Global modelling of atmospheric chemistry
special project SPDEACM interim report
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The years 2016 and 2017 brought several changes to the original SPDEACM project planning: First we had to deal with the leaving of our group member Yi Heng in February 2016, which led to the shutdown of our modelling activities in CAMS. In July 2017, Martin Schultz will change to the Supercomputing division at FZ Juelich (JSC) to focus on new pathways to earth data exploration (Schultz et al., 2016). Finally, a growing number of publications arose from our scientific work on tracer and meteorological transport modelling, all making extensive use of IFS model output. For these purposes data from historic operational forecasts as well as meteorological and chemical reanalysis products are stored in Jülich for scientific analysis. As part of a long-term obligation, data of meteorological and chemical data from the MARS and ECFS archives to the Jülich supercomputing systems is transferred regularly in near-realtime in order to serve our CAMS chemical boundary condition server.

C-IFS and IFS-MOZ

After the shutdown of FZ Jülich evolvement in the C-IFS development in 2016 our HPC usage at ECMWF could be drastically reduced, as the global models in use (ECHAM6-HAMMOZ, EMAC, ICON) are able to run on the JURECA cluster at FZ Jülich. The C-IFS-MOZ development in CAMS has been handed over to Idir Bouarar (MPI-Met Hamburg). Three scientific papers analysing results from CAMS and MACC model results could be published in 2016 (Liora et al., 2016; Kracher et al., 2016; Lyapina et al., 2016). For details see our 2016 progress report.

Data services supporting CAMS and MACC

Already since 2012 NRT data from the operational CAMS forecasts (formerly MACC forecasts) as well as from the GFAS fire emission inventory (Kaiser et al. 2012) are transferred to FZ Jülich on a daily basis and made available to the public via our OWS interface JOIN (Waychal et al. 2013; http://join.iek.fz-juelich.de/). In addition, we downloaded all chemical species concentrations from the MACC reanalysis 2003-2012 which are not publically available from the MARS archive. Tracer fields from the CAMS operational forecasts and from the MACC reanalysis are used for scientific analysis of atmospheric chemistry (Gaudel et al., 2015; Lyapina et al, 2016; Kracher et al, 2016) and serve as boundary conditions for regional air quality models (Liora et al., 2016). Currently our existing Web Coverage Service (WCS) for sharing individually tailored model results is being re-engineered to make use of rasdaman, a scalable array database technology in order to improve performance, enhance flexibility, and allow the operation of catalogue services. The WCS protocol is upgraded to WCS2.0 and the metadata shall be interfaced with the EUDAT (https://www.eudat.eu/) service structure (Stein et al., 2017). In 2017, we established a closer collaboration with Julia Wagemann (ECMWF) to share our experiences with access to complex multi-dimensional atmospheric data and with the rasdaman technology also developed at ECMWF in the framework of the EarthServer2 project.

Other studies performed with ECMWF data products

Small-scale temperature fluctuations induced by atmospheric gravity waves can trigger the formation of polar stratospheric clouds (PSCs). In a study by Hoffmann et al. (2017a) we introduced a new ten-year-long Atmospheric Infrared Sounder (AIRS) satellite record of gravity wave activity in the polar lower stratosphere to investigate this process. The analysis of temporal patterns in the data set revealed a strong seasonal cycle in wave activity with wintertime maxima at mid- and high latitudes. The analysis of spatial patterns indicated that orography as well as jet and storm sources are the main causes of the observed waves. Wave activity is closely correlated with 30 hPa zonal winds, which is attributed to the AIRS observational filter. We used the new data set to evaluate explicitly resolved temperature fluctuations due to gravity waves in the European Centre for Medium-Range Weather Forecasts (ECMWF) operational analysis (Fig. 1). It was found that the analysis reproduces orographic and non-orographic wave patterns in the right places, but that wave amplitudes are typically underestimated by a factor of 2–3 (Fig. 2).

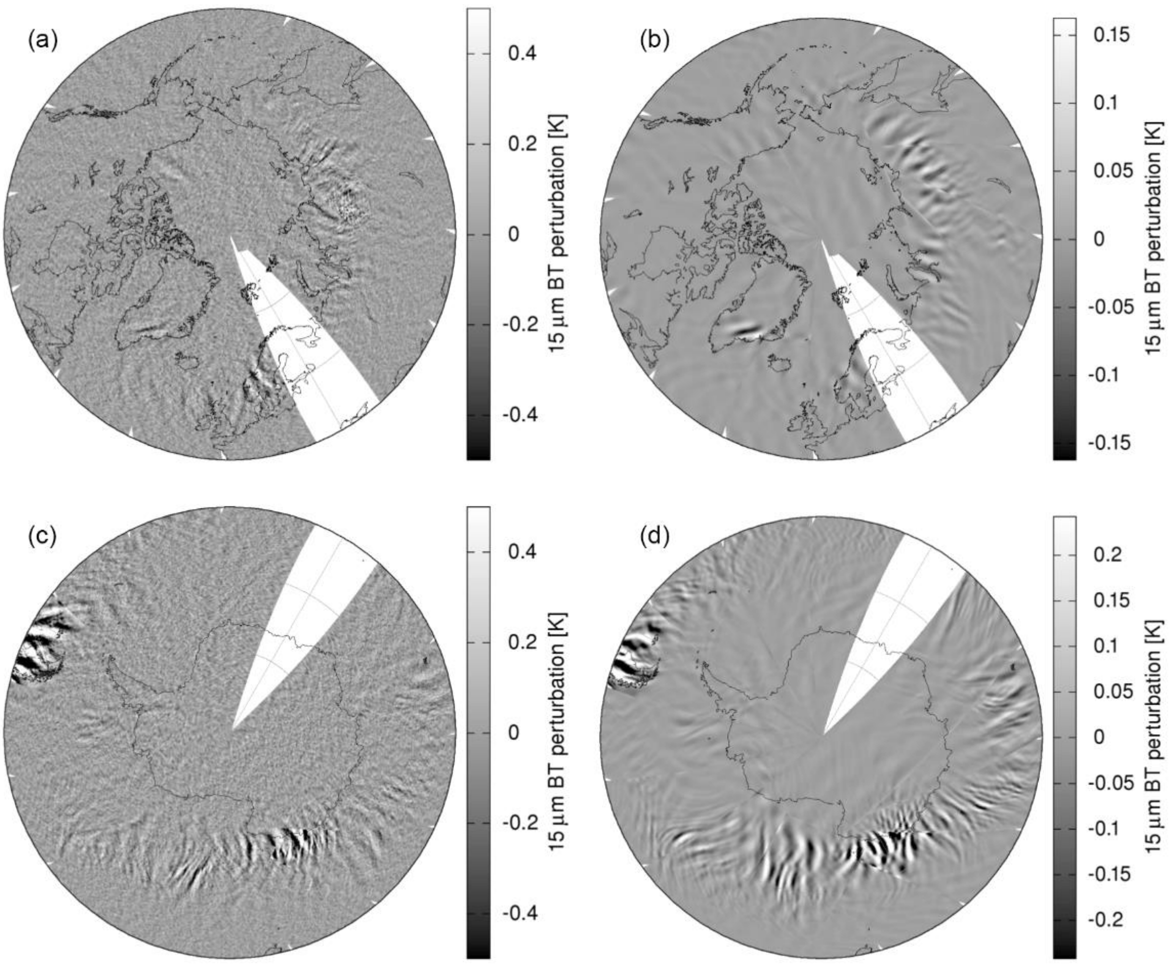

Figure 1: AIRS measurements of 15 µm brightness temperature perturbations (left) and corresponding simulations based on ECMWF operational analysis temperatures (right). Real measurements took place on 11 December 2003 from 12:00 to 24:00 UTC in the Northern Hemisphere (top) and on 22 July 2011 from 00:00 to 12:00 UTC in the Southern Hemisphere (bottom). Simulated measurements are based on synoptic data at 18:00 and 06:00 UTC, respectively.

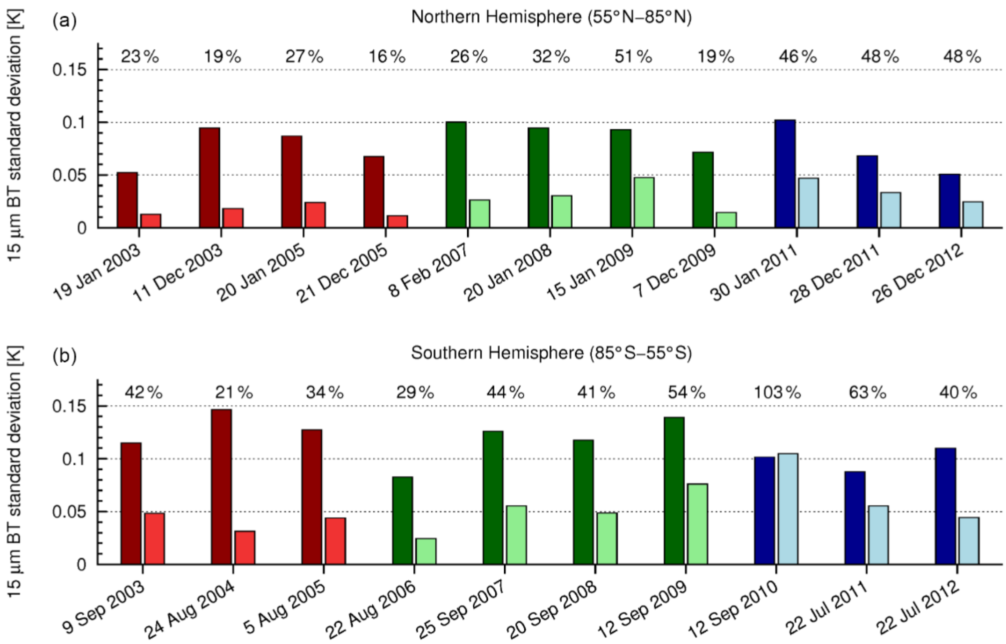

Figure 2: Peak events of gravity wave activity in individual 2003–2012 Northern and Southern Hemisphere winter seasons. The 15 µm brightness temperature standard deviations were inferred from real AIRS measurements (dark shading) or simulations based on ECMWF operational analysis data (light shading). The color coding refers to the resolution of the ECMWF data (red is T511L60, green is T799L91, and blue is T1279L91). The percentages at the top of the plots indicate the relative differences of the simulated data with respect to the measurements.

In a second study by Hoffmann et al. (2017b) we compared temperatures and horizontal winds of meteorological analyses in the Antarctic lower stratosphere. The study covered the ECMWF operational analysis, the ERA-Interim reanalysis, the MERRA and MERRA-2 reanalysis, and the NCEP/NCAR reanalysis. The comparison was performed with respect to long-duration observations from 19 superpressure balloon flights during the Concordiasi field campaign in September 2010 to January 2011 (Fig. 3). Considering the fact that the balloon observations have been assimilated into all analyses, except for NCEP/NCAR, notable differences found in the paper indicate that other observations, different forecast models, and different data assimilation procedures have significant impact on the analyses as well. We also used the balloon observations to evaluate trajectory calculations with our new Lagrangian transport model Massive-Parallel Trajectory Calculations (MPTRAC), where vertical motions of simulated trajectories were nudged to pressure measurements of the balloons. The paper is accepted for publication at ACP.

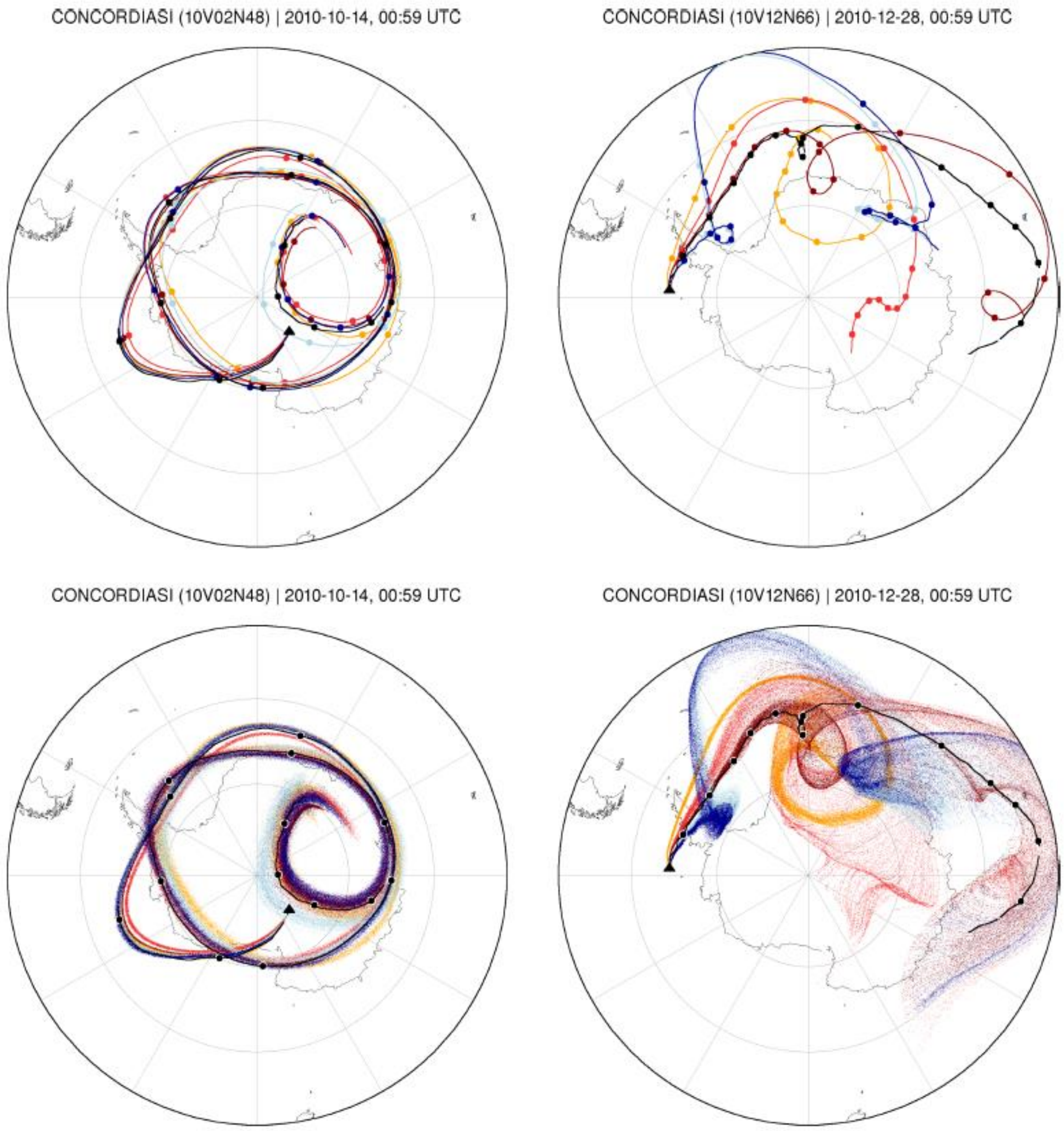

Figure 3: Examples of trajectories calculated with different meteorological analyses (dark blue: ECMWF OA, light blue: ERA-Interim, dark red: MERRA-2, light red: MERRA, orange: NCEP/NCAR) and corresponding Concordiasi balloon trajectory (black). Plot titles provide the starting times and triangles indicate the starting positions of the trajectories. Circles indicate trajectory positions at 0 UTC each day. Plots at the top show individual trajectories calculated without diffusion. Plots at the bottom illustrate dispersion simulations with diffusion being considered.

In a further study by Rößler et al. (2017) we focused on the minimization of truncation errors that originate from the use of numerical integration schemes to solve the kinematic equation of motion. We analysed truncation errors of six explicit integration schemes of the Runge Kutta family, which we implemented in the Massive-Parallel Trajectory Calculations (MPTRAC) model. The simulations were driven by wind fields of ECMWF operational analysis and forecasts at T1279L137 spatial resolution and 3 h temporal sampling. In total more than 5000 different transport simulations were performed and we quantified the accuracy of the trajectories by calculating transport deviations with respect to reference simulations using a 4th-order Runge-Kutta integration scheme with a sufficiently fine time step (Fig. 4). The selection of the integration scheme and the appropriate time step should possibly take into account the typical altitude ranges as well as the total length of the simulations to achieve the most efficient simulations. However, trying to generalize, we recommend the 3rd-order Runge Kutta method with a time step of 170 s or the midpoint scheme with a time step of 100 s for efficient simulations of up to 10 days time based on ECMWF's high-resolution meteorological data.

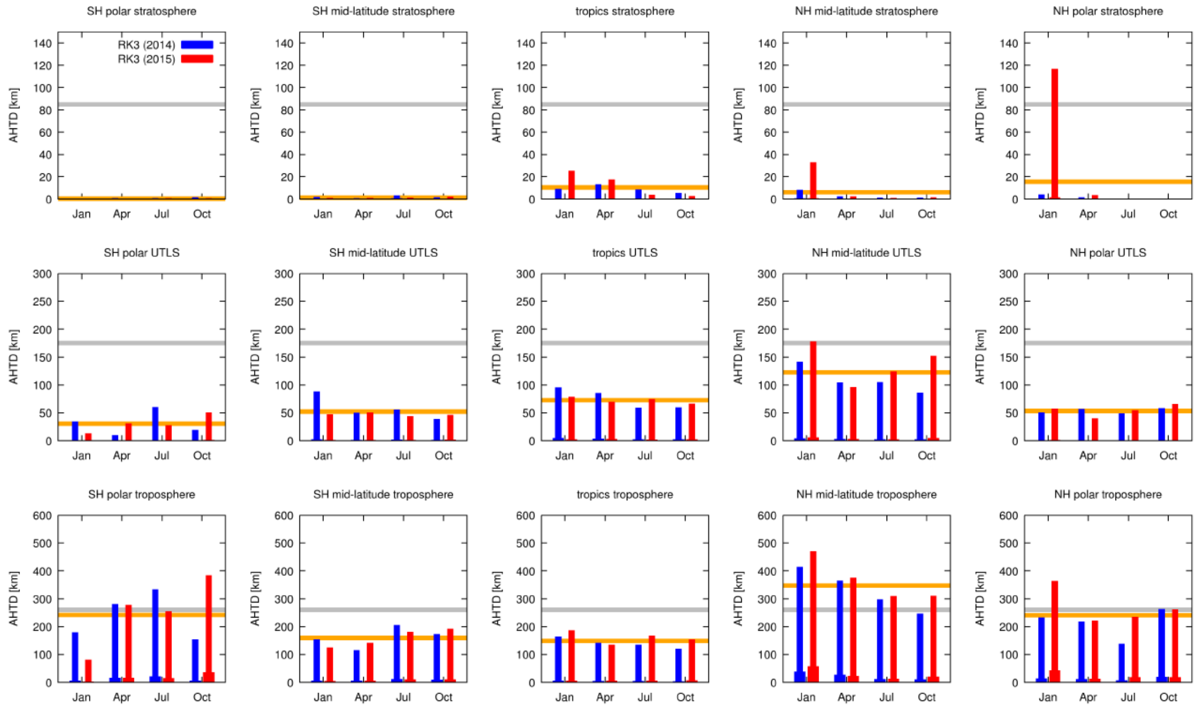

Figure 4: Mean (thin bars) and median (thick bars) horizontal transport deviations after ten days simulation time in different domains for the RK3 method and 120 s time step. Orange lines show the averages of the four months (January, April, July, and October) and both years (2014 and 2015). Gray lines show error limits based on diffusion.

For the studies of Heng et al. (2016) and Hoffmann et al. (2016) we refer to the 2016 interim report.

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