# The Influence of Local Emissions and Long-Range Transport on PM10 Hotspots in Saxony

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- **Chemistry-Transport Model MUSCAT**
  ***Aerosol Model, Numerics, Parallelization***
- **Online-Coupling COSMO-MUSCAT**
  ***Coupling scheme, Feedback, Load balance***
- **Selected Applications**
  - ***Air Quality in Saxony***
  - ***"Wild-land fire" episode (talk of M. Sofiev)***
- **Conclusion and Outlook**

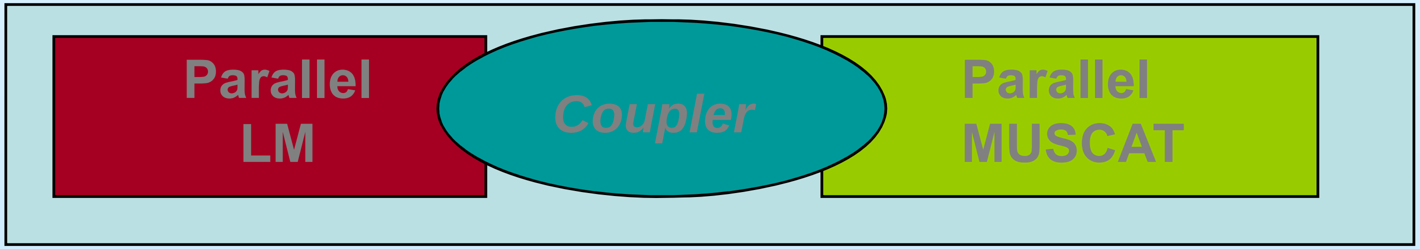
# Chemistry-Transport Model MUSCAT

**(« *MUltiScale Chemistry Aerosol Transport* »)**

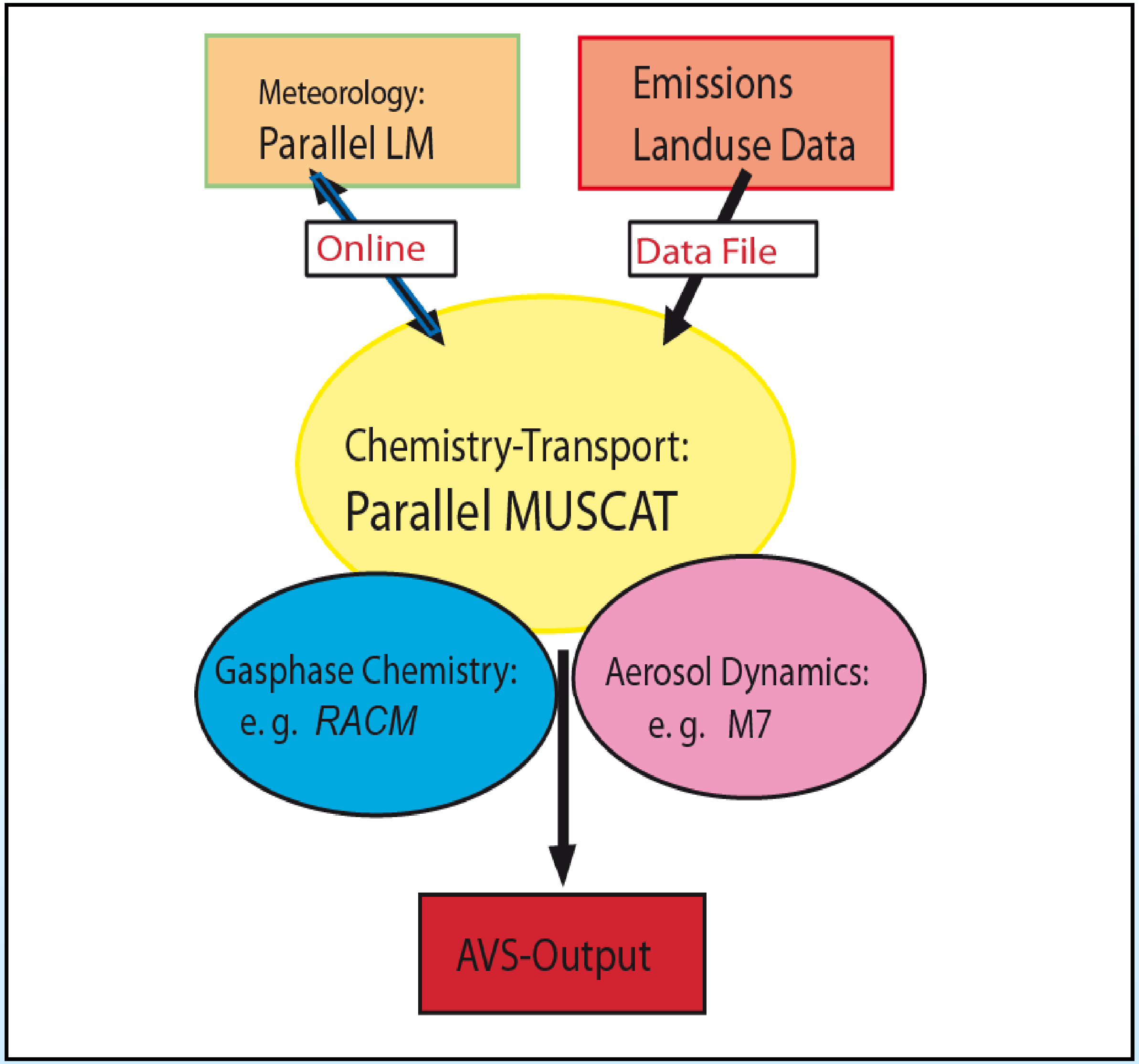
- **Described Processes**
  - **Gas phase chemistry via ASCII file (e.g. RACM-MIM2)**
  - **Modal aerosol module *or an only mass-based scheme***
  - **Dry and wet deposition, anthropogenic and biogenic emissions**

- **Numerical techniques**
  - **Multiscale grid**
  - **IMEX time-integration scheme (*BDF method for implicit part)***
  - ***Parallelization, load balancing***

- **Online coupling with COSMO *(renamed LM « Lokal-Modell »)***



# Model System COSMO-MUSCAT



## Gas phase chemistry

**Most applications: RACM-MIM2**
**(Stockwell et al, 1997; Karl et al, 2006)**

**Reaction mechanism**
**from input file:**
**High flexibility.**

**Difference to KPP *(Sandu et al.):***
- ***Data structures are generated.***
- ***KPP generates FORTRAN code.***

***No Cloud-Chemistry is included currently.***

### 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

- **Modal model MADMAcS I** ***(Wilck and Stratmann, 1997):***
  - ***Coagulation, condensation, gas uptake*** *(,nucleation)*
  - ***Equilibrium models:***
    ***ISORROPIA*** **(Nenes et al., 1998)**, EQSAM (Metzger, 2001)

  ➔ **Only for process studies !**

- **Mass-based approach:**
  ***Similar to EMEP model***

- **In both approaches: Dry and wet deposition, sedimentation**

- **Considered components: Sulphate, nitrate, ammonia, EC, POC**
  **only in mass-based approach: SS, SOA (Schell et al., 2001)**

- **SAMUM: Dust sectional (5 or 12 size bins)**

- **Work in progress: Modified M7** ***(Vignati et al, 2004, Stier et al., 2005)***
  ***Sulphate, sea salt, dust, EC, OC + nitrate, ammonia, SOA partitioning***

## Anthropogenic Emissions

- 11 SNAP codes of EMEP/CORINAIR for characterising the different anthropogenic source types (e.g., combustion in energy industry, road transport, agriculture) are used.
- The considered chemical species are the main pollutants $SO_2$, $NO_x$, CO, $NH_3$, $PM_{2.5}$, $PM_{10}$, methane, and non-methane volatile organic compounds (NMVOC).
- Area, line and point sources possible. *(Special: "cooling tower").*
- **Aerosol emissions:** Particle number and composition are generated in dependence from the corresponding SNAP (***Splitting table***).
  **(EMEP + Stier et al.+ Measurements)**

## Dust emissions scheme (*Tegen et al., 2002)*

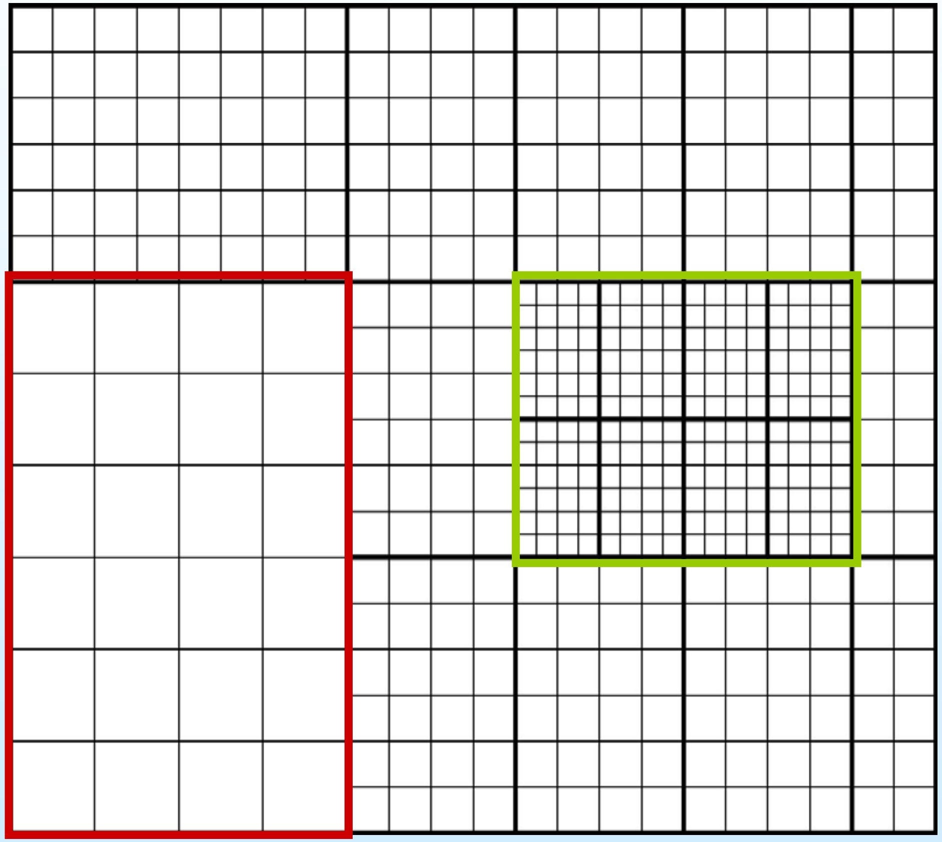
## Biogenic Emissions

- NO emissions are calculated in dependence on the vegetation type and surface temperature *(Williams et al., 1992).*
- The VOC emissions additionally depend on sunlight *(Günther et al., 1993).*

# Decomposition of Horizontal Domain

***Static grid***
***("multiblock approach")***

- **From a given rectangular grid (usually for the meteorological driver).**
- **Non-overlapping subblocks (also of rectangular type) are marked for refining or coarsening.**
- **Refinement level between neighbouring blocks is restricted to 1.**



# Numerical methods

- **Space discretization**
  - ***Staggered grid. Finite-volume techniques.***
  - ***Advection: Third-order upwind scheme (Hundsdorfer et al., 1995).***

- **Time-integration: IMEX scheme** *(Knoth & Wolke, 1998)*
  - ***Explicit second-order Runge-Kutta for horizontal advection***
  - ***Second order BDF method for the rest:*** *Jacobian is calculated explicitly, linear systems by Gauss-Seidel iterations or AMF*

# 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

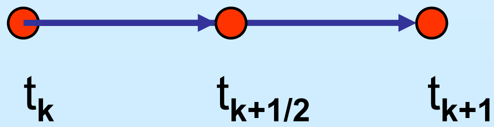

$$Y_1 = c(t_n)$$

$$Y_2 = Z_2(h_E) \quad \text{with}$$

$$\frac{dZ_2}{d\tau} = f_E(t_n, Y_1) + f_I(t_n + \tau, Z_2), \quad \tau \in [0, h_E], \quad Z_2(0) = Y_1,$$

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

IMEX–RK2



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  - ***Multirate techniques (Schlegel, 2007):*** *Only "local" CFL criteria have to be fulfilled, leads to different explicit time steps in different regions*

# Multirate approach

**CFL criteria ("Stability")**

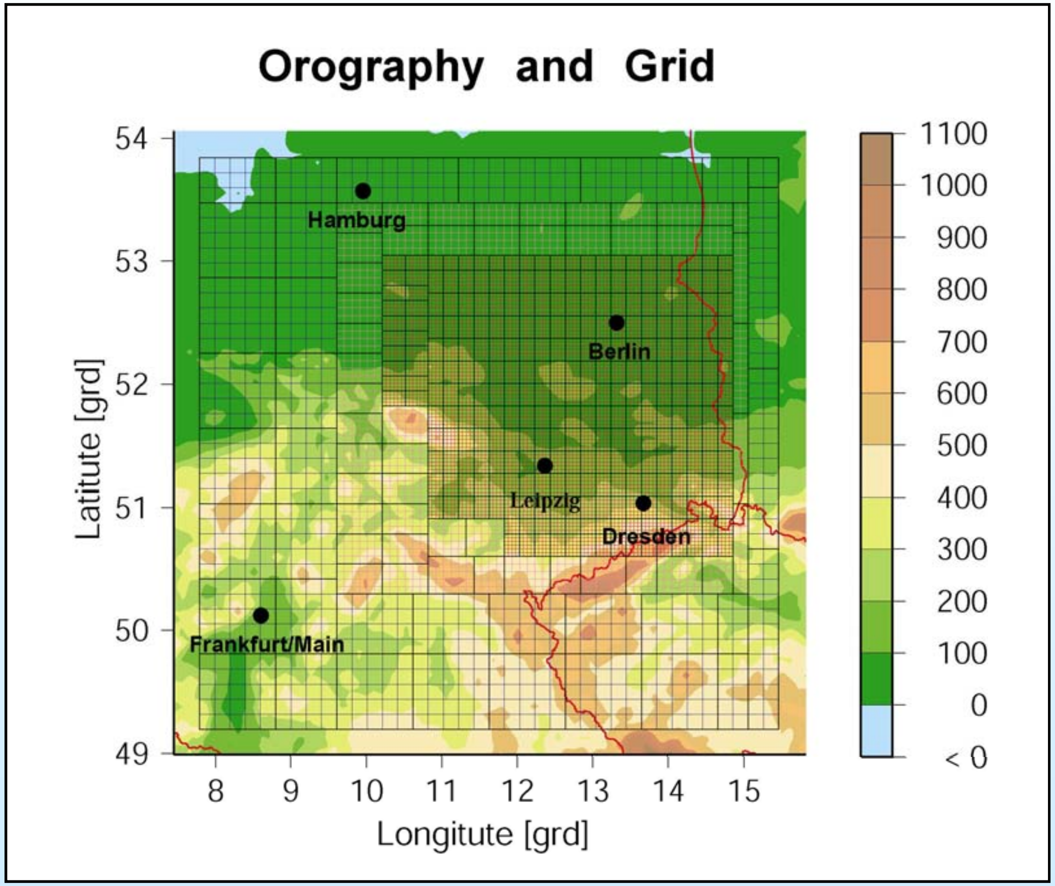
$$\Delta t_{Ex} \leq \beta \, \Delta x \, / \, u$$

β … method specific
(e.g., 0.66 for Heun2)

**CFL restricted by smallest resolution!!**

**Problem of different time steps :**

Save mass consistency and the order of the RK methods on faces with different time steps.



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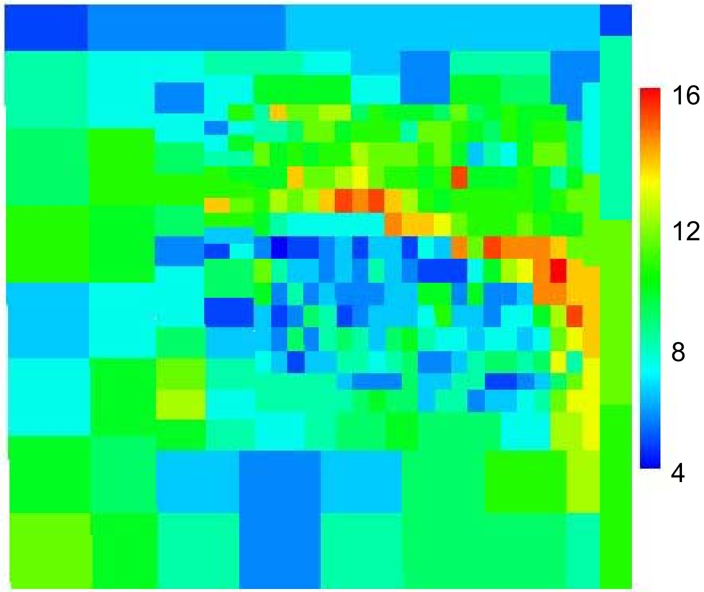
- **Time-integration: IMEX scheme** *(Knoth & Wolke, 1998)*
  - ***Explicit second-order Runge-Kutta for horizontal advection***
  - ***Second order BDF method for the rest:*** *Jacobian is calculated explicitly, linear systems by Gauss-Seidel iterations or AMF*
  - ***Automatic step size control***

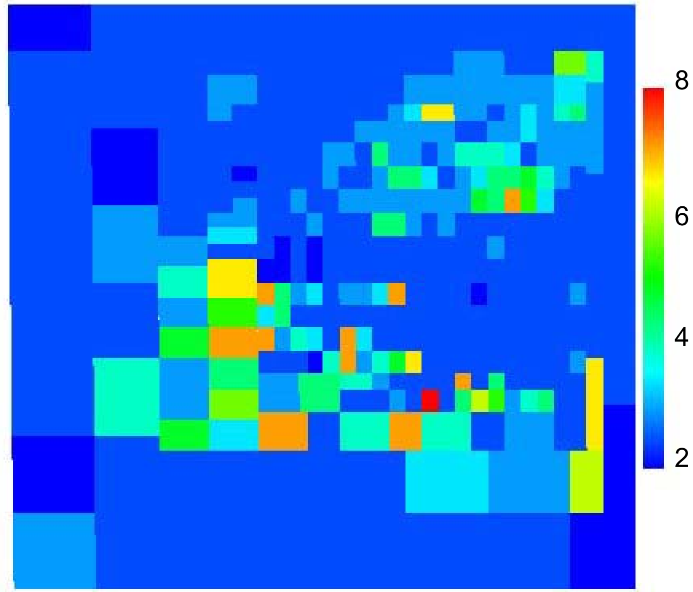
    ➔ ***different number of steps (load imbalances)***

- **Parallelization**
  - ***domain decomposition***
  - ***dynamical load-balancing by redistribution of blocks***

# Load Balancing of MUSCAT



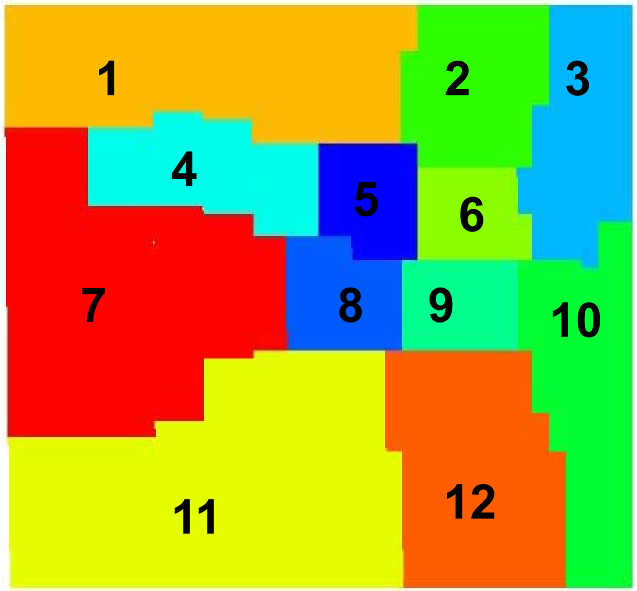

Day 1: 12:00



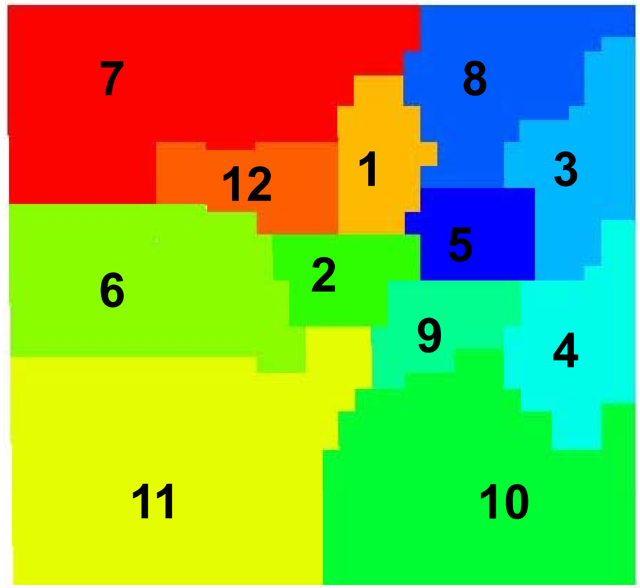

Day 1: 15:50

The number of function evaluations of each block at the start and the end time.

# Load Balancing of MUSCAT




Start



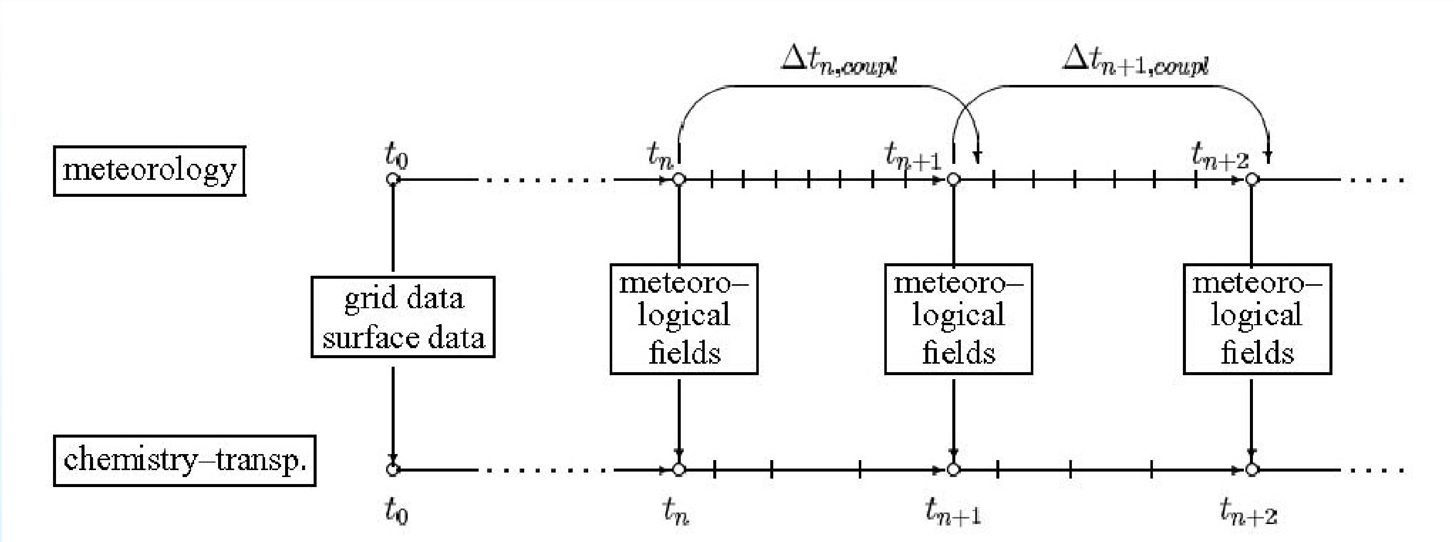

End

Start and end distribution for a run with12 MUSCAT processors

# "Local Model" (LM) of the German Weather Service
(Doms and Schättler, 1998-2003; Steppeler et al. 2003)

- **non-hydrostatic, compressible**
- **formulated with regard to a hydrostatic reference state**
- **staggered grid**
  - **horizontal: uniform, orthogonal ($\lambda$,$\varphi$)**
  - **hybrid vertical coordinate**
- **operational mode for weather forecast, regional scale**
- **boundary and initial data from GME**
- **highly parallel**
- **New operational version (prognostic TKE, multi-layer surface model, "new cloud" scheme, … ) is renamed in COSMO model (community model: e. g., Swizerland, Greece, … )**
- ***Currently version 4.0***

# Coupling Scheme (+ mass conservation)




- 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

  ➔ **necessary for mass conservation (elliptic equation by cg-method) !!**
- Separate time step size control for LM and MUSCAT

# Coupling Scheme: Mass Conservation

Discrete continuity equation is not valid for given density

$$\rho$$

and mass flux field

$$\vec{U} = (\rho u, \rho v, \rho w).$$

Modify mass flux field by

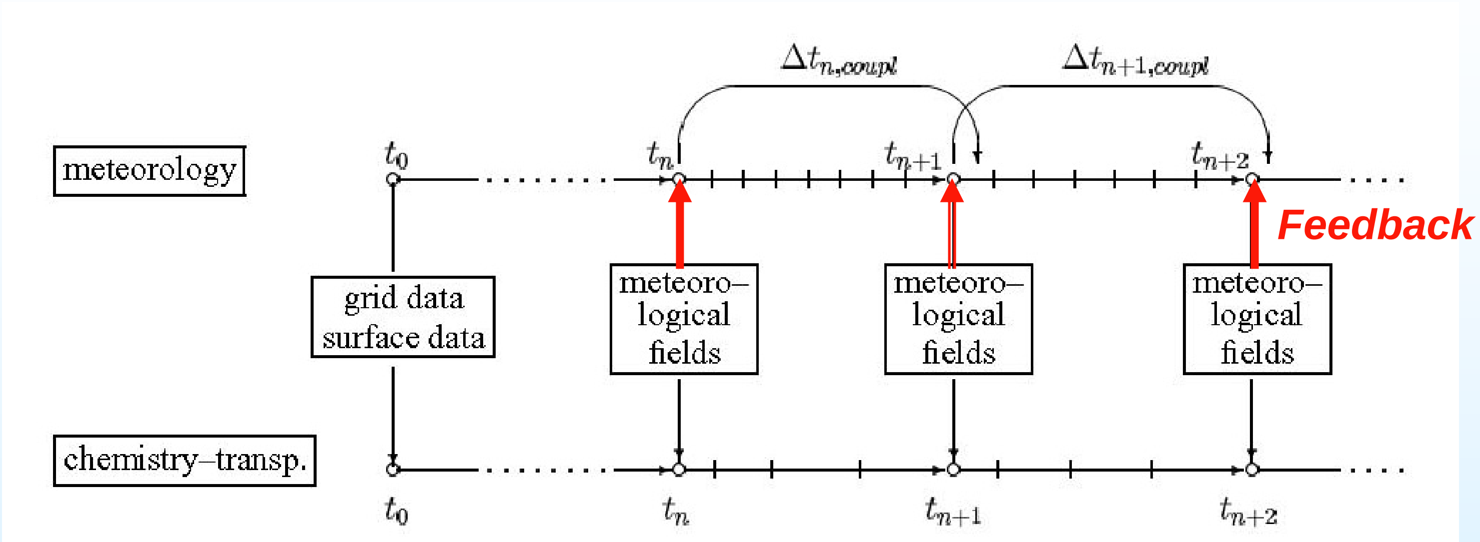
$$\left\| \vec{U}^{*} - \vec{U}^{n+1} \right\| \to \text{Min!}$$

and

$$\rho^{n+1} - \rho^{n} + \Delta t_{n} \nabla \vec{U}^{*} = 0.$$

- Projection changes all components of the mass flux field.
- Projection is done on the LM grid. Density and the mass flux field are interpolated to the composed grid without violating the continuity equation.

# Coupling Scheme (+ feedback to COSMO)

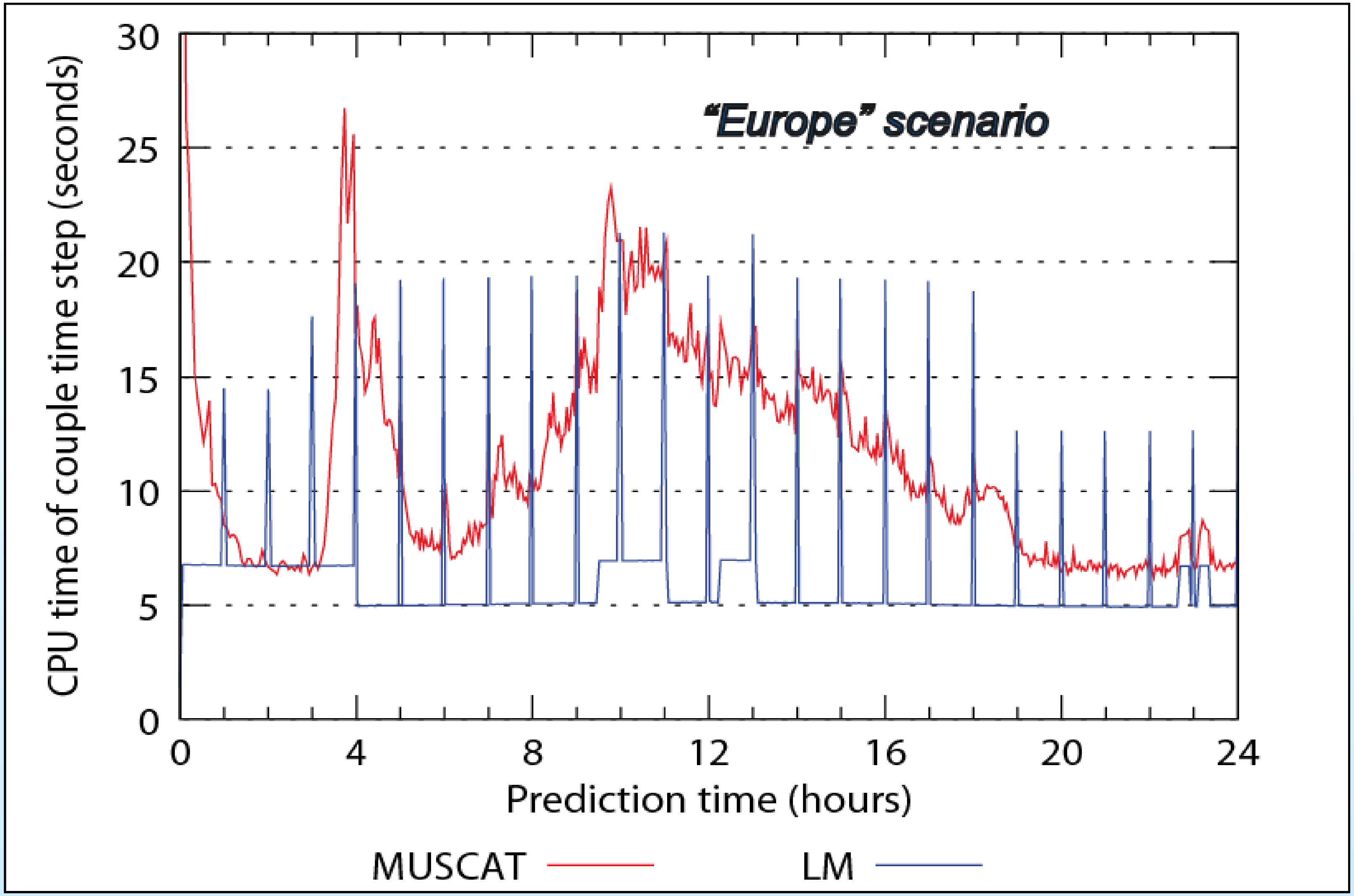



- Time interpolation of the meteorological fields:
  1. Linear interpolated in $[t_n, t_{n+1}]$ : Temperature, Density,….
  2. Time-averaged values on $[t_n, t_{n+1}]$ : Projected wind field
- Separate time step size control for LM and MUSCAT

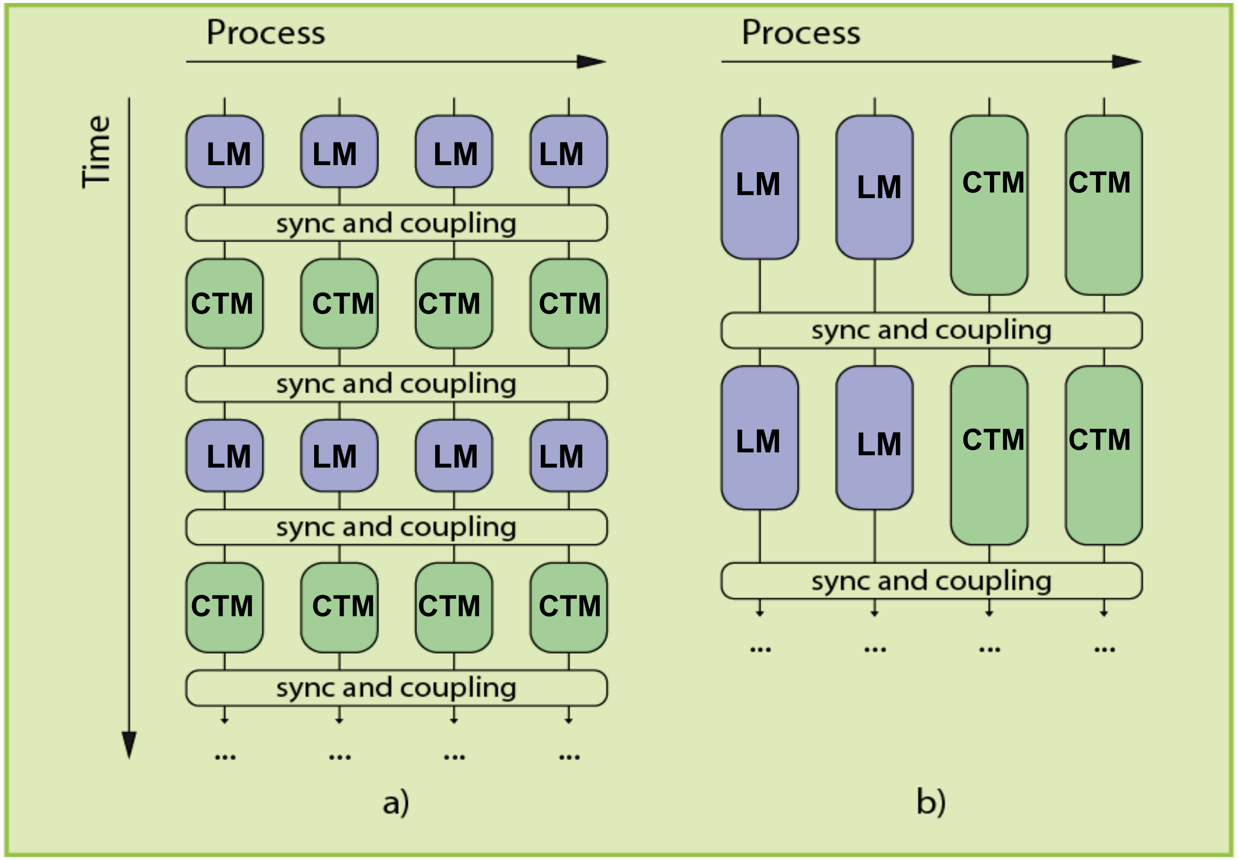
# Parallel coupling of COSMO and MUSCAT

- "concurrent" or "sequential" coupling scheme:
  - $P_{LM}$ for **LM** *(MPI_COM_MET)*
  - $P_{CTM}$ for **MUSCAT** *(MPI_COM_CTM)*
- Each model use its own domain decomposition:
  - LM rectangular
  - MUSCAT distribution of blocks
- LM and MUSCAT use its own "topology" for communication ("optimal" for used decomposition)
- MDE library for data transfer.
- Projection of wind fields by parallel cg-method.

# Performance Analysis II



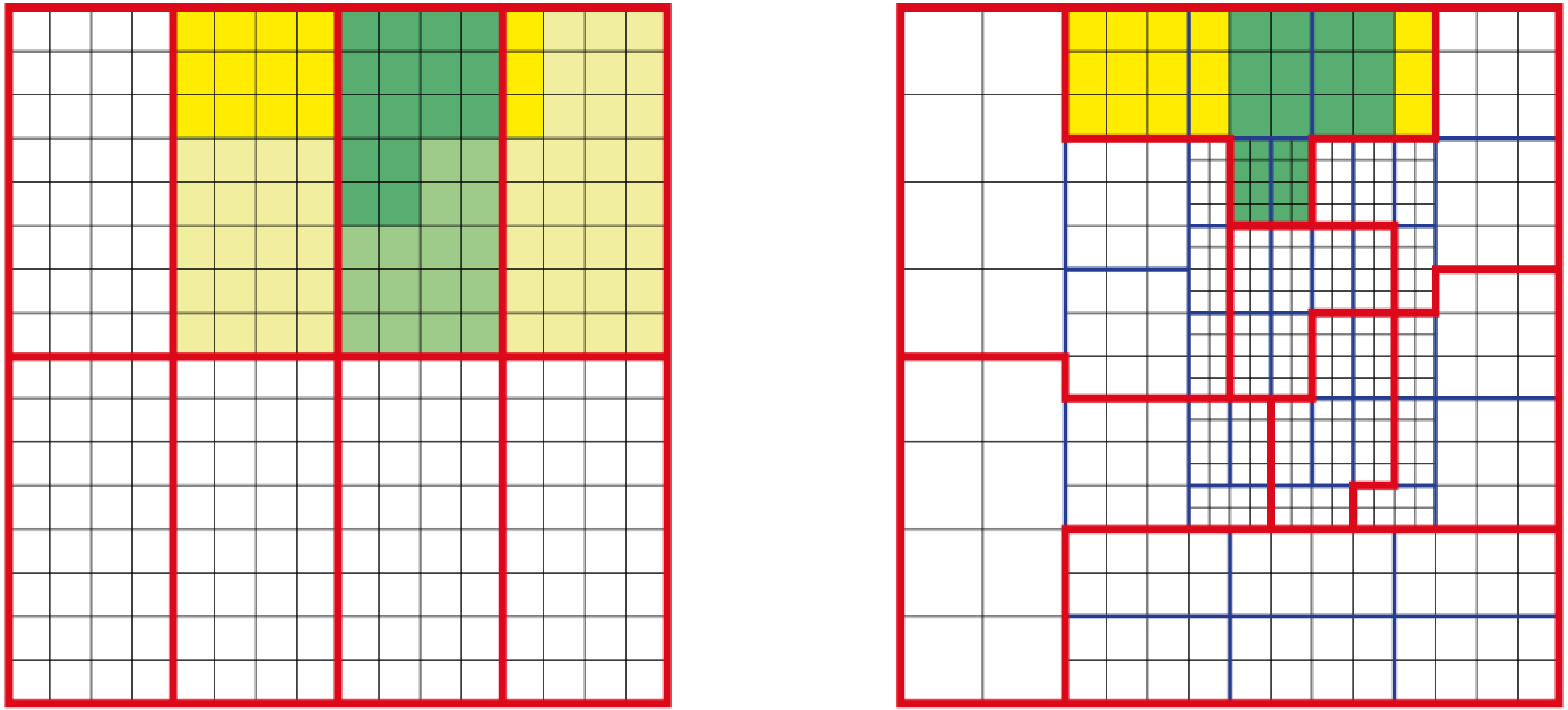
# Sequential vs. Concurrent Coupling




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

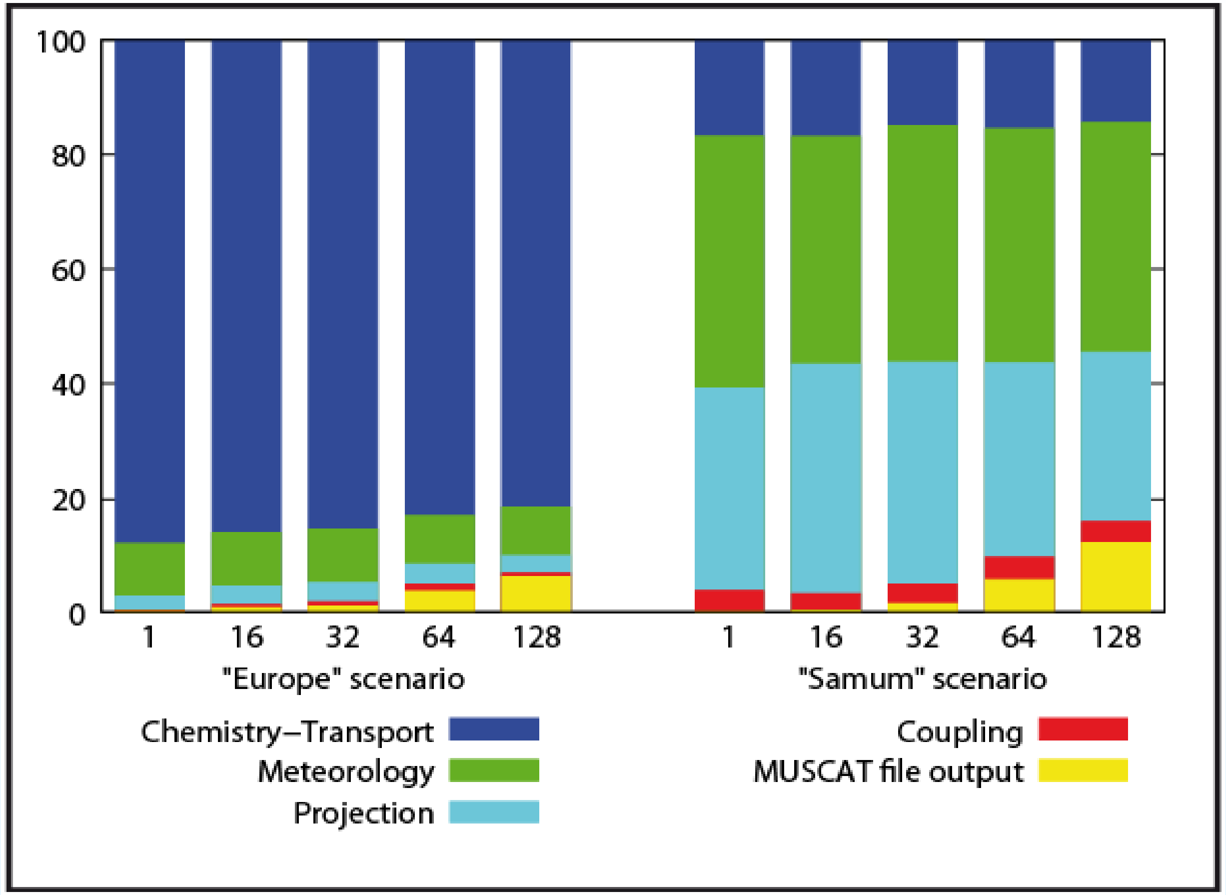
*Lieber & Wolke (2007)*

# Coupling Scheme: Grid Structure



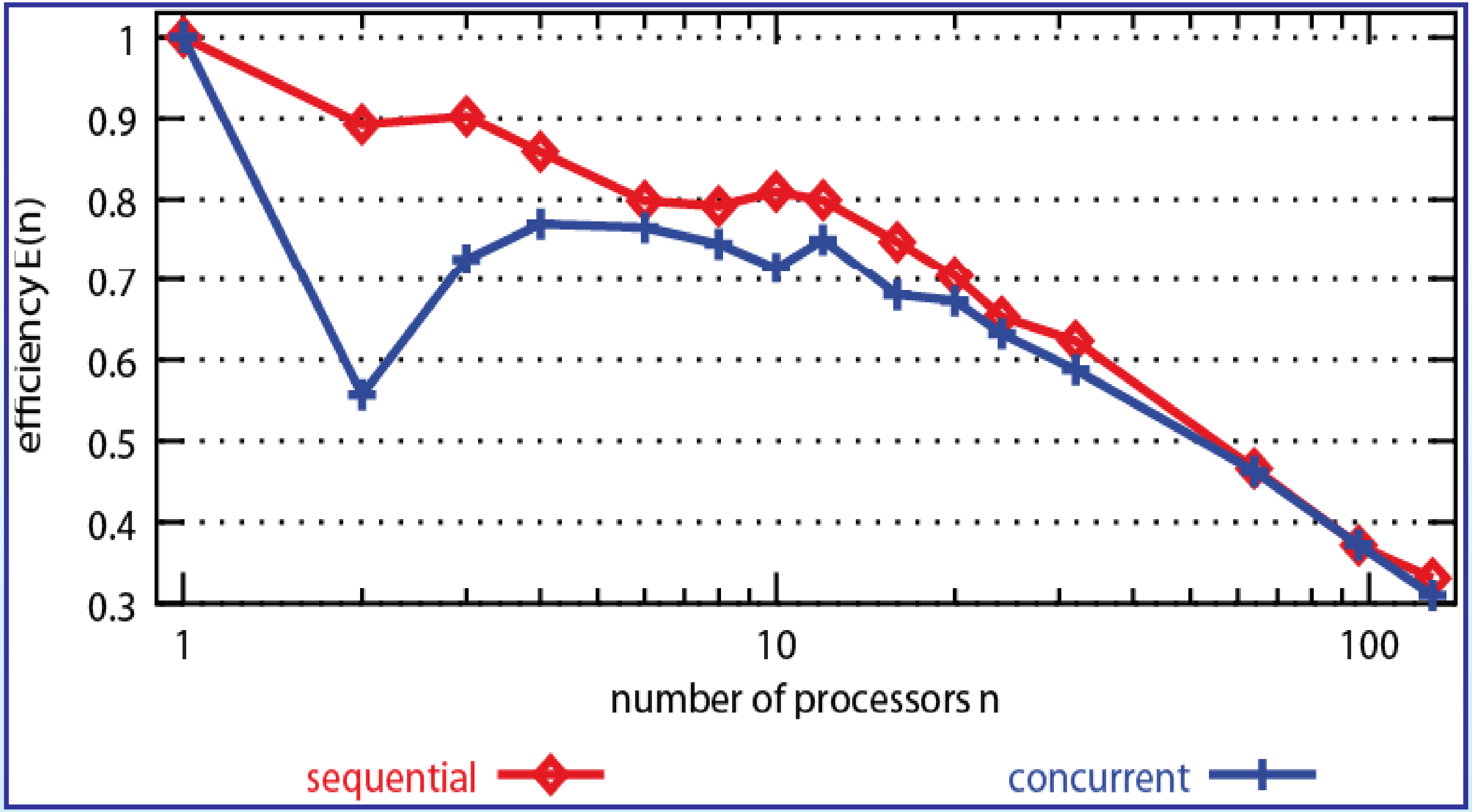
Multiblock data structures : LM (left) and MUSCAT (right)

# Performance Analysis I




Workload percentage of LM-MUSCAT components for different processor numbers using the sequential coupling (IBM p690).

## Parallel efficiency for the “Europe“ scenario



# Air quality applications

LfUG Saxony (measurement campaign)

"The influence of long range transport on PM10 hot spots in the Dresden area"

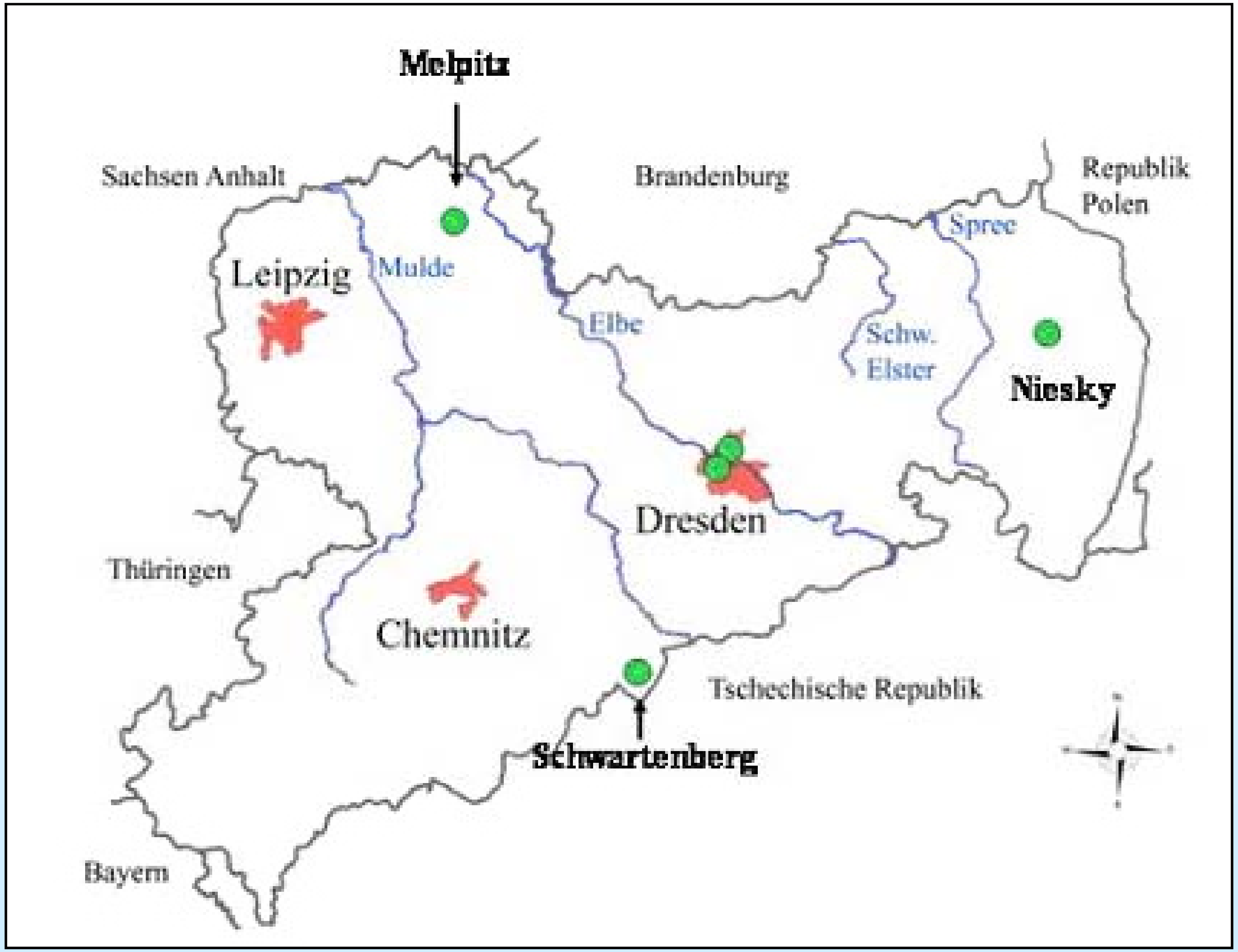
Period: 01.09.2006 – 31.08.2007

Approach: Take 24 hour samples by "High Volume Samplers", in time steps of 4 days, 5 measurement sites, analysis of mass and chemical composition.

Additional: Saxonian and UBA stations. *Modelling ?!*

Here: Focus on 15. October and 19. October 2006.

# Location of Measurement Sites




Rural:

*Melpitz, Niesky, Schwartenberg*

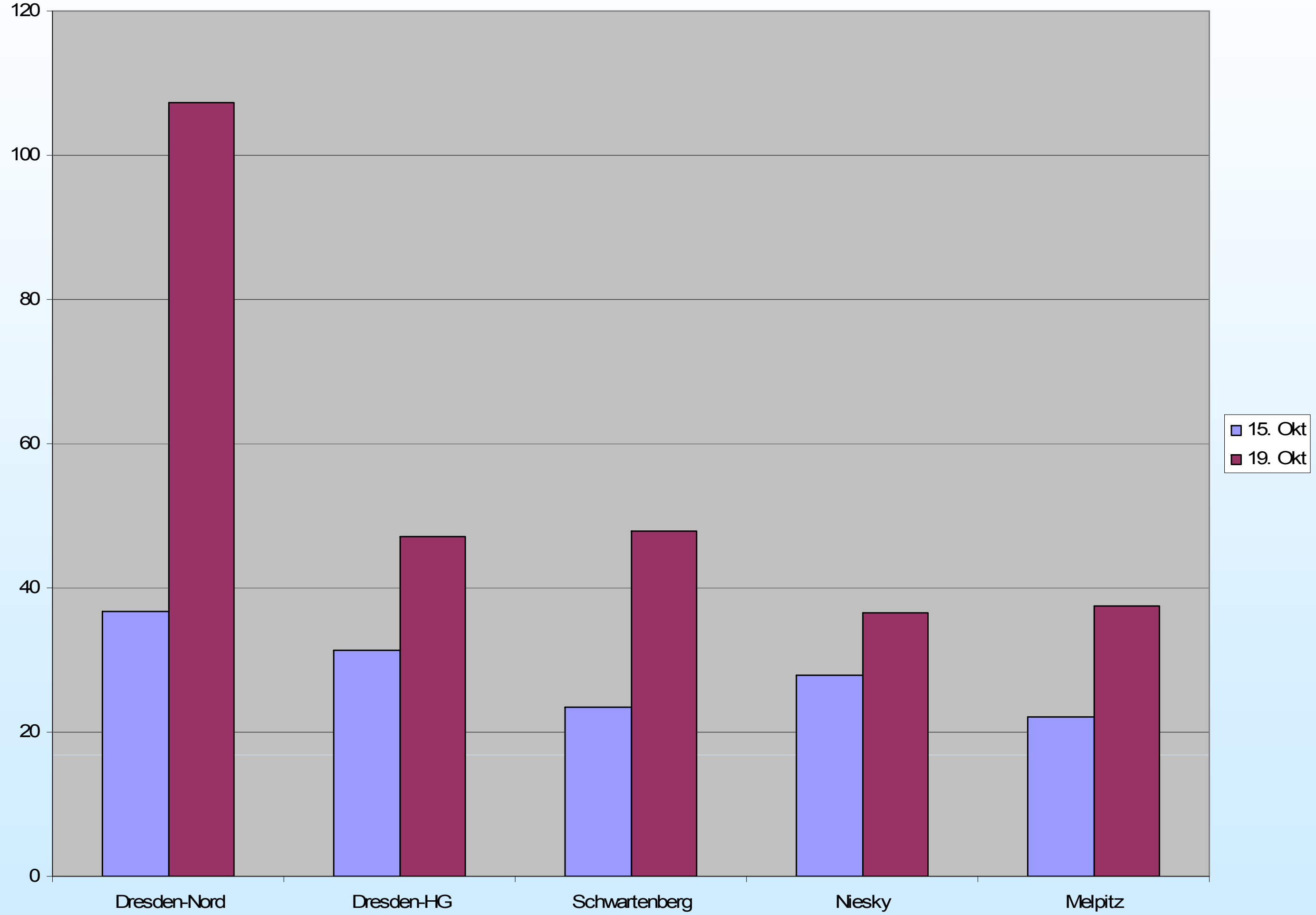
Urban:

*Dresden-HG*

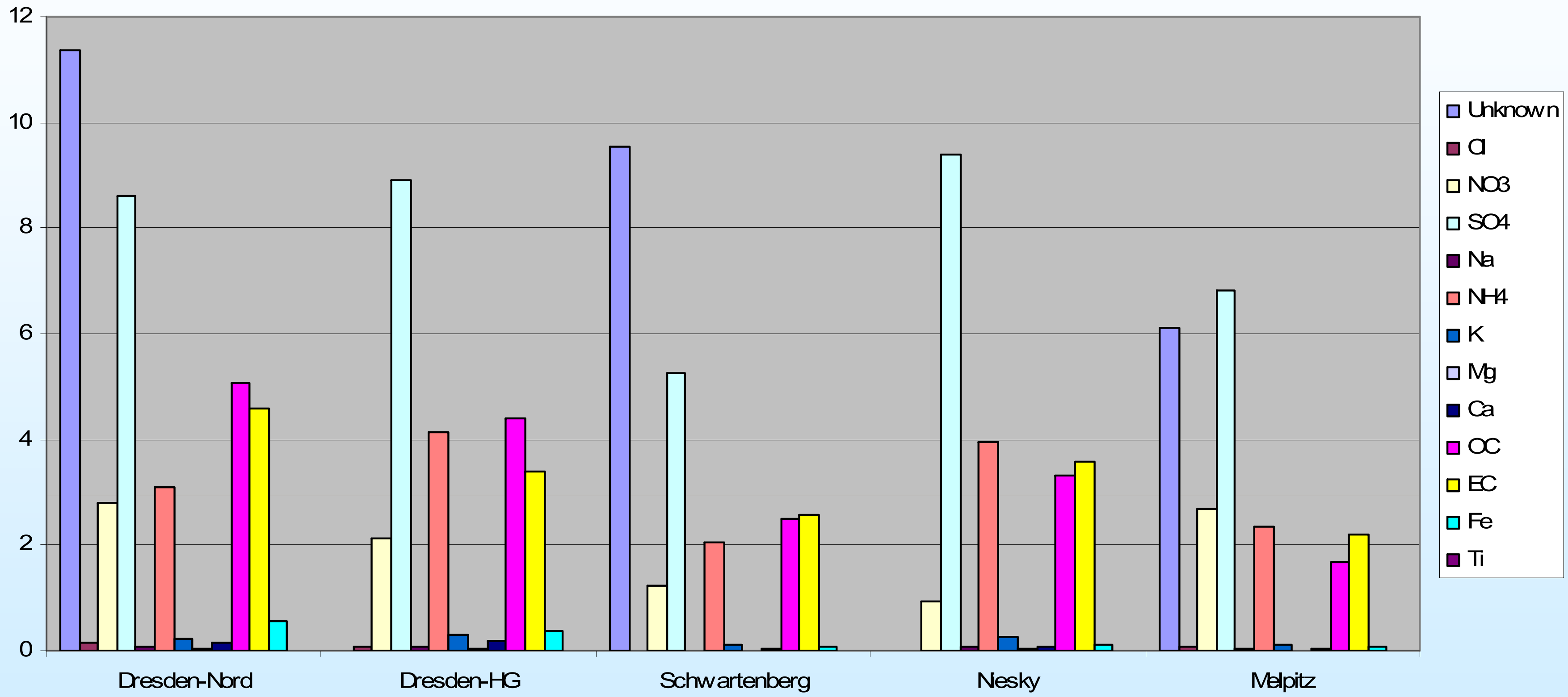
Urban-Traffic:

*Dresden-Nord*

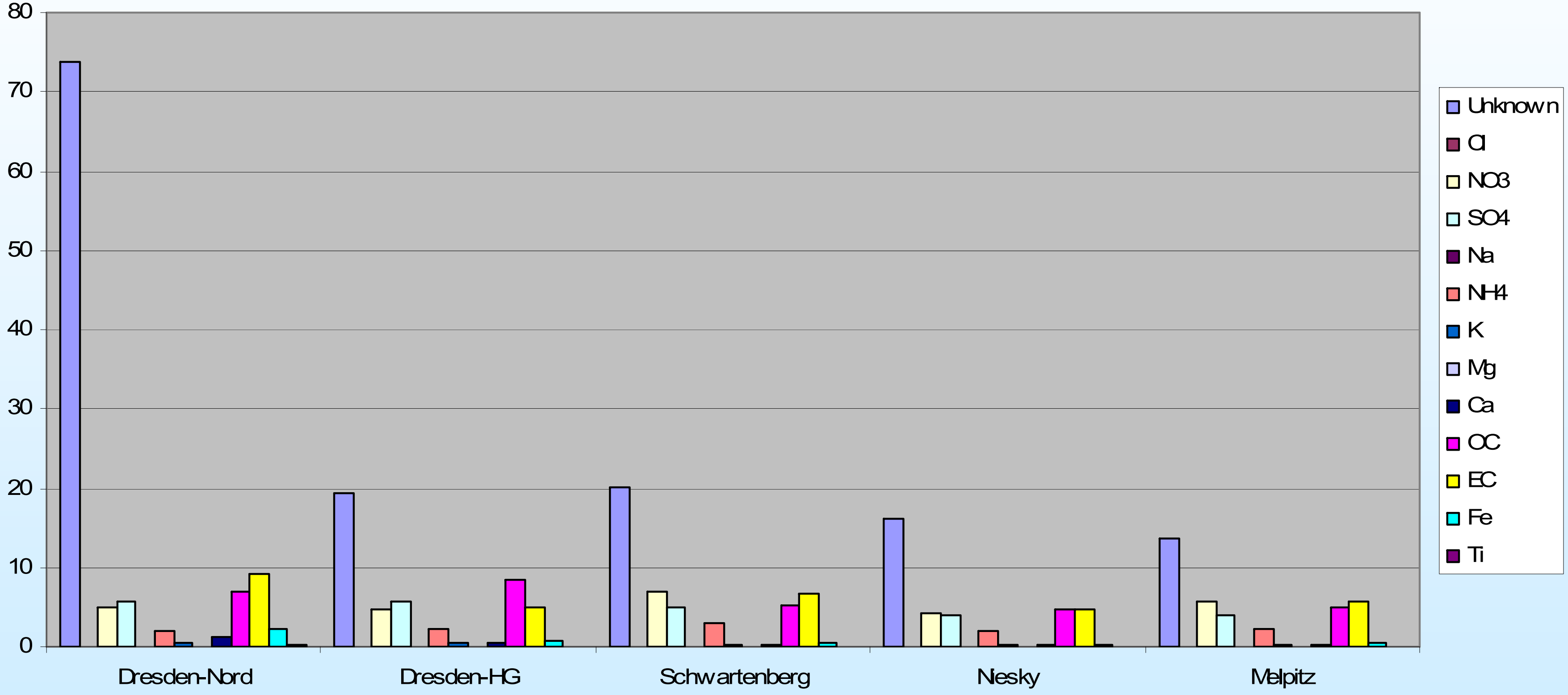
# PM10 [µg/m3]


120
100
80
60
40
20
0
Dresden-Nord
Dresden-HG
Schwartenberg
Niesky
Melpitz
15. Okt
19. Okt

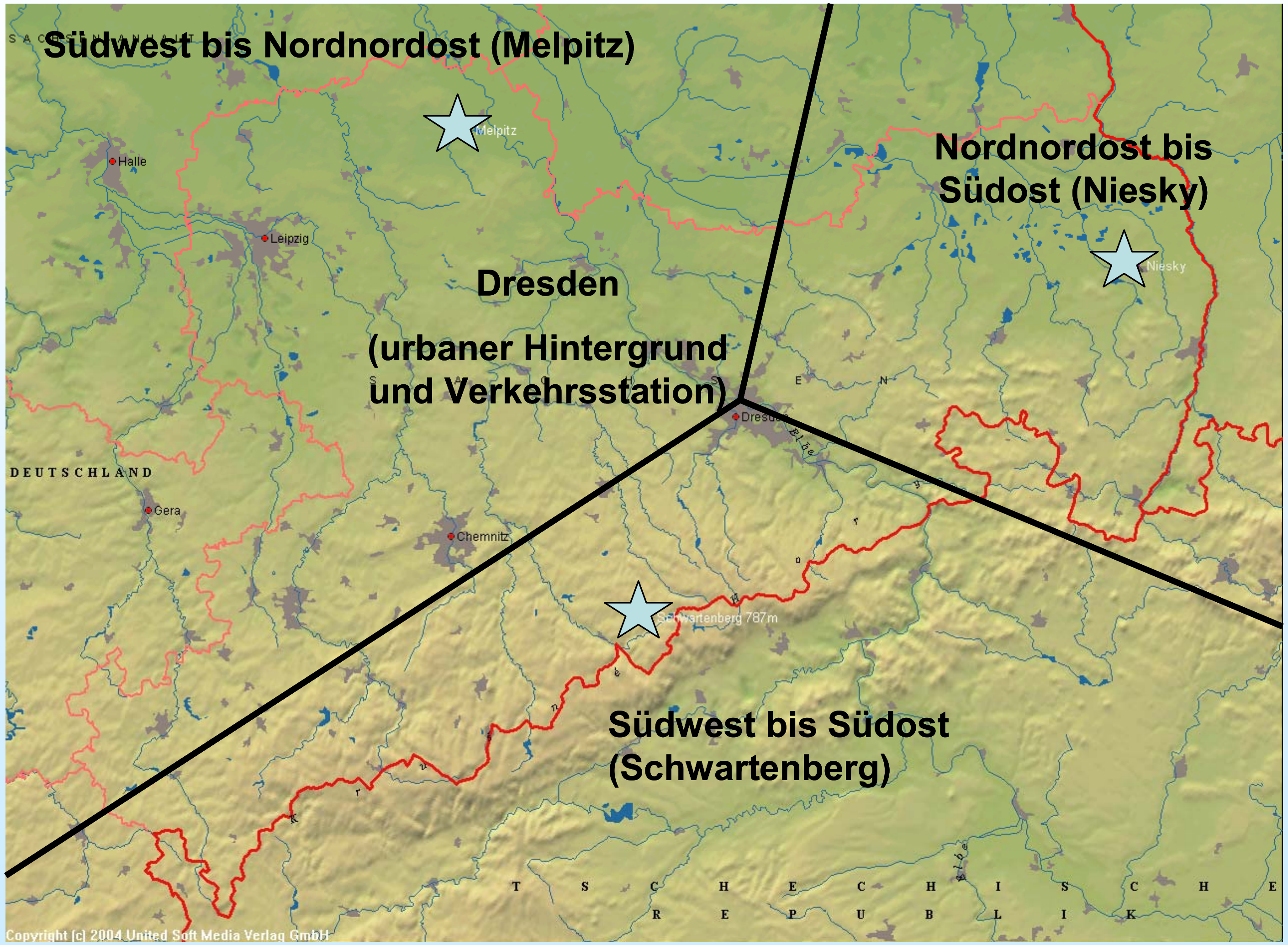
# Particle Composition (15.10.2006)



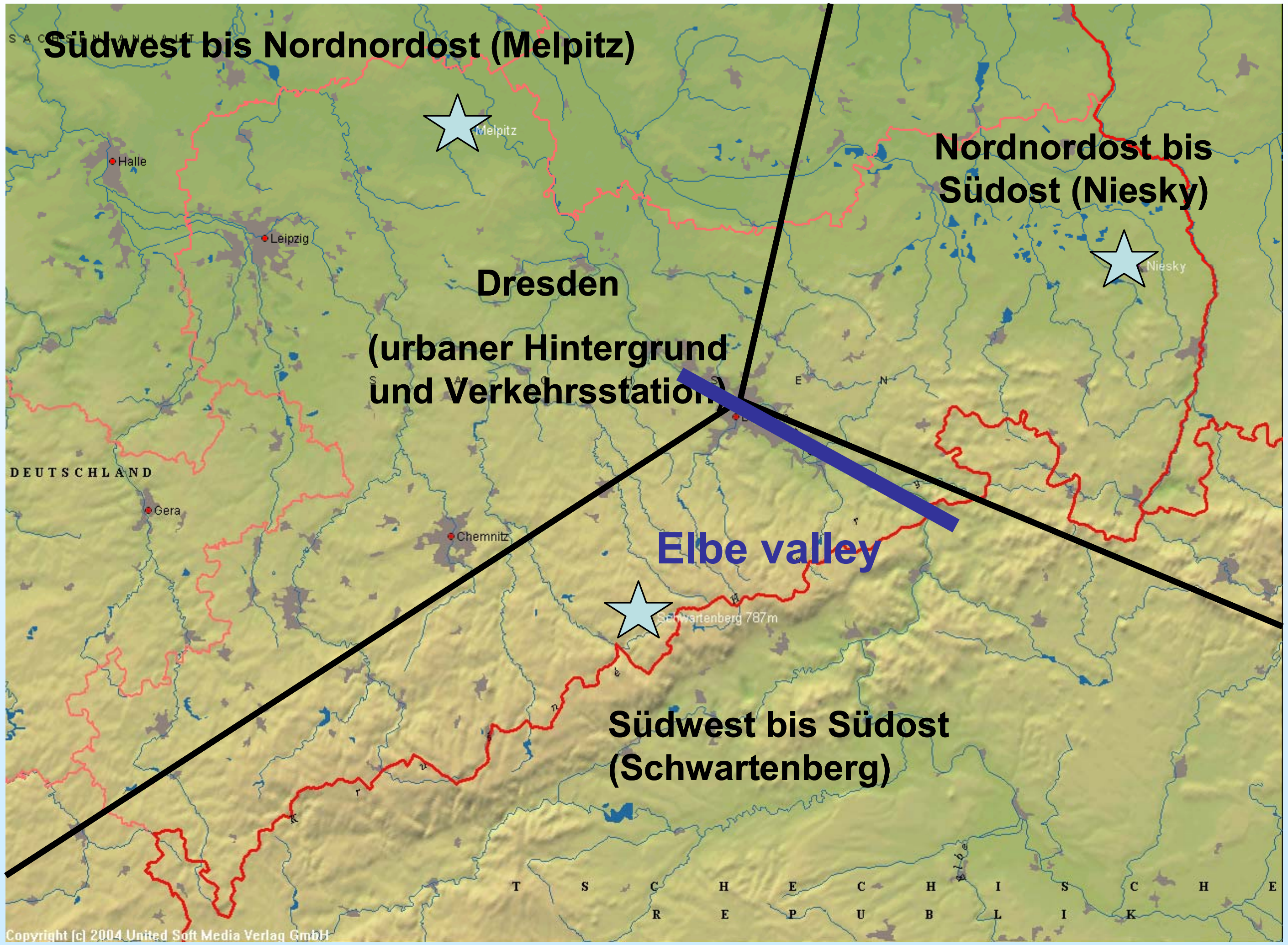
# Particle Composition (19.10.2006)



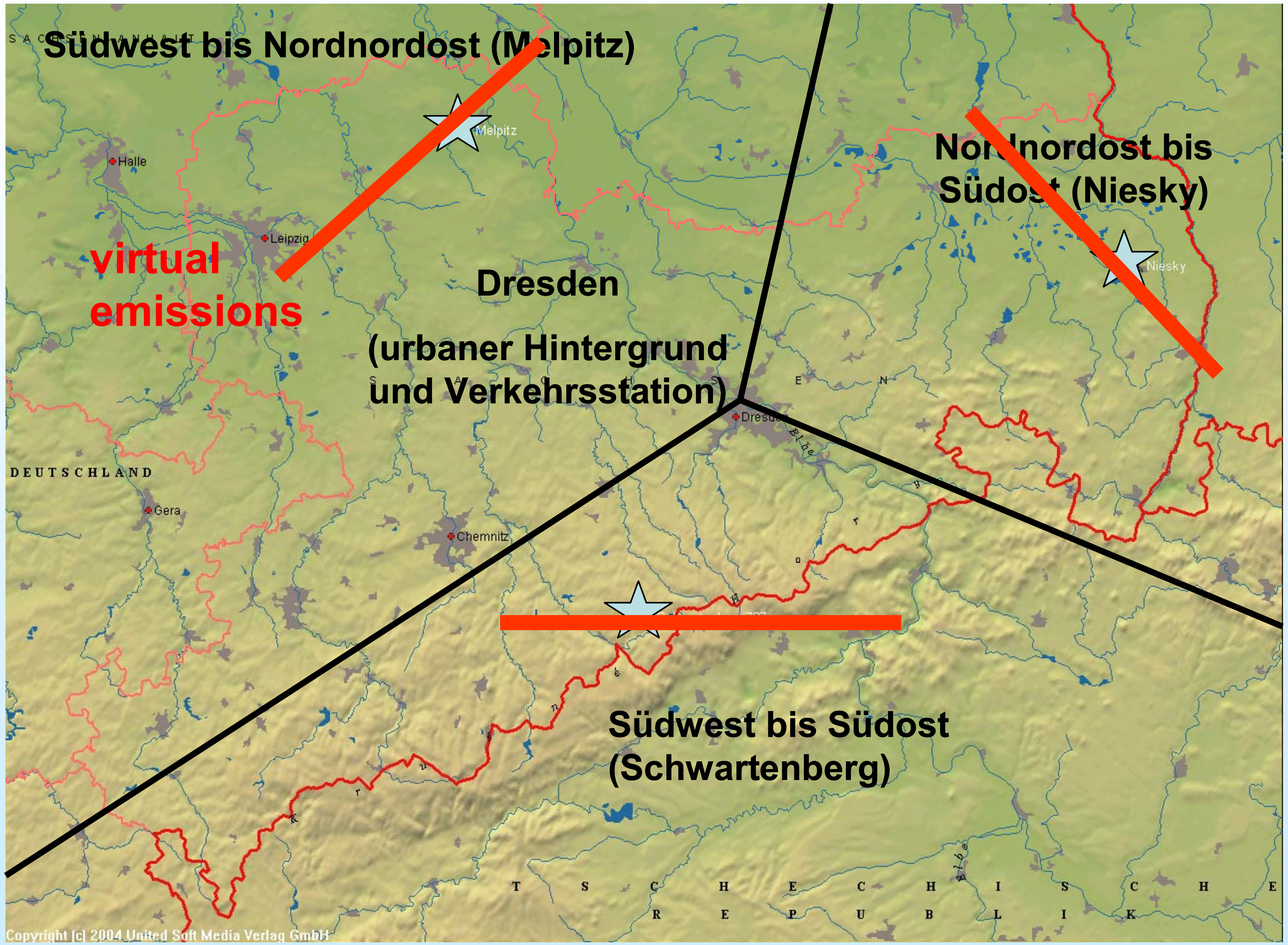
# Classification according to wind direction



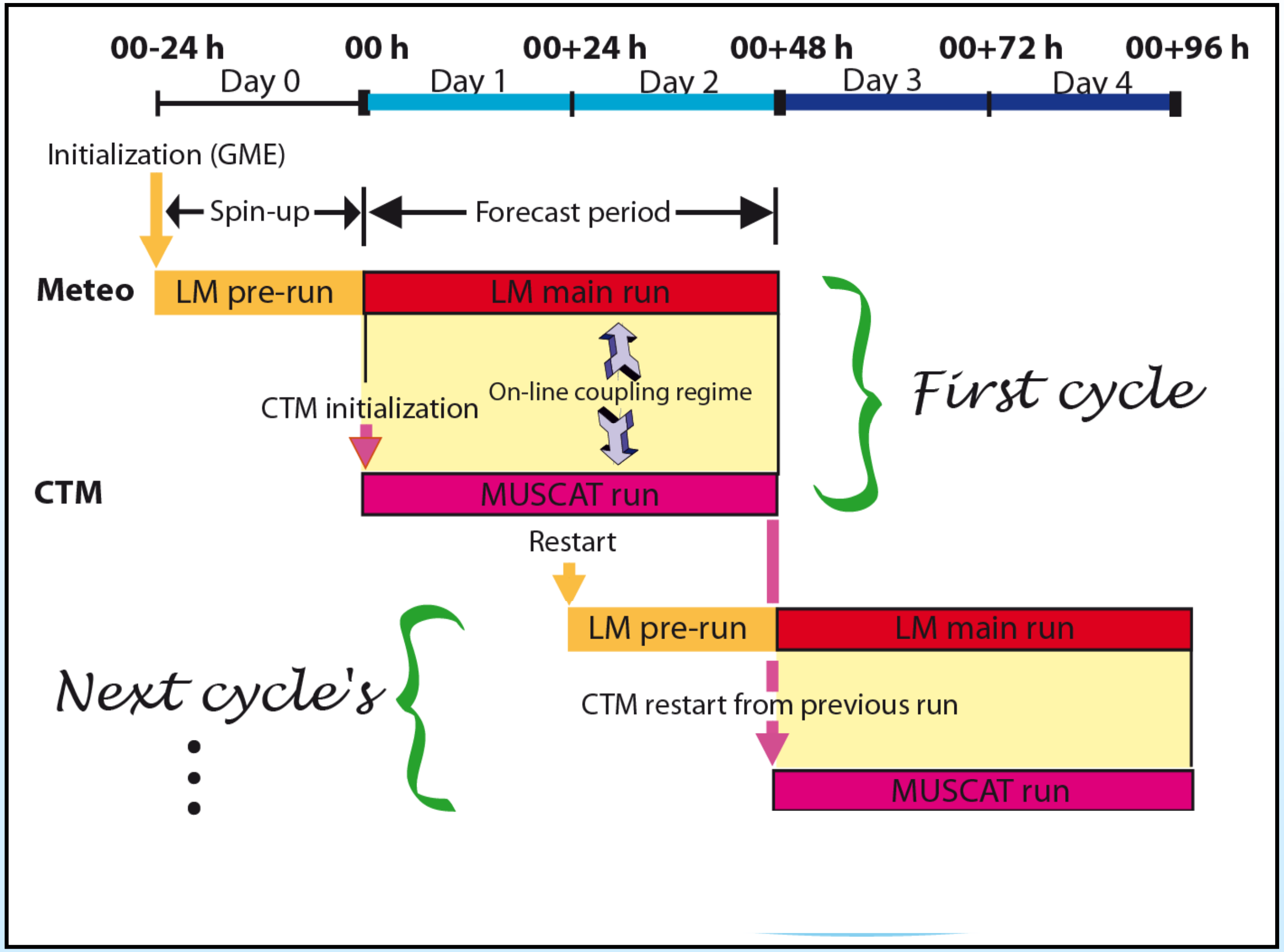
# Meteorological situation



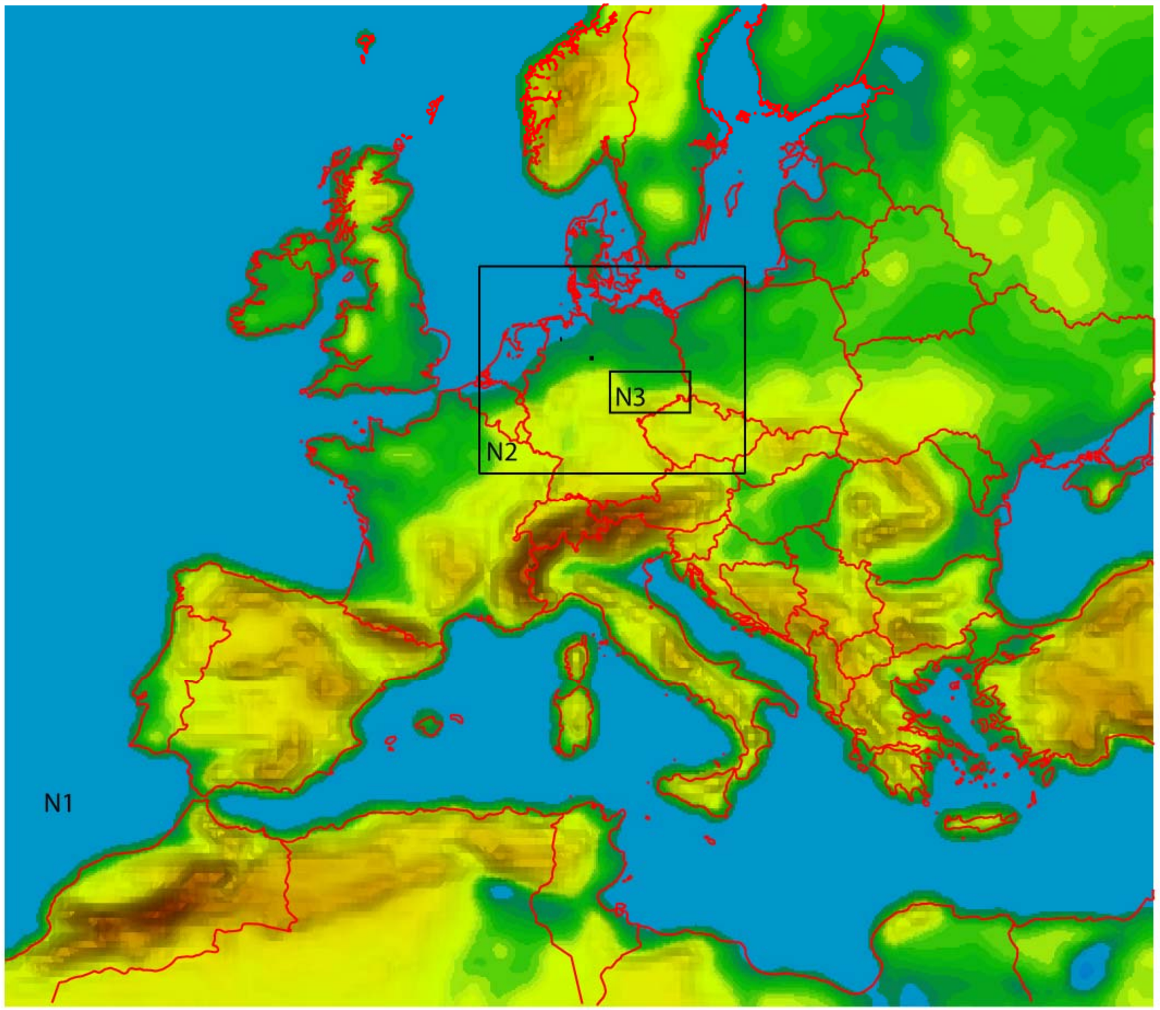
# Tracer simulations to characterize meteorology



# Time Schedule for Model Runs



# LM Grid Nesting




**<u>Size resolution</u>**

**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**

**<u>Time period:</u>**

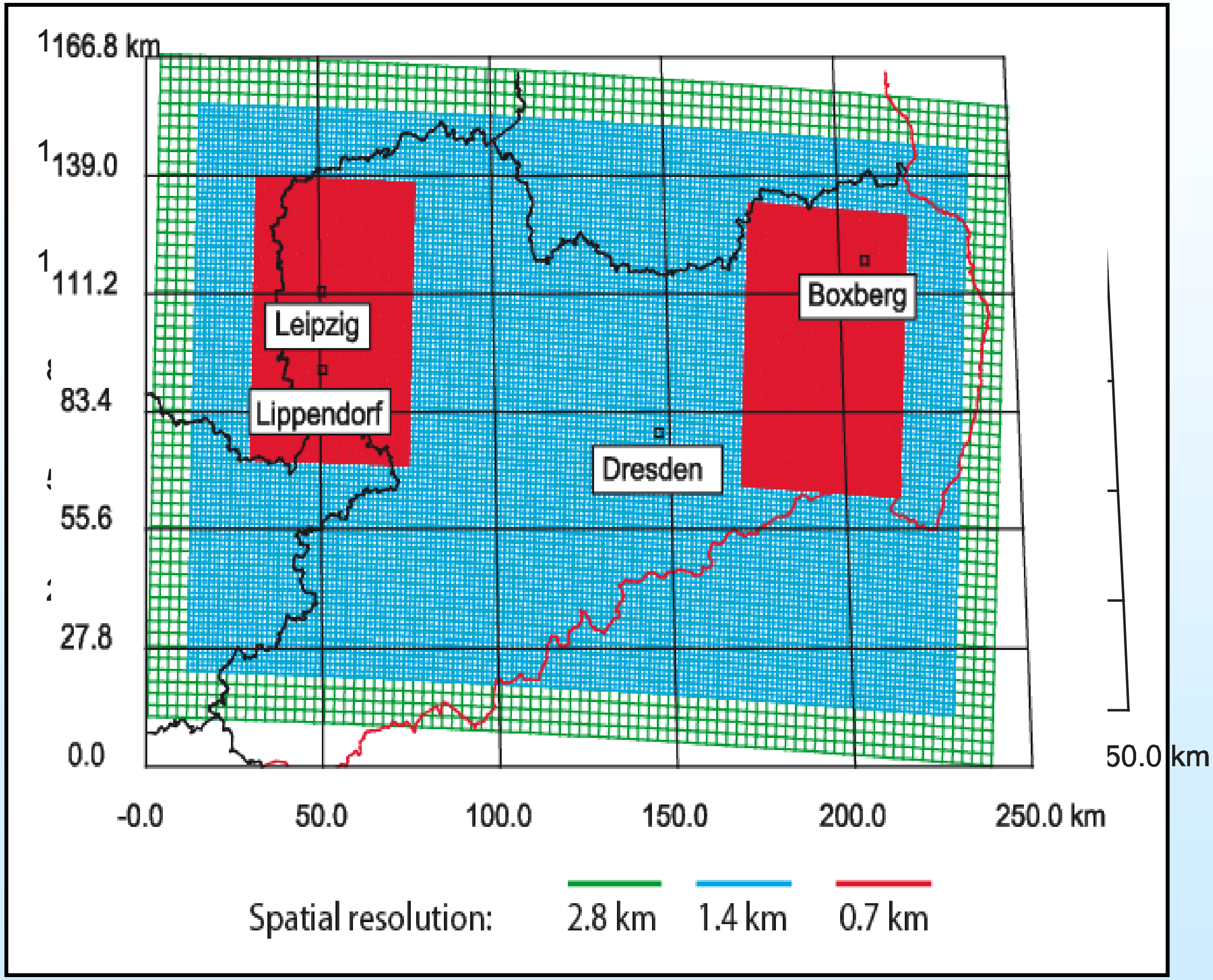
**12. – 19. October 2006**

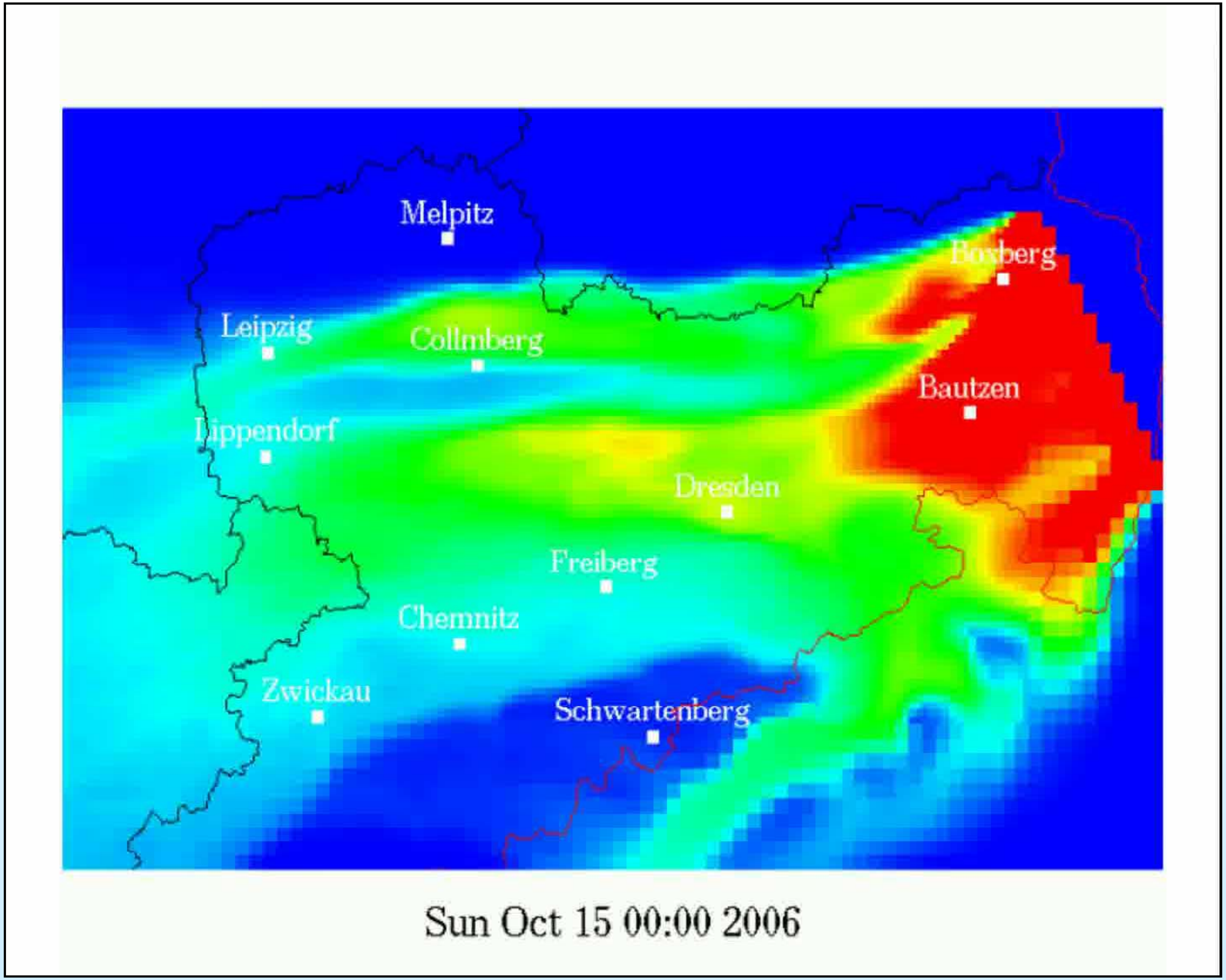
**N1 runs to generate appropriate boundary values !**

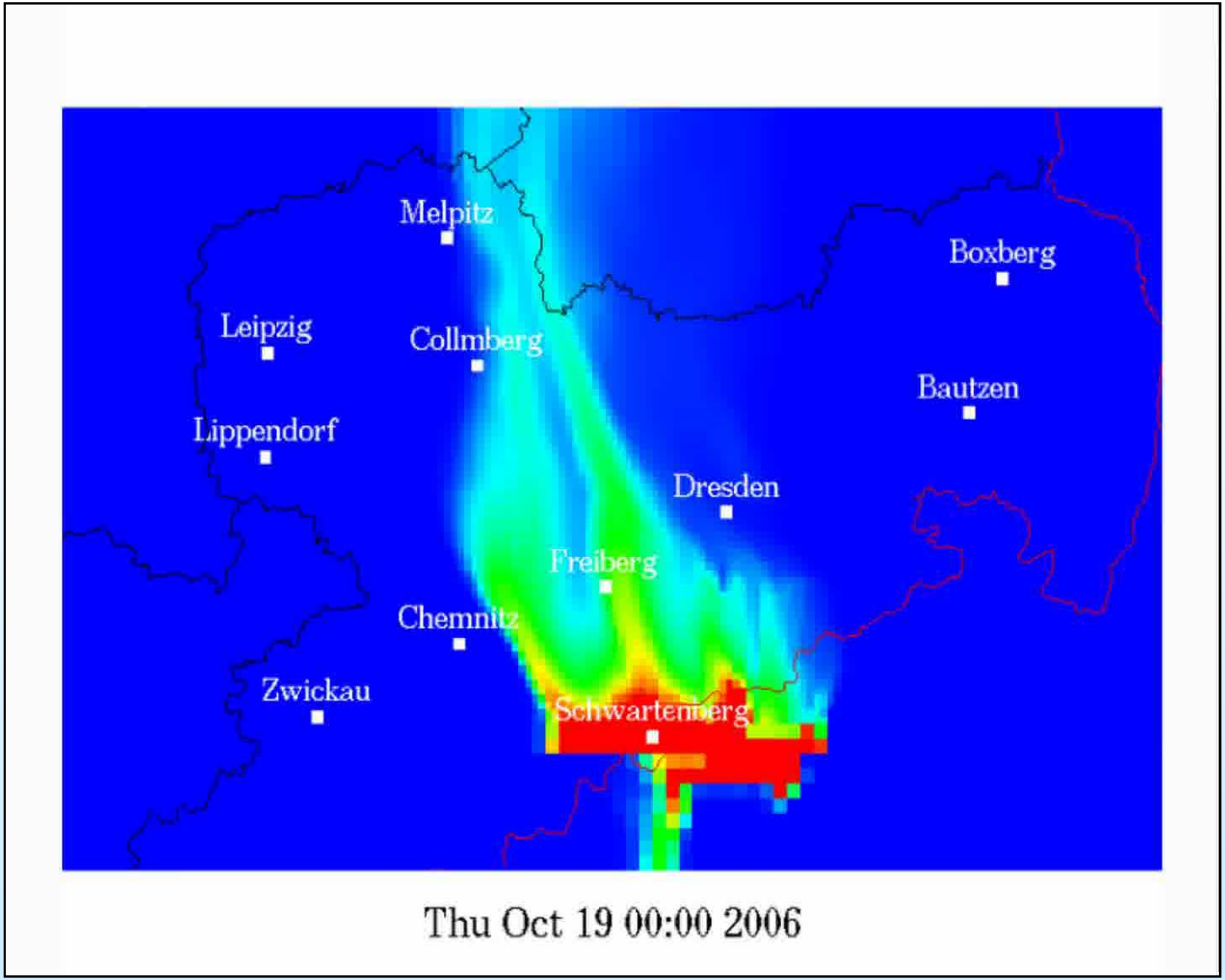
# Example of N3 Grid of MUSCAT

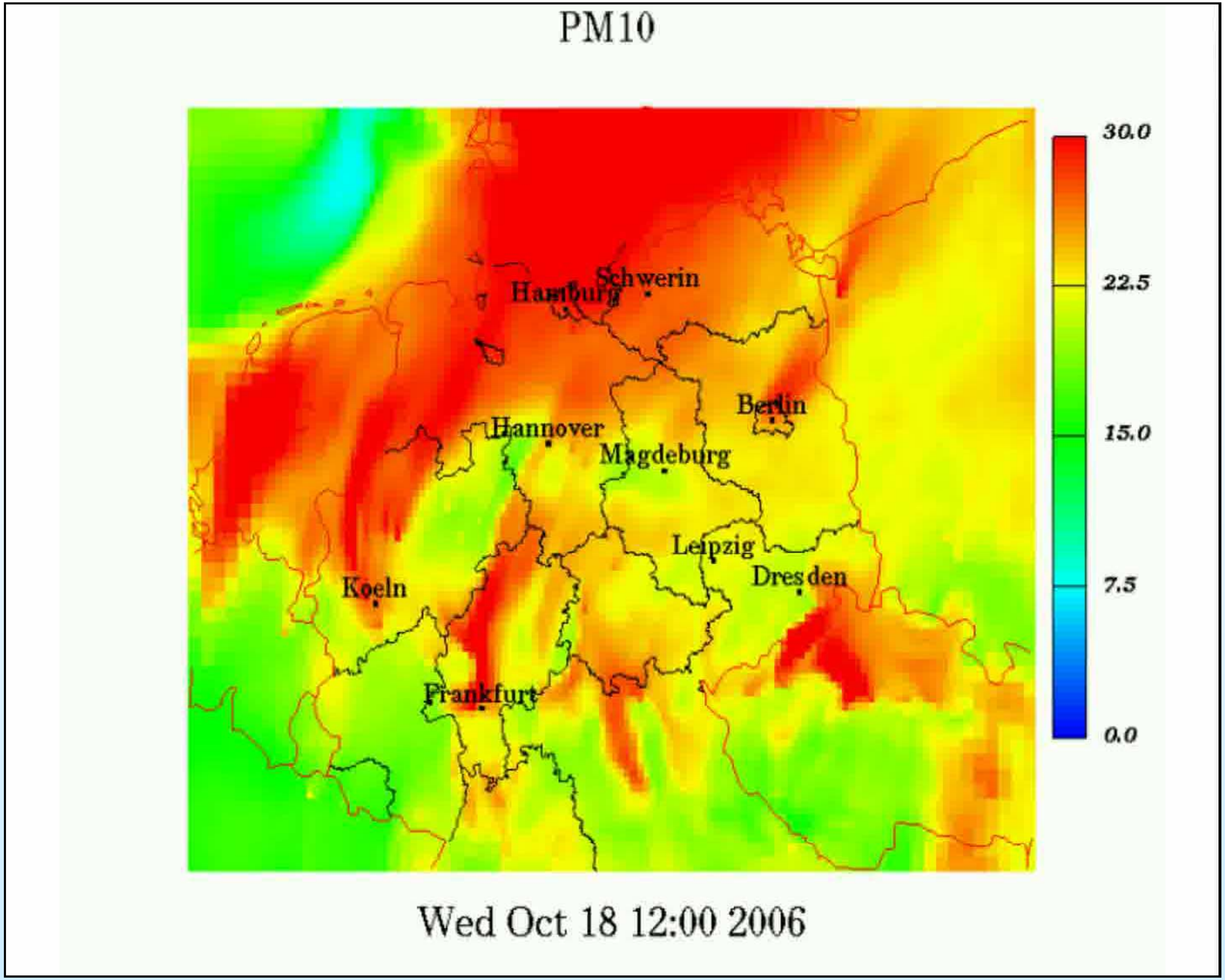
**Here:**

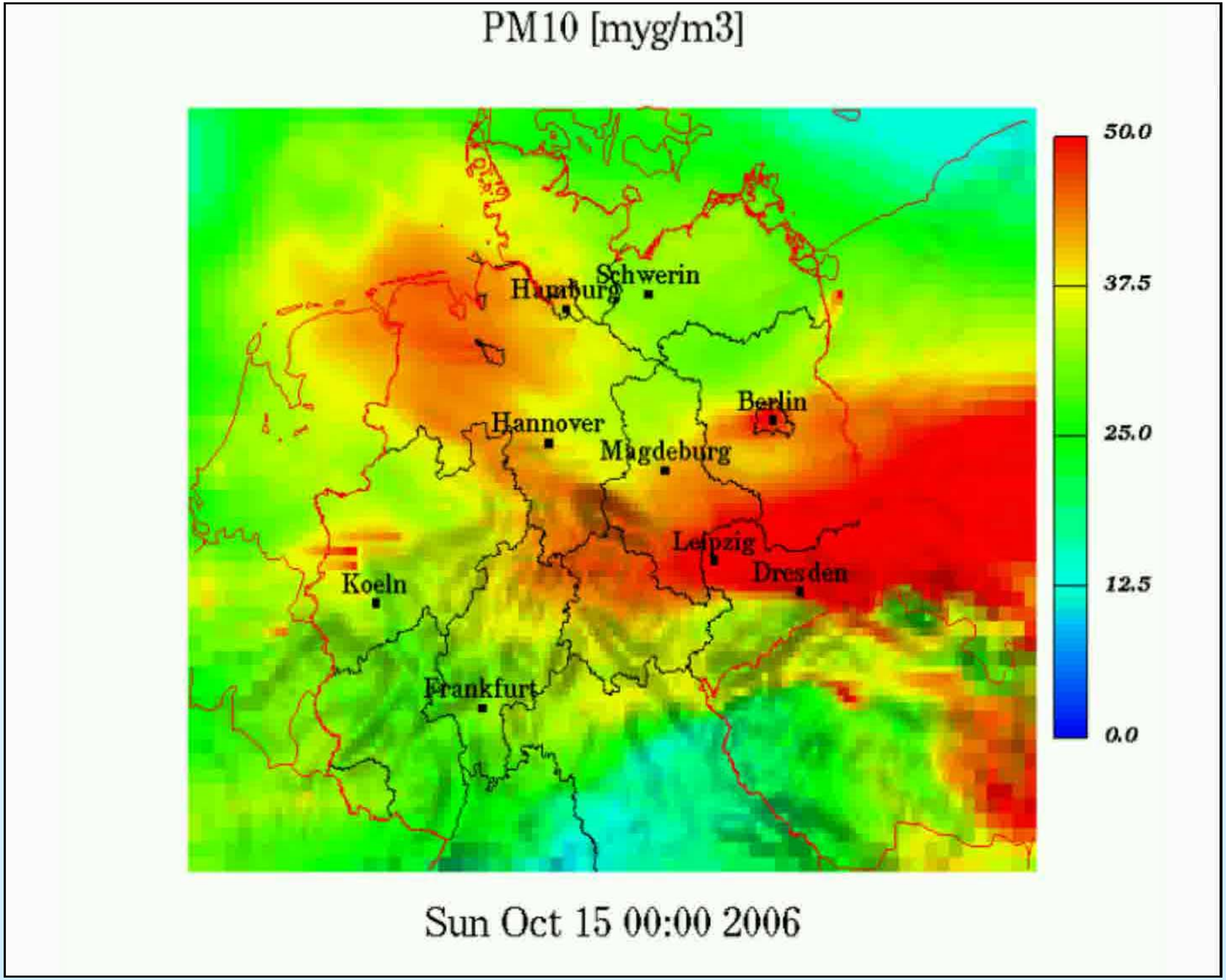
**Only 2.8 km and 1.4 km resolution !**



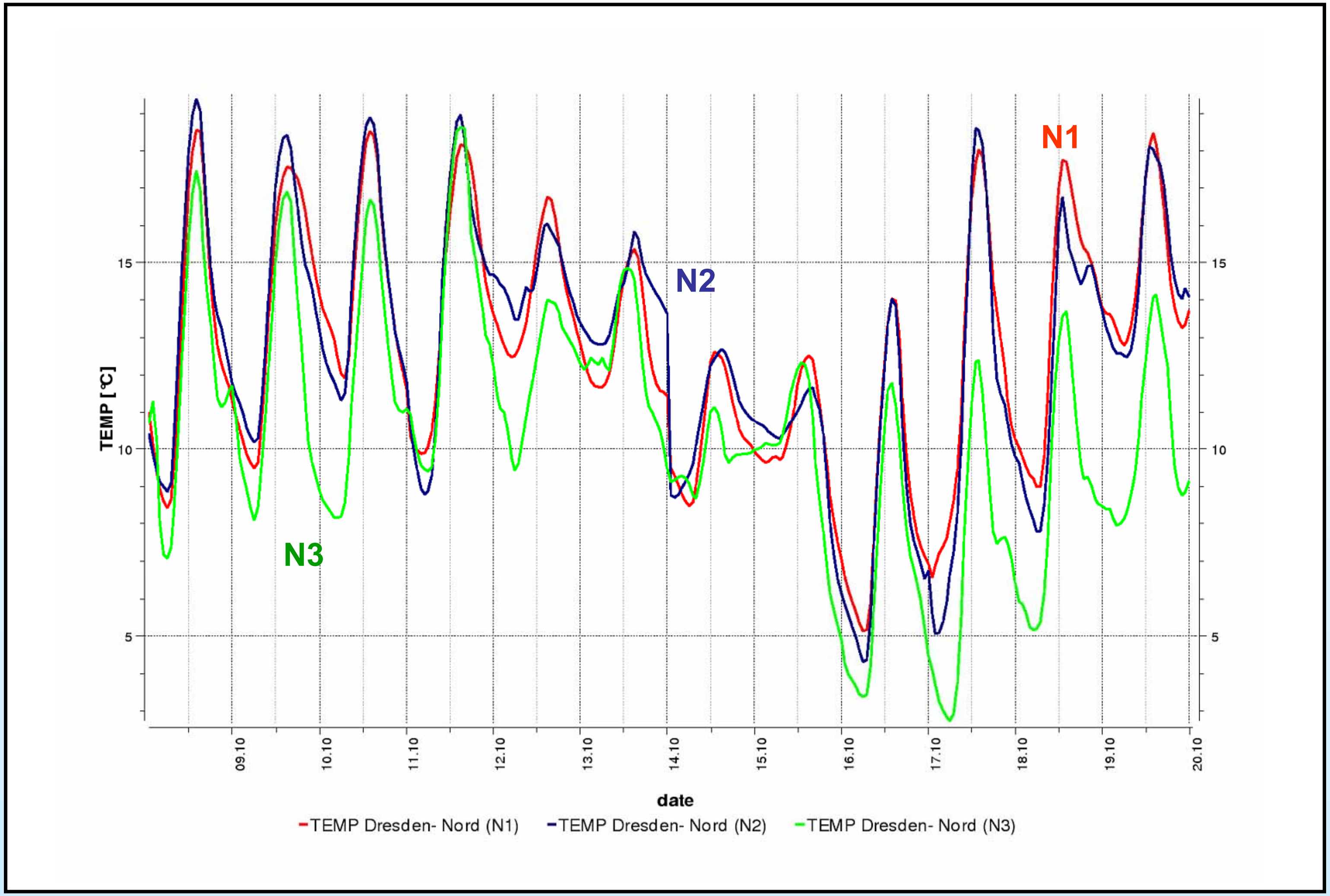

Melpitz
Boxberg
Leipzig
Collmberg
Bautzen
Lippendorf
Dresden
Freiberg
Chemnitz
Zwickau
Schwartenberg
Sun Oct 15 00:00 2006


Melpitz
Boxberg
Leipzig
Collmberg
Bautzen
Lippendorf
Dresden
Freiberg
Chemnitz
Zwickau
Schwartenberg
Thu Oct 19 00:00 2006

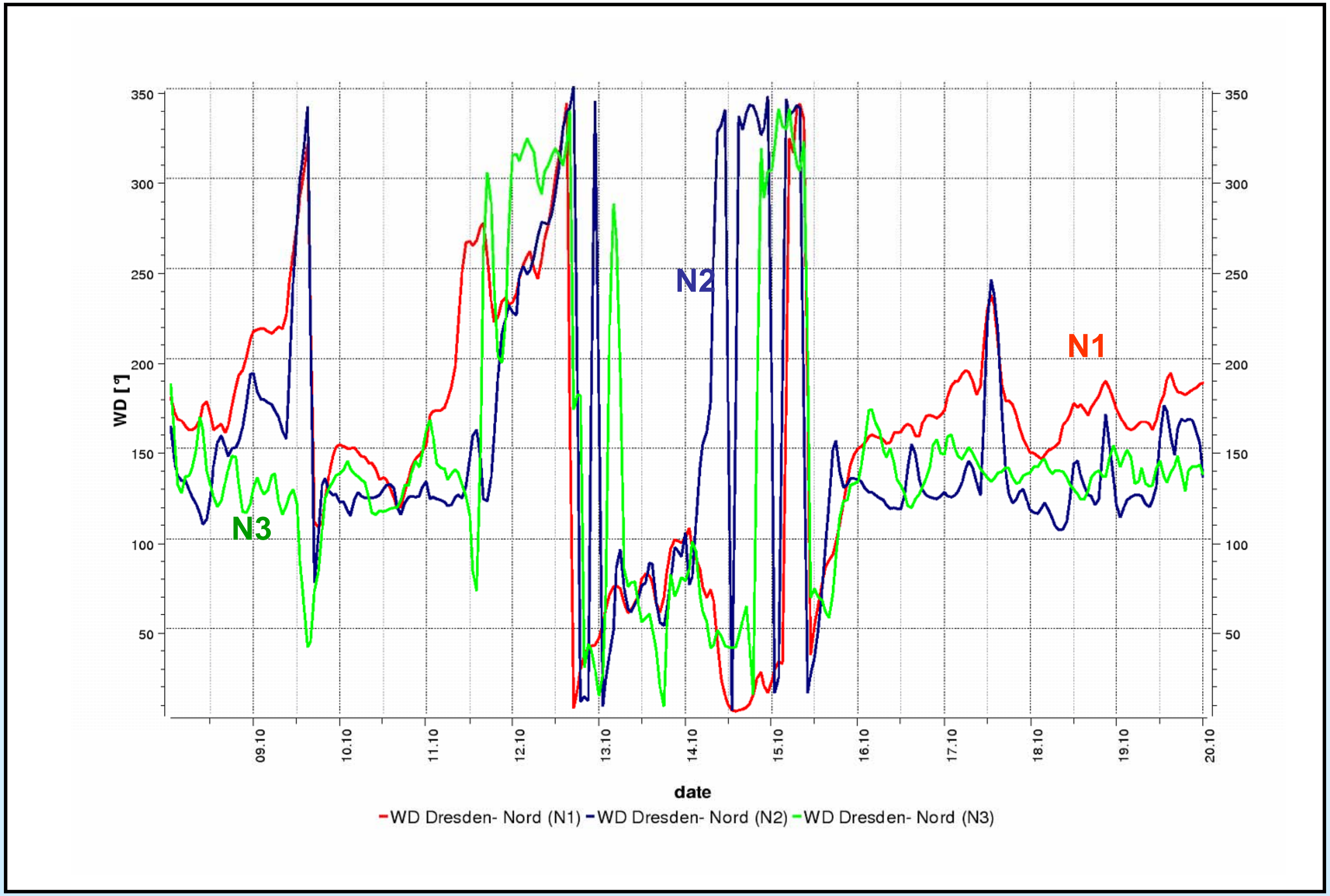

PM10
30.0
22.5
15.0
7.5
0.0
Schwerin
Hamburg
Berlin
Hannover
Magdeburg
Leipzig
Dresden
Koeln
Frankfurt
Wed Oct 18 12:00 2006


PM10 [myg/m3]
Schwerin
Hamburg
Berlin
Hannover
Magdeburg
Leipzig
Dresden
Koeln
Frankfurt
50.0
37.5
25.0
12.5
0.0
Sun Oct 15 00:00 2006

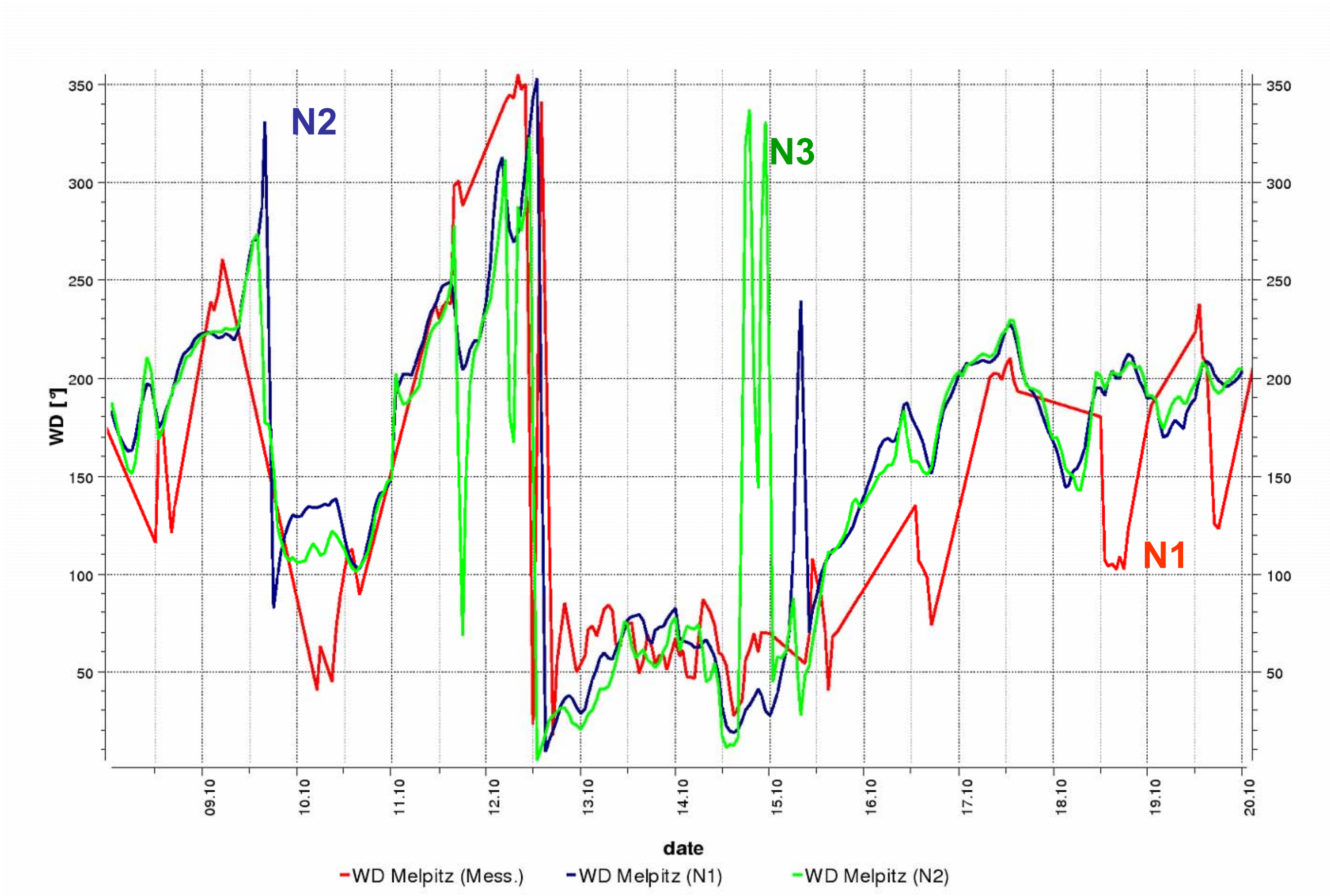
# Temperature [K], Dresden-Nord



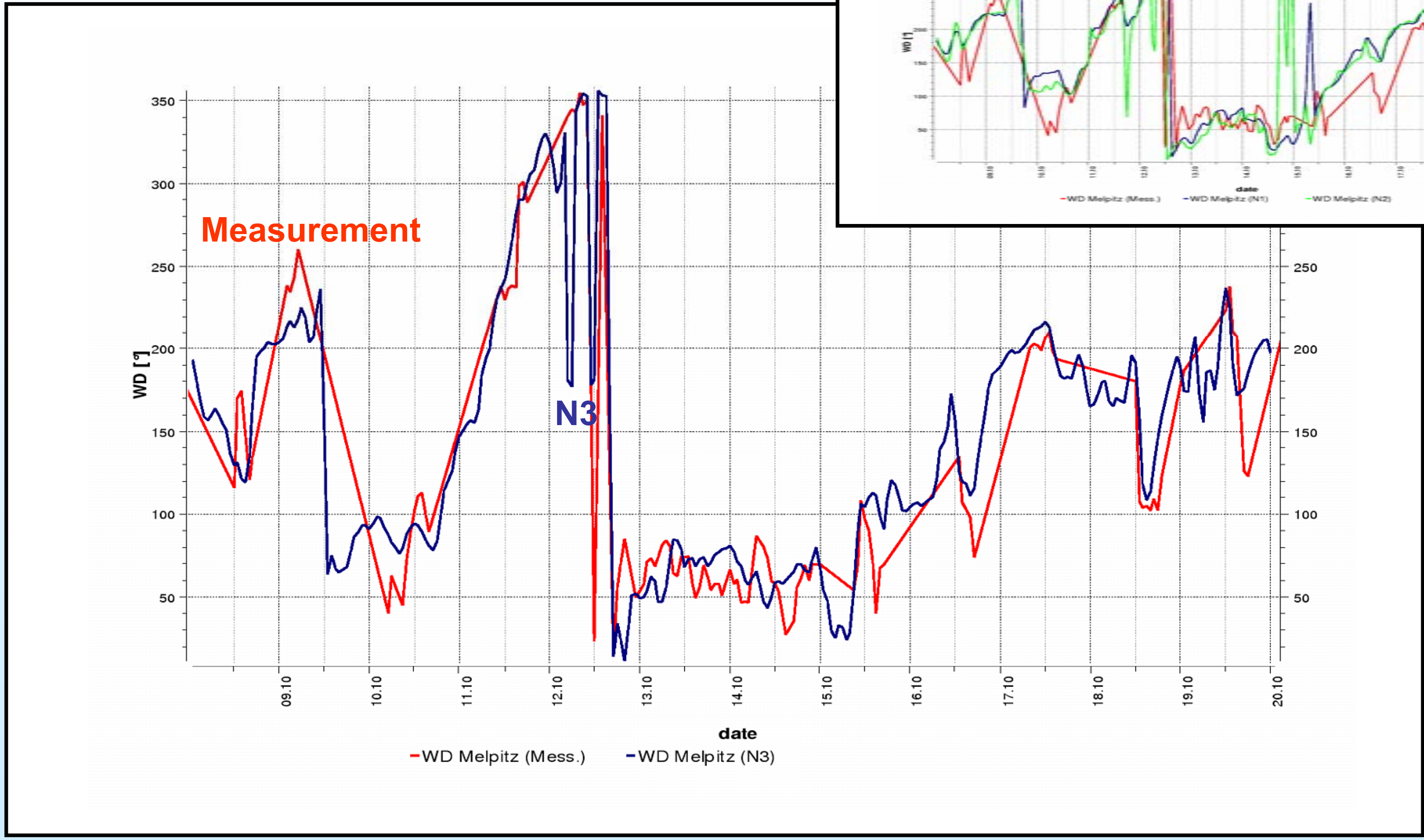
# Wind direction [°], Dresden-Nord

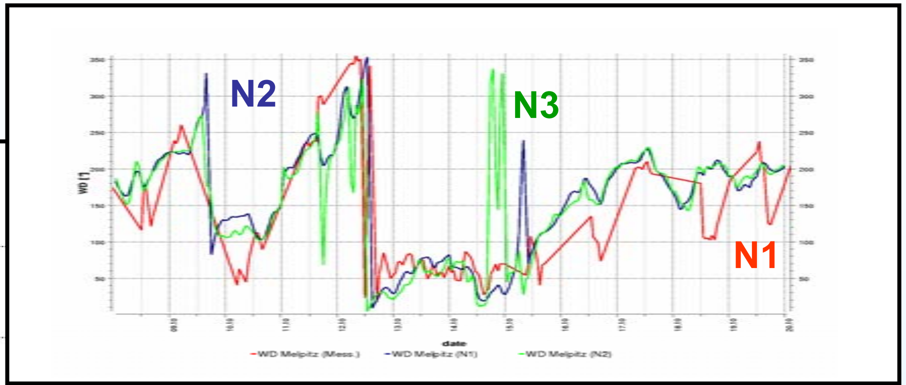


# Wind direction [°], Melpitz

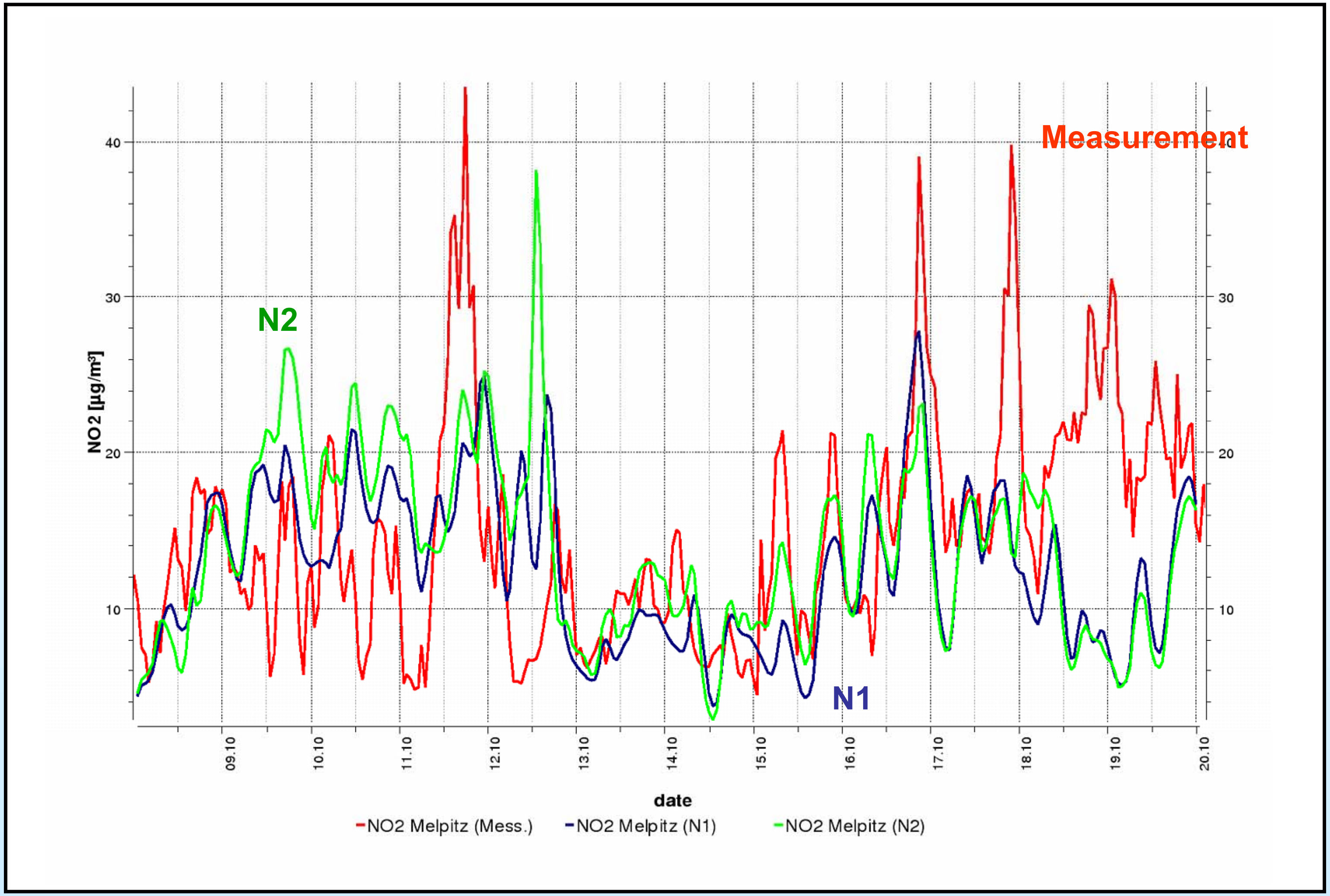


# Wind direction [°], Melpitz

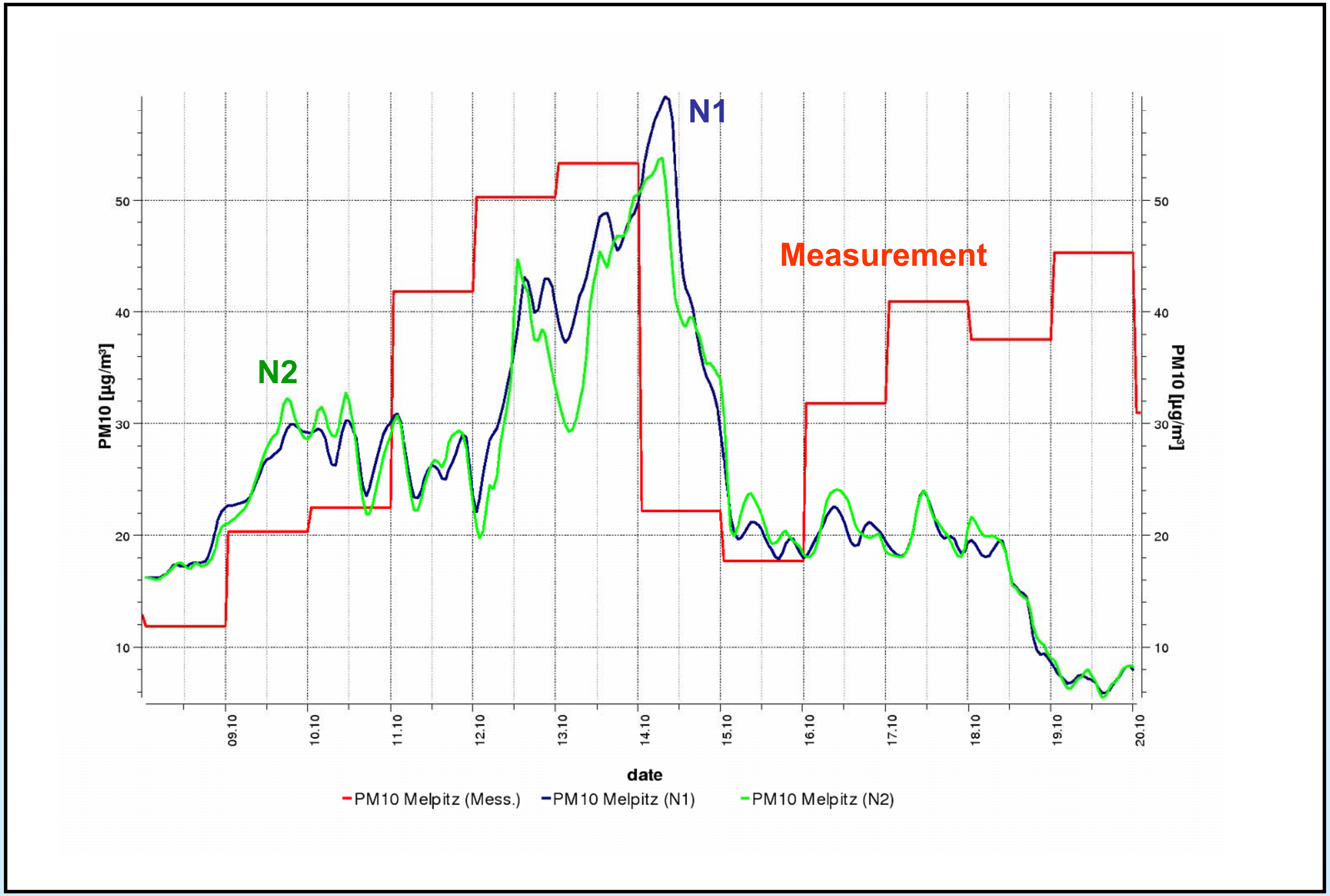


# NO2 [µg/m3], Melpitz



# PM10 [µg/m3], Melpitz



# “Land-Fire“ Episode

Question:

The influence of land-fire emissions in Russia on hotspots in Saxony in the beginning of May 2006 ?

COST 728, Model intercomparison (Mikhail Sofiev)

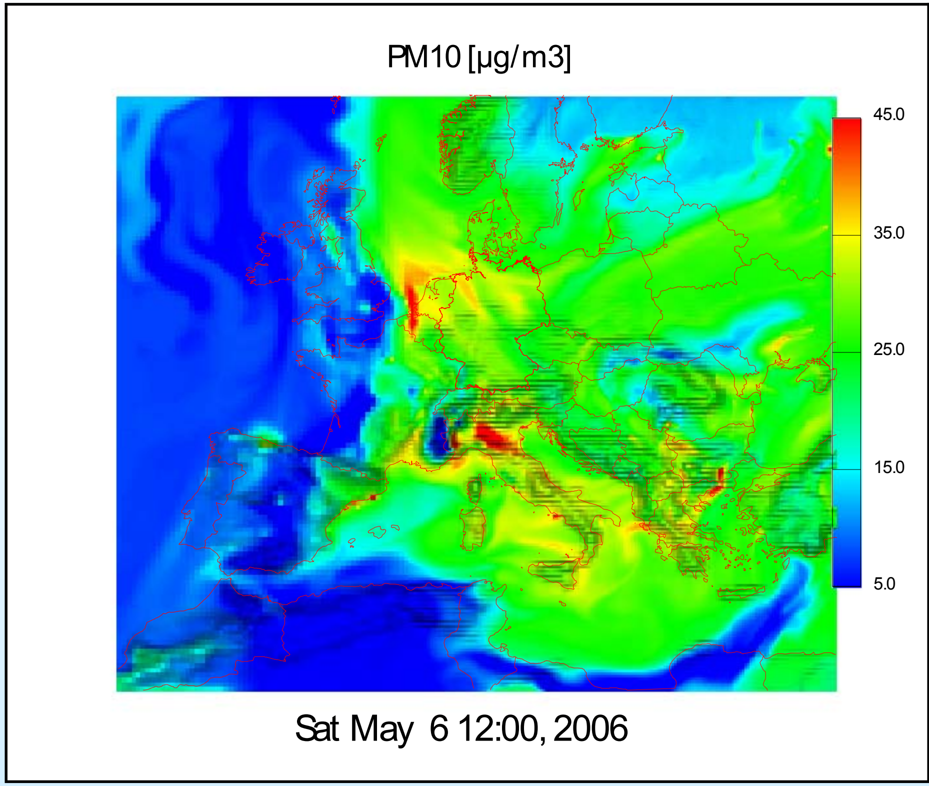
Simulation area: N1

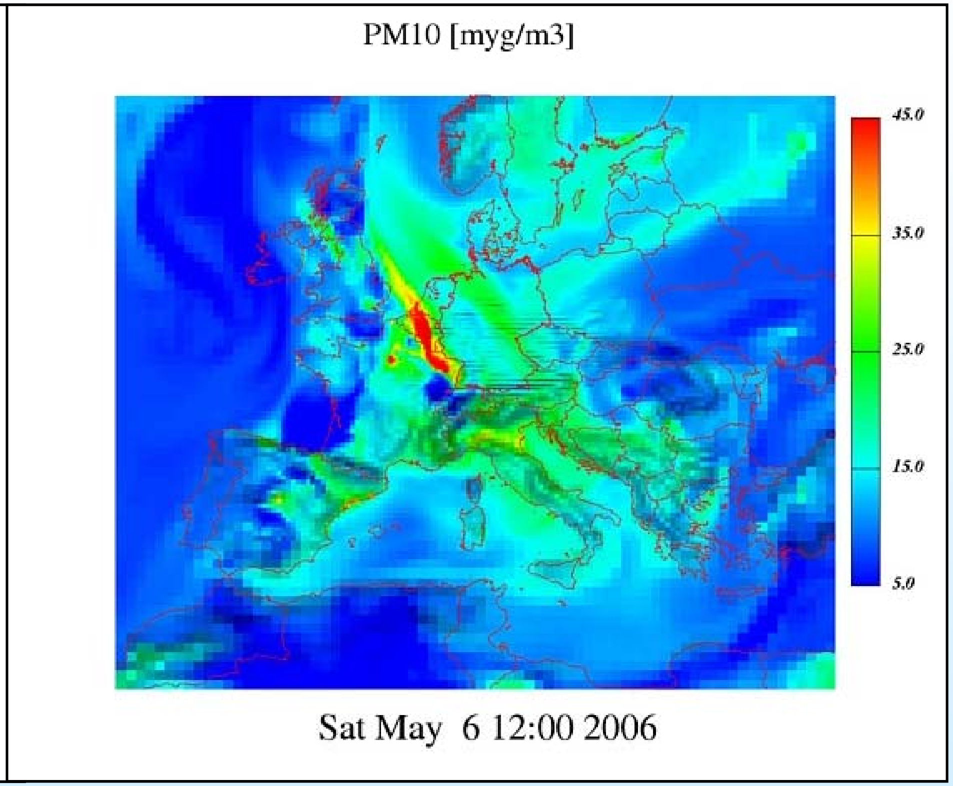
Simulation period: 15.04.2006 – 15.05.2007

Emissions: PM2.5 ( ⇨ gas phase, PM10, EC, POC, …)

Focus on 2. May – 10. May 2006.

# “Land-Fire“ Episode (15.04.-12.05.2006)

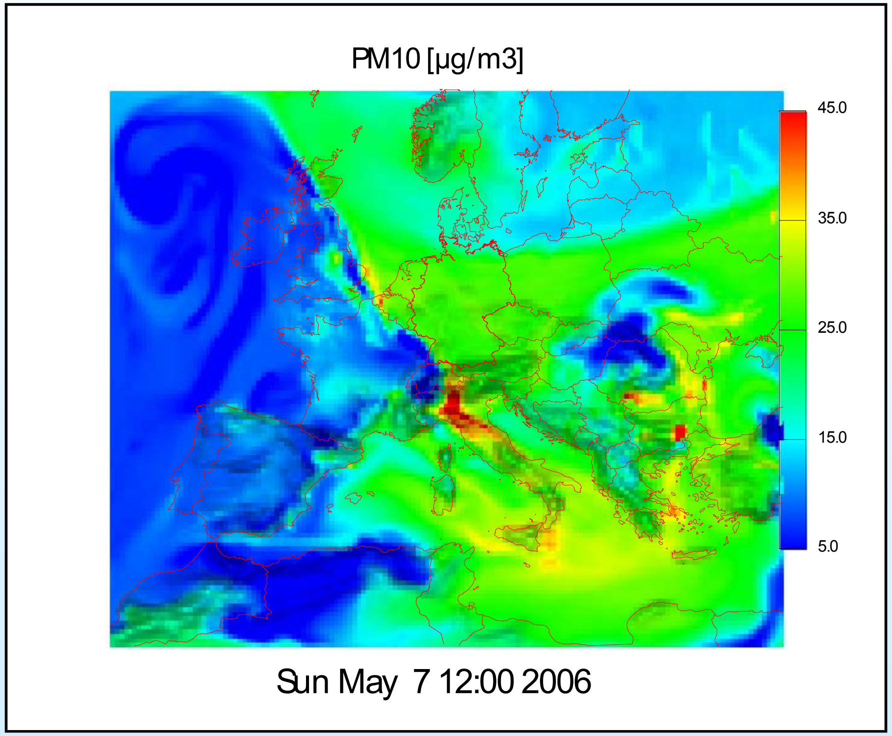


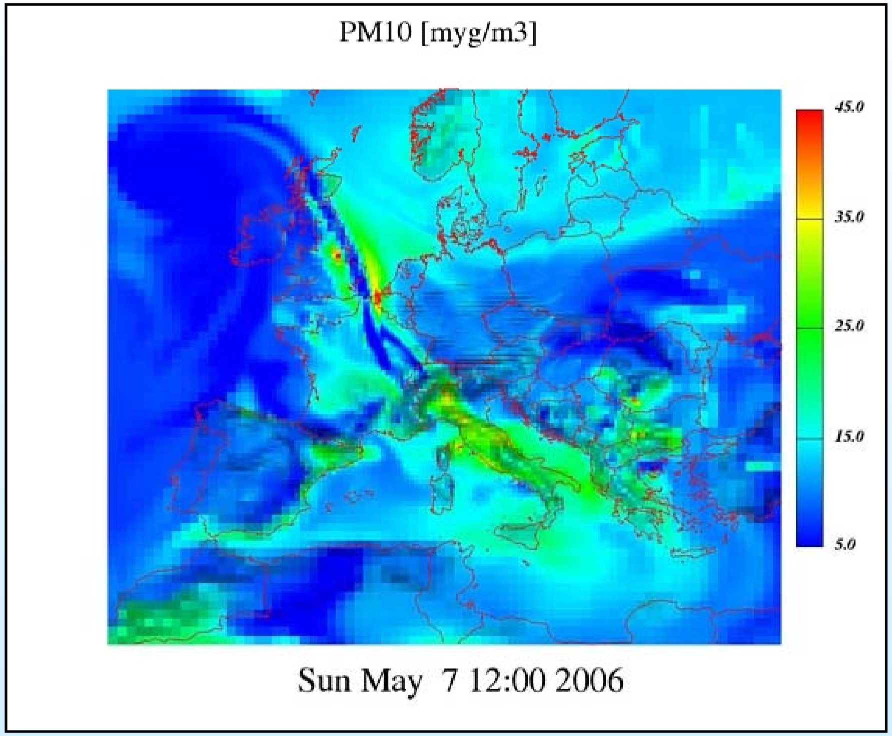

“land-fire“ emissions included

not included

# “Land-Fire“ Episode  (15.04.-12.05.2006)

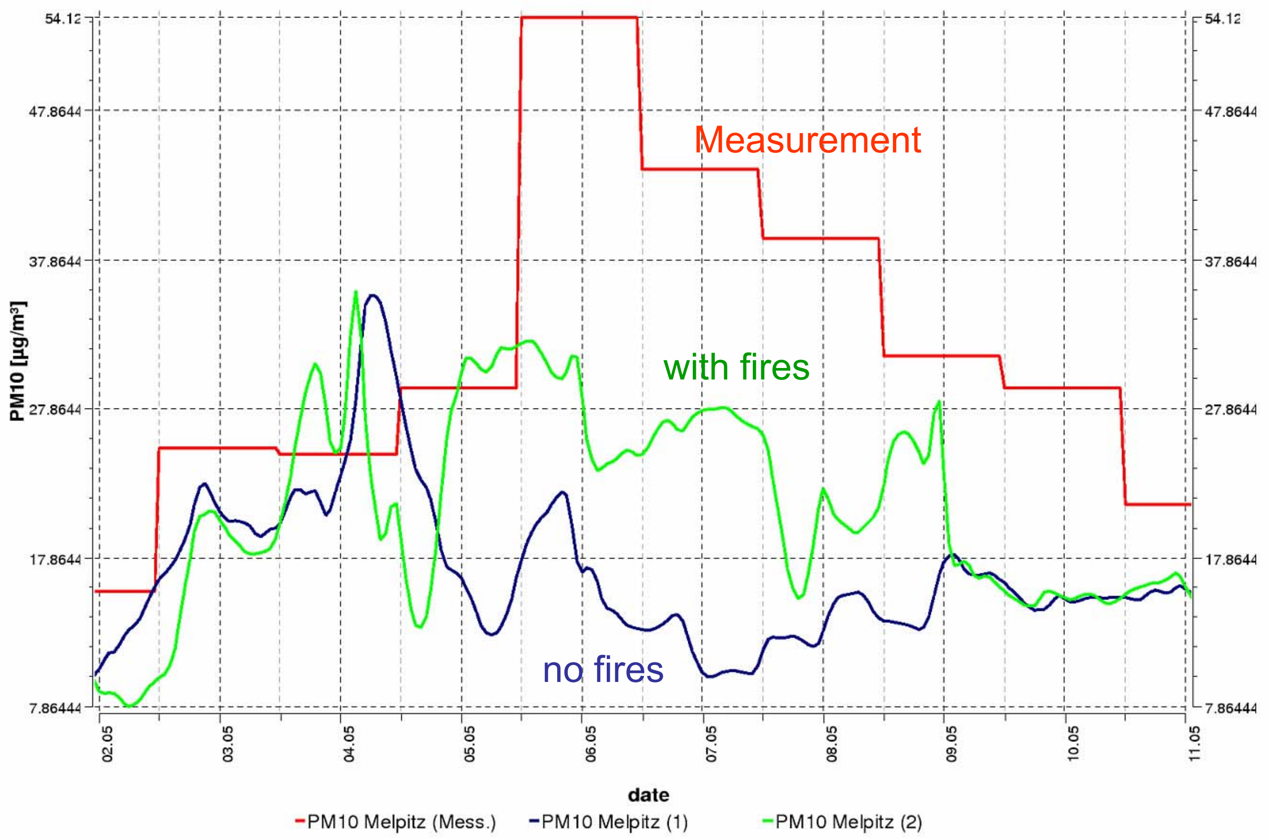



“land-fire“ emissions included

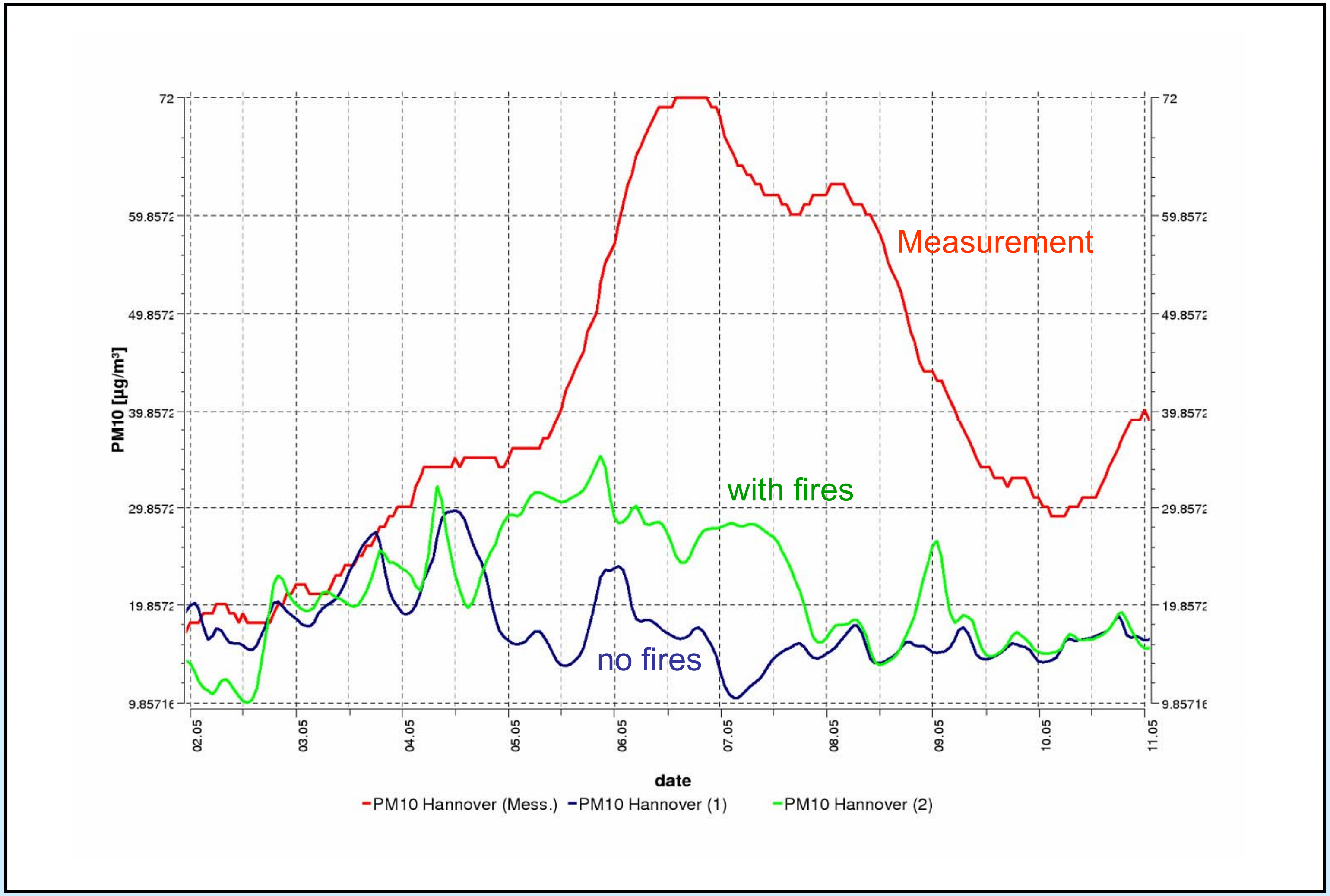



not included

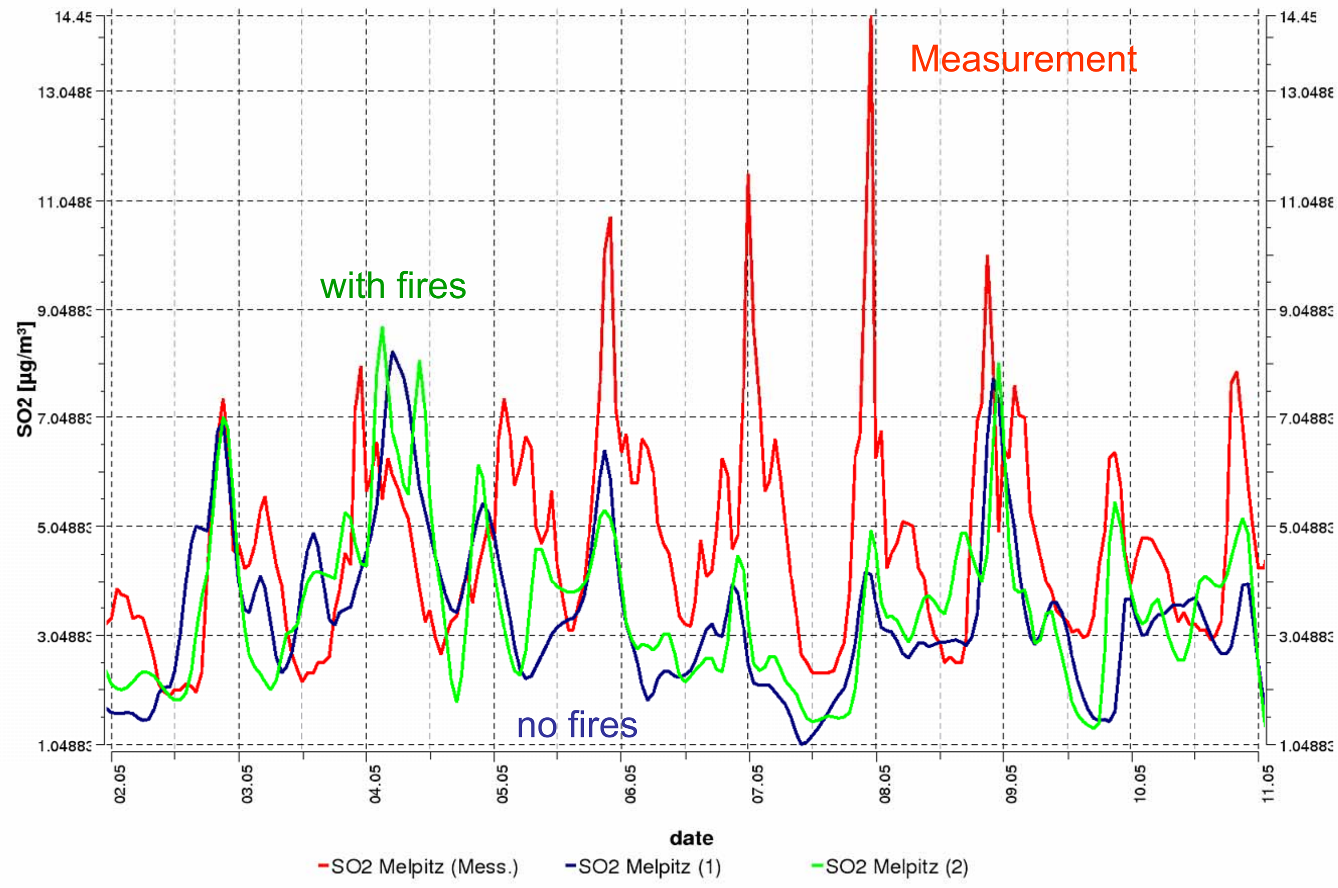
# PM10 [µg/m3], Melpitz



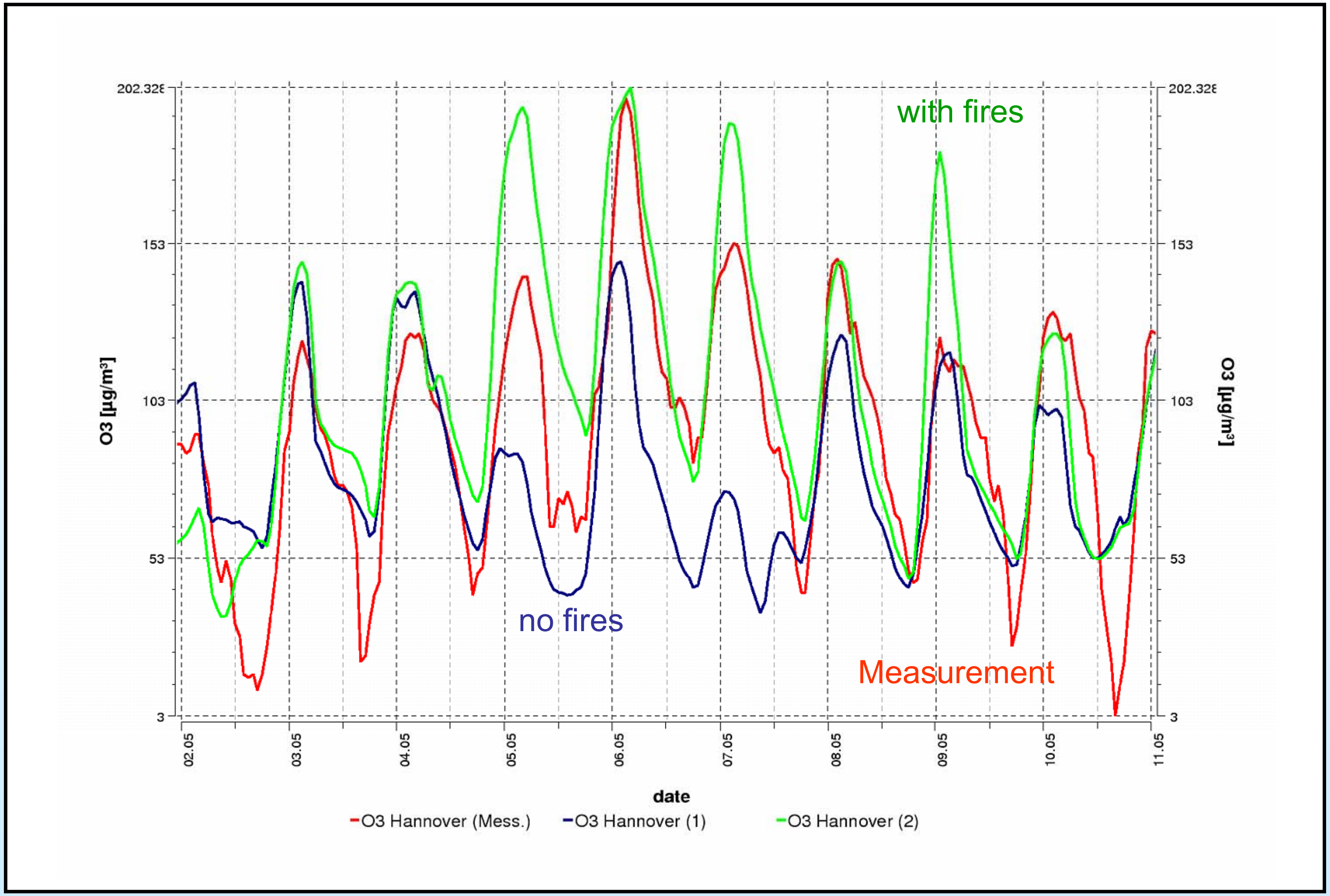
# PM10 [µg/m3], Hannover



# SO2 [µg/m3], Melpitz



# O3 [µg/m3], Hannover



# Outlook

**Dust modelling**

1. Refinement of the dust emission scheme and dust source areas, convective transport of dust (SAMUM II)
2. Processing of Saharan dust (aging), comparison with EARLINET data

**Multiphase processes in clouds**

Spectral Mikrophysics in LM (SPP1167)

DFG-Proposal "Parallelizing cloud processes in LM":
*dynamical data structures , load balancing , "multirate" time integration (together with TU Dresden)*

Laboratory work at IfT (LACIS, CAPRAM-development)

*We thank the LfUG Saxony, the ZIH Dresden, the ZAM Jülich for support and the DWD for cooperation.*

# Thank you!