The new model system ICON-MUSCAT – first European air quality simulations

**BERND HEINOLD, OSWALD KNOTH, JENS STOLL, RALF WOLKE,
CHRISTA ENGLER, BIRGIT HEINRICH, JACOB SCHACHT, WOLFRAM SCHRÖDER,
THOMAS STÖTER[#]**

Leibniz Institute for Tropospheric Research (TROPOS), Leipzig, Germany
 # Now at Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany

COSMO / CLM / ICON / ART User Seminar 2017
March 2017 **|** *DWD, Offenbach, Germany*

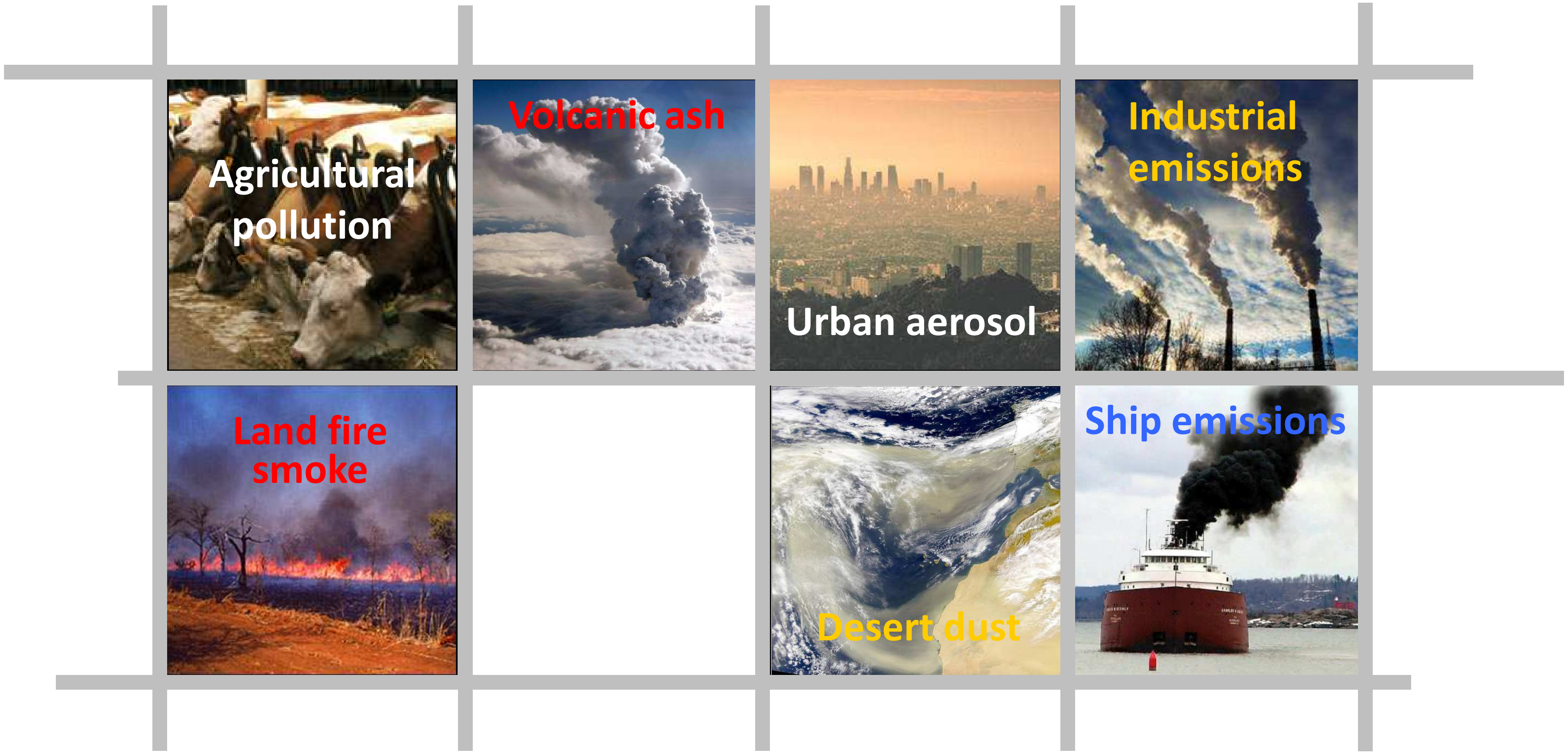
Member of the Leibniz Association

TROPOS
Leibniz Institute for Tropospheric Research

Motivation

- Air pollutants from local sources and long-range transport seriously affect the local climate, the ecosystem and human health.

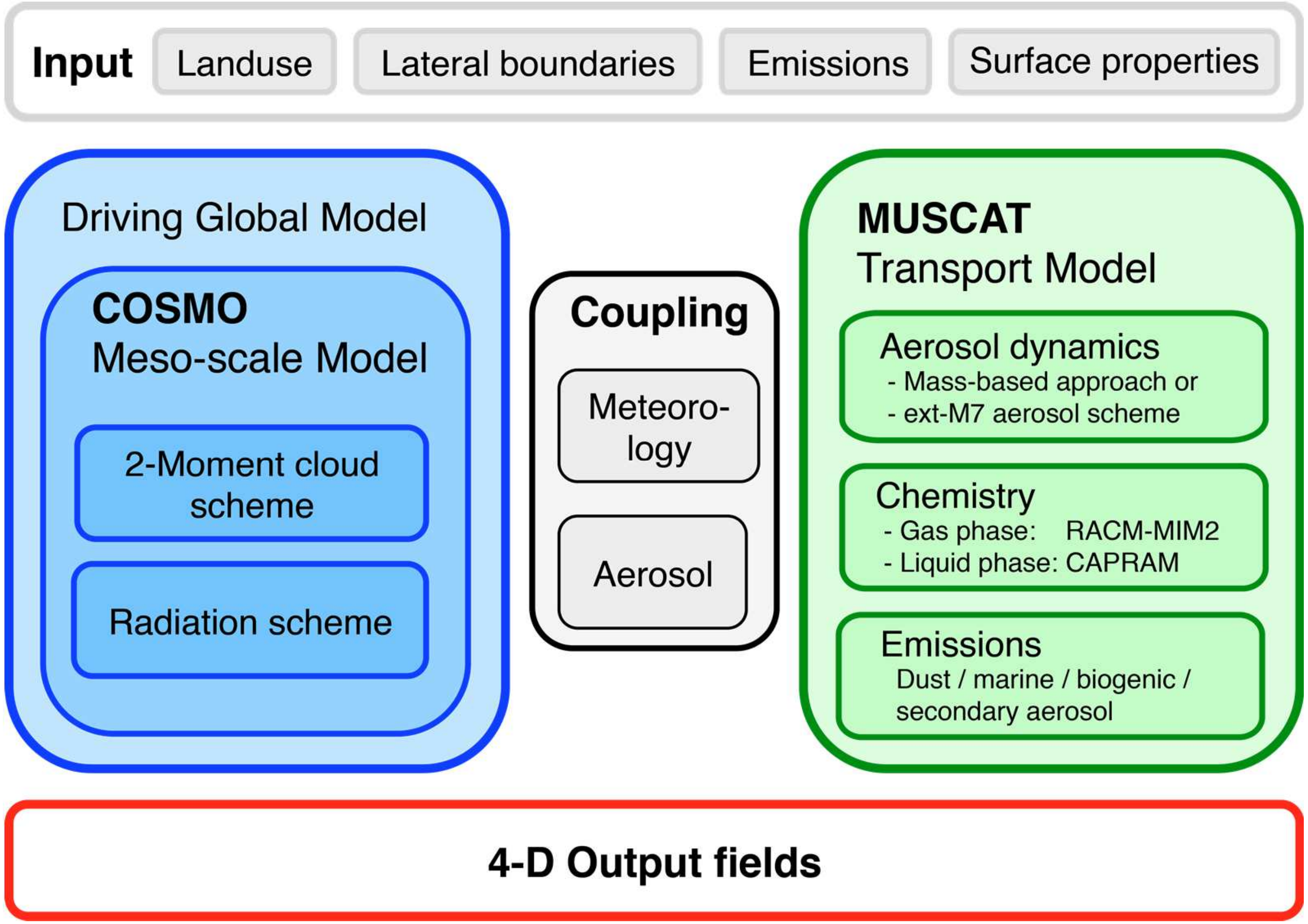
- 3D aerosol-chemistry modeling can help understanding the complex multiphase atmospheric processes involved.



Outline

- Motivation
- The multiscale aerosol-chemistry transport model MUSCAT
- Coupling of ICON and MUSCAT
- First air quality simulations – Melpitz Column 2015
- Summary and Outlook

Model system COSMO-MUSCAT



Wolke et al., 2012

Model system COSMO-MUSCAT

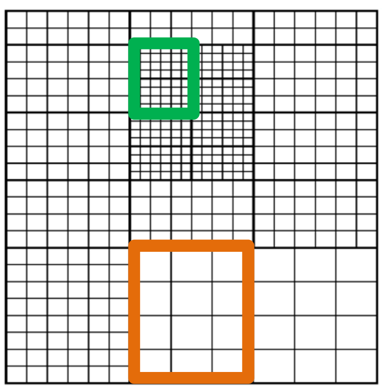
- **Chemistry ("read in")**
  - Gas phase: RACM (Stockwell et al., 1997) + MIM2 (Taraborelli et al., 2009)
  - Aqueous phase: CAPRAM
- **Aerosol model**
  - Mass-based approach (similar to EMEP) OR
  - Modal scheme M7 (Vignati et al., 2004) extended by nitrate and ammonium and SIA by ISORROPIA I (Nenes et al., 1998)
  - Dust: sectional, 5 size bins (Tegen et al., 2002; Heinold et al., 2011)
- **Dry and wet deposition, sedimentation**
- **SOA scheme:** Modified SORGAM (Schell et al., 2001; Li et al., 2013)
- **Emissions**
  - Anthropogenic (11 snaps, area + point, land fires)
  - Biogenic (Steinbrecher et al., 2009)
  - Sea salt (Sofiev et al., 2013)

Numerical approaches in MUSCAT

- **Spatial discretization**
  - Staggered grid, Finite-volume techniques
  - Advection: **Third-order upwind scheme**

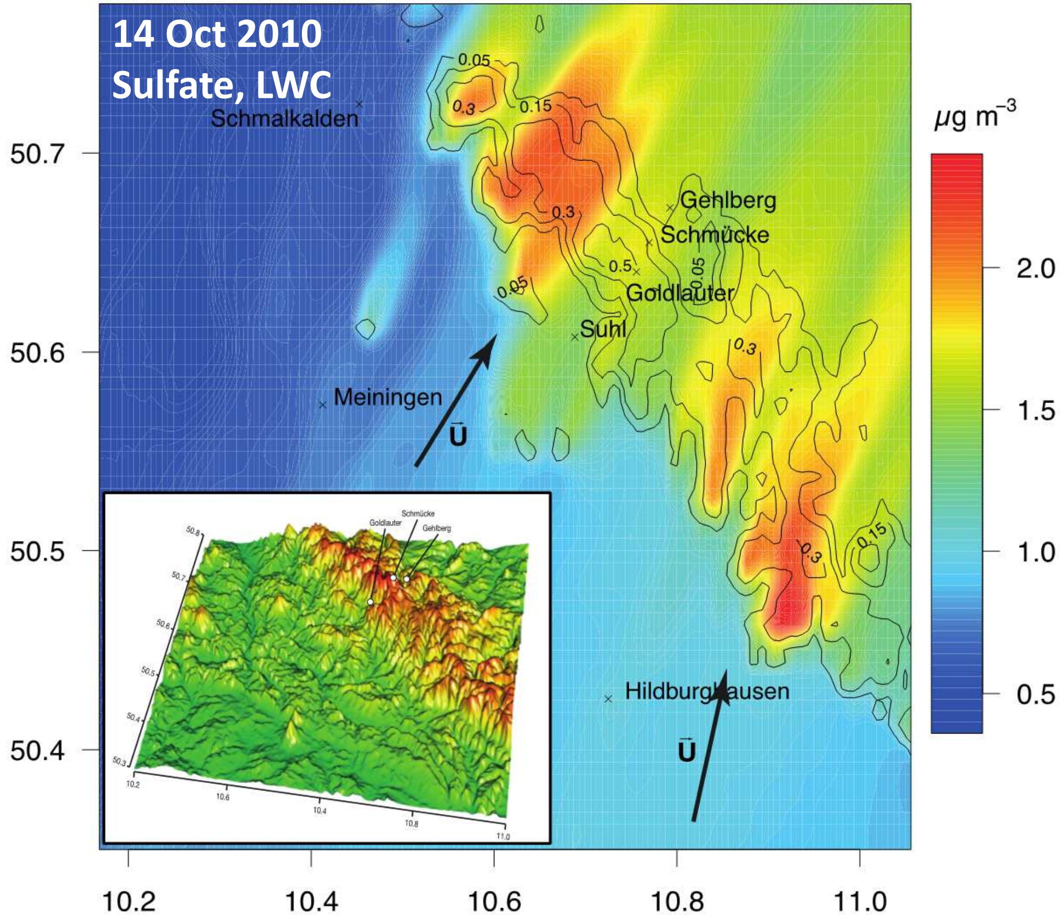
- **Time integration: IMEX scheme**
  - Explicit second-order Runge-Kutta for horizontal advection
  - Second order BDF method for the rest: **Jacobian is calculated explicitly**, linear system by Gauss-Seidel iterations
  - Automatic time-step control

- **Parallelization**
  - **Domain decomposition**
  - **Dynamical load-balancing** by redistribution of blocks



Hill Cap Cloud Thuringia 2010 (HCCT-2010)

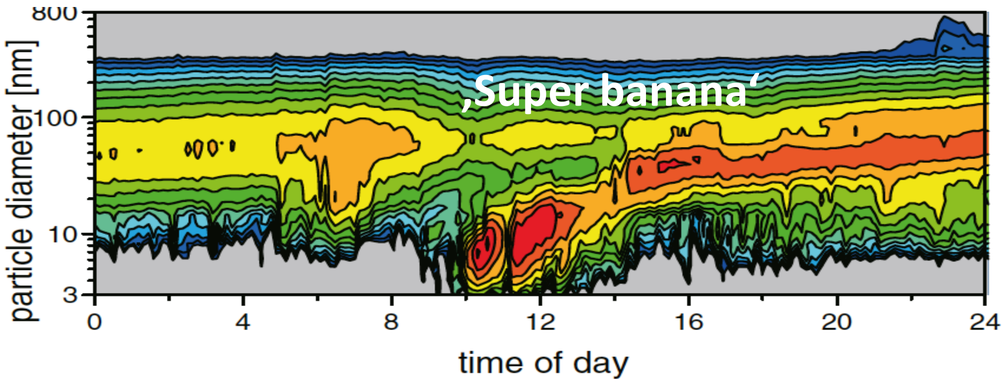
A ground-based integrated study of chemical aerosol-cloud interaction

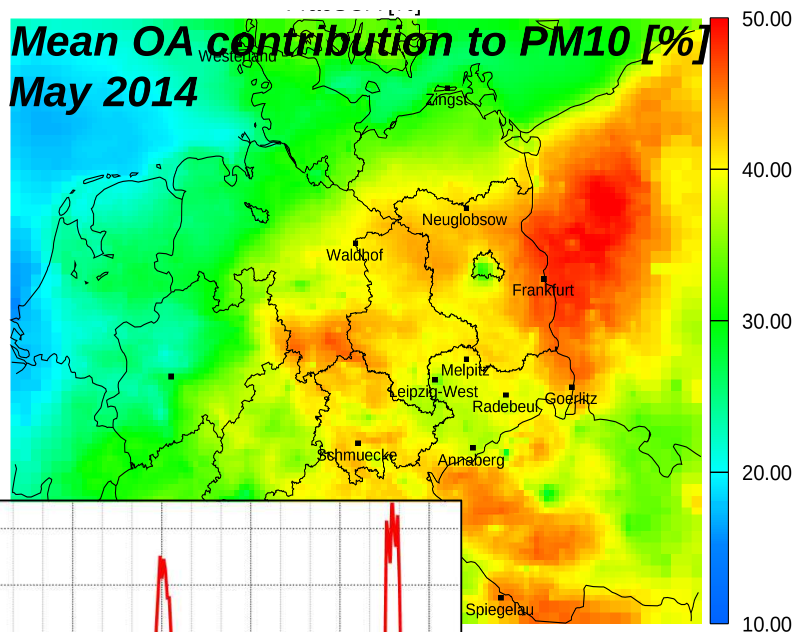


- 3-site ground-based **Langrangian experiment at Mt. Schmücke**, Germany, to study physico-chemical **multiphase processing of aerosol** particles during orographic cloud events; focus on organic particles and gas phase oxidants.

3D modelling of SOA formation

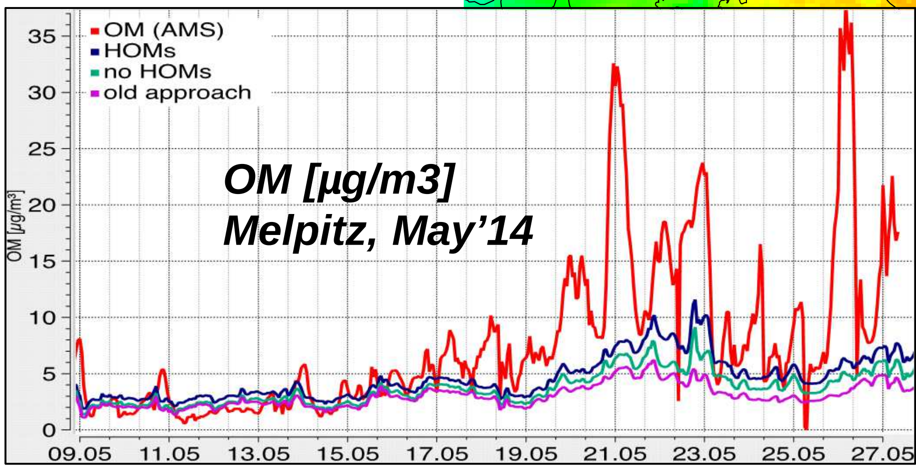
Towards a better representation of secondary particle formation





‚Super bananas‘

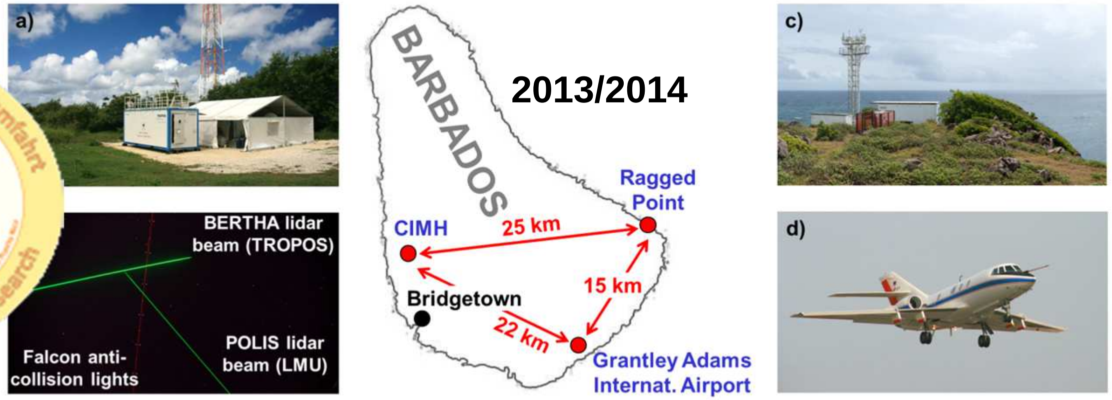
Major particle formation events as observed, e.g., in Melpitz in Jun 2013/ May 2014

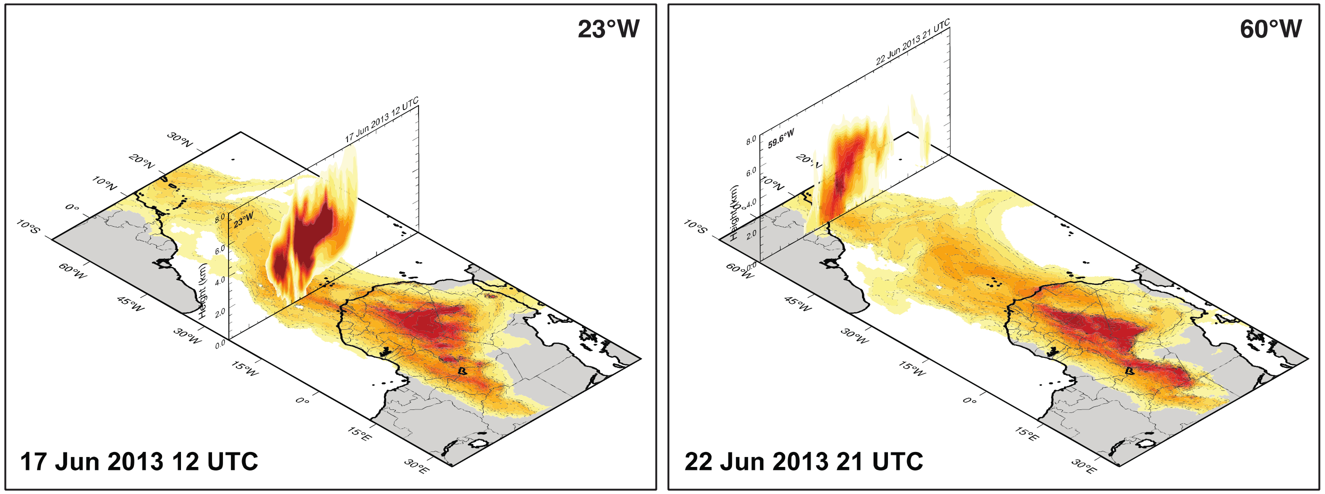


- Investigating different ways to improve the model representation of SOA formation; evaluation against timely highly resolved measurements.

SALTRACE (www.pa.op.dlr.de/saltrace)

Saharan Aerosol Long-range Transport & Aerosol-Cloud-Interaction Experiment





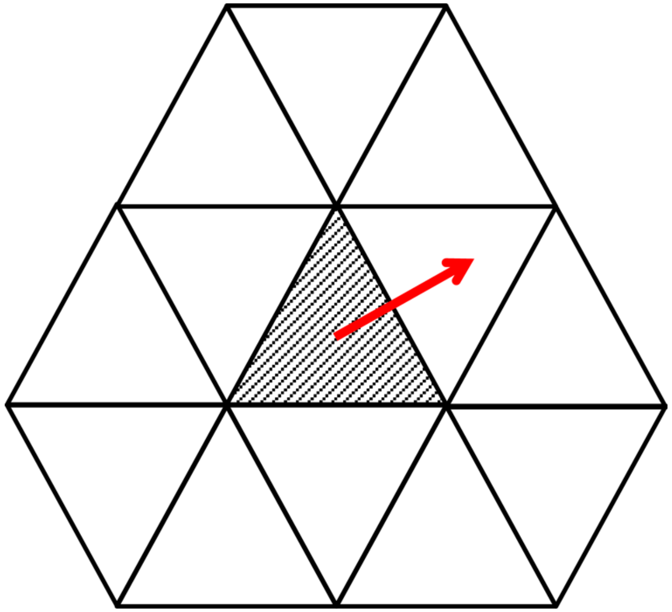
- German initiative to study the **long-range transport of Saharan dust** into the Caribbean focusing on **particle aging**, mixing, and **removal processes**, as well as **aerosol-cloud-radiation interactions**.

Online coupling of ICON and MUSCAT

- Additional Eulerian transport scheme
- Advection scheme “third-order upwind”
- Runge-Kutta IMEX scheme: horizontal transport explicitly, vertical transport and chemistry implicitly
- #ifdef MUSCAT compiler directives in ICON subroutines
- Separate MUSCAT subdirectory
- ICON-style namelist for MUSCAT

```
&MUSCAT_nml
 MUSCAT                  = .true.
 MUSCAT_lvadv_tracer     = .true.
 MUSCAT_lhadv_tracer     = .true.
 MUSCAT_Chemie= 1
 MUSCAT_dust             = 0
 MUSCAT_drydep           = 1
 MUSCAT_wetdep= 1
 MUSCAT_areaemiss        = 1
 MUSCAT_pointemiss       = 0
 MUSCAT_input_name       = "maccIcon"
 MUSCAT_aemiss_file      = "muscatICONEmiss.nc“
 MUSCAT_latbc            = 1
 MUSCAT_dt_latbc         = 10800
/
```

Advection scheme



- Polynomial interpolation, different stencils
- Outgoing flux from corresponding edge value
- Realized with tools from ICON
- Other stencils possible

TROPOS

IMEX time integration scheme

$$c' = f_E(t,c) + f_I(t,c)$$

where $f_E(t,c)$ represents the horizontal advection and $f_I(t,c)$ includes the vertical transport processes and the chemistry.

IMEX–Heun2

$$Y_1 = c(t_n)$$

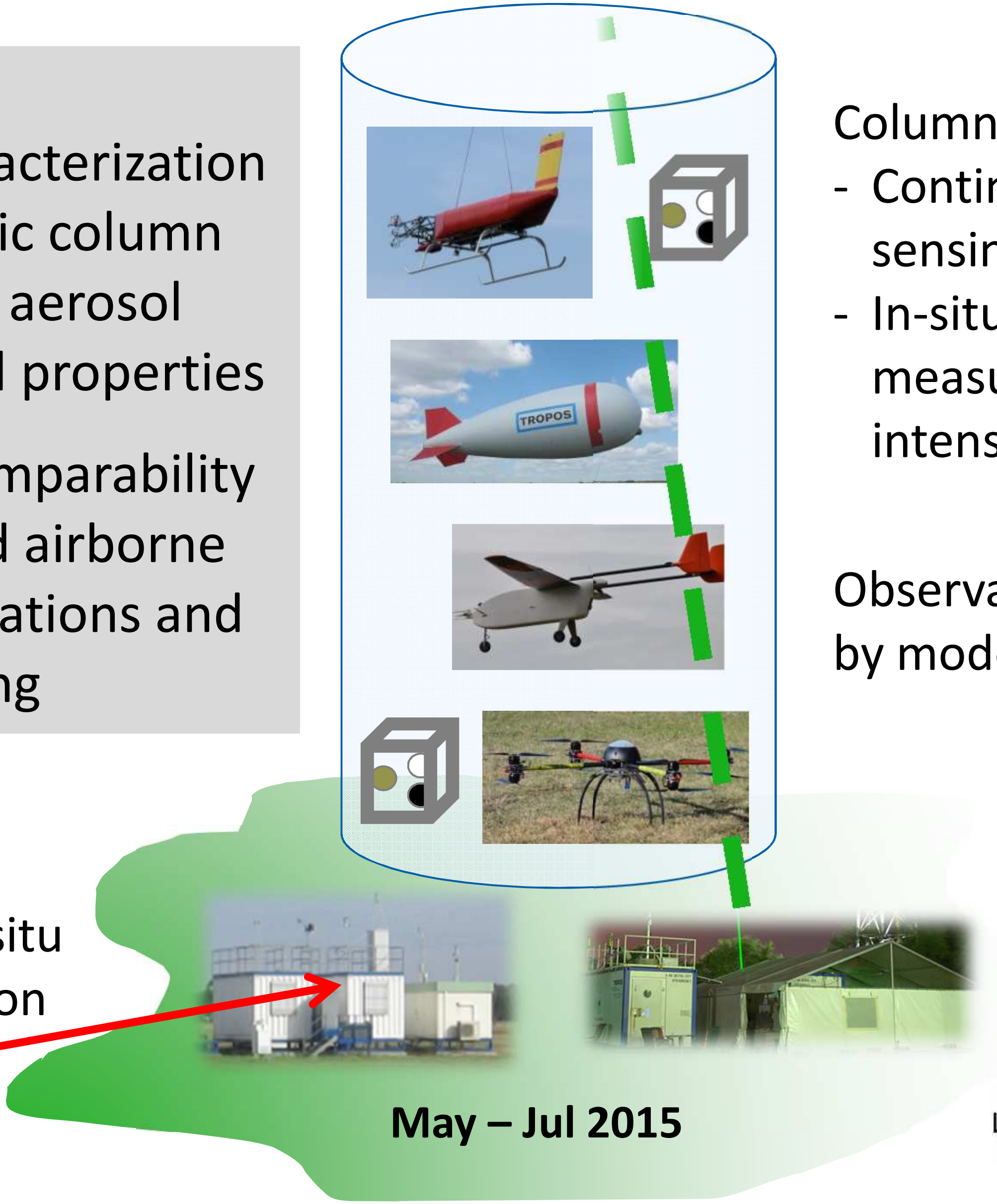
$$\begin{aligned} Y_2 &= Z_2(h_E) \quad \text{with} \\ &\frac{dZ_2}{d\tau} = f_E(t_n, Y_1) + f_I(t_n+\tau, Z_2), \quad \tau \in [0, h_E], \quad Z_2(0) = Y_1, \end{aligned}$$

$$Y_3 = \frac{h_E}{2}\left(f_E(t_n+h_E, Y_2) - f_E(t_n, Y_1)\right) + Y_2,$$

IMEX–RK2

Test case – Melpitz Column Experiment

Goals:
- Detailed characterization of atmospheric column with focus on aerosol and its optical properties
- Evaluating comparability of ground and airborne in-situ observations and remote sensing



Column:
- Continuously by remote sensing (lidar, radar...)
- In-situ airborne measurements during intensive periods

Observations completed by modelling studies

Very detailed in-situ characterization on ground

TROPOS
Leibniz Institute for Tropospheric Research

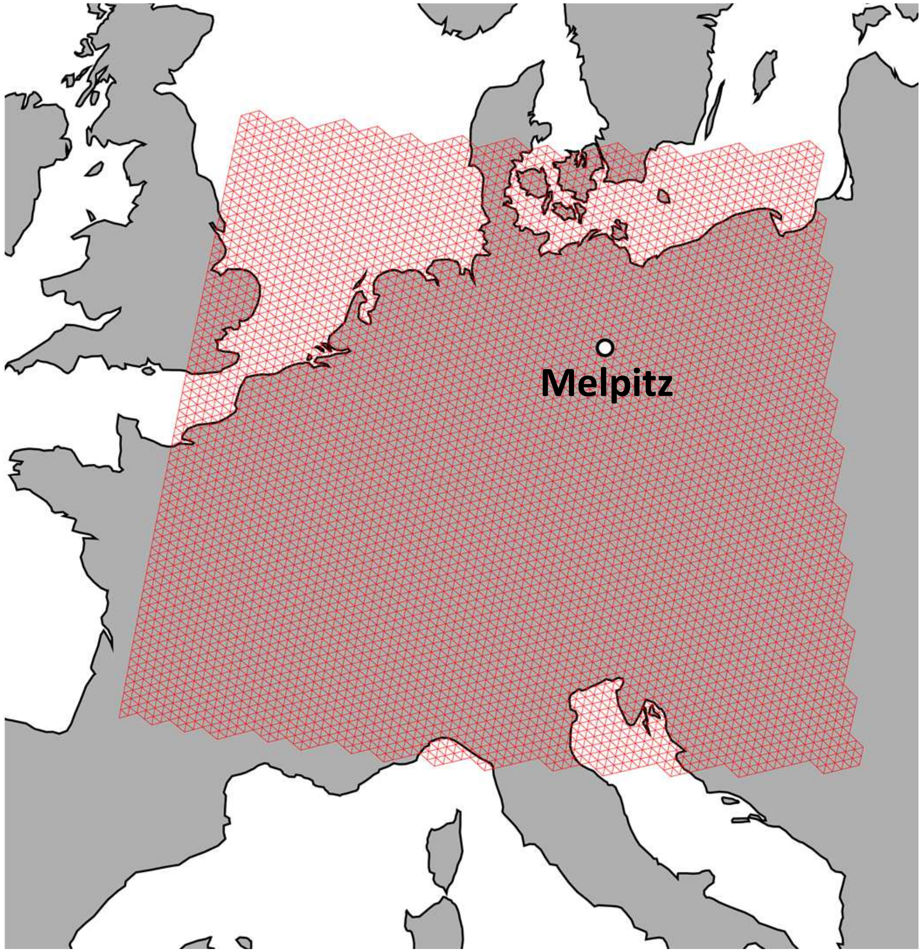
Melpitz Column

Intensive field campaign: May – Jul 2015, follow-up campaign in Jan/Feb 2017

Melpitz

- TROPOS' rural background site 40 km NE of Leipzig, member of ACTRIS network
- Long-term (> 20 yr) physico-chemical aerosol characterization, including analysis for ions, OC/EC and specific organics

Model setup – Melpitz Column 2015



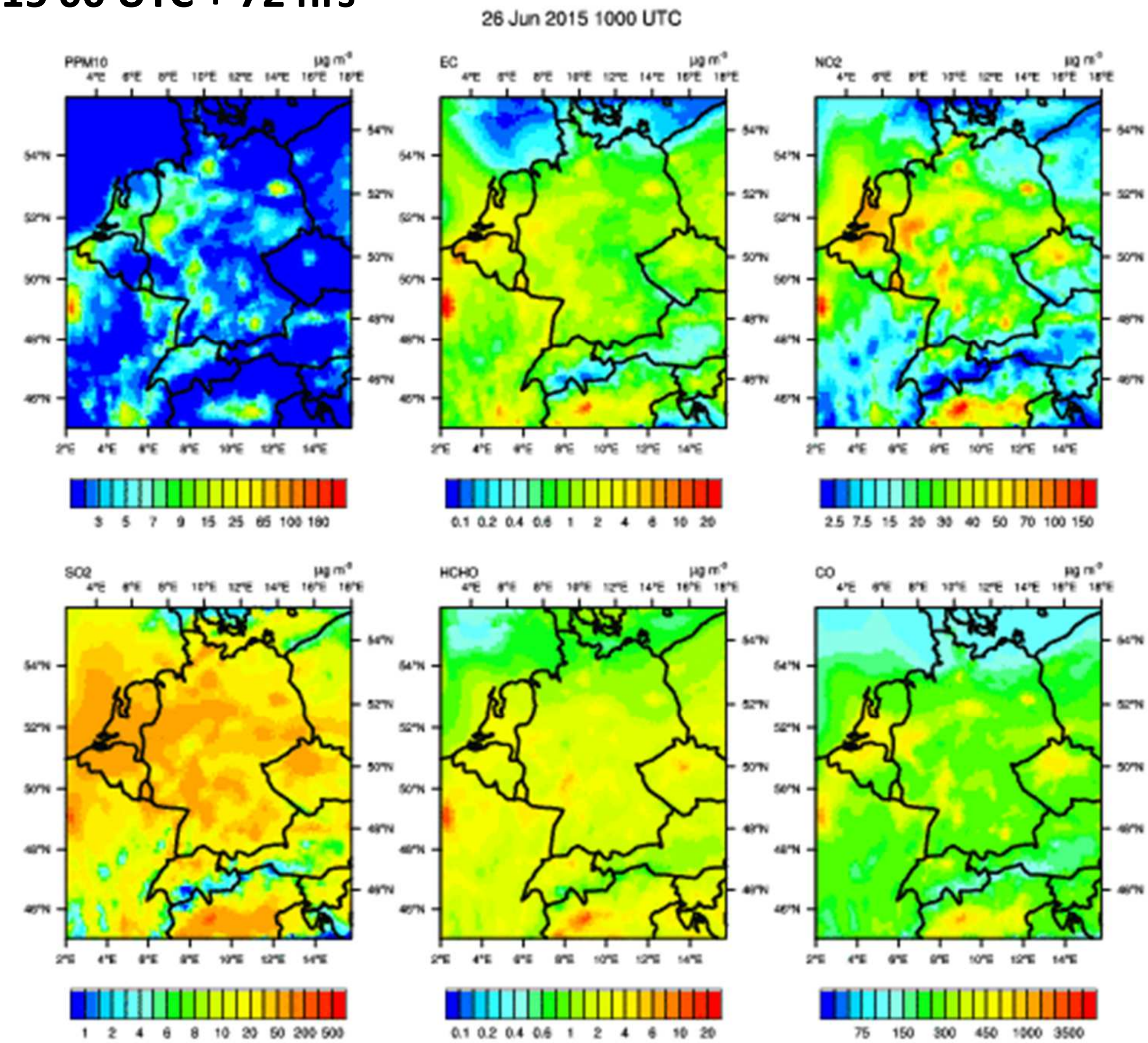
- Meteorology: ICON nwp-2.0.15
- Transport scheme MUSCAT
- Horizontal grid: R3B07 (13 km), 60 vertical layers
- Initial / boundary conditions: ECMWF-IFS, MACC
- Emission inventory: MACC 2009 (7.5 km) / IIASA 2010 (30km)
- Chemistry: RACM-MIM2 (99 gas species, 274 reactions)

Period of interest:

1st May – 15th Jul 2015

First ICON-MUSCAT results

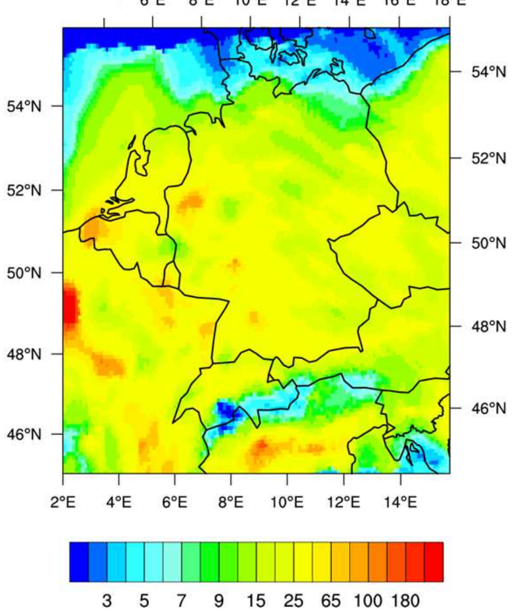
26 Jun 2015 00 UTC + 72 hrs

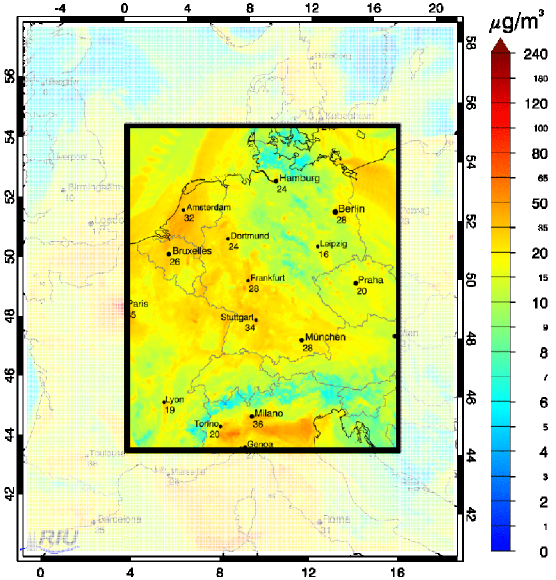


ICON-MUSCAT vs. EURAD forecast

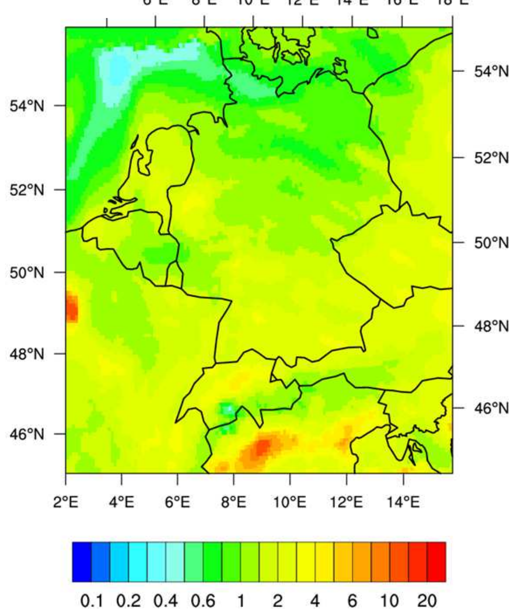
Surface level
28 Jun 2015

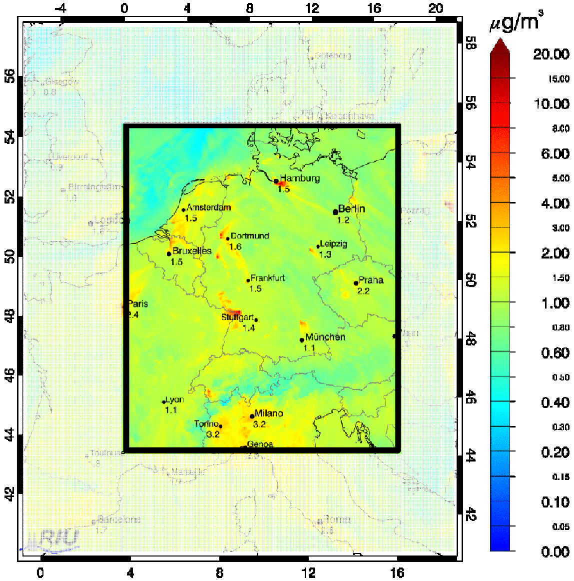
PM10



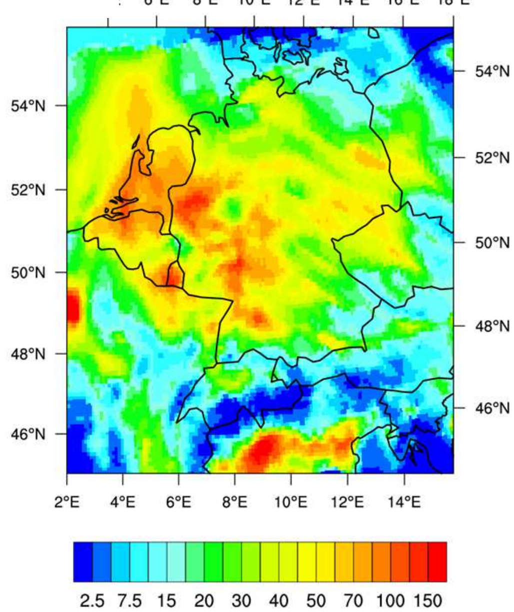


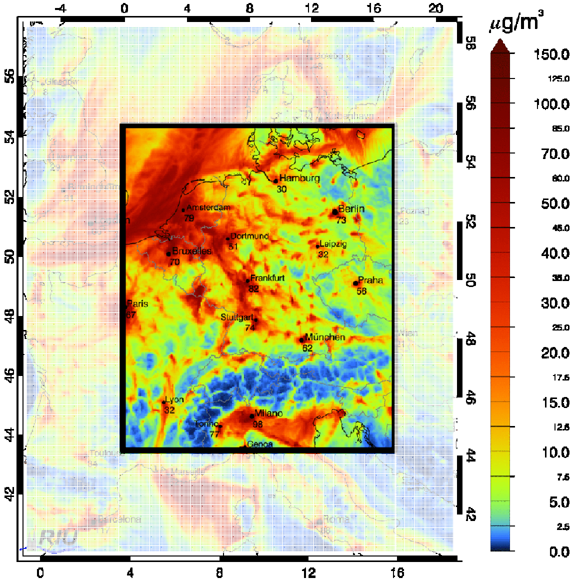
HCHO



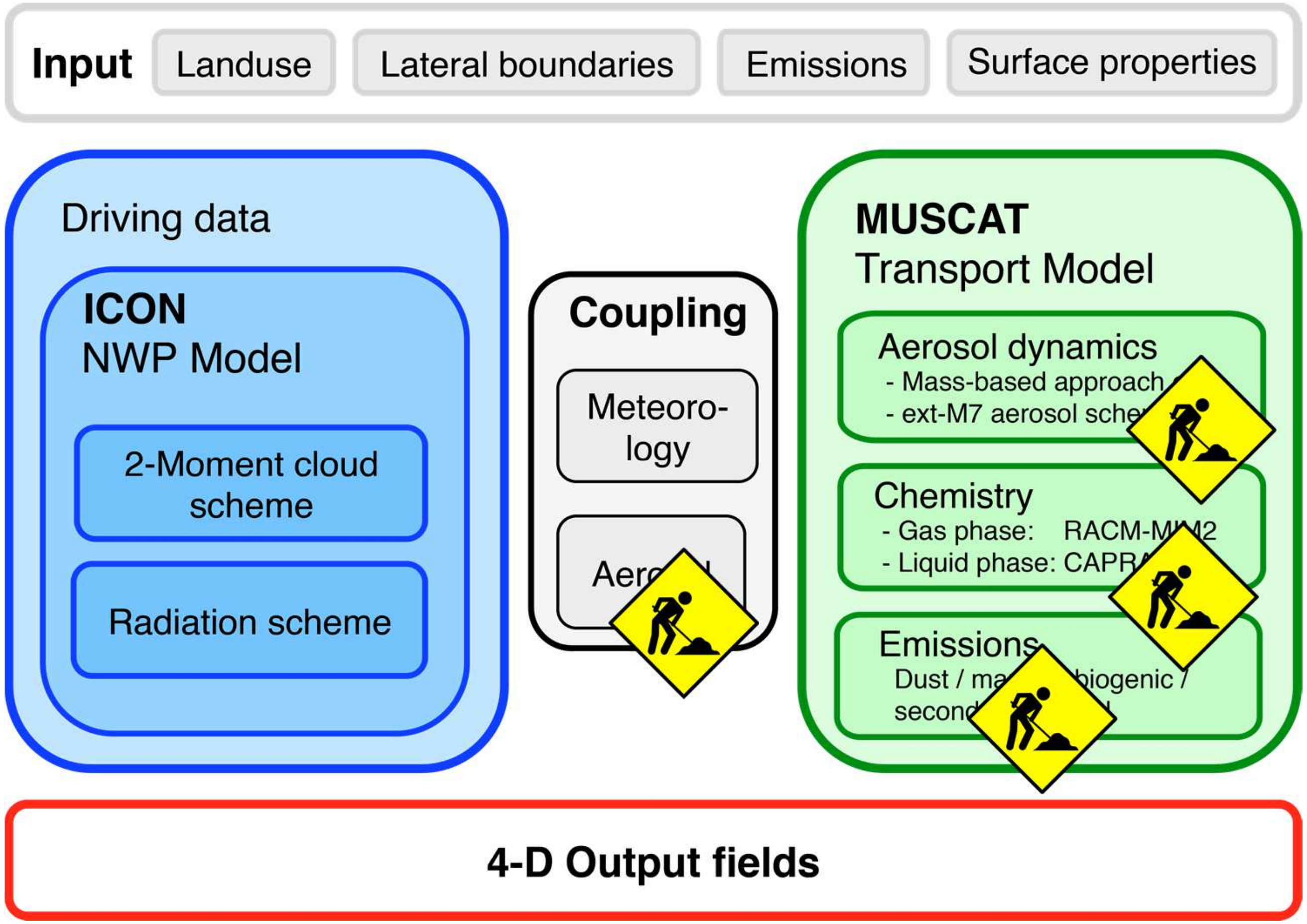


NO2





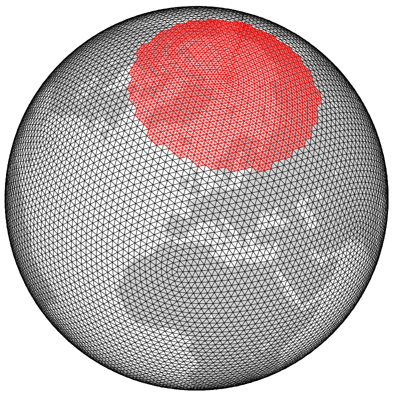
Summary



- The aerosol-chemistry-transport code has been coupled to the ICON model.
- First air pollution simulations demonstrate the principle functionality of the new model system.

Next steps and plans for the future

- Complete functionality of MUSCAT model
  - Automatic time-step control
  - Biogenic and marine aerosol emissions and secondary aerosol formation
  - Aerosol feedback on radiation and cloud microphysics in ICON
  - Nesting capability
- Intensive testing, including comparisons to observations and COSMO-MUSCAT simulations
- Global & Arctic-focused aerosol simulations within the DFG-Transregio (AC)³ – **ArctiC Amplification: Climate Relevant Atmospheric and SurfaCe and Feedback Mechanisms**



ICON grid with Arctic nest

TROPOS