

# The Mesoscale Air Quality Model System COSMO-MUSCAT

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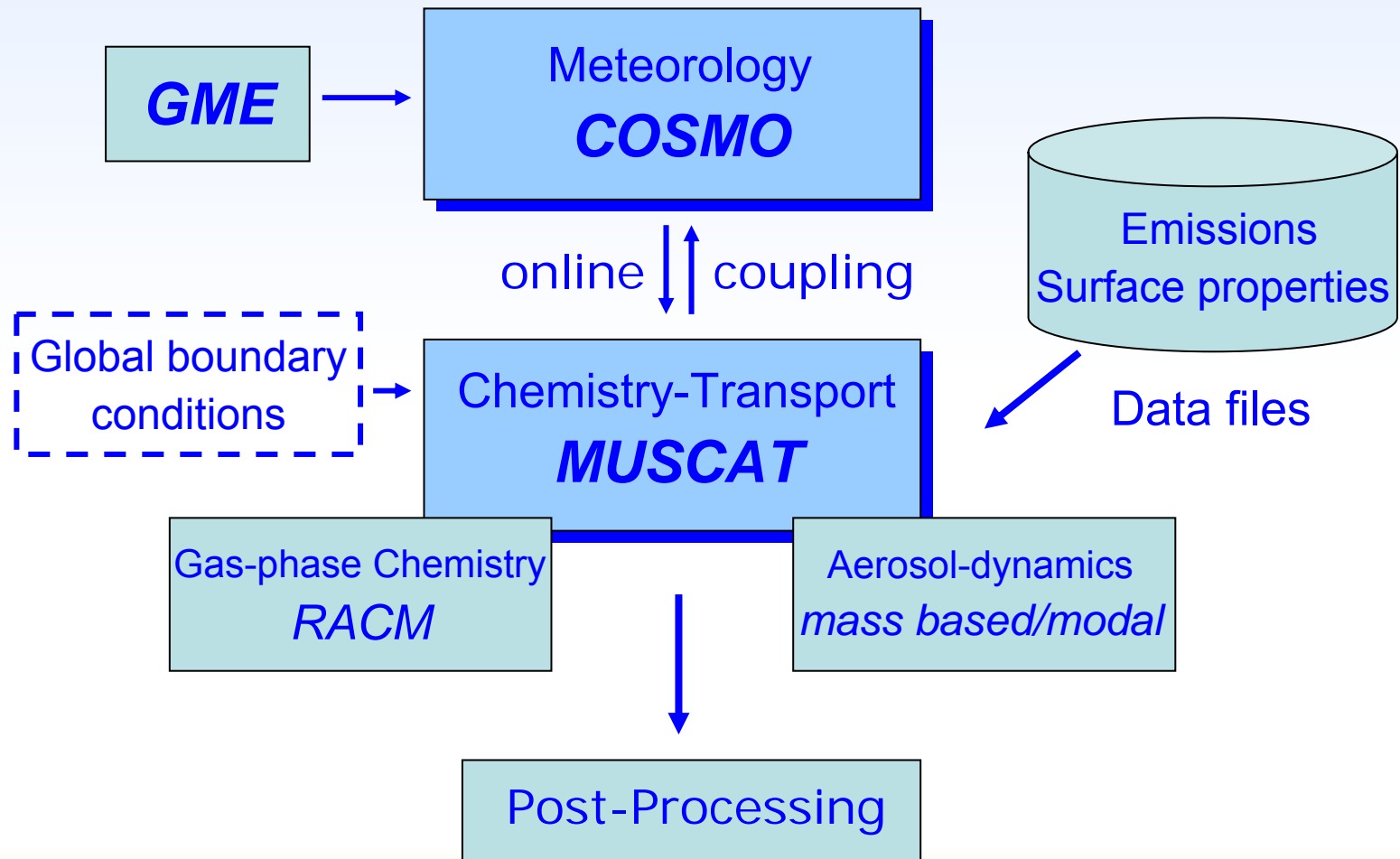
# Motivation

- Continuing interest in atmospheric physico-chemical processes and aerosol dynamics:
  - Air quality monitoring
  - Research on impacts on natural and human environments, feedback mechanisms
- Mesoscale atmospheric chemistry transport models allow insight into these very complex and still poorly understood processes



# Model system COSMO-MUSCAT

MULTIScale Chemistry Aerosol Transport (Wolke et al., '04)



# Gas phase chemistry

- Most applications: RACM-MIM2  
> 70 species, > 200 reactions  
(Stockwell et al., '97; Karl et al, '06)
- Reaction mechanism from  
input file: **High flexibility**
- **Currently, no cloud chemistry**

## Example of a Chemistry Input-File

```
#----- Bsp.sys -----  
#  
#-----  
#--- GAS PHASE  
#-----  
#  
CLASS: GAS  
NO2 - O3PX + NO  
PHOTABC: A: 7.67e-03 B: 1.773179e-00 C: 0.77233e-00  
  
CLASS: GAS  
O3PX + NO - NO2  
TROE: KO: 9e-32 N: 1.5 KINF: 3e-11 M: 0  
  
CLASS: GAS  
O3PX + NO2 - NO + [O2]  
TEMP1: A: 6.50E-12 E/R -120.0  
  
CLASS: GAS  
O1D + [H2O] - HO + HO  
CONST: A: 2.20E-10  
  
CLASS: GAS  
HNO4 - HO2 + NO2  
TROEQ: KO: 1.80E-31 N: 3.2  
KINF: 4.7E-12 M: 1.4 KO: 2.1E-27 B: 10900  
  
CLASS: GAS  
HO2 + HO2 - H2O2  
SPEC4: C1: 2.3E-13 C2: 600 C3: 1.7E-33 C4: 100
```

# Aerosol Model

- Mass-based approach (similar to EMEP model)  
**or**
- Modal model M7 (Vignati et al., '04; Stier et al., '05):
  - 4 internal-mixed and 3 external modes
  - Sulphate, sea salt, dust, EC, OC
- Dry and wet deposition, sedimentation
- Considered components:
  - Sulphate, nitrate, ammonia, EC, POC, dust, sea salt
  - **Only in mass-based approach: SOA** (Schell et al., 2001)
- Wind-blown mineral dust:
  - Sectional, 5 – 8 size bins
- Under progress: “modified M7”:
  - Sulphate, sea salt, dust, EC, OC + **nitrate, ammonia, SOA partitioning**

# Emissions

- Anthropogenic Emissions
  - Area, line and point sources (special: “cooling towers”)
  - Following EMEP/CORINAIR: PM<sub>2.5</sub>, PM<sub>10</sub>, SO<sub>2</sub>, NO<sub>x</sub>, CO, NH<sub>3</sub>, CH<sub>4</sub>, and non-methane volatile organic compounds (NMVOC)
  - Aerosol emissions: Particle number and composition depend on corresponding SNAP (EMEP)
- Dust emission scheme (Tegen et al., '02)
- Land fire emissions using MODIS fire products (Justice et al., '02)
- Biogenic Emissions
  - NO emissions in dependence on vegetation type and surface temperature (Williams et al., '92)
  - VOC emissions additionally depend on sunlight (Günther et al., '93)

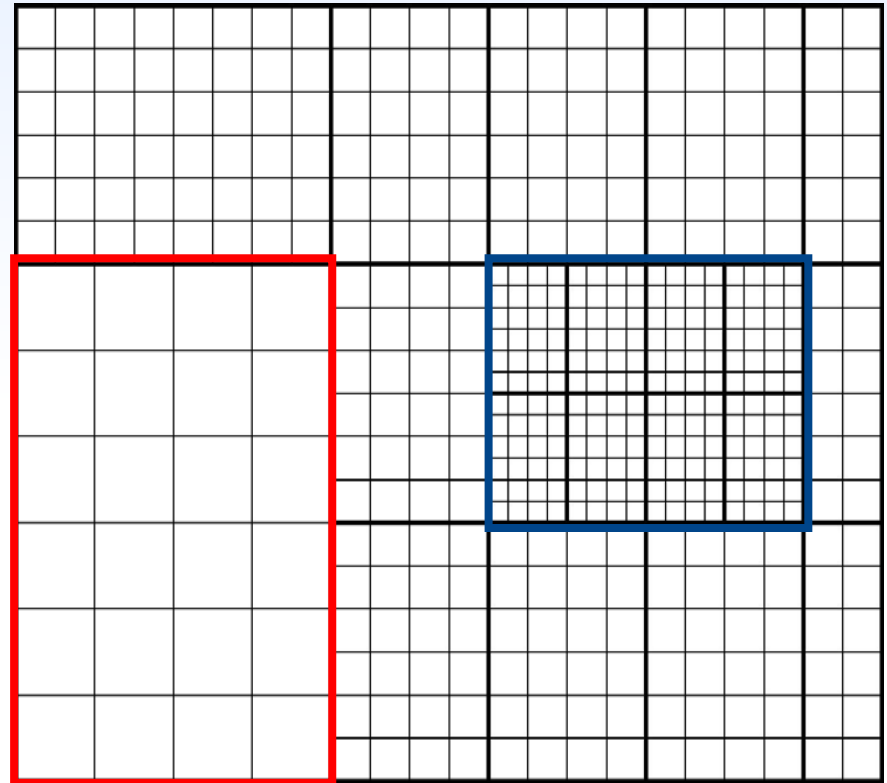
# Numerical methods

- Space discretization
  - Staggered grid, finite-volume techniques
  - Advection: 3<sup>rd</sup>-order upwind scheme (Hundsdoerfer et al., '95)
- Time-integration: IMEX scheme (Knoth & Wolke, '98)
  - Explicit 2<sup>nd</sup>-order Runge-Kutta for horizontal advection
  - 2<sup>nd</sup>-order BDF method for the rest: Jacobian is calculated explicitly, linear systems by Gauss-Seidel iterations or AMF
  - Automatic step size control
    - ➔ different number of steps (load imbalances)
- Parallelization
  - Domain decomposition
  - Dynamical load-balancing by redistribution of blocks

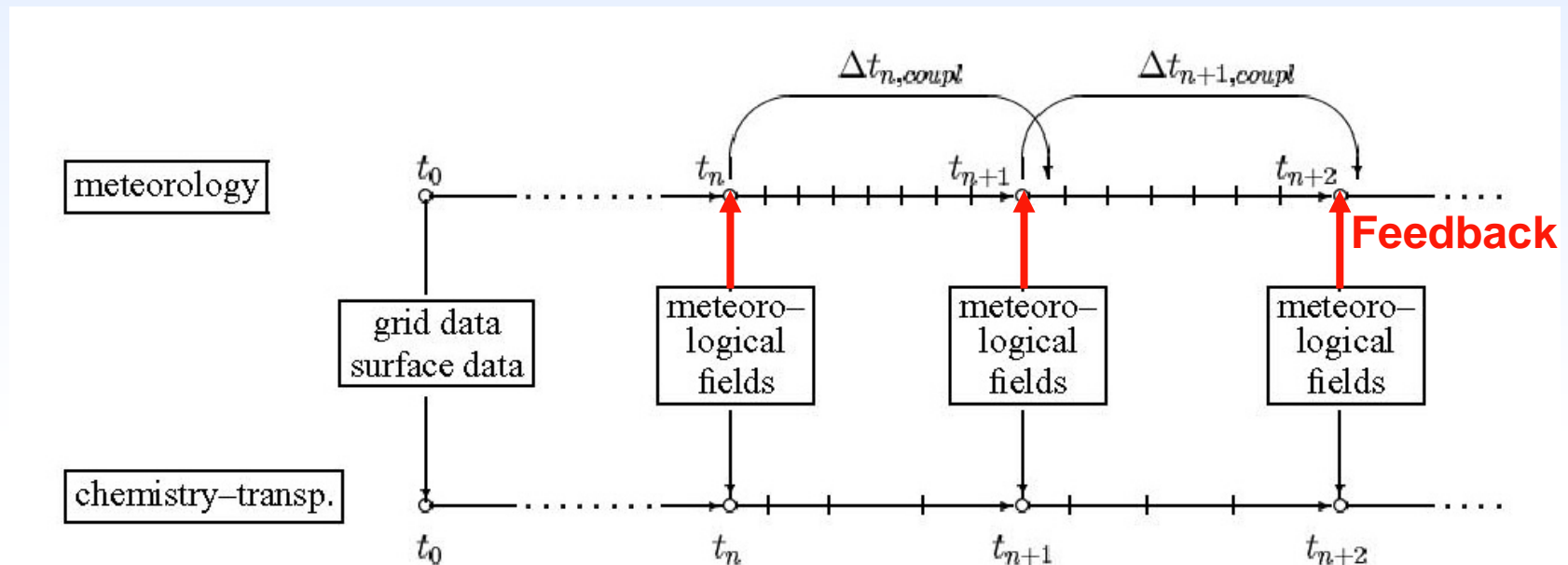
# Horizontal domain decomposition

## Static grid ("multiblock approach")

- From a given rectangular grid (of the meteorological driver)
- Non-overlapping, rectangular subblocks marked for refining or coarsening
- Refinement level between adjacent blocks restricted to 1

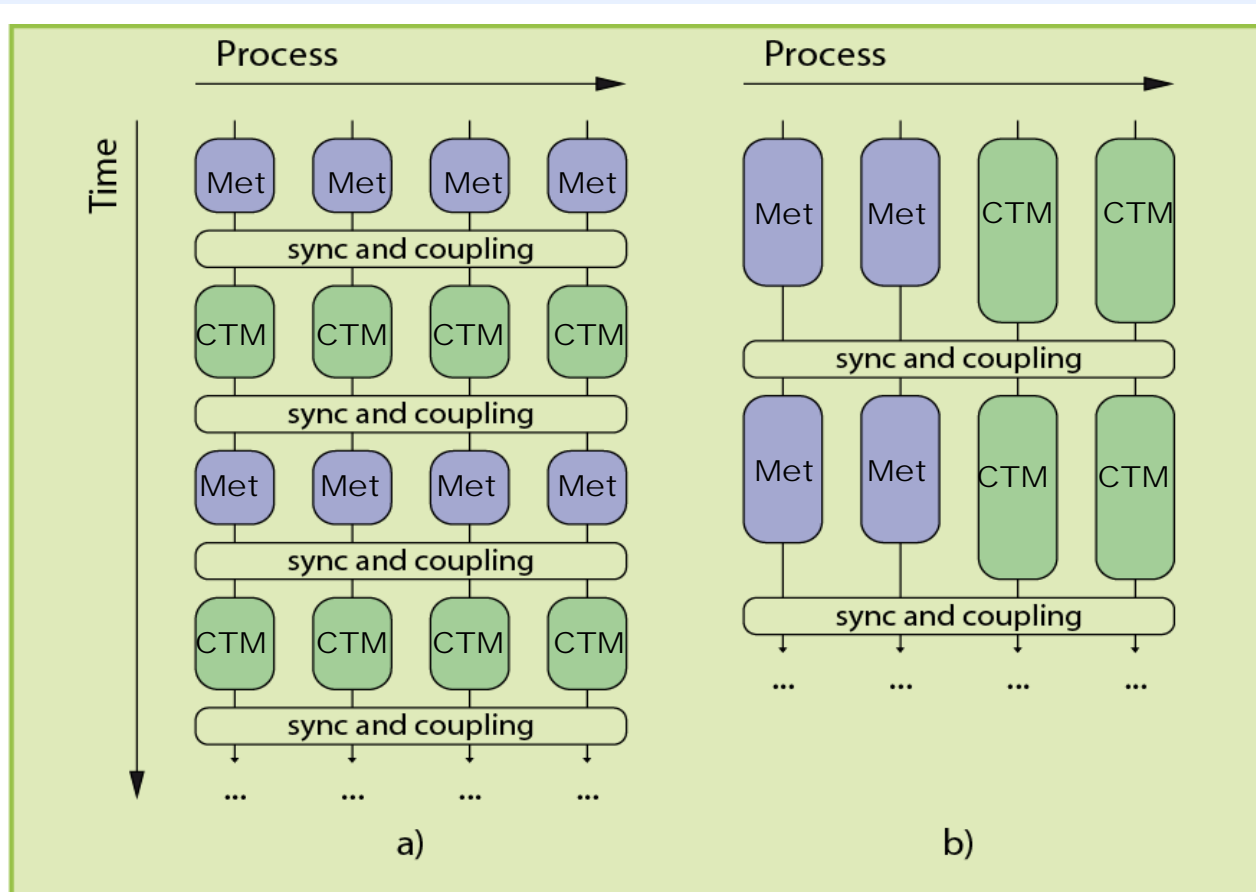


# Coupling scheme (+ feedback to COSMO)



- Time interpolation of the meteorological fields:
  1. Linear interpolated in  $[t_n, t_{n+1}]$ : Temperature, Density, ...
  2. Time-averaged values on  $[t_n, t_{n+1}]$ : Projected wind field
- Separate time step size control for COSMO and MUSCAT

# Coupling strategy



Coupling scheme for model systems: a) sequential, b) concurrent.

(Lieber & Wolke '08)

# Air quality applications

- LfUG Sachsen

Examination of the contribution of two large brown-coal fired power stations in Saxony to the formation of secondary particles (PM<sub>10</sub>)

- UBA

Peaks of number concentrations in urban regions

- LA Niedersachsen

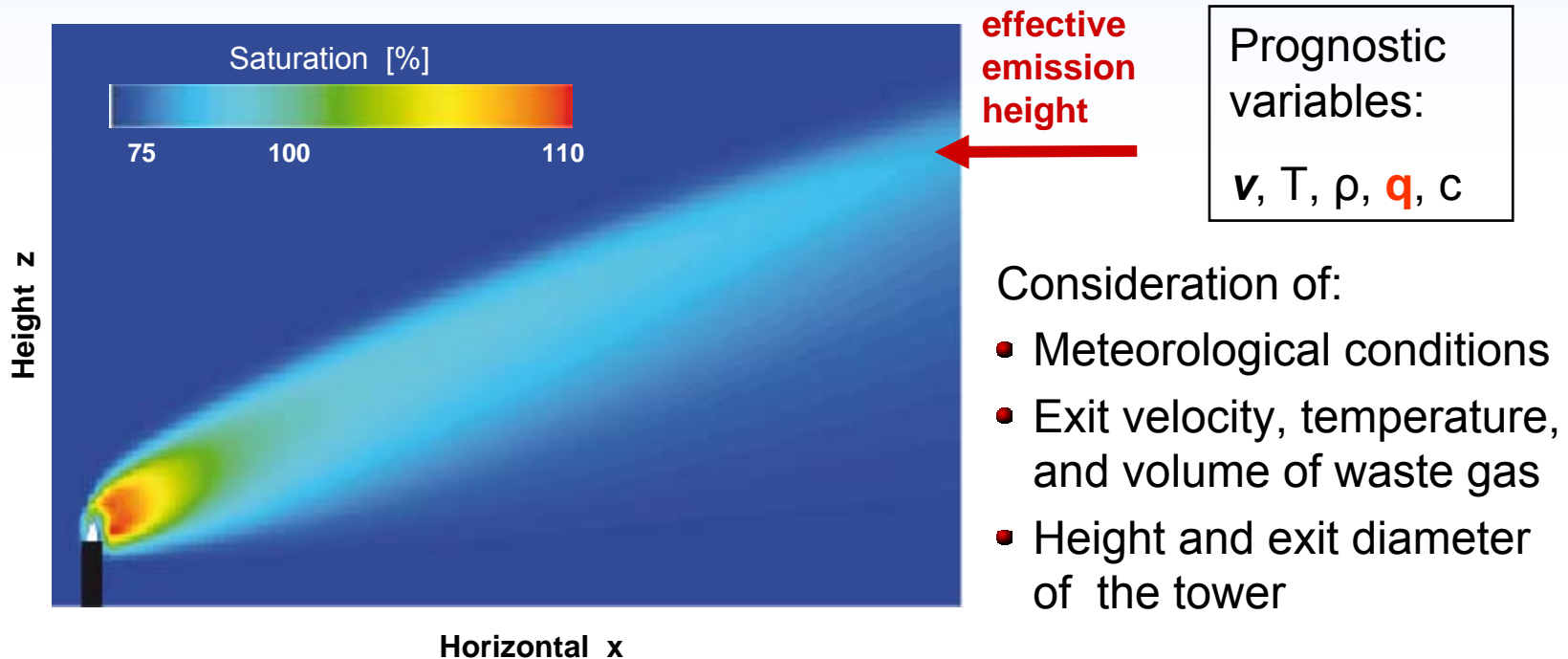
Influence of ammonia emissions on impact of particulate matter



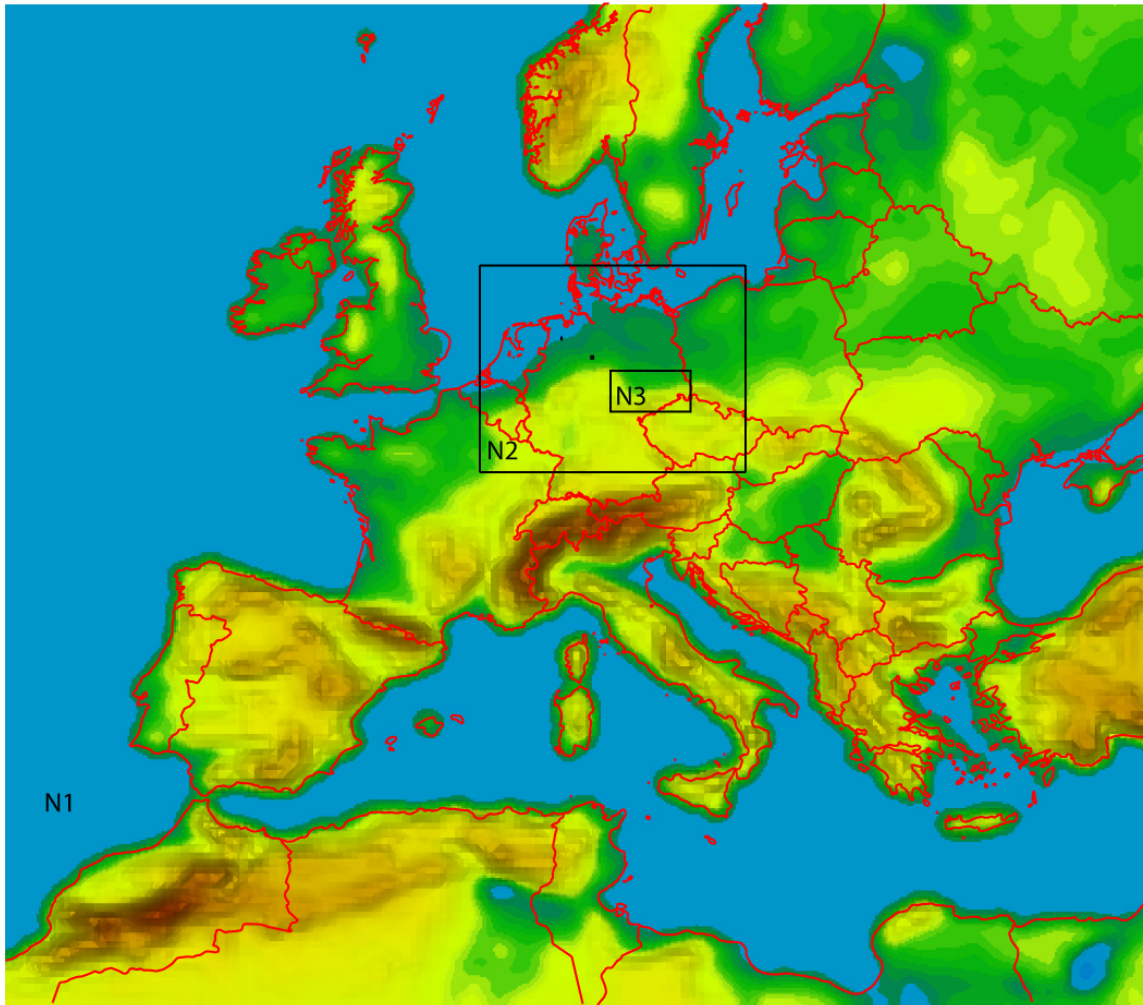
# Cooling tower emissions

Cooling tower model S/P (Schatzmann & Policastro, '84)

- Integral hydro-dynamical model, based on PDE of fluid dynamics
- Conservation of mass, momentum, energy, **water**, and inert pollutants



# LM grid nesting



## Grid resolution:

N1: 16 km x 16 km  
40 vertical layers

N2: 8 km x 8 km  
50 vertical layers

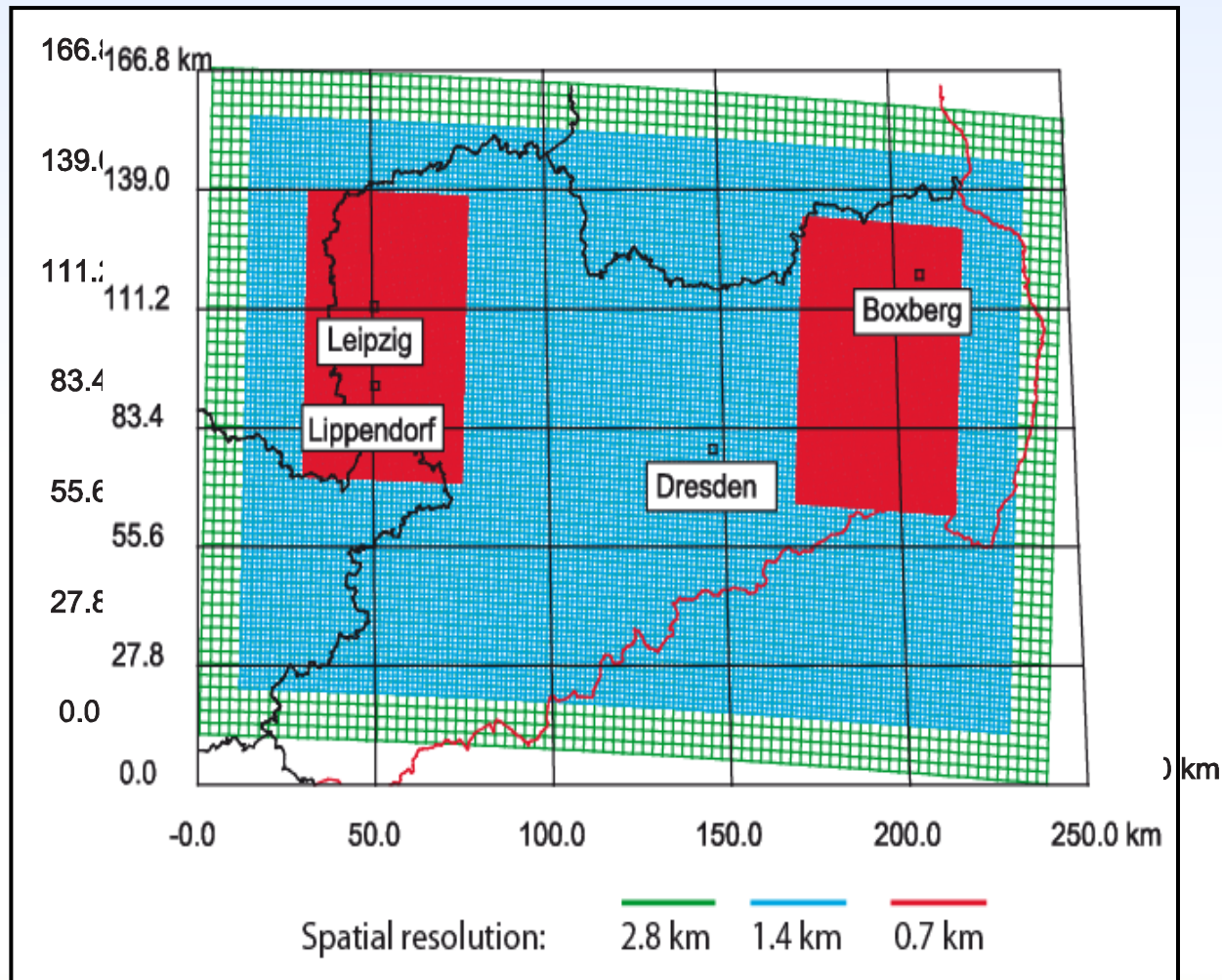
N3: 2.8 km x 2.8 km  
50 vertical layers

## Time period:

August 10 – 24, 2002

Appropriate boundary  
values from N1 run!

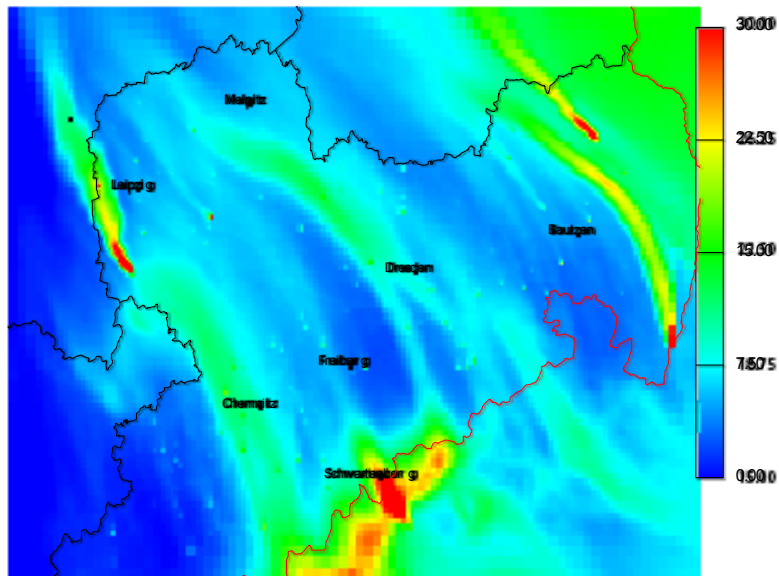
# N3 grid of MUSCAT



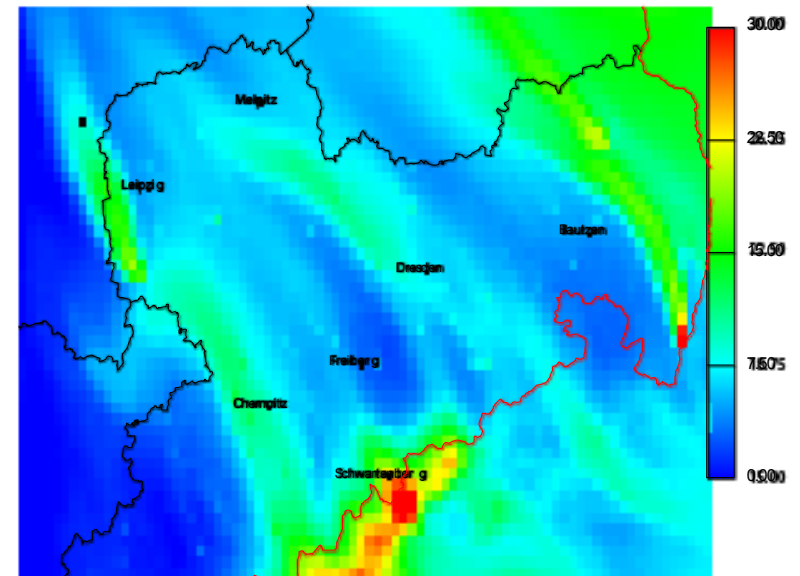
# Comparison of different resolutions

PM10 ( $\mu\text{g}/\text{m}^3$ )

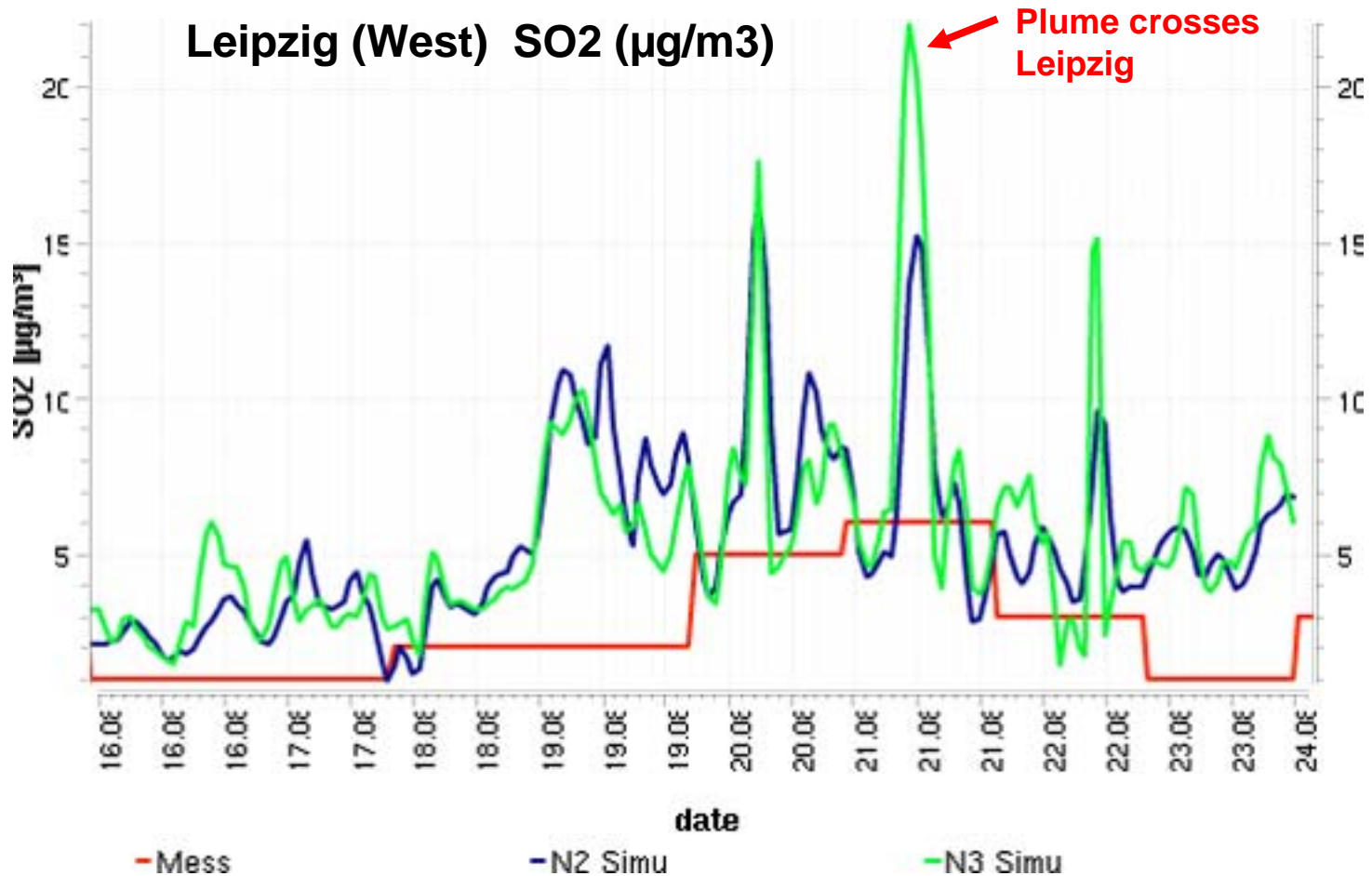
standard version



run with coarser grid resolution

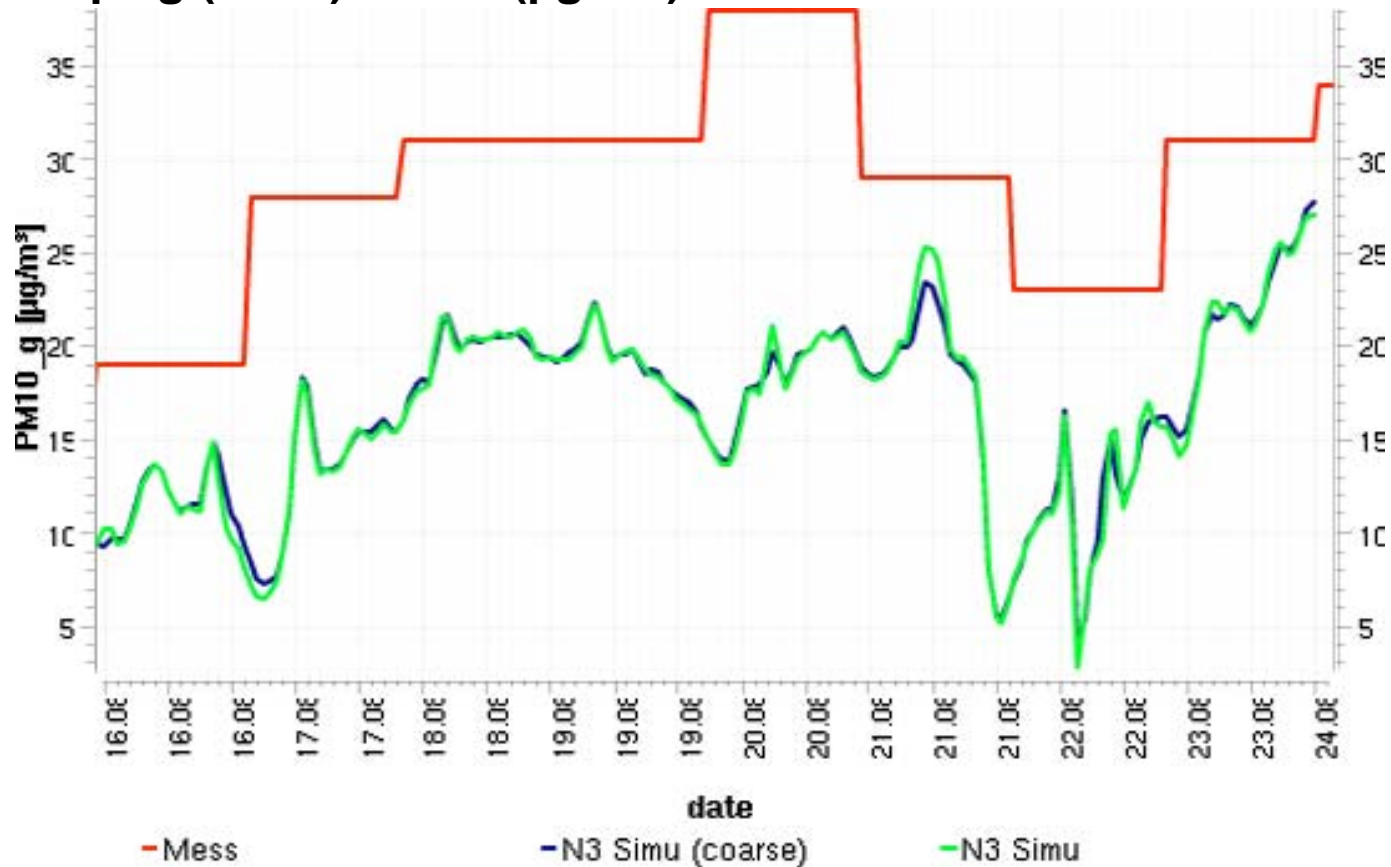


# Grid resolution LM (N2-N3)



# Grid resolution MUSCAT

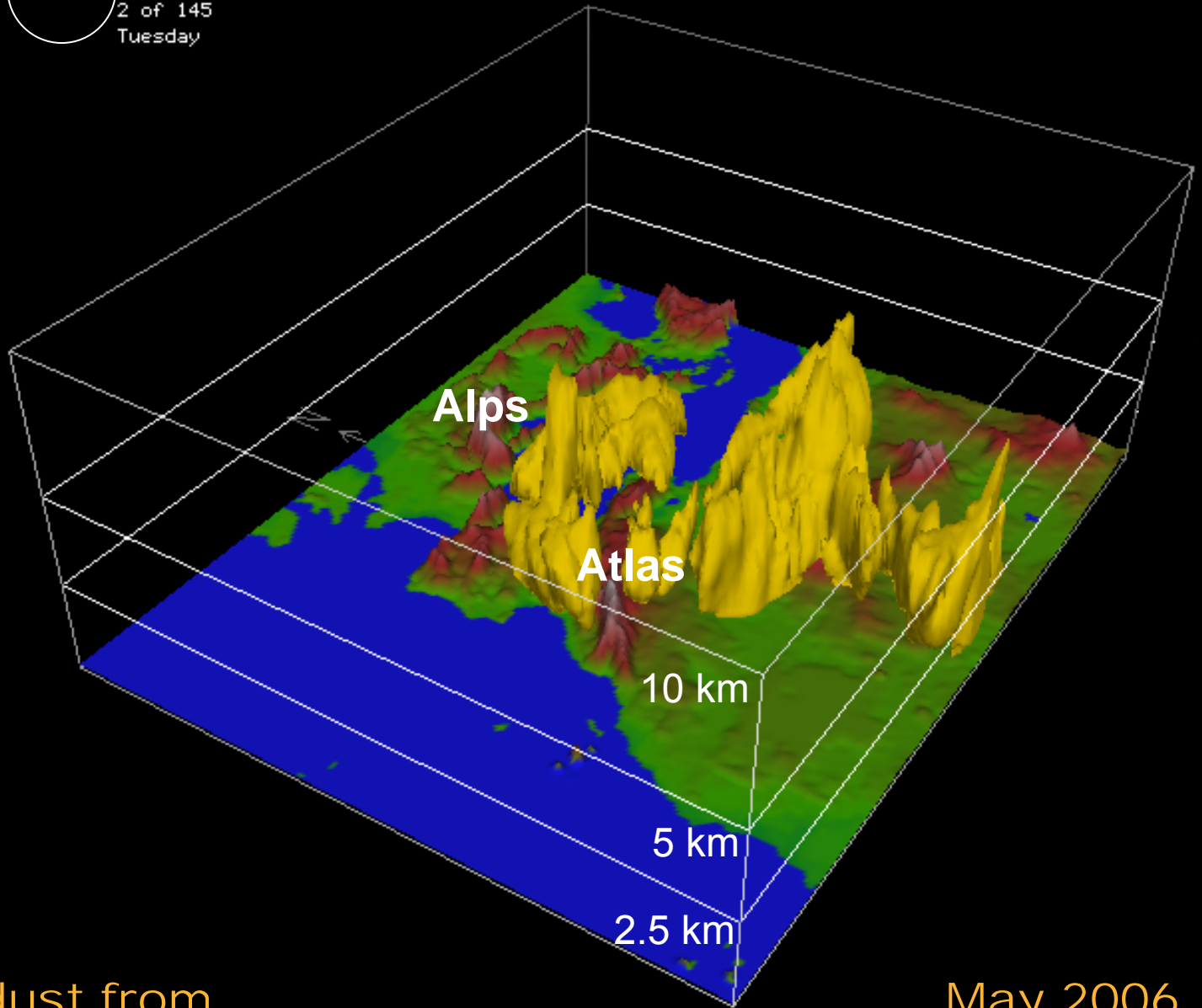
Leipzig (West) PM10 ( $\mu\text{g}/\text{m}^3$ )



# SAMUM Project

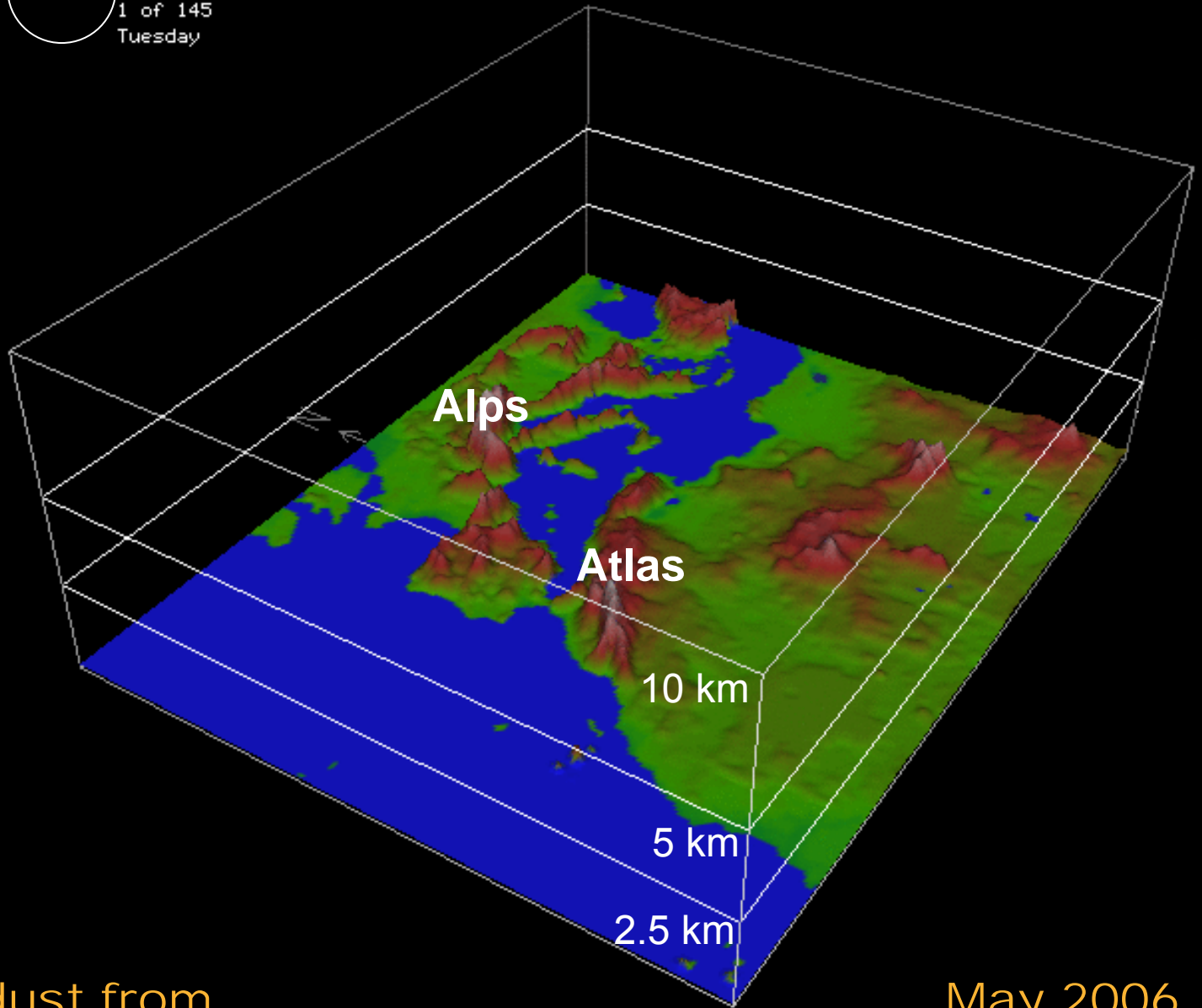
## SAharan Mineral dUst experiMent

- DFG research group  
(IfT, DLR, TU Darmstadt, U. Mainz, U. München, U. Bremen)
- Investigation of radiative properties of pure & mixed Saharan desert aerosol
- SAMUM I (2004-2007) & SAMUM II (2007-2010)
- Field campaigns:
  - Ground-based/air-borne in-situ & remote sensing measurements
  - Morocco, May/June 2006
  - Cape Verde, January/February 2008



Saharan dust from  
LM-MUSCAT simulations

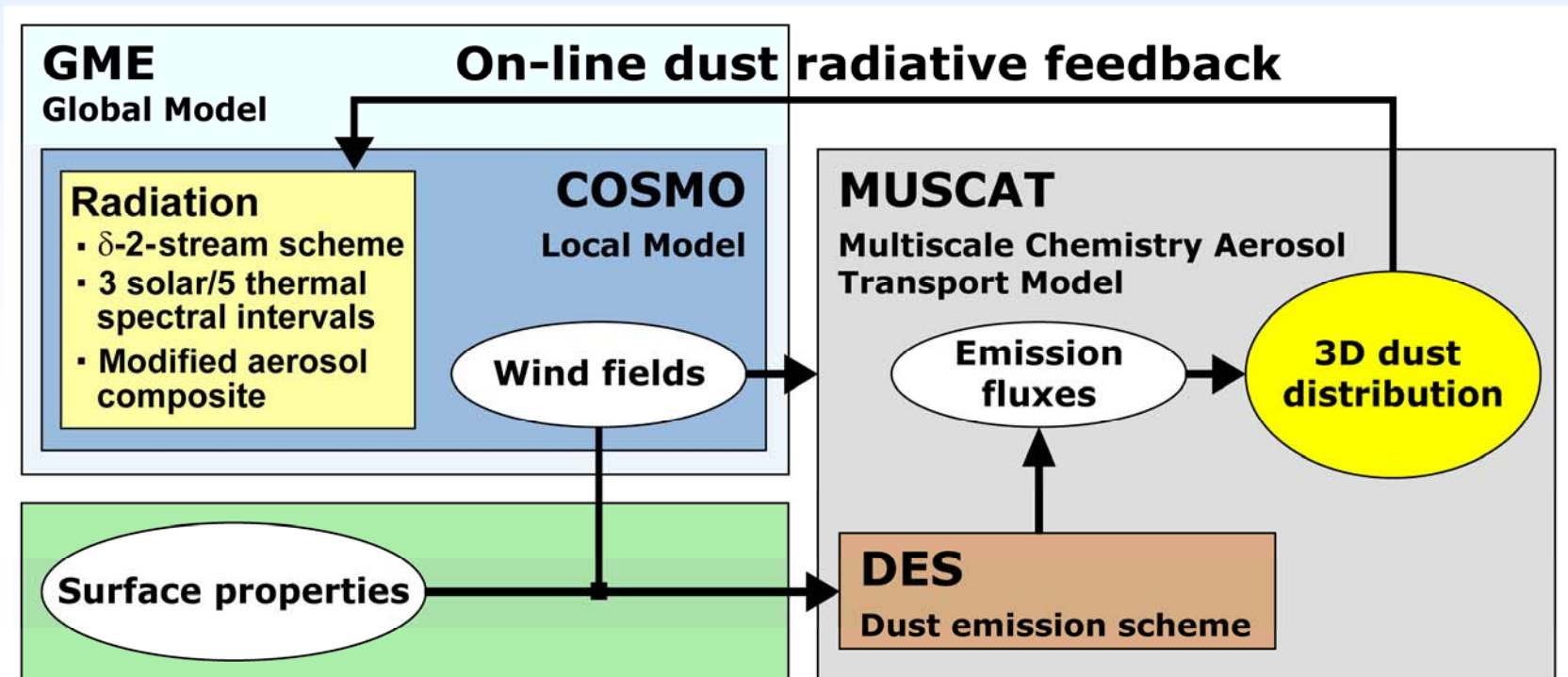
May 2006



Saharan dust from  
LM-MUSCAT simulations

May 2006

# Dust radiative feedback

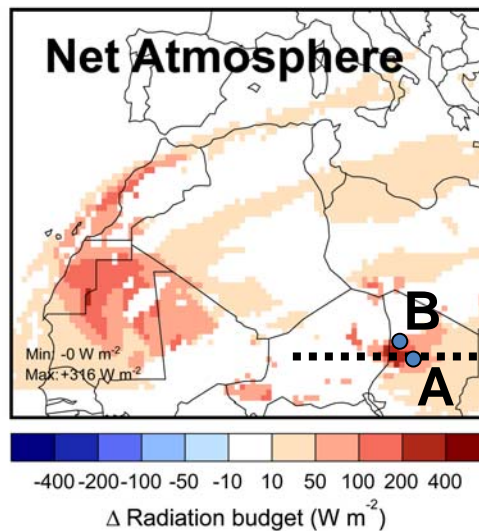
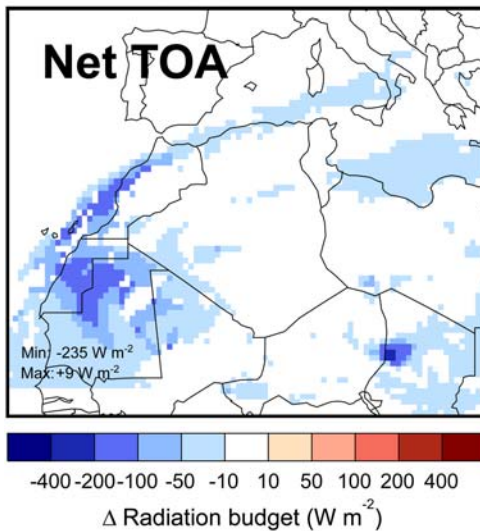
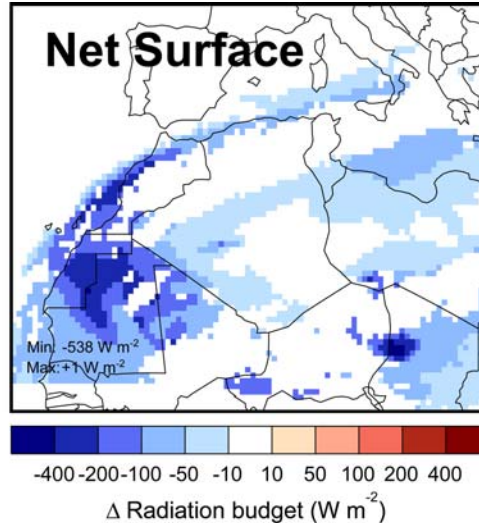
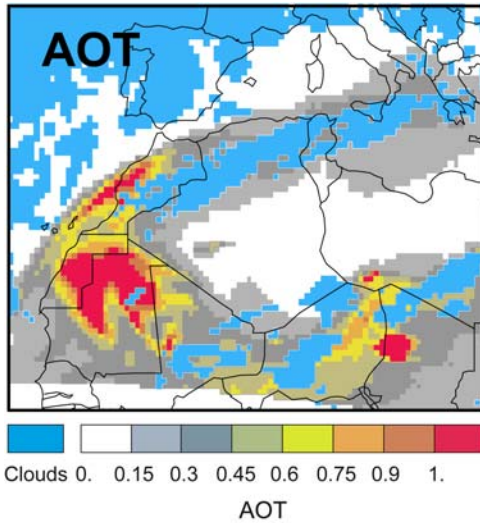


(Helmert et al., '07; Heinold et al. '07/'08)

„Absorbing dust“ 2% hematite, 98% kaolinite (Sokolik & Toon, '99)

# Radiative effects of Saharan dust

06-05-20, 12 UTC



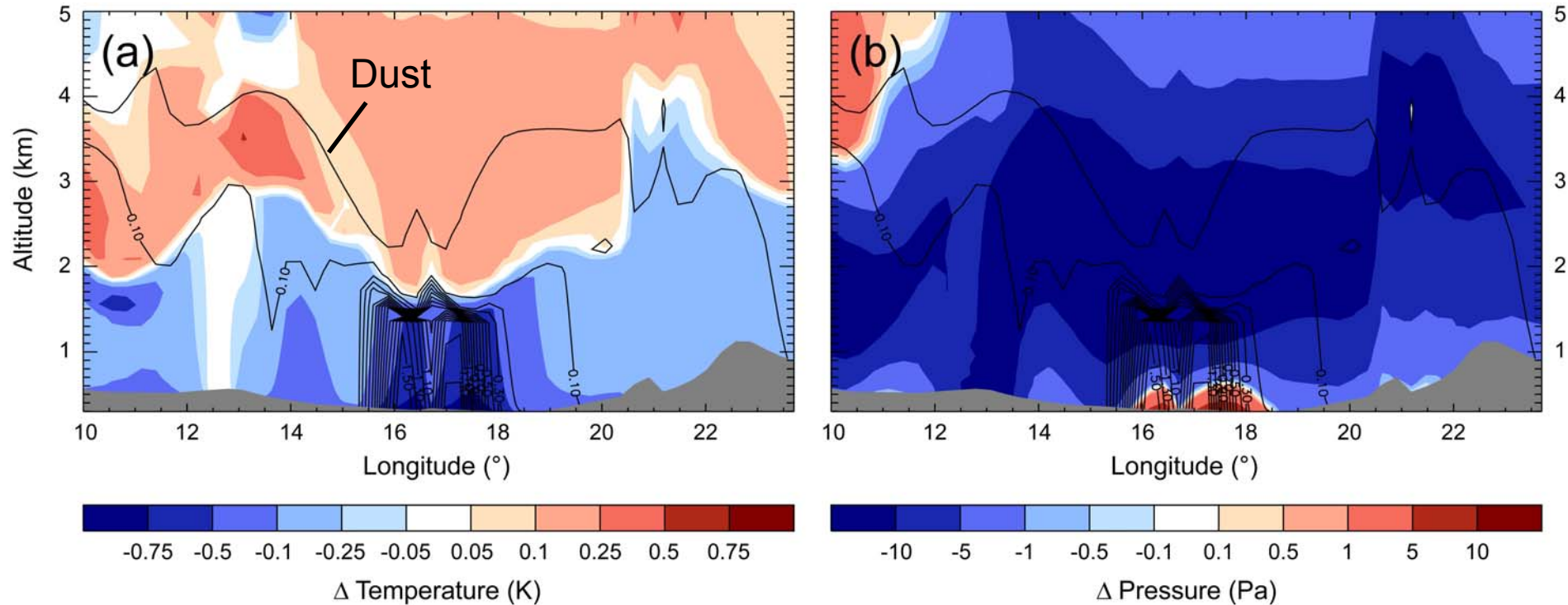
16.8° N

# Effect on stratification, Bodélé

Temperature differences

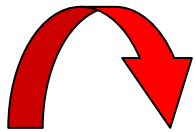
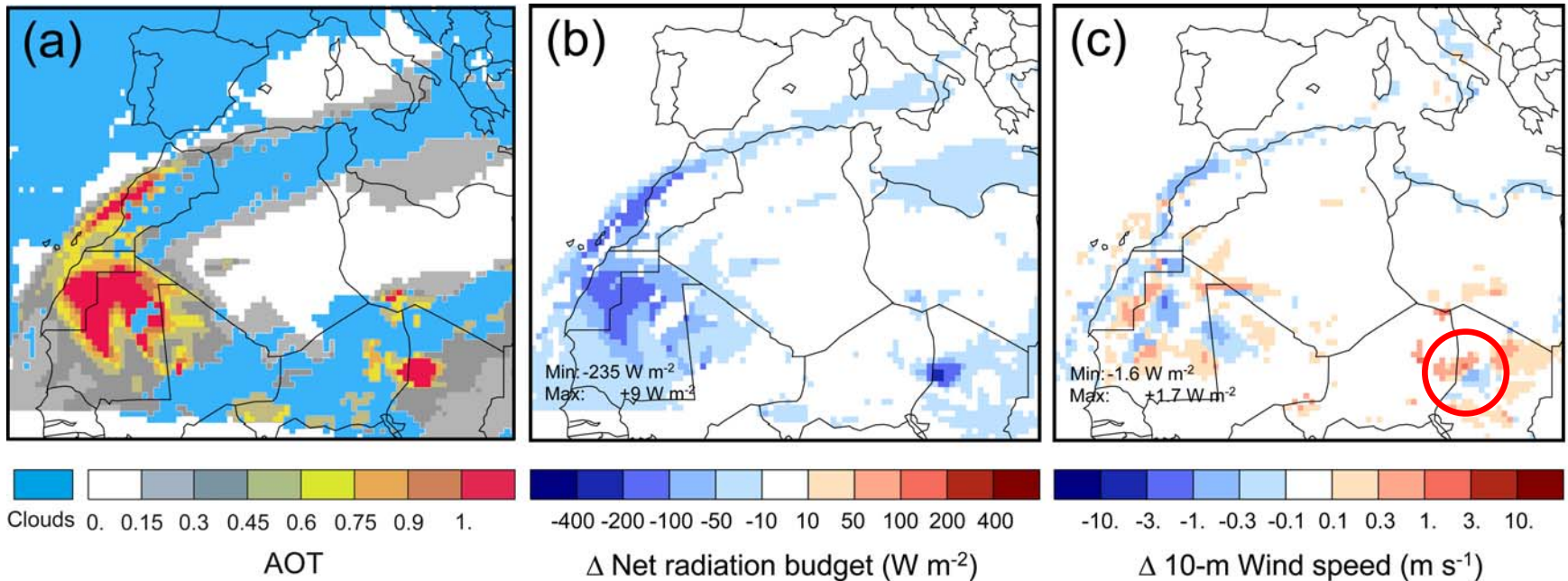
Pressure differences

in model results  
with dust feedback – without



# Effect on surface winds

06-05-20, 12:00 UTC



Positive & negative dust radiative feedback upon wind fields

# Summary

- COSMO-MUSCAT – a useful modeling system for:
  - Air quality applications
  - Integration and interpretation of measurement results
  - Study of feedback mechanisms
  - Identification of relevant effects
- Multiblock grid techniques and IMEX time integration schemes ensure an efficient treatment of transport, chemistry and aerosol dynamics
- High flexibility due to modular model architecture

[http://projects.tropos.de/cosmo\\_muscat](http://projects.tropos.de/cosmo_muscat)

## *Acknowledgement*

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