DKRZ – project 617
Atmospheric chemistry process modelling (new developments)

S. Brinkop[1], V. Grewe[1], P. Jöckel[1], A. Kerkweg[2]

[1]Institute for Atmospheric Physics, DLR, Oberpfaffenhofen
[2] Institute for Atmospheric Physics, University of Mainz

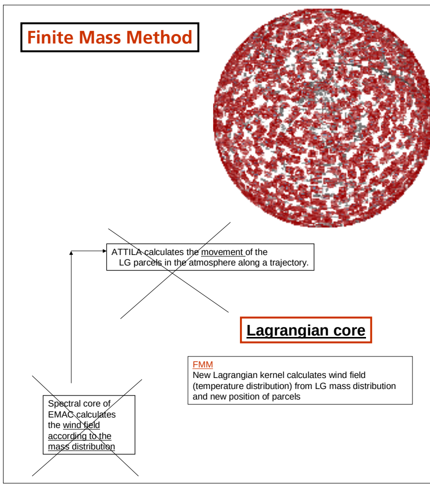
617 is a DKRZ project which develops new concepts for modelling atmospheric chemistry.

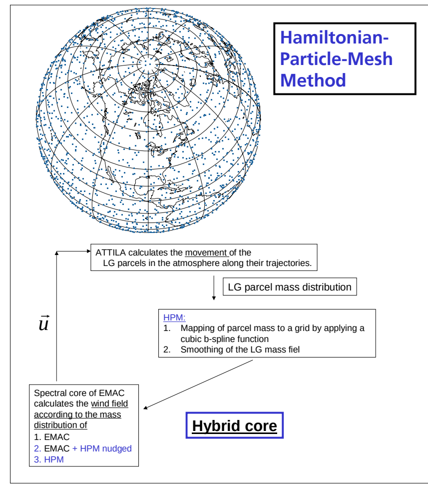
Development of a Lagrangian dynamical core

Two appropriate methods are developed and tested according to their applicability. The **Finite Mass method** (Yserentant, 1997) and the **Hamiltonian Particle Mesh method** (Frank and Reich, 2004) should be extended to be applicable on the sphere and subsequently be tested in EMAC/ATTILA (ECHAM5/MESSy, Jöckel et al., 2013). ATTILA being the Lagrangian tracer transport model (Reithmeier and Sausen, 2002).

The **Finite Mass Method** divides the mass of the atmosphere into small mass packets. These mass packets move under the influence of internal and external forces and the law of thermodynamics and adopt their shape, volume and orientation in space to the local flow behaviour.

In the **Hamiltonian-Particle Mesh** method the Lagrangian parcels remain centroids without extension and are mapped to a mesh. The transfer of information between grid and parcels is realized by cubic splines.



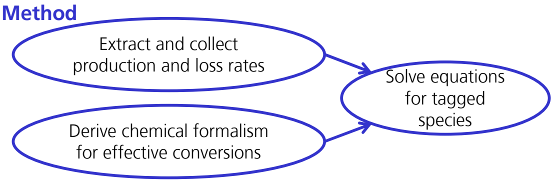


Ozone-chemistry diagnostics: Tagging

Objective

The atmospheric ozone concentration is determined by emissions of precursors, like nitrogen oxides (NO_x) and non-methane-hydrocarbons (NMHC), stratospheric ozone production, chemical loss and dry deposition on the ground. The ozone diagnostic, called **tagging**, is an **accounting mechanism**, which follows the reaction pathways and **attributes ozone concentrations to various sources like, stratospheric production, lightning, traffic, biomass burning, industry, etc.**

Method



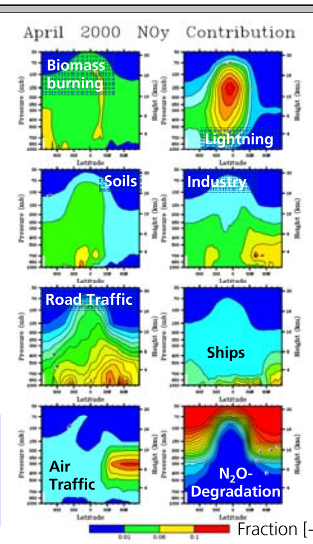
Results:

The figure shows the contribution of ten different sources of nitrogen oxides (NO_y) to its concentration. Lightning and biomass burning have a large contribution in the tropics, however at different altitudes.

The air traffic contribution is basically located at the respective flight levels on the Northern Hemisphere. Nitrogen oxides in the stratosphere are produced by degradation of nitrous oxide (N_2O). The contribution from ship emissions are mostly confined to the marine boundary layer.

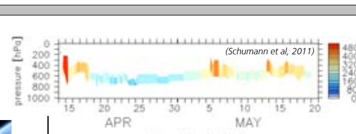
Next Steps:

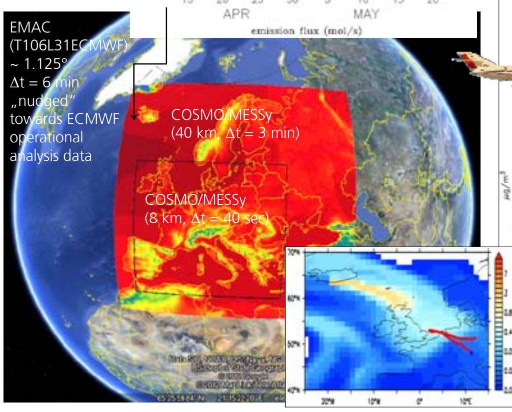
The tagging scheme has been implemented for NO_y, PAN, NMHC, CO, O_3, OH and HO_2. The results are currently verified.



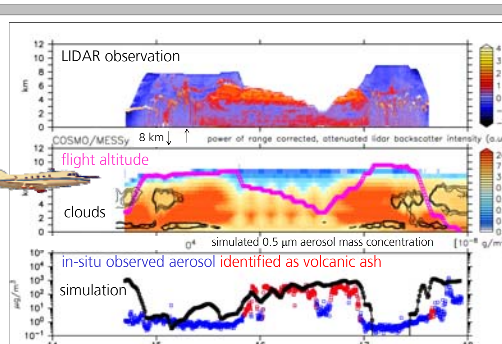
Campaign supporting modelling

One way to regionally increase the model resolution is by nesting a limited area model into a global model or into a coarser resolved limited area model. In MECO(n) (**ME**SSy-fied **EC**HAM and **CO**SMO models nested **n**-times) an arbitrary number of COSMO/MESSy (*Kerkweg & Jöckel, 2012a*) instances can be nested **on-line** into the global ECHAM/MESSy Atmospheric Chemistry (EMAC, Jöckel et al., 2010) model and/or into each other. **On-line** means that the different model instances communicate (so far **one-way**) via the message passing interface (MPI) based Multi-Model-Driver (MMD, *Kerkweg & Jöckel, 2012b*) during run-time. After successful meteorological evaluation (*Hofmann et al., 2012*), the tracer transport as prerequisite for a full atmospheric chemistry evaluation, is evaluated by simulating the Eyjafjallajokull eruption plume in 2010.





0.5 µm aerosol column density [mg/m²]



Above: Inter-comparison of LIDAR (top) and in-situ (bottom) observations with the simulated (COSMO/MESSy , innermost instance) ash cloud (0.5 µm aerosol). The purple line shows the flight altitude of the DLR-Falcon (D-CMET).

Left: 0.5 µm aerosol column density simulated by the 2nd COSMO/MESSy instance (~ 8km resolution); the red line shows the flight path of the DLR-Falcon (D-CMET).

References:
- Jöckel et al., Geosc. Model Dev., 2010
- Kerkweg & Jöckel, Geosc. Model Dev., 2012a, b
- Hofmann et al., Geosc. Model Dev., 2012
- Schumann et al., Atmos. Chem. Phys., 2011