Coupled time-integration of atmospheric chemistry-transport processes by using multirate implicit-explicit schemes

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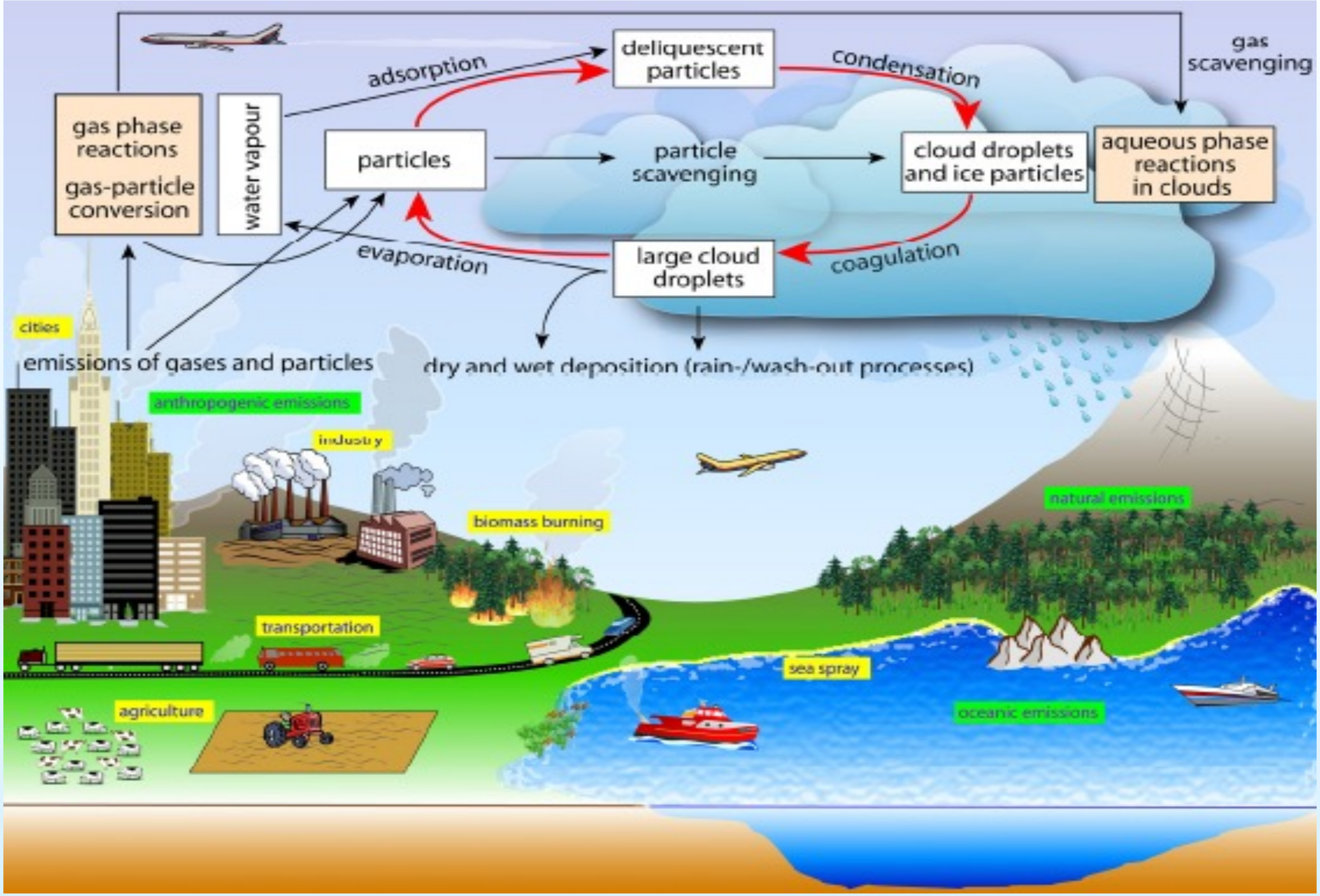
Outline

- **Introduction**
- **Model system COSMO-MUSCAT**
- **Numerics**
  - Model coupling
  - Static grid nesting (“multiblock” approach)
  - Time integration (IMEX scheme, multirate)
- **Air quality application *(“cooling towers” in Saxony)***
- **Conclusions**

Tropospheric Processes



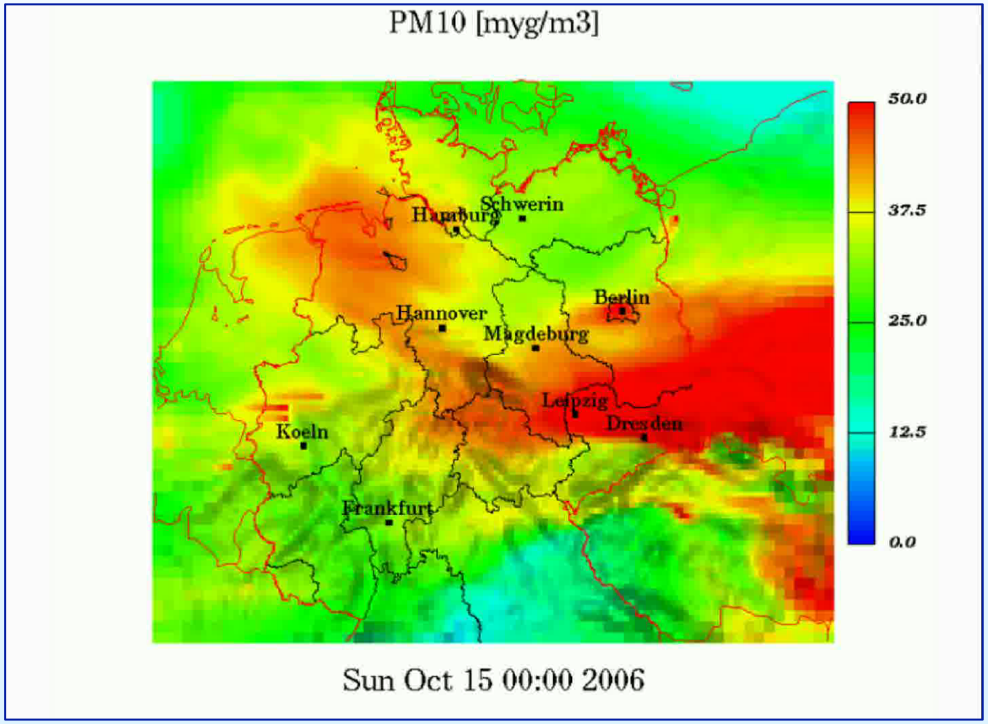
Schrödner (2009)

TROPOS

Focus:

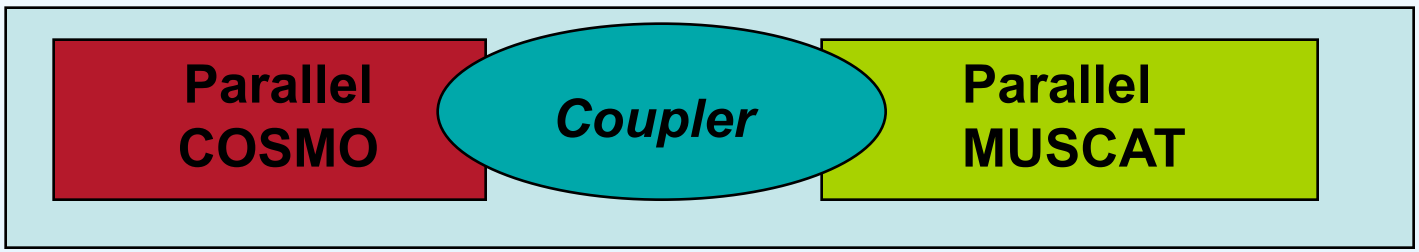
- ***Process studies of tropospheric multiphase system***
- ***Interactions aerosols – clouds – radiation***
- ***Climate-relevant processes***
- ***Air quality***
- ***Impact on human health and ecosystems***

"Air Quality": *Particulate Matter Hotspots*
(*Long Range Transport*)



Chemistry-Transport Model MUSCAT
(« *MUltiScale Chemistry Aerosol Transport* »)

- Transport and chemical transformation of gas phase pollutants and particles in the atmosphere
- Online coupling with COSMO



- Applied from regional to urban scale
- Mainly used in forecast mode without data assimilation and nudging
- Direct and semi-direct feedback is implemented.

The Meteorological Model COSMO
(COnsortium for Small-scale Modeling)
(DWD: Doms, Schättler, et al. 1998-2014; Baldauf et al. 2011)

- non-hydrostatic, compressible
- formulated with regard to a hydrostatic reference state
- staggered grid
  - horizontal: uniform, orthogonal
  - rotated Lambda-Phi grid
  - hybrid vertical coordinate
- operational mode for weather forecast, regional scale
- boundary and initial data from GME
- highly parallel
- Usually: Operational setup (Version: 5.01)
  prognostic TKE, multi-layer surface model, …

Chemistry Transport Model System COSMO-MUSCAT

Gas phase ("*read in*"):

- **RACM** *(Stockwell et al., 1997)* **+**
- **MIM2** *(Karl et al., 2006)*

Aerosol model:

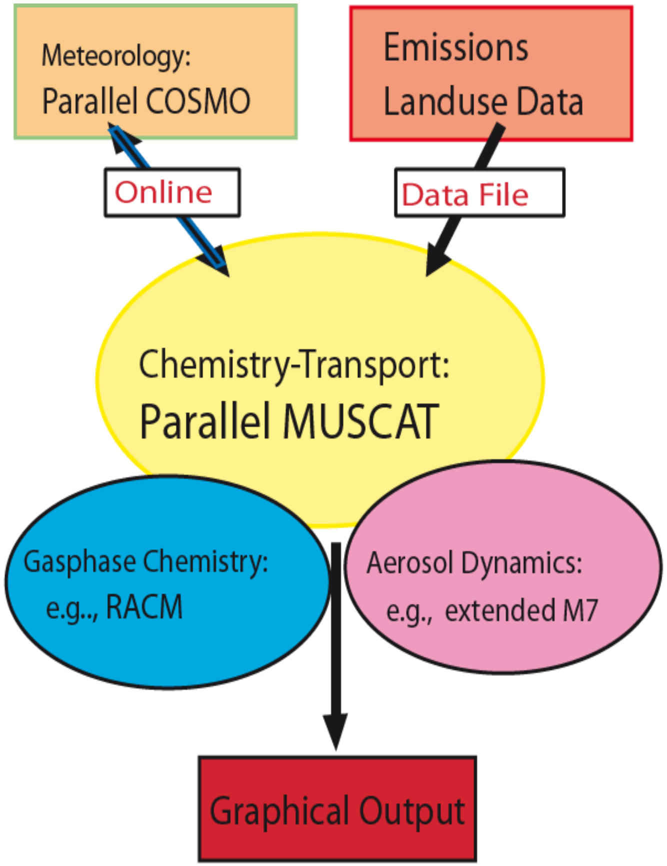
- **Mass-based approach (e.g., *EMEP*) *or***
- **Modal approach M7 *(Vignati et al, 2004)*:**
  - **4 internal-mixed and 3 external modes**
  - **sulphate, sea salt, dust, EC, OC**

  extended by
  - **nitrate and ammonium**
  - **SIA by *ISORROPIA* *(Nenes et al., 1998)***
  - **SOA by SORGAM *(Schell et al., 2001)***
- **Dust: sectional (5 bins)**

Dry and wet deposition, sedimentation

Emissions:

- **Anthropogenic (11 snaps, area + point, fires)**
- **Biogene *(Steinbrecher et al., 2007)***
- **Seasalt *(Sofiev et al., 2013)***



The coupled model system COSMO-MUSCAT

Reaction system from input file:

High flexibility

Gas phase mechanism:

RACM-MIM2

95 species, 245 reactions

(Stockwell et al, 1997; Karl et al, 2006)

Currently, cloud-chemistry is included!

C3.0RED

(up to 110 aqueous species in each droplet class)

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
```

Advection-Diffusion-Reaction Equations

Mass balance equation in flux form:

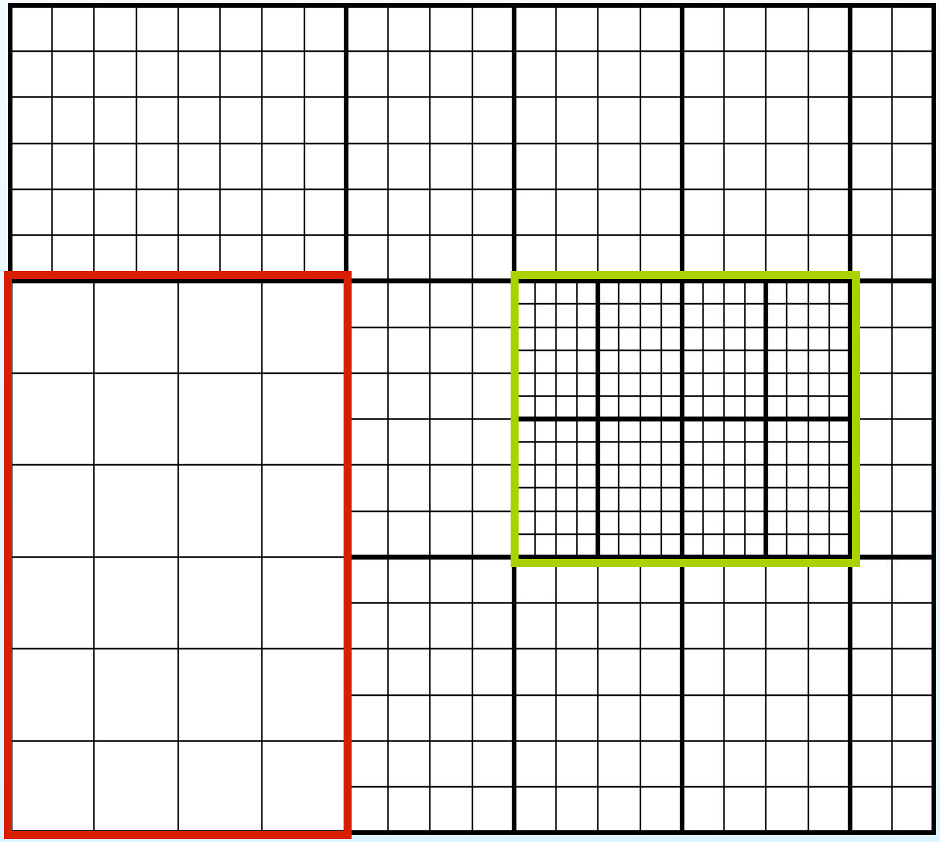
$$\frac{\partial c}{\partial t} + div(\vec{v}\rho\frac{c}{\rho}) = div(K\rho\nabla\frac{c}{\rho}) + R(c;T,q) + Q_c$$

c	…	*vector of species concentrations*
$\vec{v}$	…	*wind vector*
ρ	…	*density of air*
T, q	…	*temperature, humidity*
R	…	*chemical reaction terms*
Q	…	*external sources (emissions)*

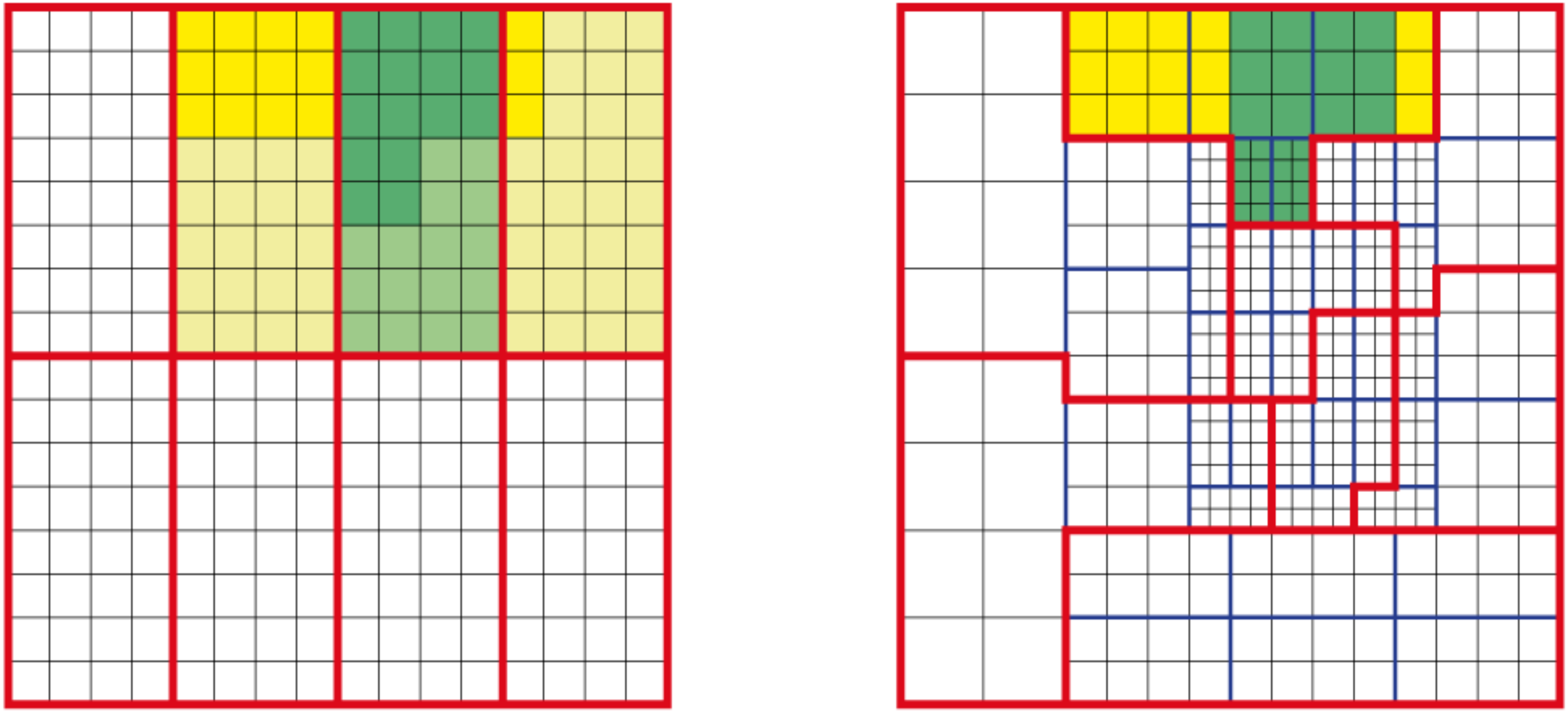
Decomposition of Horizontal Domain

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.

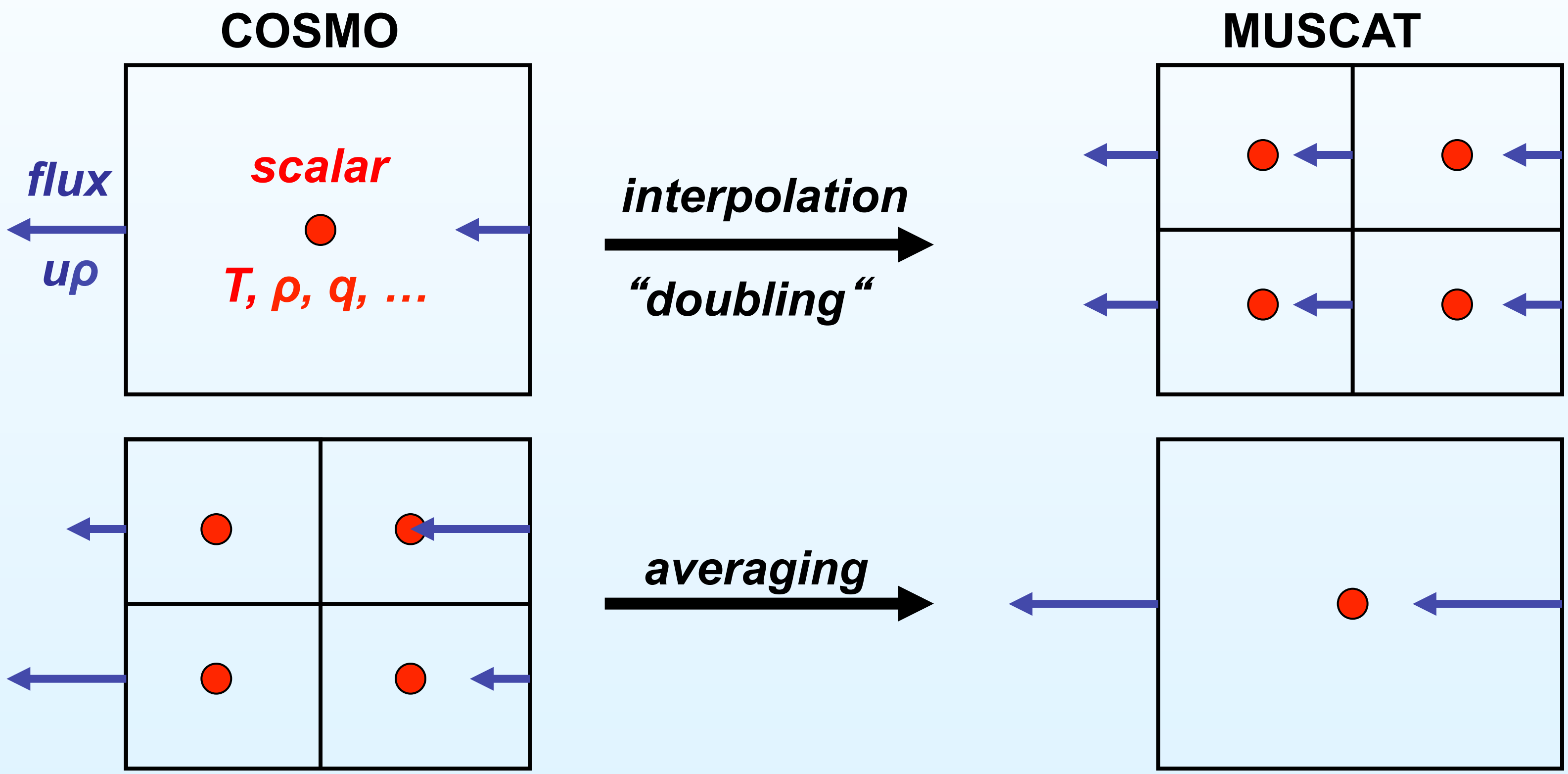


Coupling Scheme: Grid Structure



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

Spatial grid transformation of meteorological arrays



Finite volume approach saves mass conservation if this is fulfilled in the original COSMO grid !!

Numerical methods

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

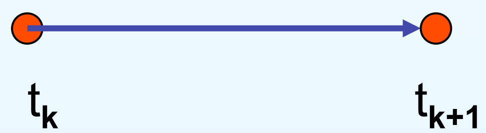
- **Time-integration: IMEX scheme** *(Knoth & Wolke, 1998)*
  - ***Explicit second-order Runge-Kutta for horizontal advection***
  - ***Second order BDF method for the rest:*** *Jacobian is calculated explicitly, linear systems by Gauss-Seidel iterations or AMF*

IMEX Time Integration Scheme

$$c' = \boxed{f_E(t,c)} + \boxed{f_I(t,c)}$$

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

<u>IMEX–Heun2</u>

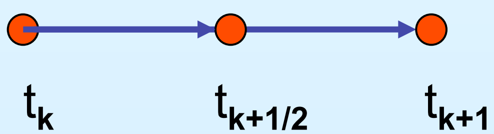


$$Y_1 = c(t_n)$$

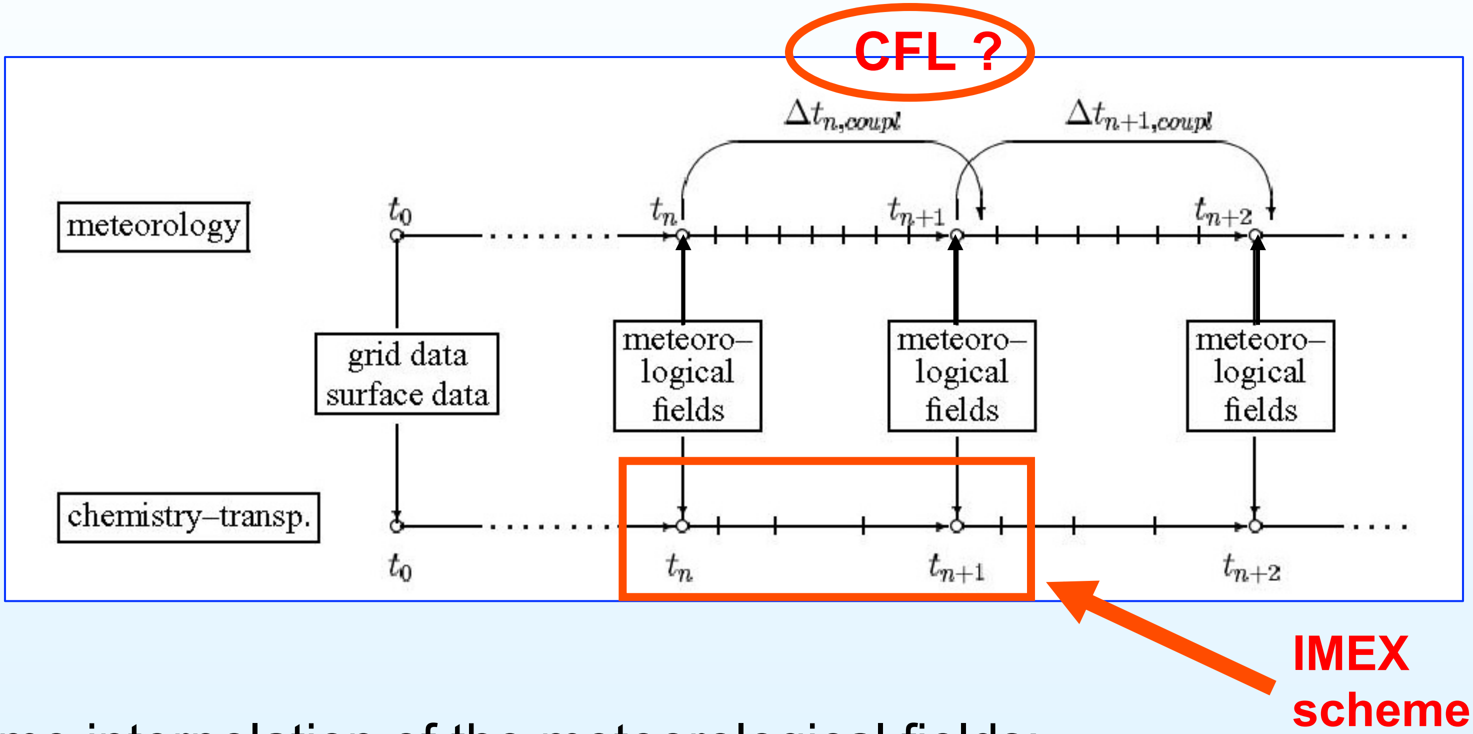
$$\begin{aligned} Y_2 &= Z_2(h_E) \quad \text{with} \\ & \frac{dZ_2}{d\tau} = f_E(t_n, Y_1) + f_I(t_n + \tau, Z_2), \quad \tau \in [0, h_E], \quad Z_2(0) = Y_1, \end{aligned}$$

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

<u>IMEX–RK2</u>



Coupling Scheme in Time



- 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

Multirate approach

CFL criteria (“Stability“)

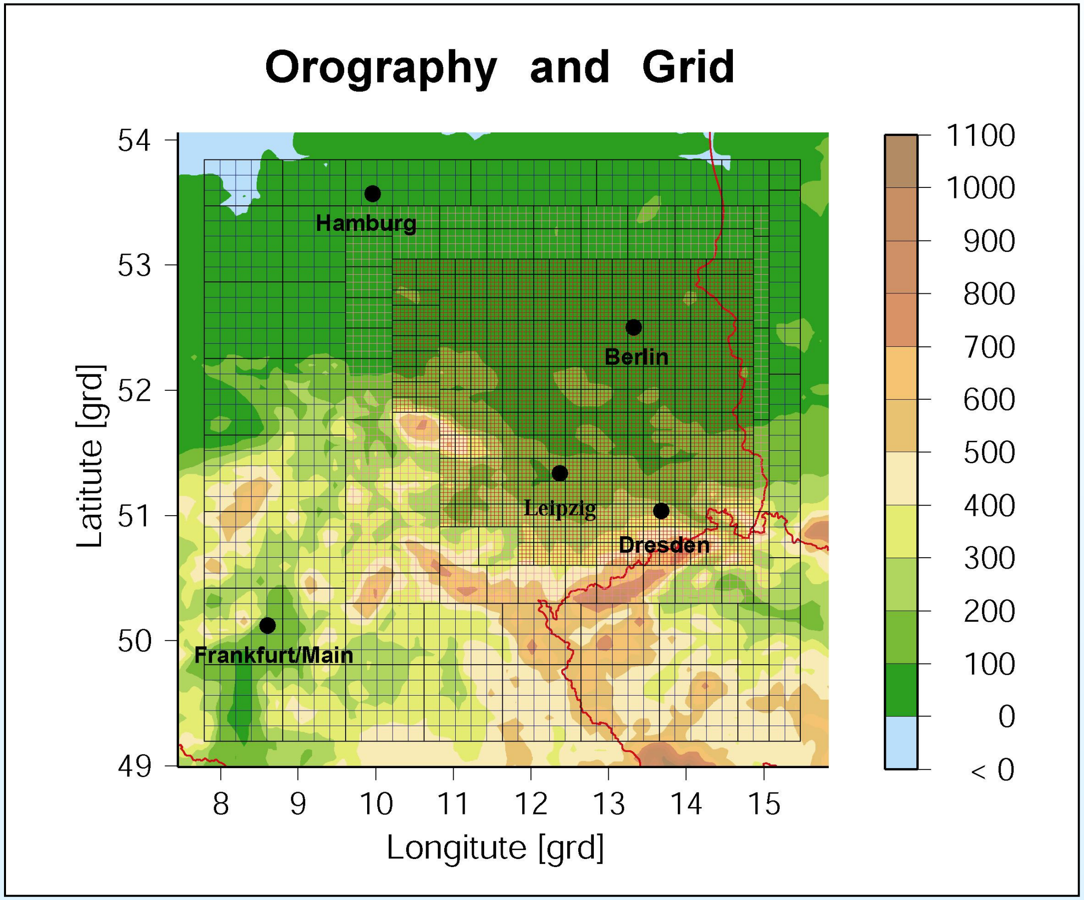
$\Delta t_{Ex} \leq \beta\, \Delta x / u$

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

CFL restricted by smallest resolution resolution!!

Problem of different time steps :

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



Basic idea:

$$c' = f_{Slow}(t,c) + f_{Fast}(t,c) + f_I(t,c)$$

Recursive Flux Splitting Multirate (RFSMR) Approach

$$W_1 = w_0, \quad (1)$$

$$r_i = \sum_{j=1}^{i-1} \left(a_{ij} - a_{i-1,j}\right) G\left(W_j\right), \quad (2)$$

$$v_i\left(\tau_{i-1}\right) = W_{i-1}, \quad (3)$$

$$\frac{dv_i}{\mathrm{d}\tau} = \frac{1}{c_i - c_{i-1}} r_i + F\left(v_i\right), \quad (4)$$

$$\tau \in \left[\tau_{i-1}, \tau_i\right], \quad i = 2, \ldots, s+1,$$

$$W_i = v_i\left(\tau_i\right), \quad (5)$$

$$w_1 = W_{s+1}, \quad (6)$$

- Eq. (4) can be solved by an **IMEX scheme (recursively).**
- Order conditions are derived:
  - *Second if all base methods of second order*
  - *For third order an additional condition have to be fulfilled.*

Schlegel et al., 2012

Numerical methods

- **Space discretization**
  - ***Staggered grid. Finite-volume techniques.***
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- **Time-integration: IMEX scheme**
  - ***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*

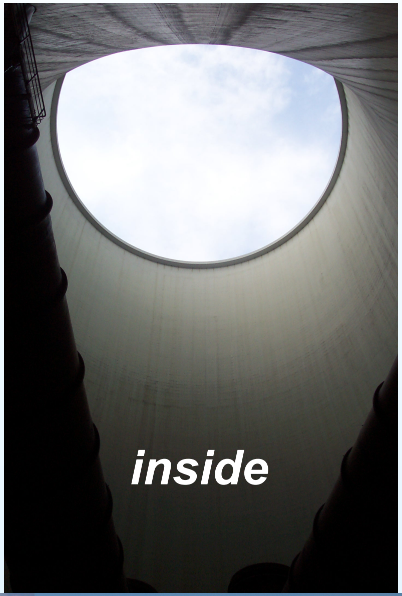
  - ***Multirate techniques (Schlegel et al., 2012):*** *Only "local" CFL criteria have to be fulfilled, leads to different explicit time steps in different regions*

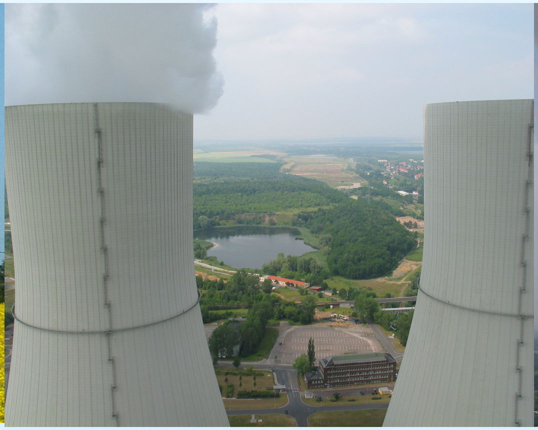
    ➔ ***Tested for air quality applications.***

Air Quality Applications

- **"Cooling Towers induced Particulate Matter (PM)"**
  - **The contribution of two large brown-coal fired power stations in Saxony to the formation of secondary PM was examined.**
  - **The highest contribution of PM in a narrow plume in the lowest modelling layer on a warm summer day is about 10 µg/m3.**
  - **About 90% of this PM are secondary formatted ammonia sulphate.**

Hinneburg et al. (2009)



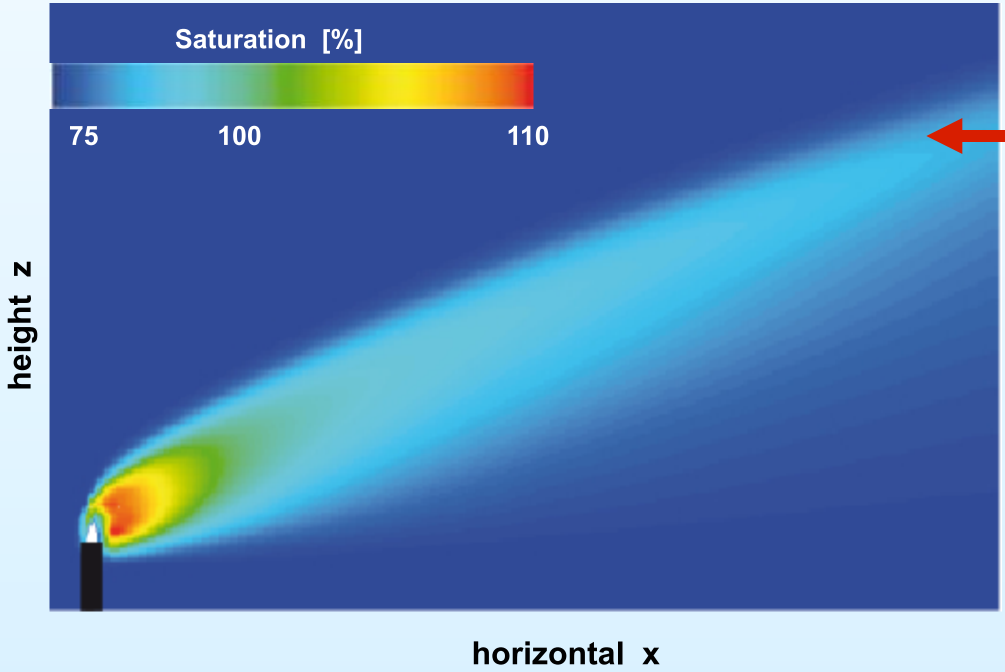


Treatment of Cooling Tower Emissions

Cooling tower model S/P ***(Schatzmann and Policastro, 1984)***:

• integral hydrodynamical model, based on PDE of fluid dynamics

• conservation of mass, momentum, energy, **water,** and inert pollutants



effective emission height

Prognostic variables:

$\boldsymbol{v}$, T, ρ, **q**, c

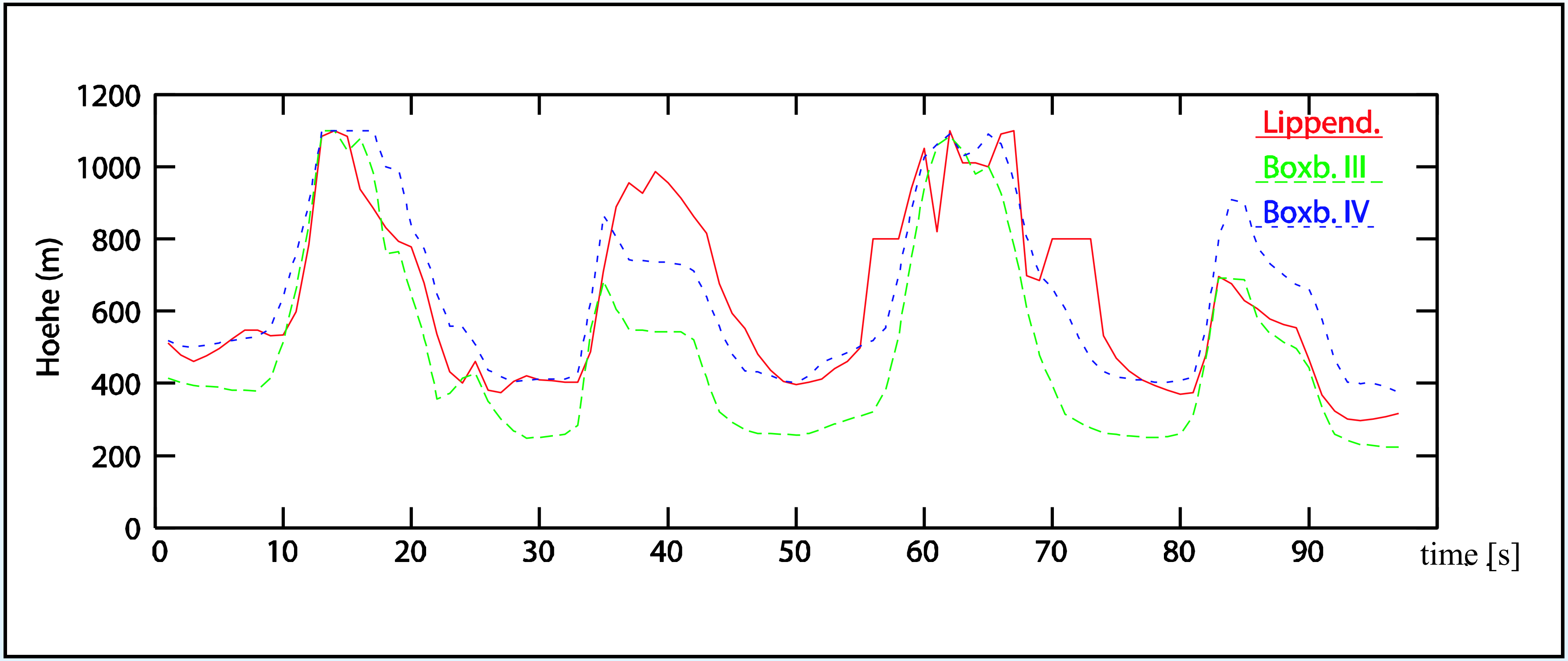
Consideration of

• meteorological conditions

• exit velocity, temperature, and volume of waste gas

• height and exit diameter of the tower

Treatment of Cooling Tower Emissions

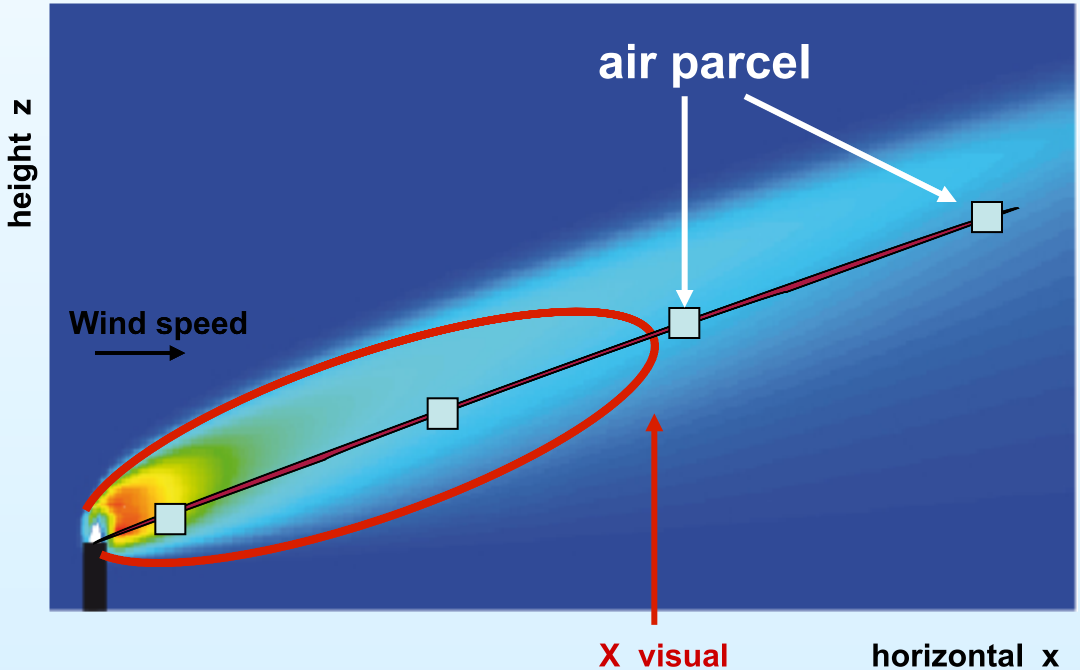


Effective emission height (Summer: 23.-26.08.2002)

Near-Source Processes

Air parcel model SPACCIM ***(Wolke et al., 2005)***:

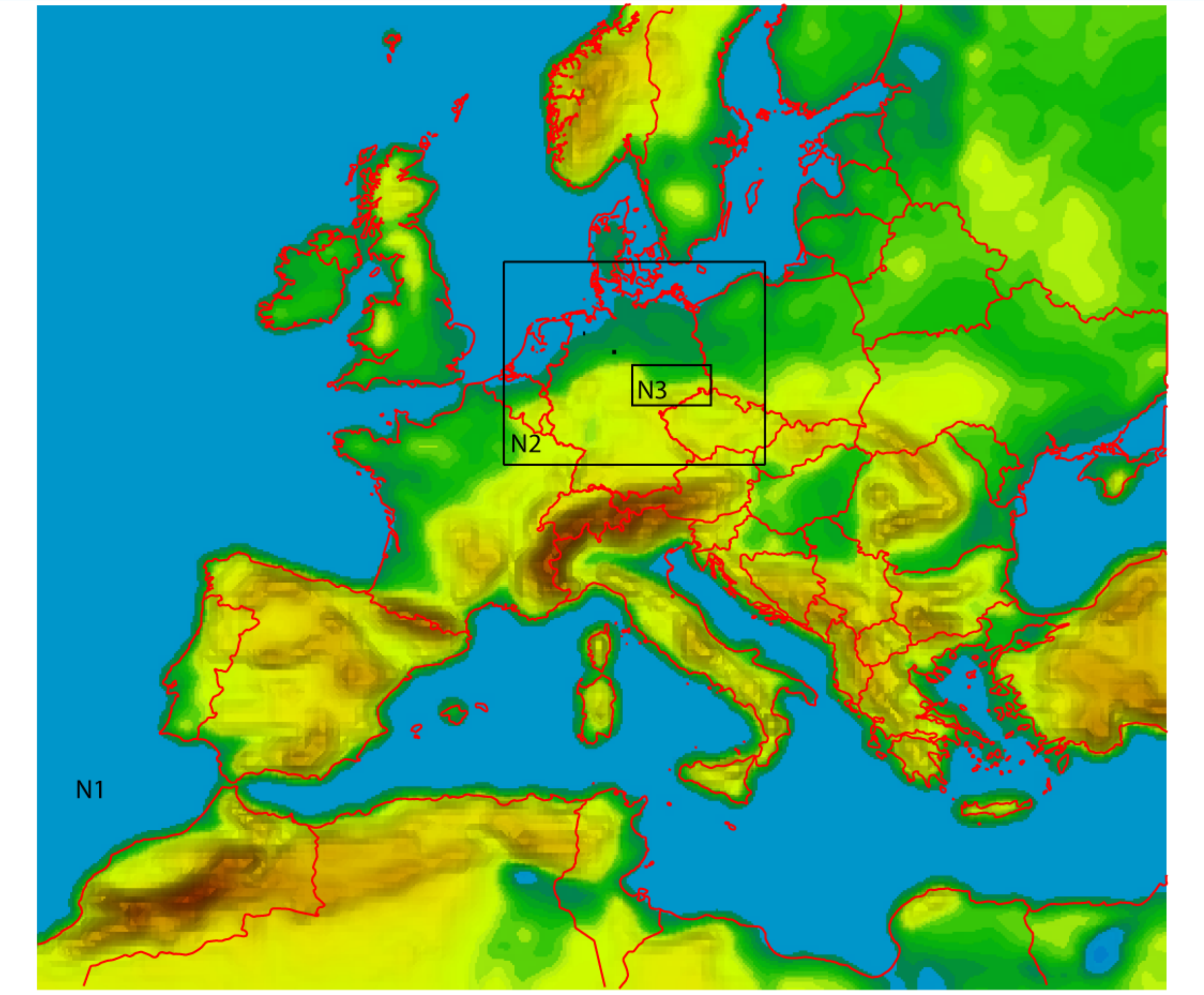
- combines detailed microphysics and complex multiphase chemistry
- size-resolved treatment of activation, mass transfer and aqueous phase chemistry



Sensitivity study:
- wind speed
- particle populations (number, size, composition)
- surrounding conditions and mixing

→ **High variability and No measurements**

COSMO Grid Nesting



Size 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:

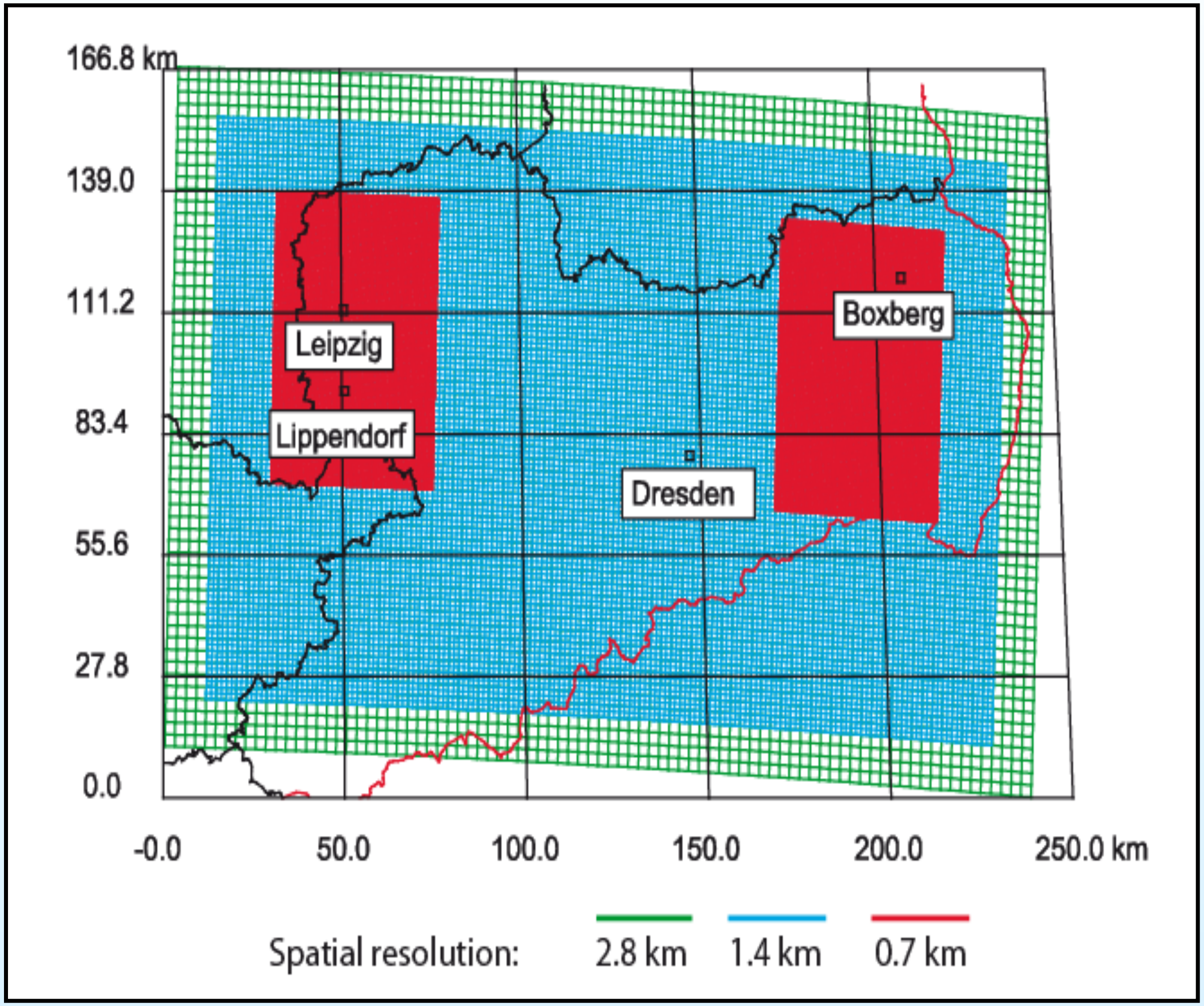
10. – 24. August 2002
(additional measurements)

Chemistry:

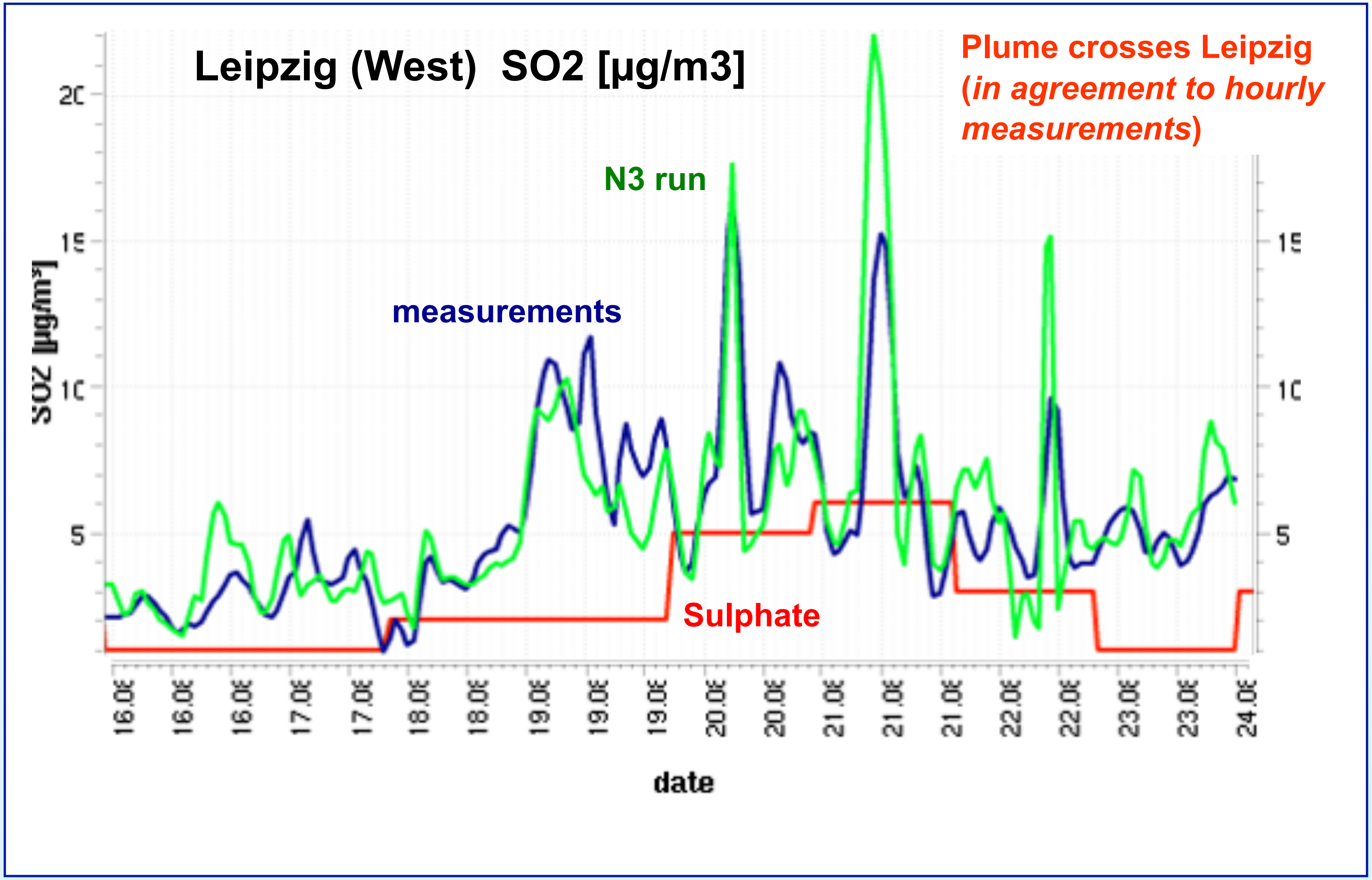
RACM-MIM2 **+ SIA**

N1 runs to generate appropriate boundary values !

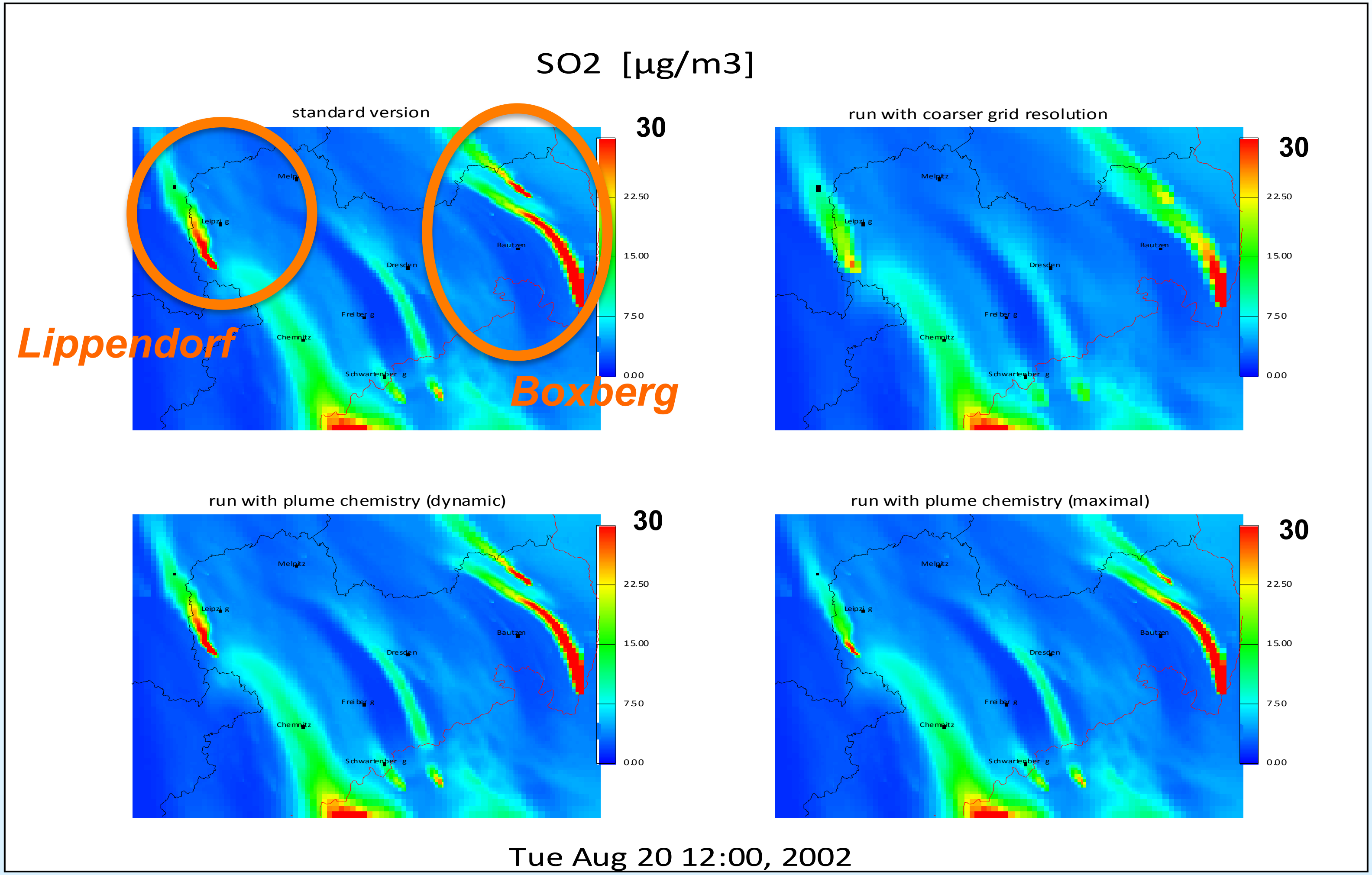
N3 Grid Structure of MUSCAT (*original*)



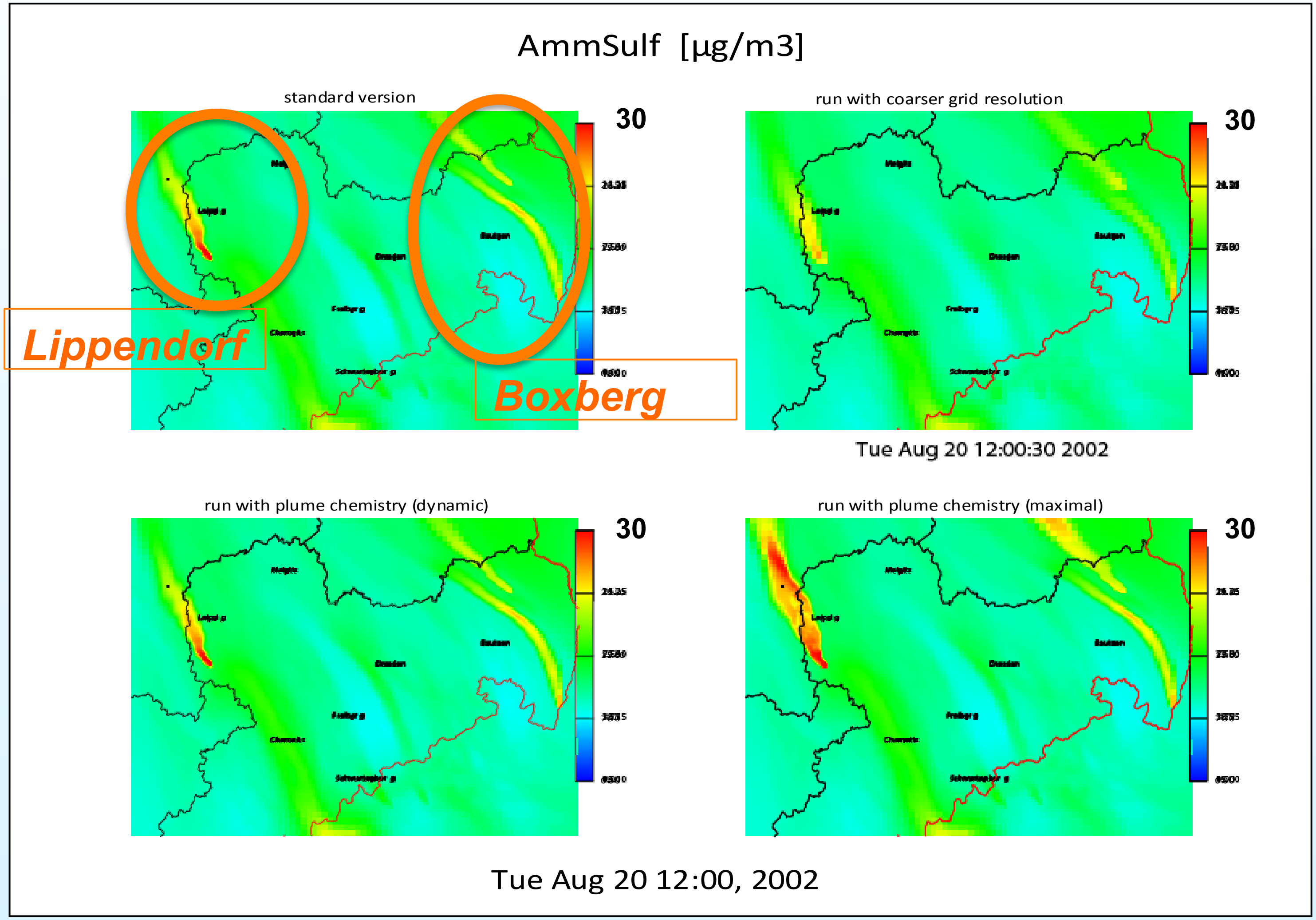
Comparison with Measurements



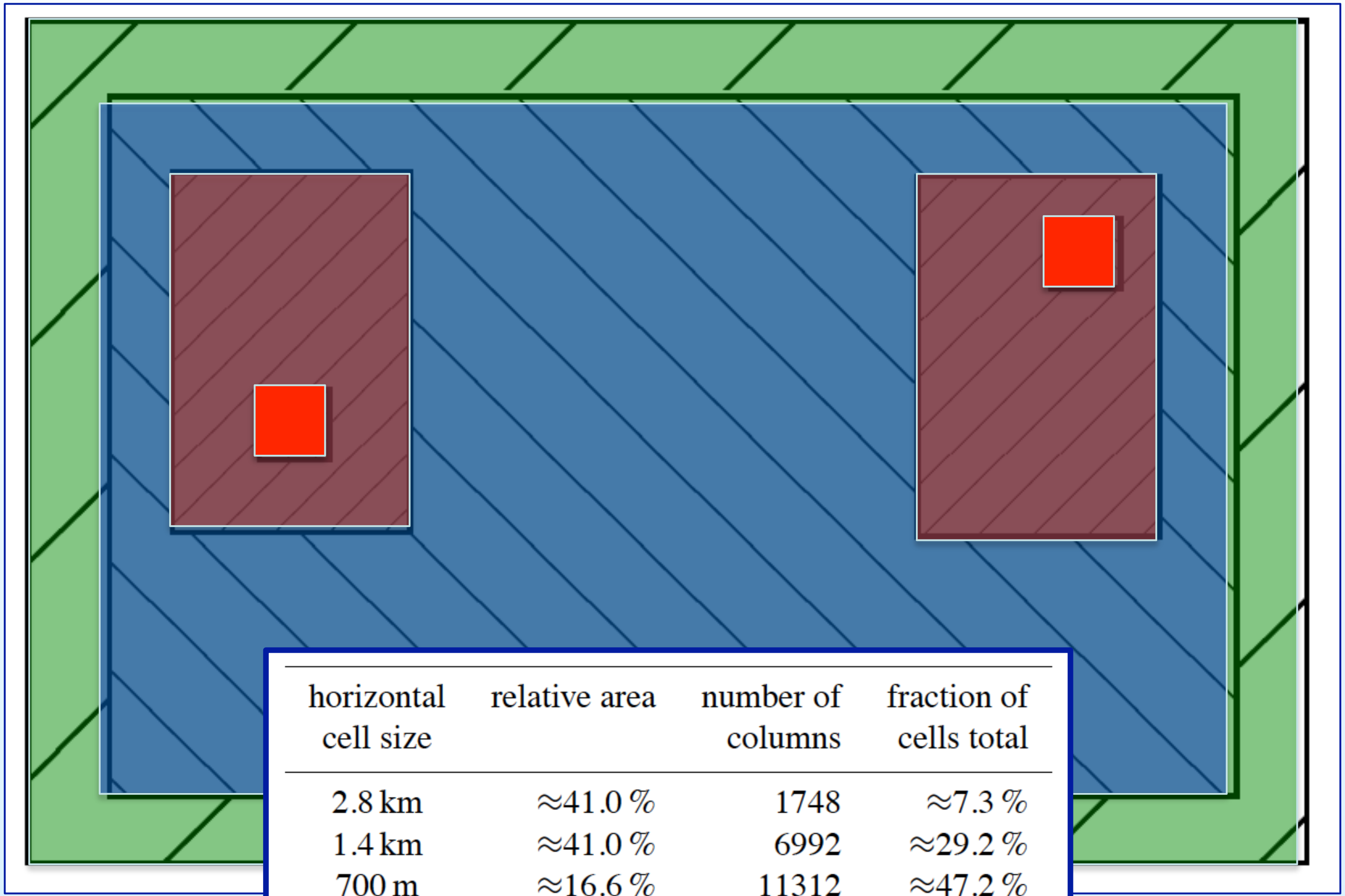
Comparison of Different SIA Schemes



Comparison of Different SIA Schemes

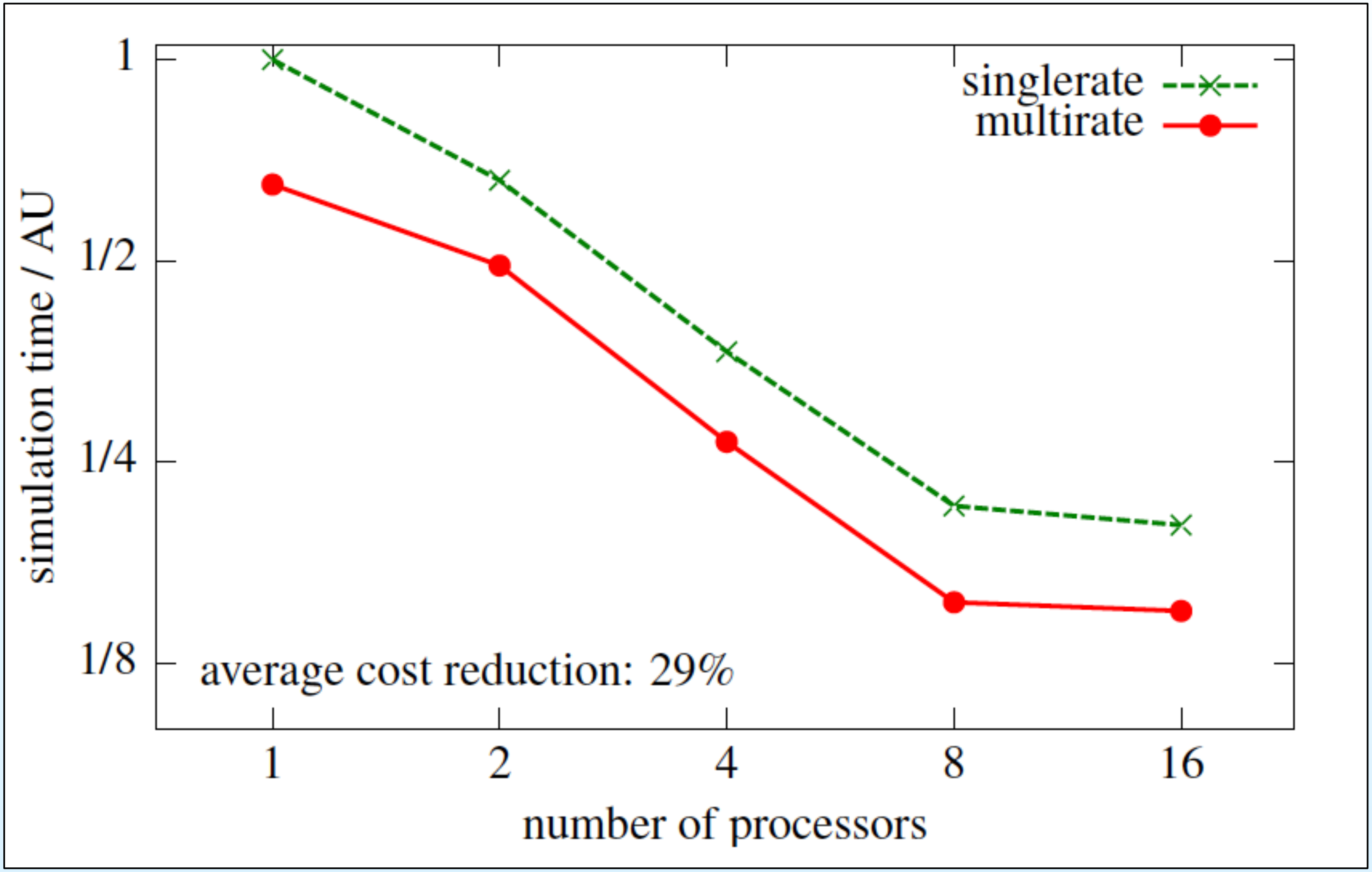


Modification of MUSCAT Grid



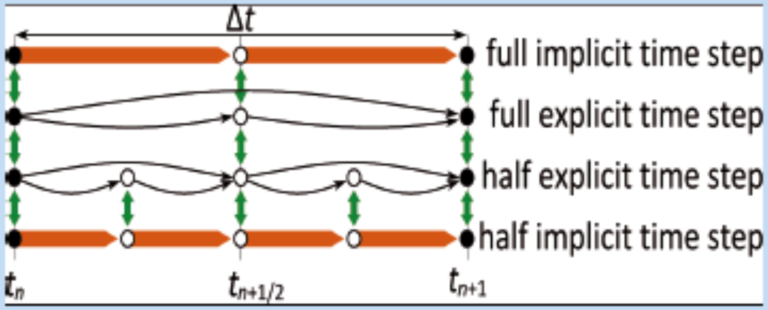
horizontal cell size	relative area	number of columns	fraction of cells total
2.8 km	≈41.0 %	1748	≈7.3 %
1.4 km	≈41.0 %	6992	≈29.2 %
700 m	≈16.6 %	11312	≈47.2 %
350 m	≈1.4 %	3904	≈16.3 %

Cooling Tower Run: Multirate vs. Singlerate



Recursive Flux Splitting Multirate (RFSMR)

Multirate Runge-Kutta scheme based on Heun2



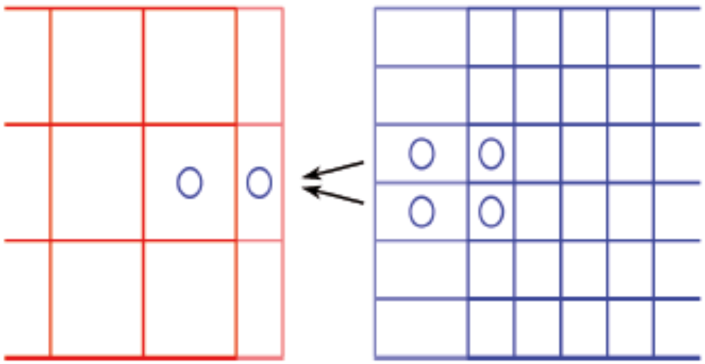
0		
½	½	
	0	1

	slow			
0				
¼	¼			
½	½	0		
¾	¼	0	½	
	0	0	1	0

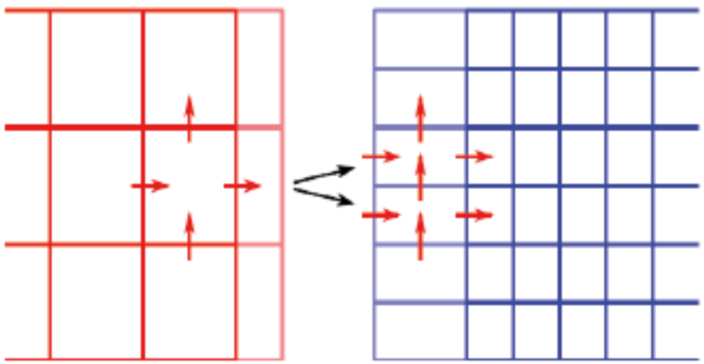
	fast			
0				
¼	¼			
½	0	½		
¾	0	½	¼	
	0	½	0	½

Data transfer for two refinement levels

concentration exchange after
summation stage on fine grid



flux exchange after
flux calculation on coarse grid

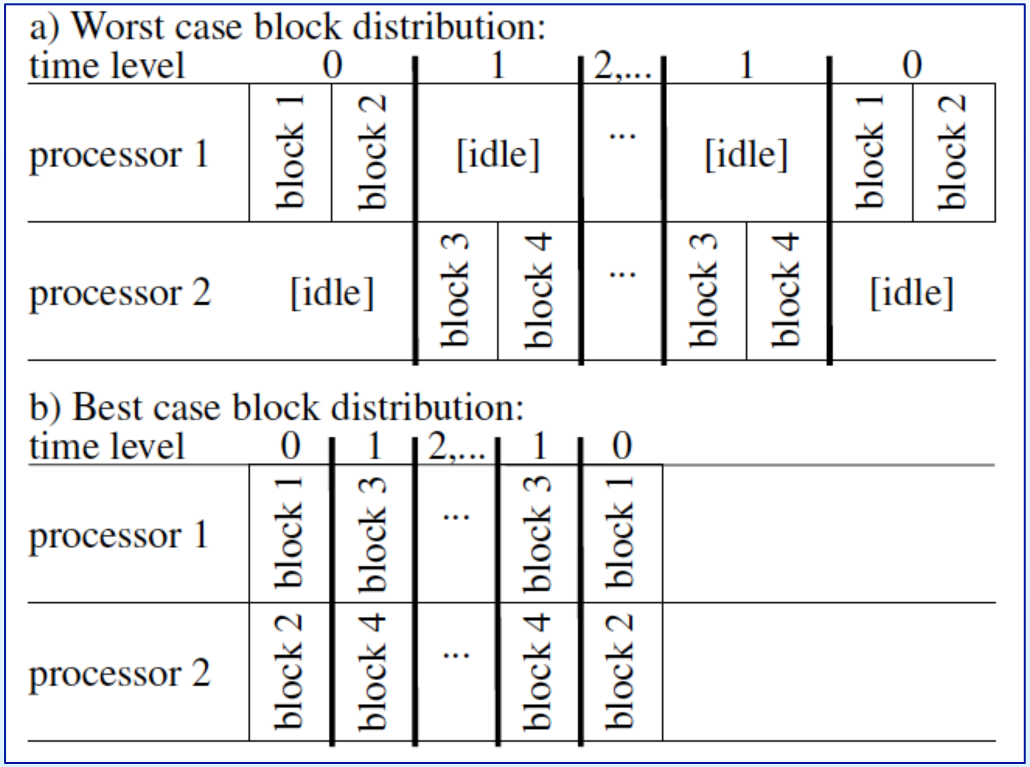


Load Balancing

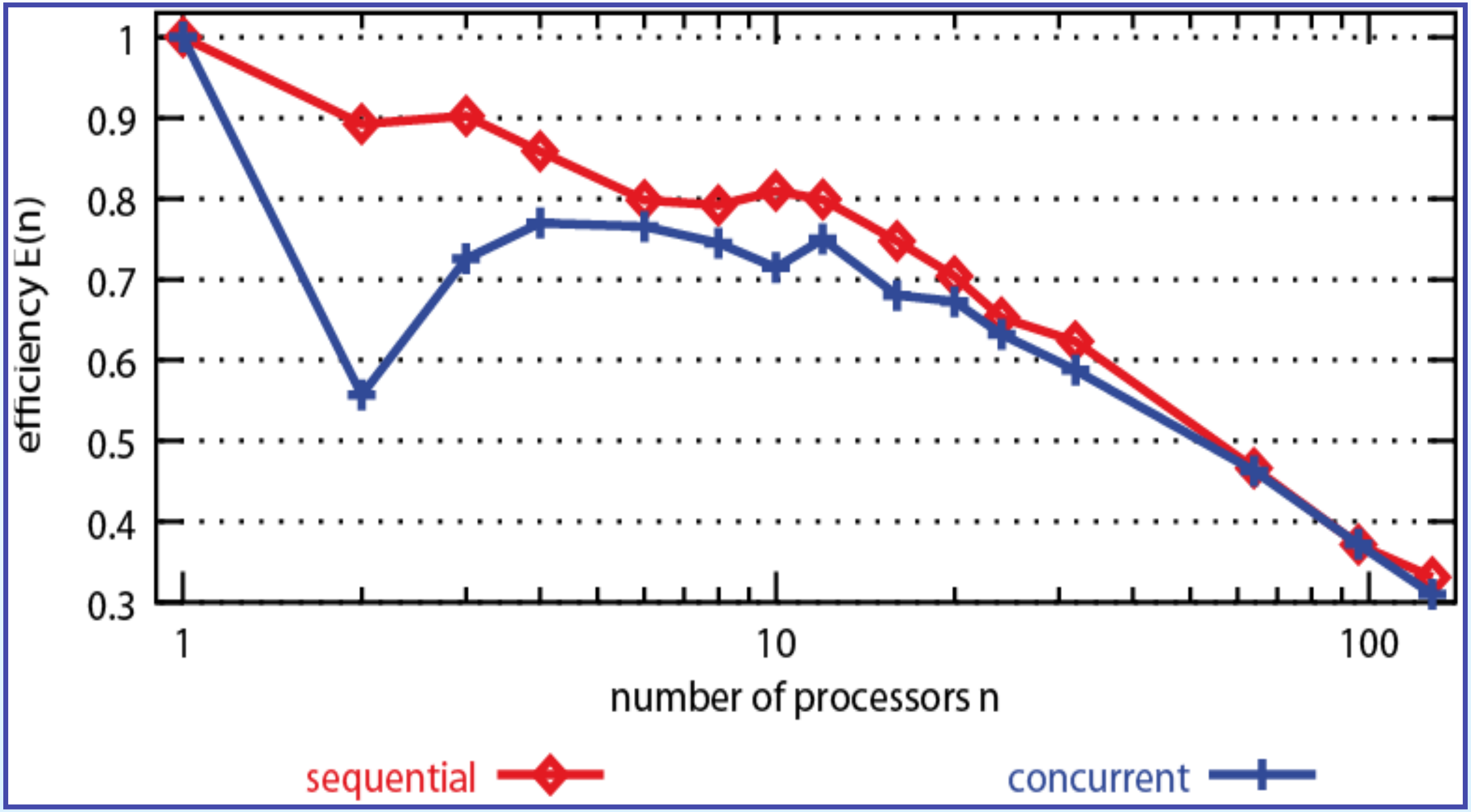
Imbalances are caused by time step control of blockwise implicit integration (large emissions, clouds)

→ **load balancing (using *ParMetis*)**

Additional imbalances by Multirate:



Parallel efficiency for the “Europe“ scenario



Conclusions

- **Multiblock grid techniques and IMEX time integration schemes are suitable for an efficient treatment of scale interactions.**

- **Outlook (*multirate time integration)*:**
  - ***considering of the cloud heterogeneity in space and time***
  - ***dynamical data structures, load balancing***

Acknowledgement

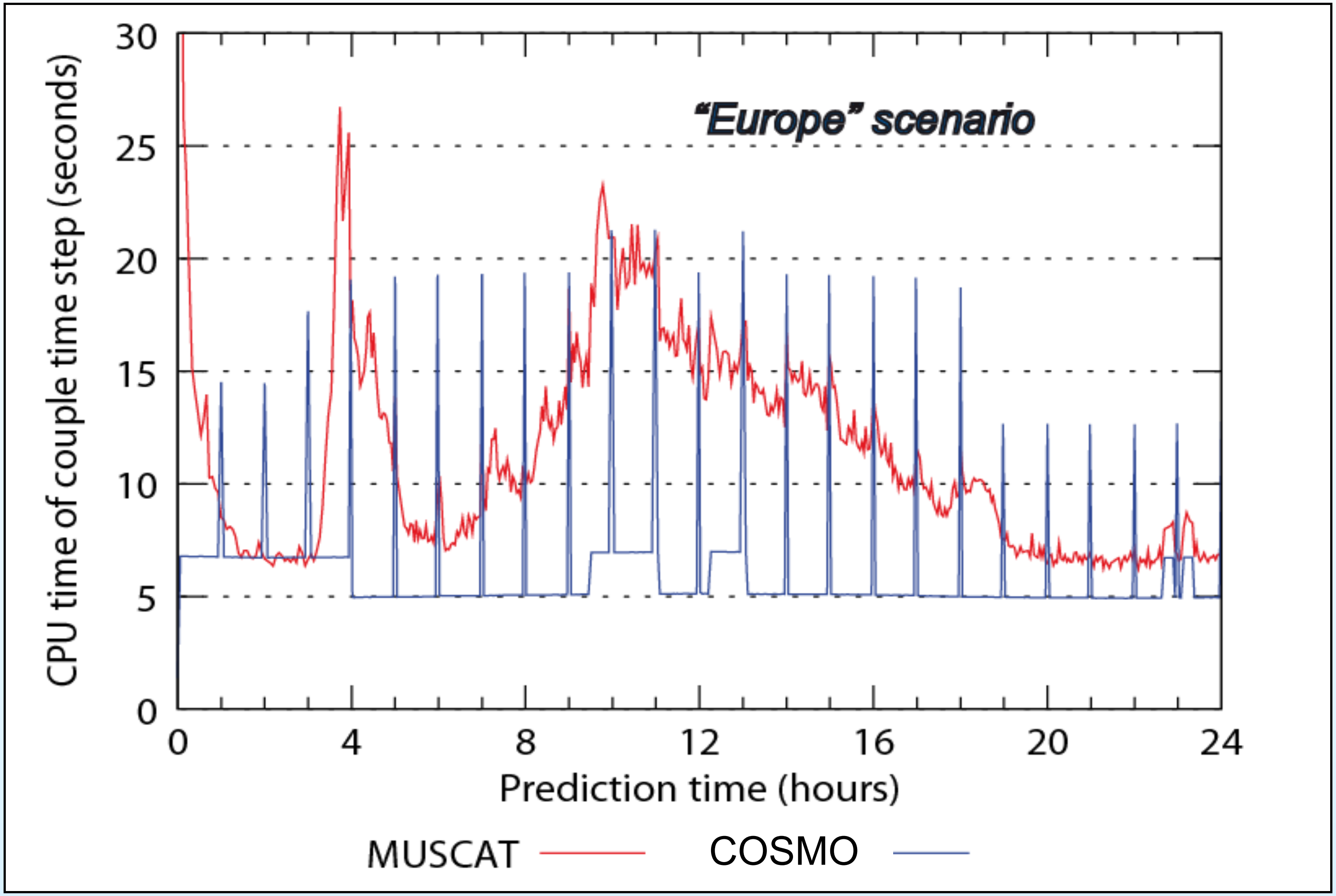
This work was supported by the LfUG Saxony, NIC Jülich and the ZIH Dresden. Furthermore, we thank the German Weather Service for their cooperation.

Thank you!

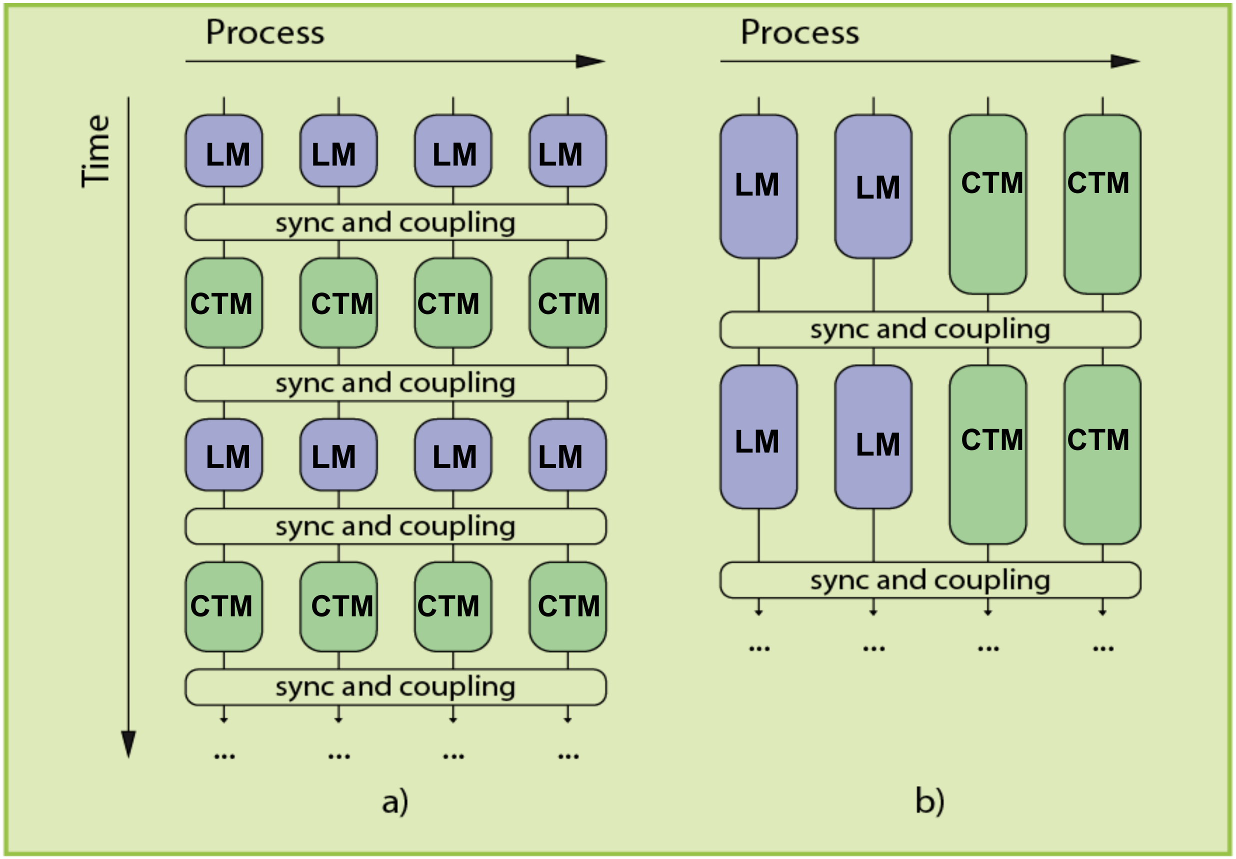
Parallel coupling of COSMO and MUSCAT

- "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 I



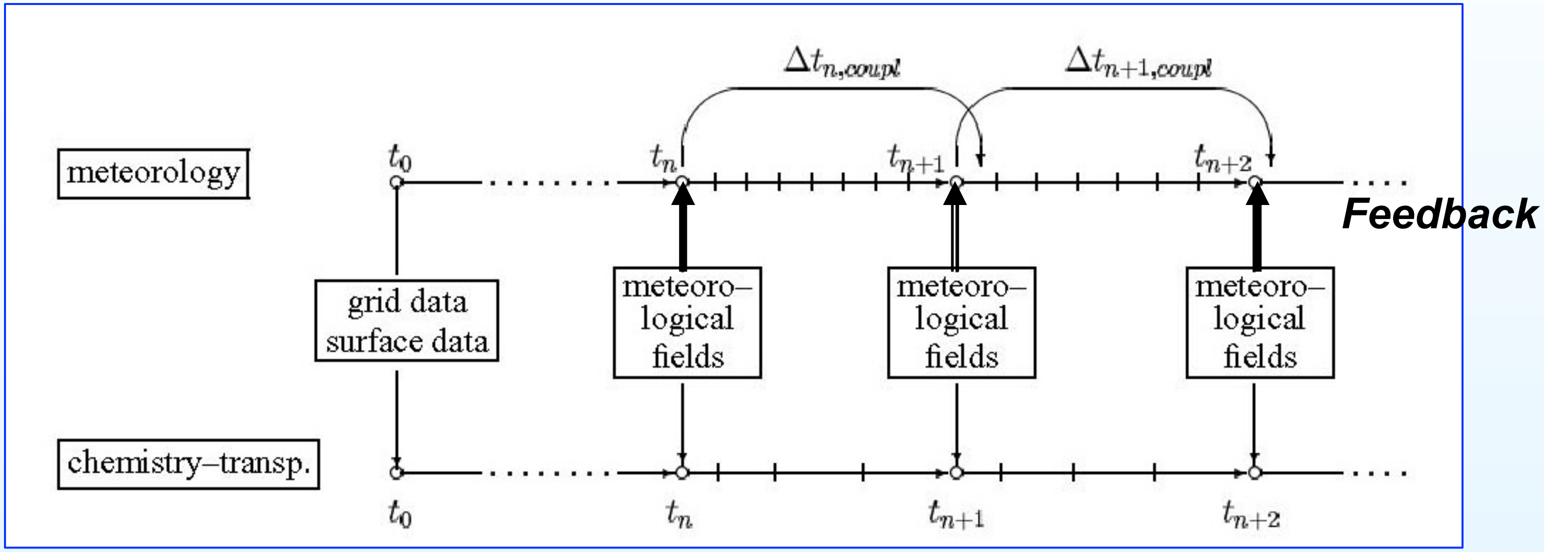
Sequential vs. Concurrent Coupling



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

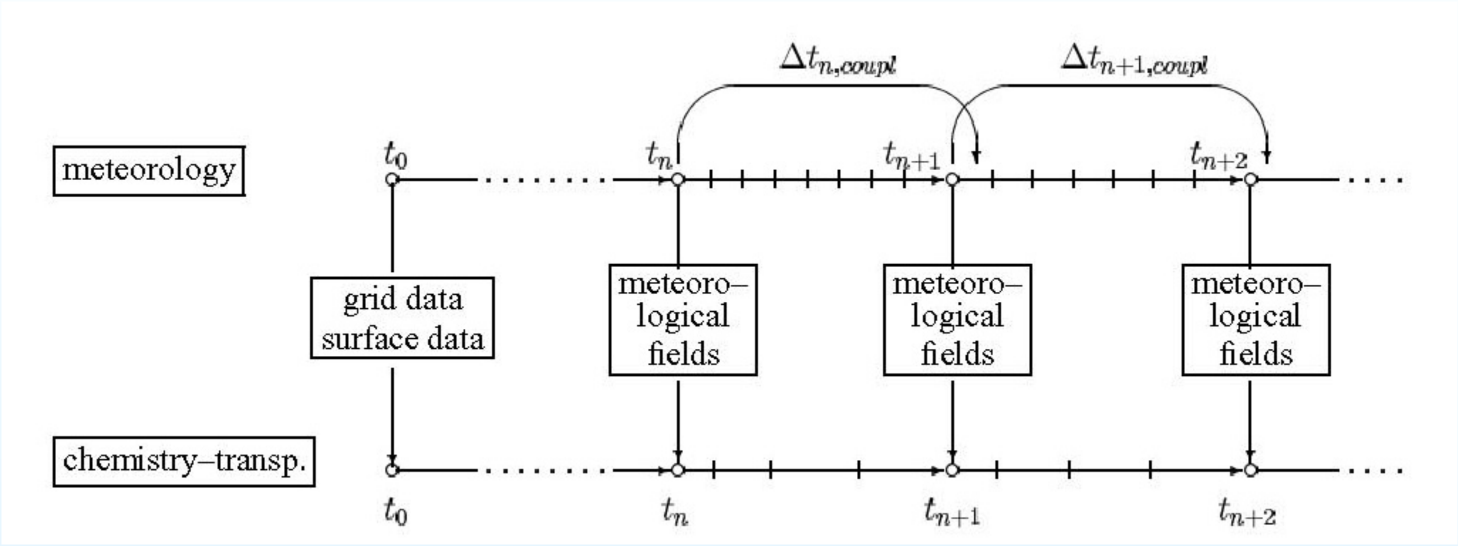
Lieber & Wolke (2007)

Coupling Scheme



- 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 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

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

and

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

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

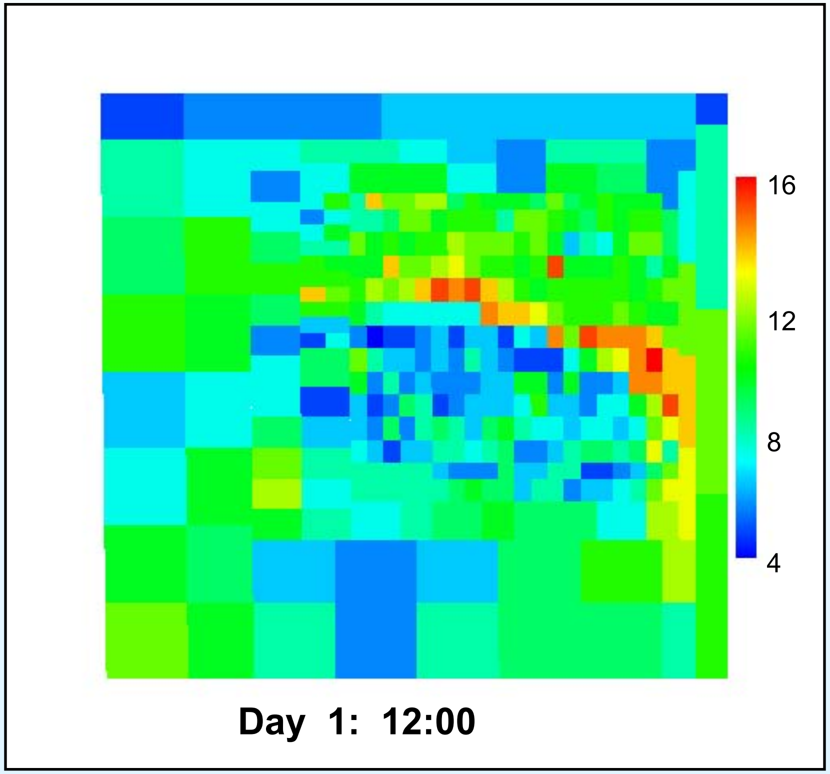
Numerical methods (Implicit integration)

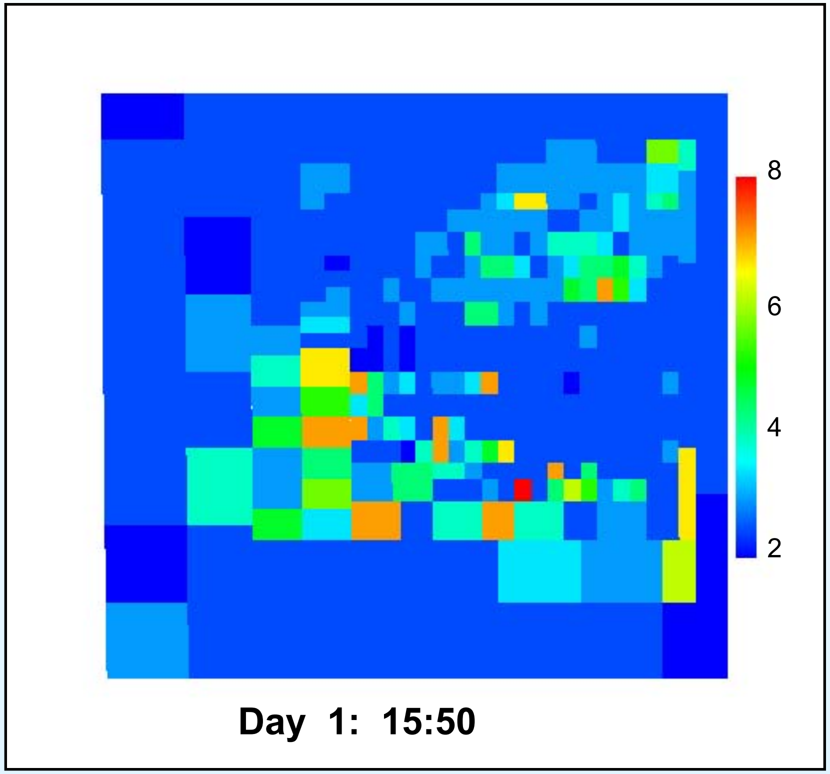
- **Space discretization**
  - ***Staggered grid. Finite-volume techniques.***
  - ***Advection: Third-order upwind scheme (Hundsdorfer et al., 1995).***

- **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*
  - ***Automatic step size control***
    - ➔ ***different number of steps (load imbalances)***

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

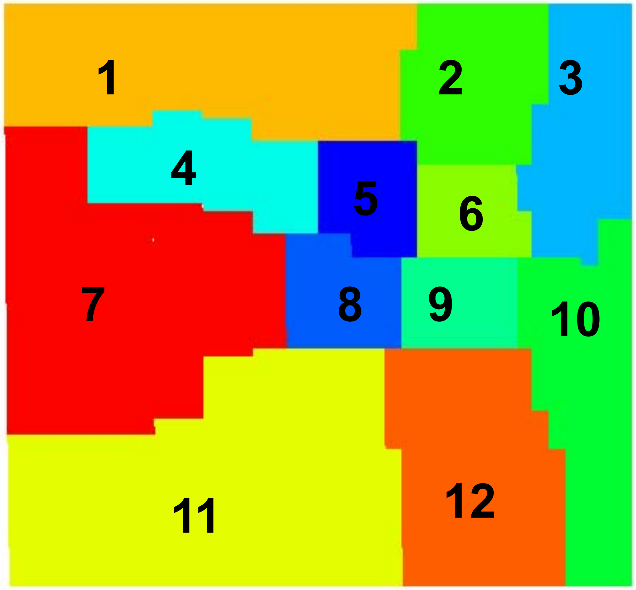
Load Balancing of MUSCAT



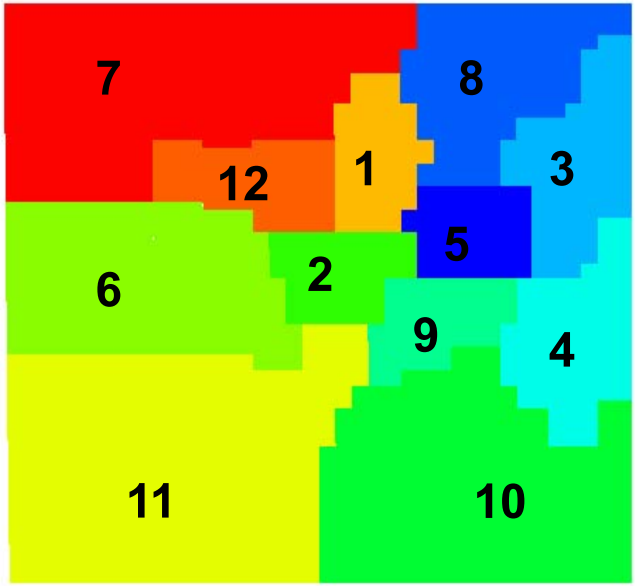


The number of function evaluations of each block at the start and the end time.

Load Balancing of MUSCAT



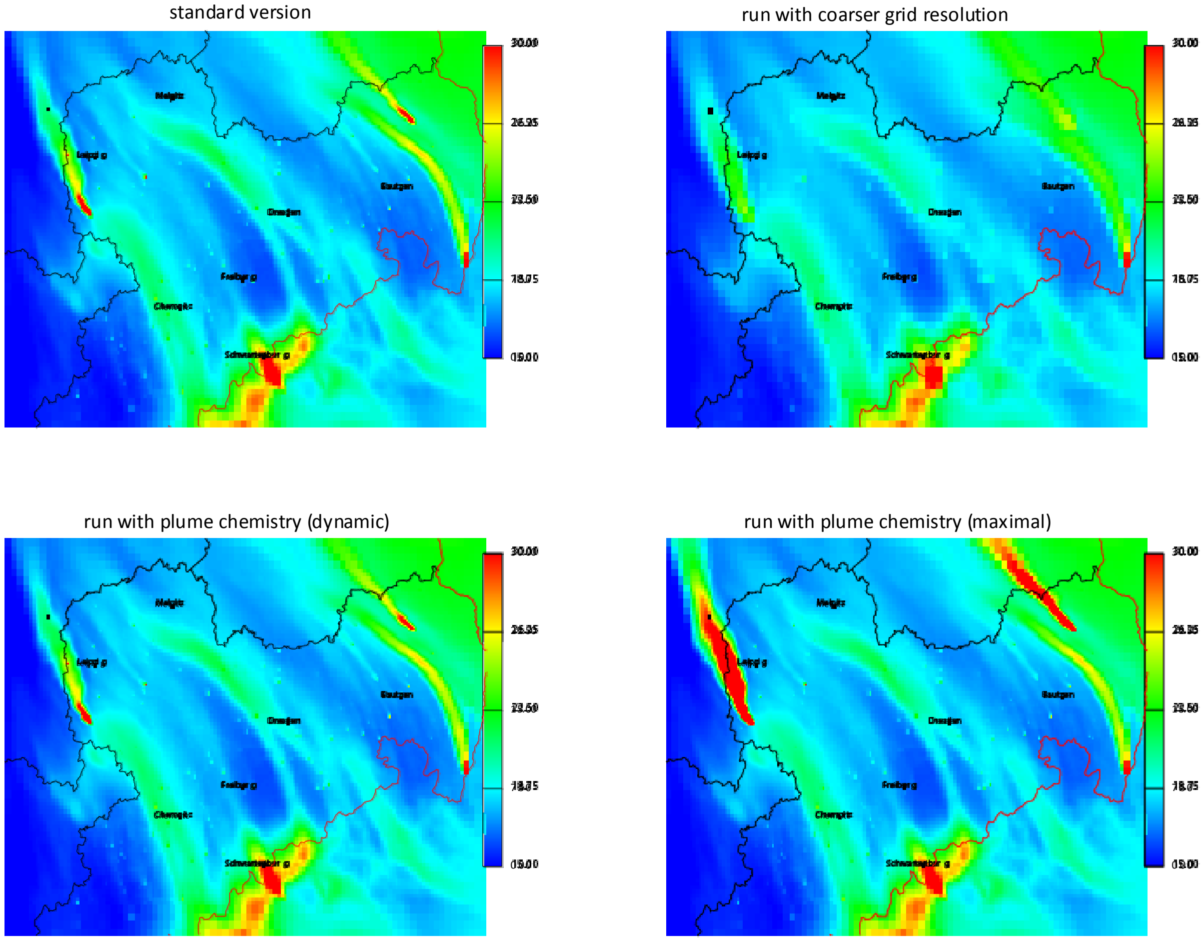
Start



End

Start and end distribution for a run with12 MUSCAT processors

PM10 [µg/m3]



Tue Aug 20 12:00, 2002

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)*.

IMEX Time Integration Scheme

- **Coupled implicit integration of**

$$c' = f_{Gas}(t,c) + f_{Hen}(t,c) + f_{Aqua}(t,c) + f_{TFrac}(t,c) \qquad (1)$$

gas phase — *phase transfer* — *aqueous phase* — *microphysical transport*

- **BDF method** (modified LSODE, *Hindmarsh 1983*)

Linear Systems

$$(I - \square\ \square t\ J)\ \square c = b \qquad (2)$$

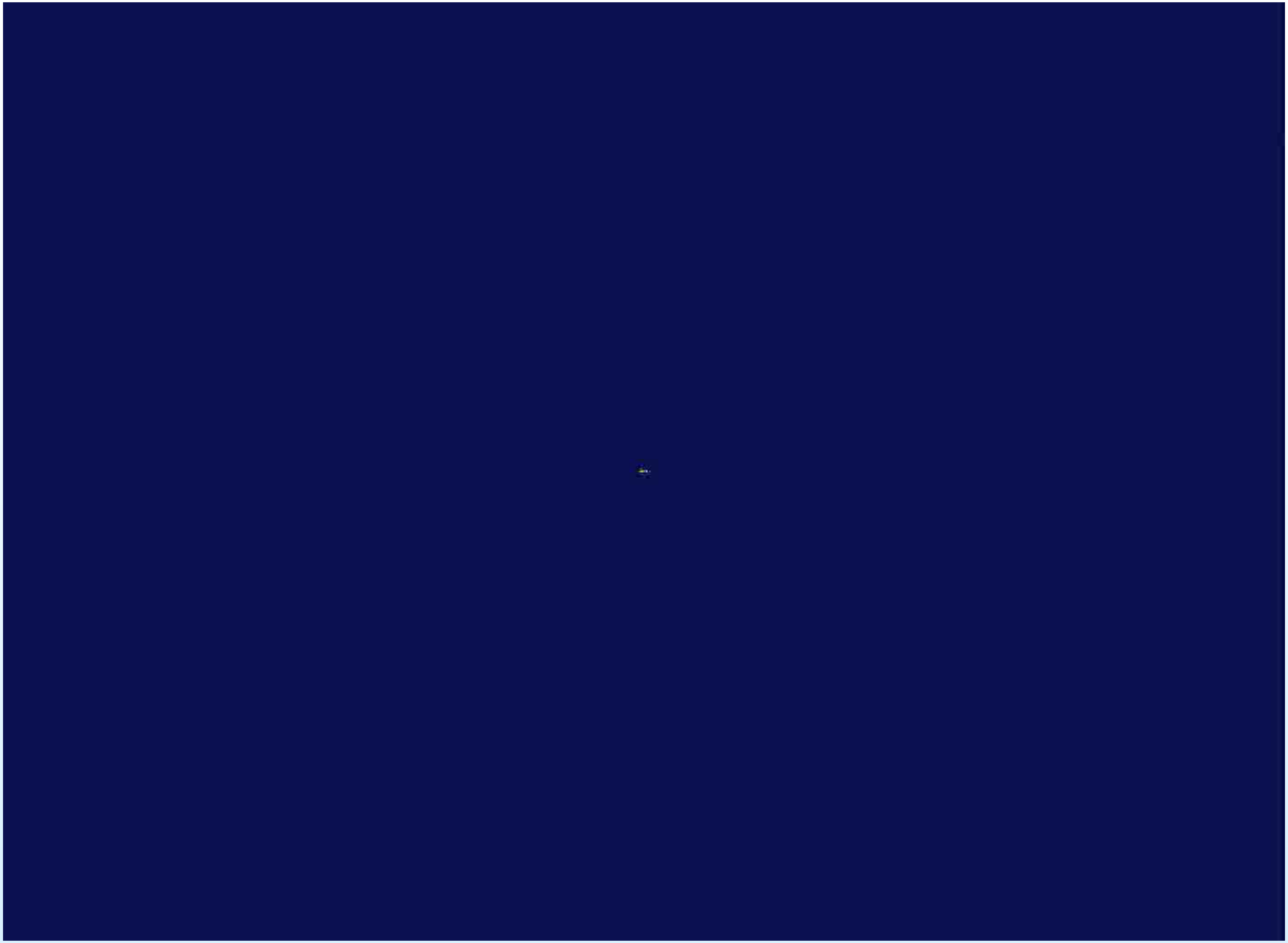
Jacobian

$$J = J^{Gas} + J^{Hen} + J^{Aqua} + J^{TFrac} \qquad (3)$$

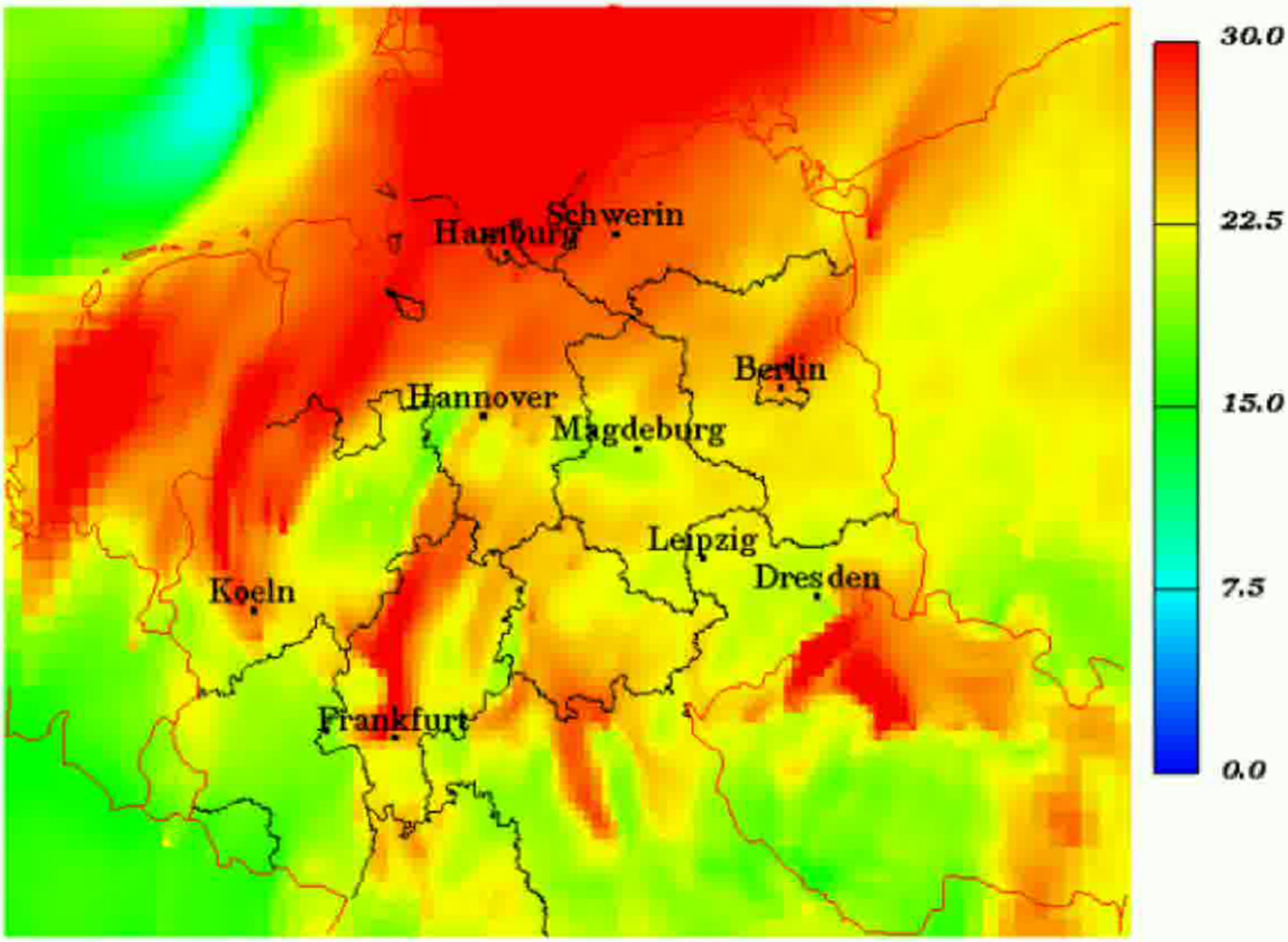
$$J^{Gas} + J^{Hen} + J^{Aqua} =: J^{Chem}$$

Numerical methods in MUSCAT

- **Spatial discretization**
  - Method of Lines: (MBE) → Large system of ordinary differential equations in time
  - 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, a linear system by Gauss-Seidel iterations or AMF methods
  - Automatic time-step control
- **Parallelization**
  - Domain decomposition
  - Dynamical load balancing



PM10



Wed Oct 18 12:00 2006