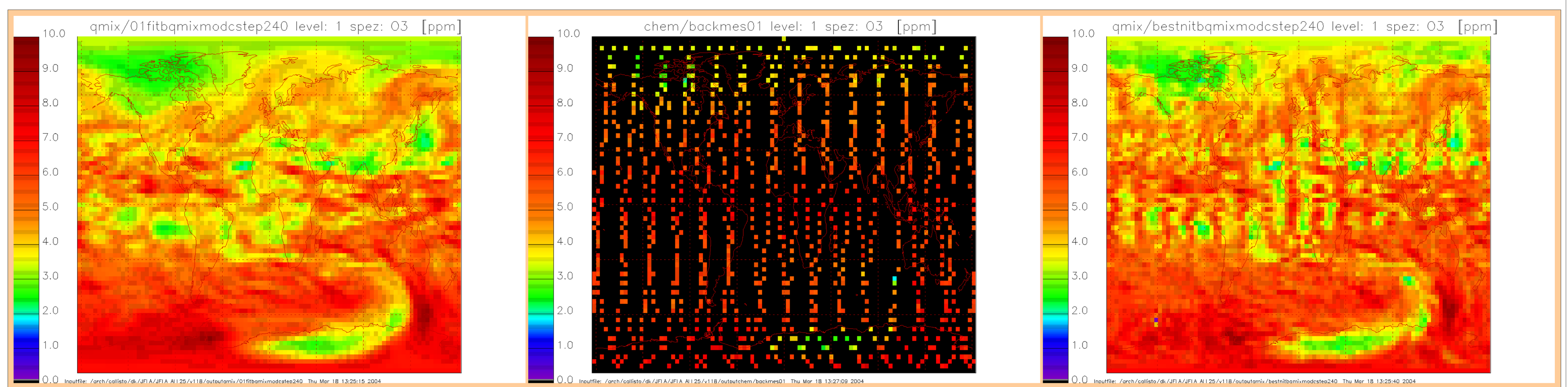


Figure 5 (Ozone assimilation):

Left hand side: Ozone distribution at 25 km altitude on Nov.5, 00UTC after 12h CTM integration, initialisation with ROSE analysis. Center: ENVISAT ozone measurements for 25 km altitude between Nov.4, 12 UTC and Nov.5, 12 UTC, all datasets combined and averaged on a 2° by 2° grid. Right hand side: Assimilation result, combining background knowledge (left) and measurements (center). Improvement is especially noticeable in the equatorial region where the model concentrations are lower. In this region, the satellite tracks are visible as the curvature penalty term was chosen to be small. Two MIPAS ESA profiles were ignored due to their unrealistically low errors.

First experiments with ESA MIPAS standard data and non-operational data provided by the IMK and the IFE groups were carried out for Nov. 4/5, 2003 and 25 km altitude with the AMMOC-CTM. The model was initialised with the ROSE analysis provided by DFD. In one experiment, all measurements were used. For comparison, three experiments were carried out where each data set was used separately. In this way, it was possible to determine the origin of certain effects (such as the blue spot in the Antarctic Sea in figure 5 which is caused by MIPAS ESA data). For performance reasons, all experiments had to be limited to 15 iterations even though the cost function did not seem to have reached its minimum at that point. Figure 5 shows the improvement of the ozone distribution in the middle of the 24h assimilation interval. The improvement for CH_4 and H_2O was similar. HNO3 measurements and analysis are displayed in figure 6. Figure 7 displays the temporal evolution of the trace gas mixing ratios at a selected grid box at 142.5°E, 30°N along with the measurements available for this grid box. In this case the analysis agrees with the measurements within the error margins for several species. By an increase of the number of iterations of the minimisation routine, we expect to achieve better compliance of model and observations.

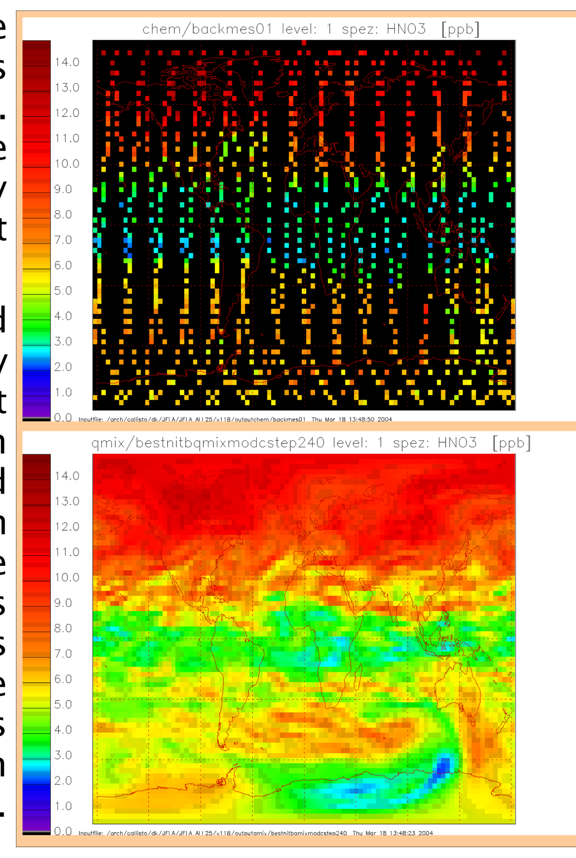


Figure 6 (HNO_3 assimilation):
Top: ENVISAT HNO3 measurements for 25 km altitude between Nov.4, 12 UTC and Nov.5, 12 UTC, all datasets combined and averaged on a 2° by 2° grid.
Bottom: analysis on Nov.5, 00 UTC.

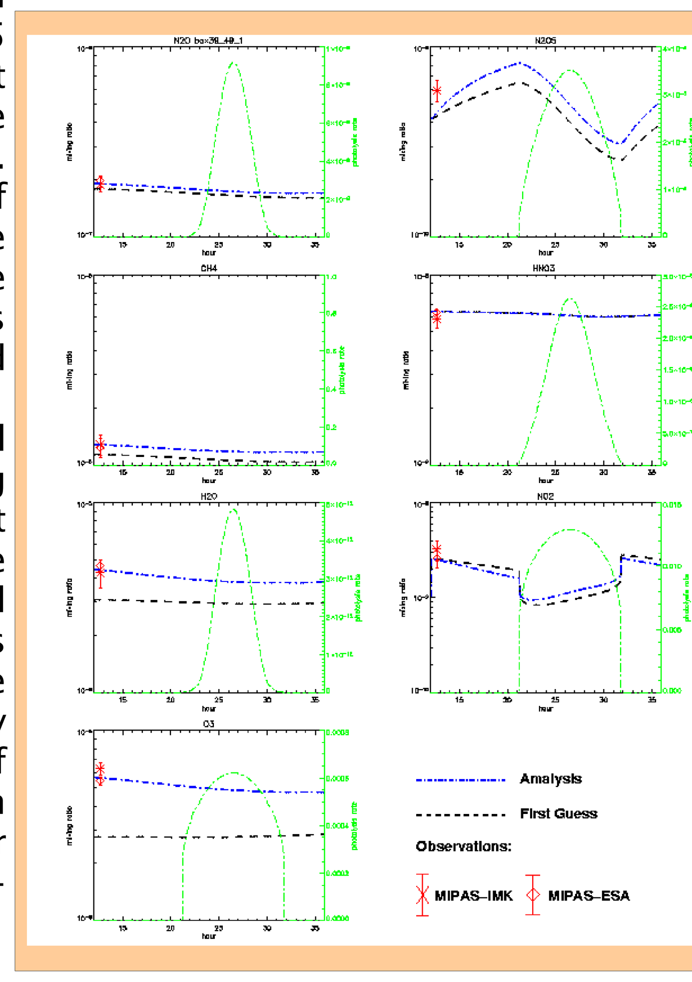


Figure 7: Temporal evolution of trace gas concentrations (mixing ratios) at 142.5°E, 30°N for (top left to bottom right) N_2O, N_2O_5, CH_4, HNO_3, H_2O, NO_2, and O_3. Shown is the model trajectory without assimilation in black and the analysis in blue as well as the available measurements MIPAS ESA and MIPAS IMK. Photolysis rates in green indicate day and night.

State of the project:

By continuously improving ENVISAT data quality of concentrations as well as respective errors, analysis products will become increasingly reliable. During this process, software status is shifting from development to optimisation. This mainly includes preconditioning adaption and data input quality control.

SACADA post-AFO 2000 application:

SACADA will run operationally at DFD and will serve as a German contribution to GMES activities; the icosahedral concept fits into the ICON initiative in preparation of the post-ECHAM5 era (COSMOS-2); flexibility of grid design allows for later extension to the troposphere with local refinements (convergence with SATEC4D objectives).

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ENVISAT CARING FOR THE EARTH

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