The online-coupled atmospheric-chemistry-aerosol model LM-MUSCAT

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Outline of the Talk

- **Coupling LM-MUSCAT**
  Coupling scheme, Data transfer
- **Chemistry-Transport Code**
  Gasphase, Aerosol, Emissions, Numerics, Parallelization
- **Projects**
  SAMUM, CityDelta, "air quality"
- **Future projects**
  Local dust, refined aerosol module ,heterogeneous chemistry

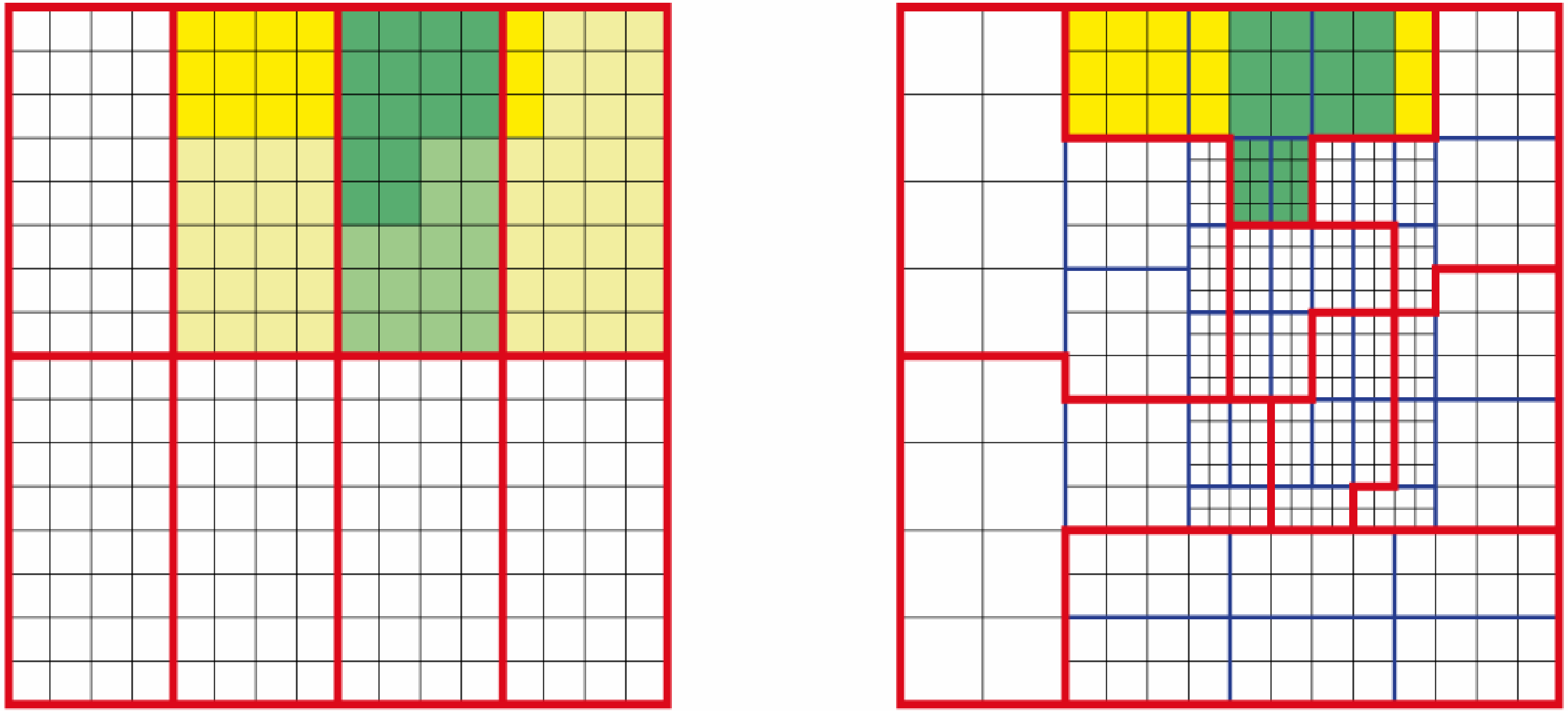
"Local Model" (LM) of the German Weather Service

- non-hydrostatic
- compressible
- formulated with regard to a hydrostatic reference state
- prognostic thermodynamic variables are temperature T and pressure p
- nonconservative formulation
- staggered grid
  - horizontal: uniform, orthogonal (λ,φ)
  - hybrid vertical coordinate
- regional scale
- boundary and initial data from GME

"Local Model" (LM) of the German Weather Service

- uniform grid in the horizontal
- rotated pole
- fixed time step, mainly dictated by the jet stream
- parallelization by horizontal domain decomposition
- highly parallel

Coupling Scheme Grid Structure



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

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

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

and

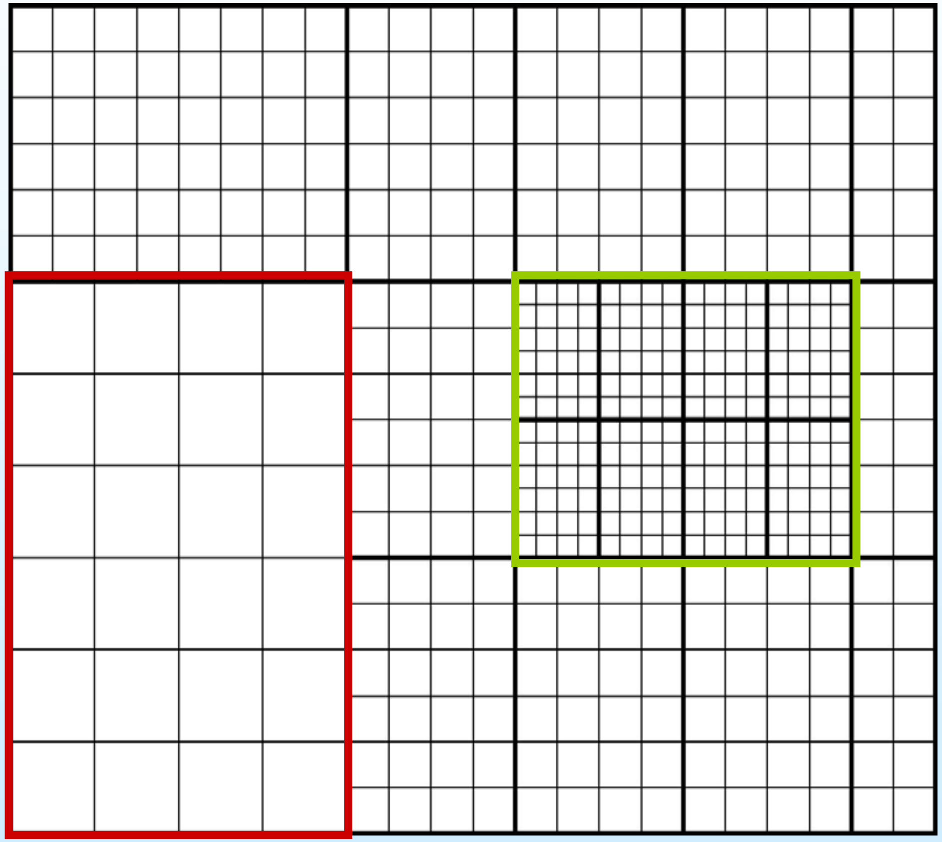
$$\rho^{n+1} - \rho^{n} + \Delta t_n \nabla \vec{U}^{*} = 0.$$

- 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.

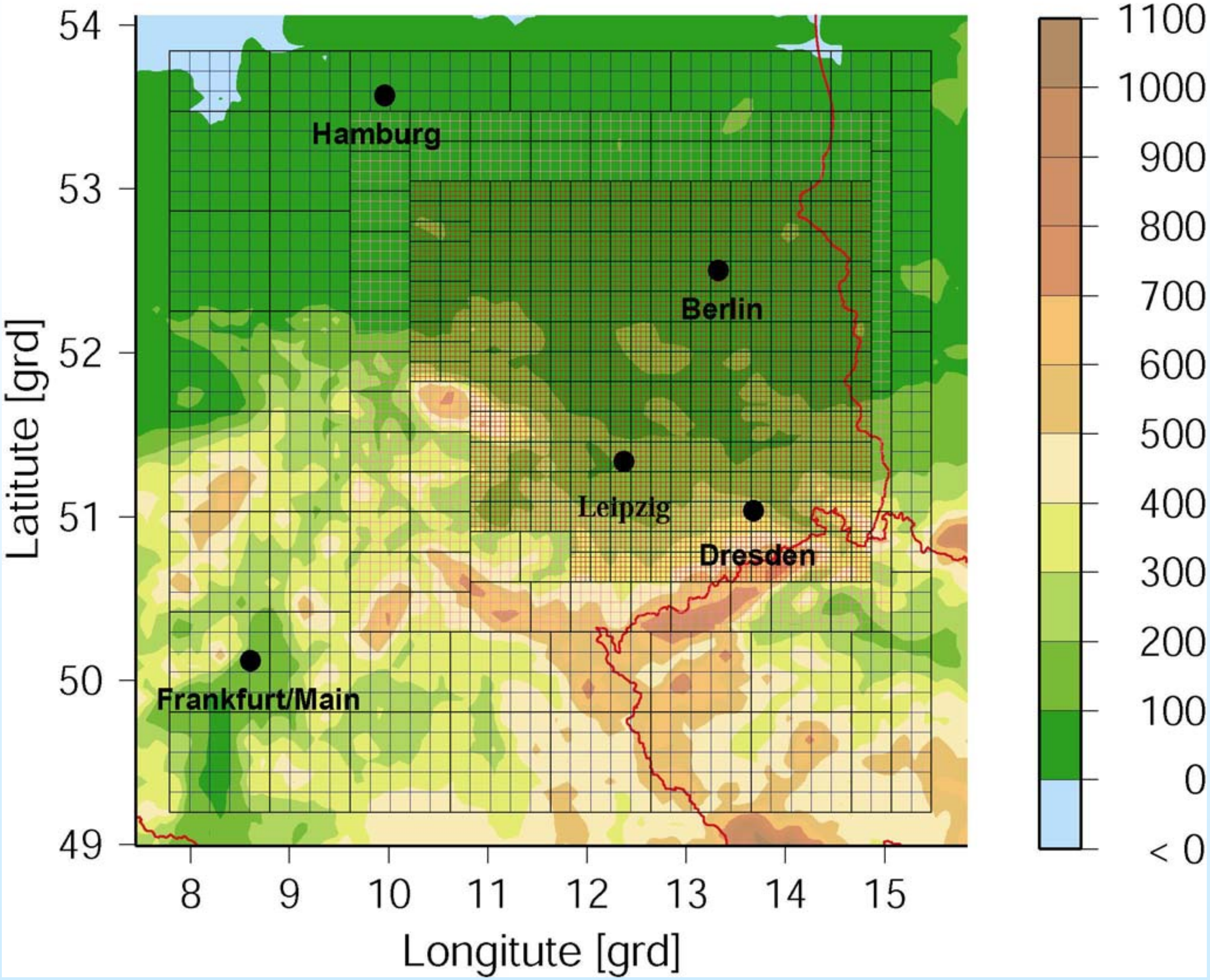
Decomposition of horizontal domain for MUSCAT

Static grid
(“multiblock approach“)

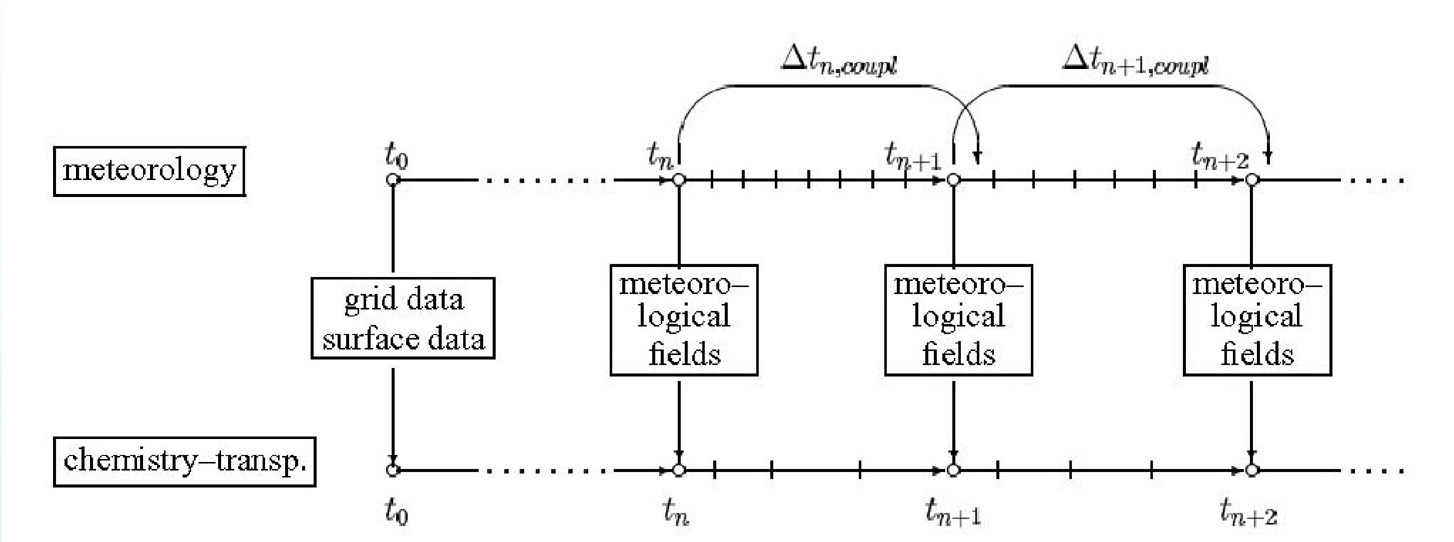
- From a given rectangular grid (usually
  for the meteorological driver).
- Non-overlapping subblocks (also of rectangular type) are marked for refining or coarsening.
- Refinement level between neighbouring blocks is restricted to 1.



Orography and Grid



Coupling Scheme in Time

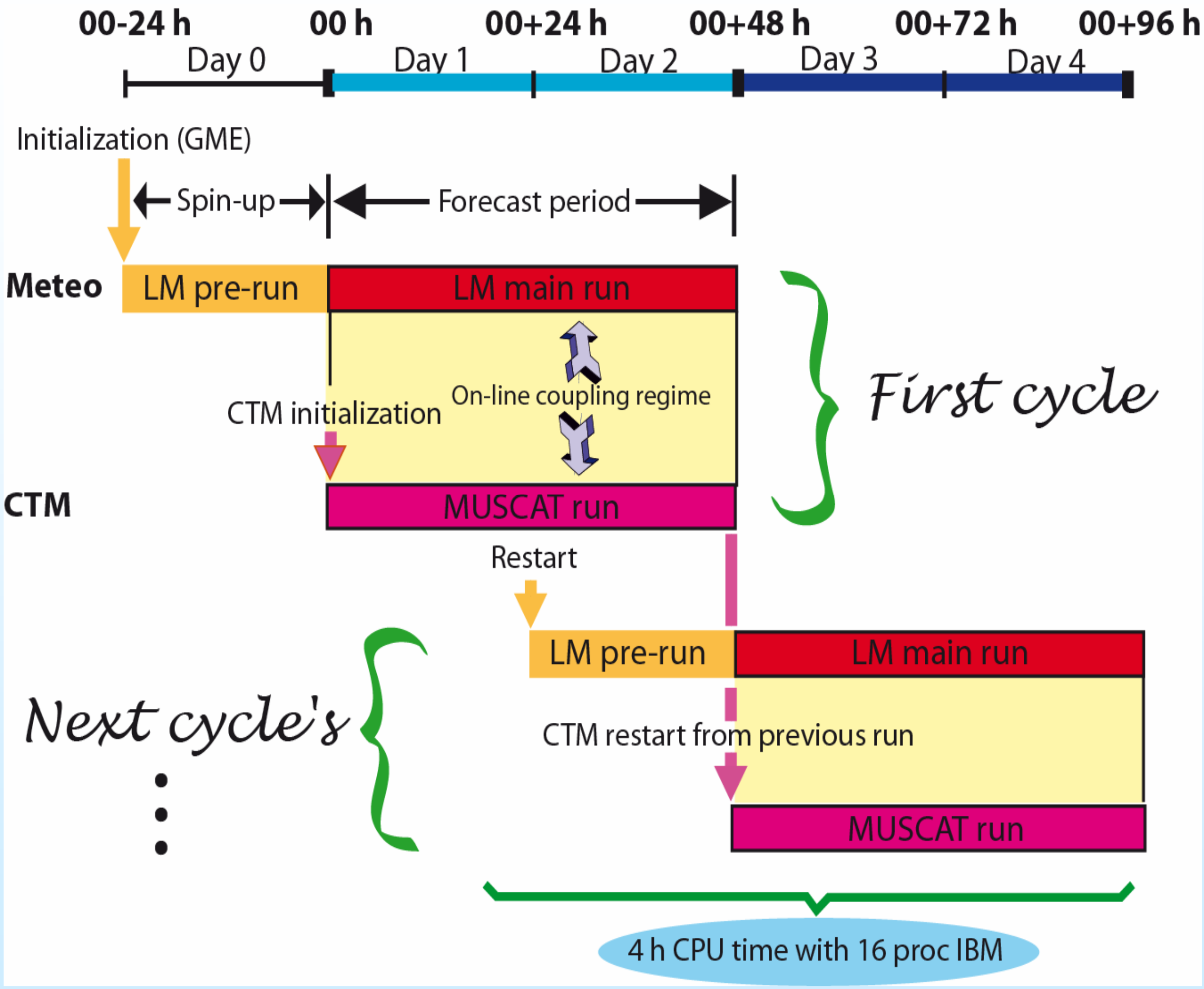


- Time interpolation of the meteorological fields:

1. Linear interpolated in $[t_n, t_{n+1}]$: Temperature, Density,….
2. Time-averaged values on $[t_n, t_{n+1}]$: Projected wind field

→ necessary for mass conservation !!

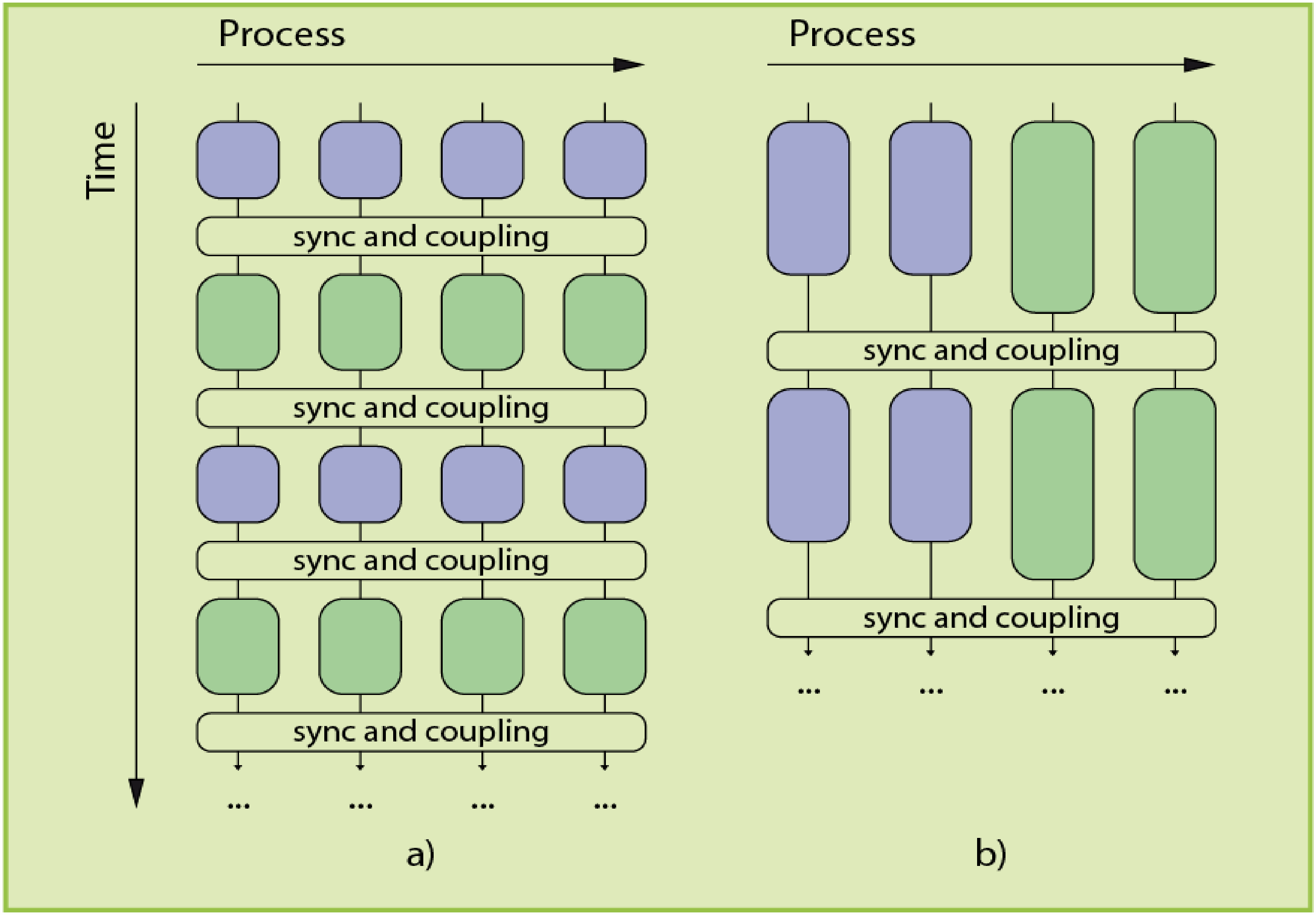
- Separate time step size control for LM and MUSCAT



00-24 h
00 h
00+24 h
00+48 h
00+72 h
00+96 h
Day 0
Day 1
Day 2
Day 3
Day 4
Initialization (GME)
Spin-up
Forecast period
Meteo
LM pre-run
LM main run
First cycle
On-line coupling regime
CTM initialization
CTM
MUSCAT run
Restart
LM pre-run
LM main run
Next cycle's
CTM restart from previous run
MUSCAT run
4 h CPU time with 16 proc IBM

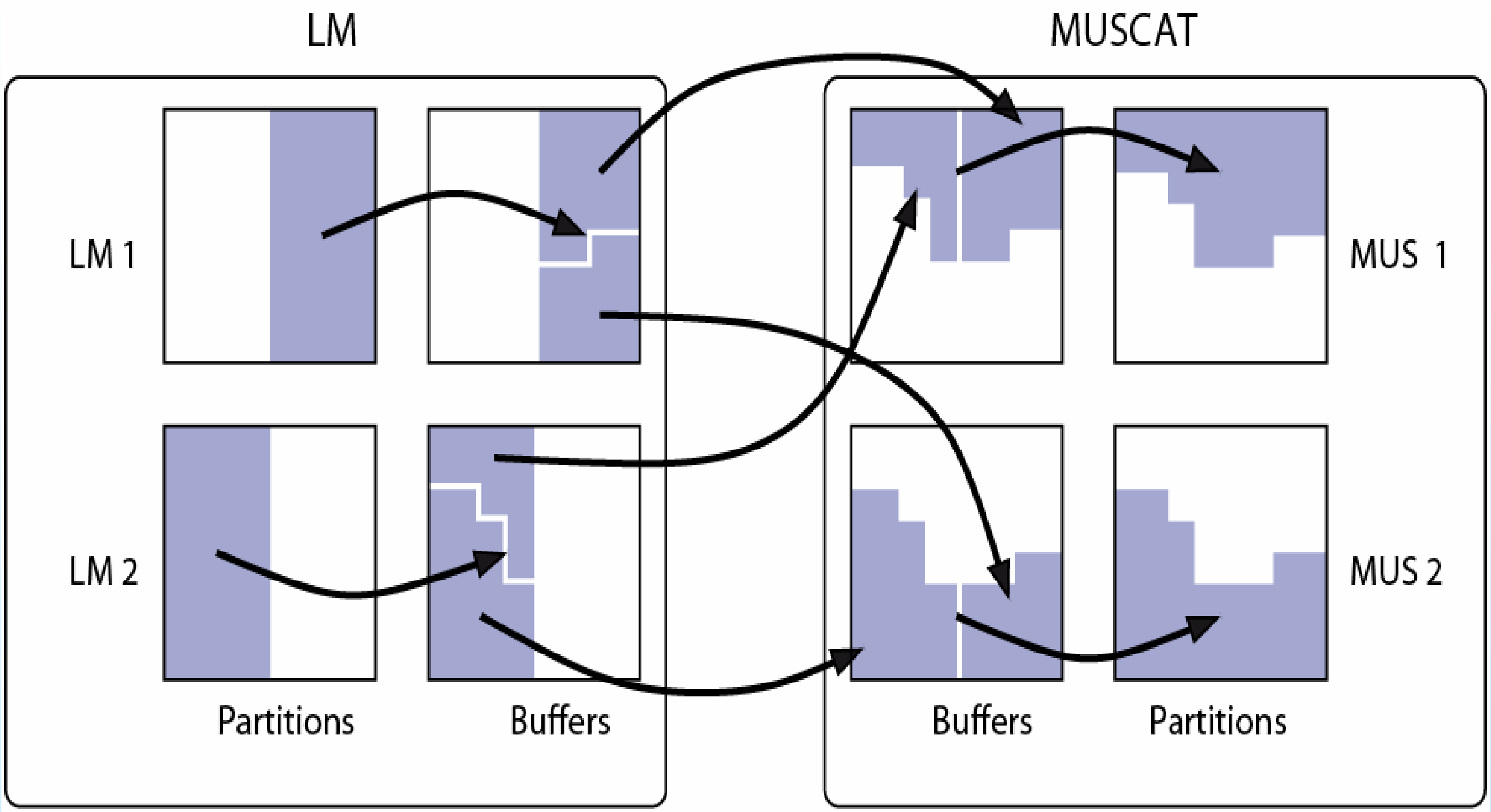
Parallel coupling of LM and MUSCAT

- “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.

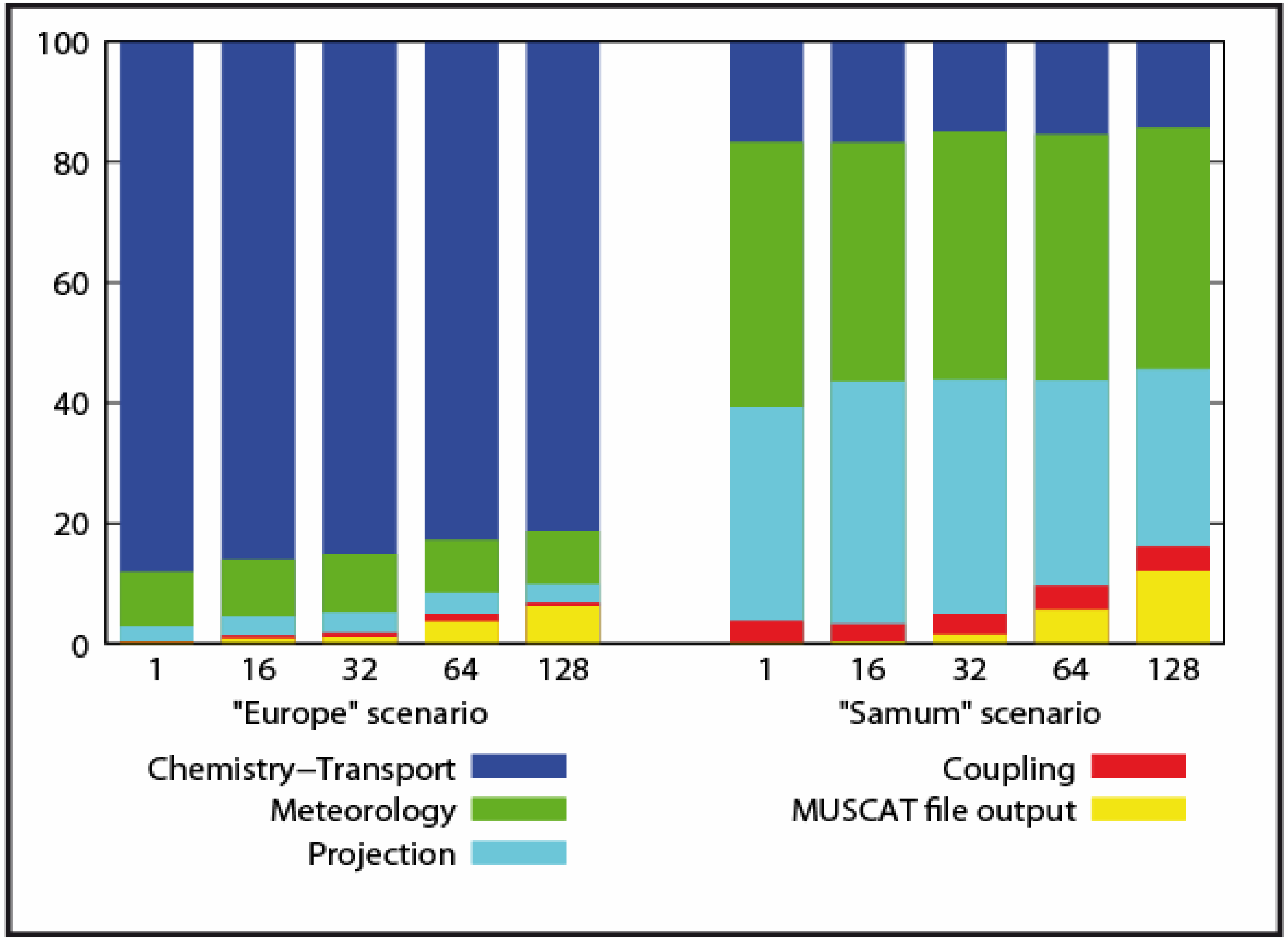


Coupling scheme for model systems: a) sequential, b) concurrent. The letters A and B represent one model code each.

Lieber (2005)

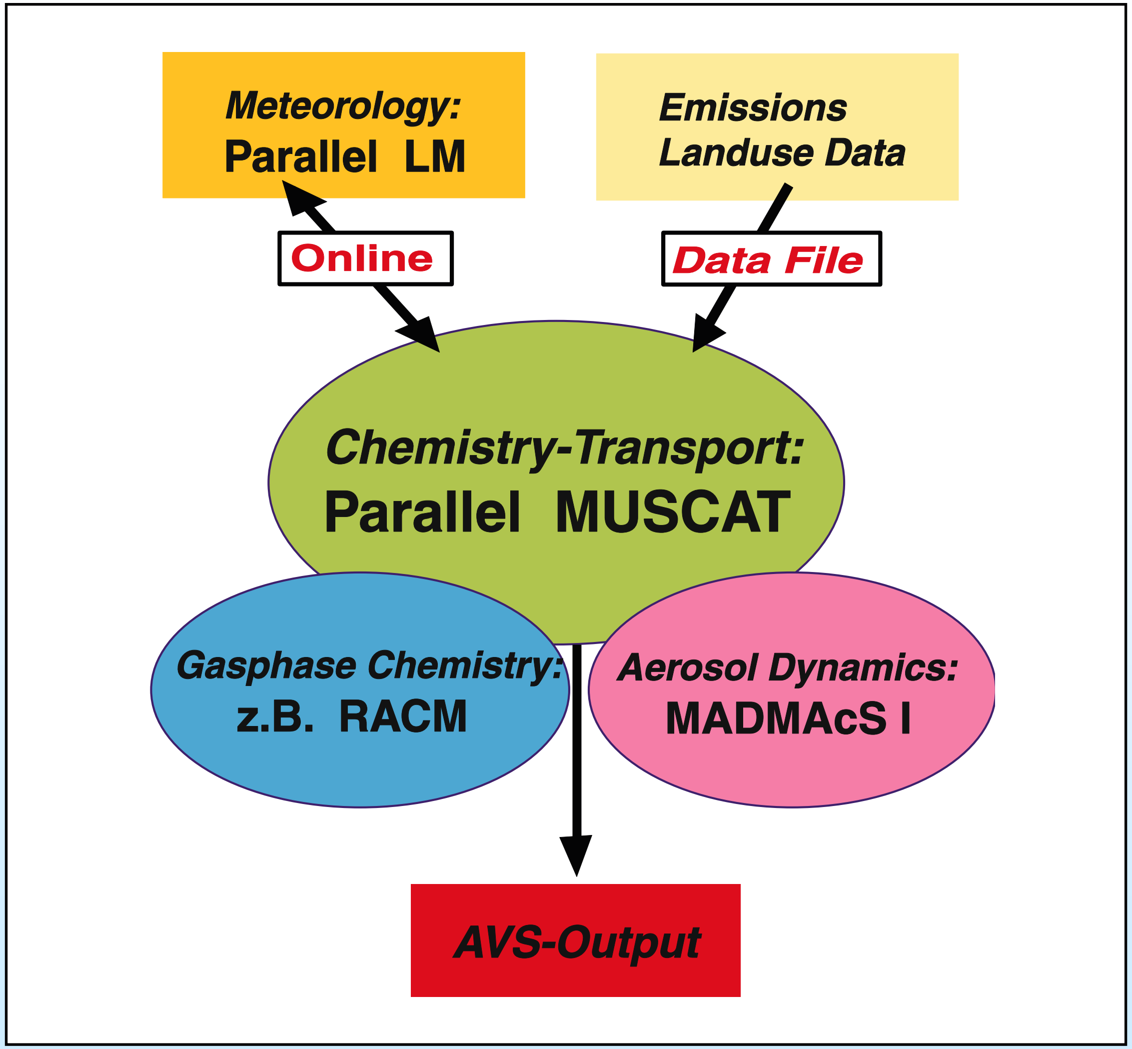


MDE approach to exchange required data between LM and MUSCAT.



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

Model System LM-MUSCAT



Numerical methods in MUSCAT

- Space discretization
  - Staggered grid. Finite-volume techniques.
  - Advection: Third-order upwind scheme (Hundsdorfer et al., 1995).
- 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 solved by Gauss-seidel iterations or AMF
  - Automatic step size control
    - ➔ different number of steps (load imbalances)
- Parallelization

  domain decomposition, load-balancing

Gas phase chemistry

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.

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 that in EMEP Eulerian model (MADE 50)

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

  Considered components: Sulphate, nitrate, ammonia, EC
  (no SOA ➔ M7 approach)

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

- **SAMUM: Sectional (5 or 12 size bins)**

Emissions

Anthropogenic Emissions

- The considered chemical species are the main pollutants SO2, NOx, CO, NH3, PM2.5, PM10, methane, and non-methane volatile organic compounds (NMVOC).
- Area, line and point sources possible. *(Special: “cooling tower”).*
- 11 SNAP codes of EMEP/CORINAIR for characterising the different anthropogenic source types (e.g., combustion in energy industry, road transport, agriculture) are used.
- Aerosol emissions: Particle number and composition of are generated in dependence from the corresponding SNAP.

Dust emission scheme

- Developed by Tegen et al. (2002) , taking paleo- and temporal lake beds as preferential source into account.

SAMUM Joint Project

Subject: "Radiative Effects of Desert Aerosol"

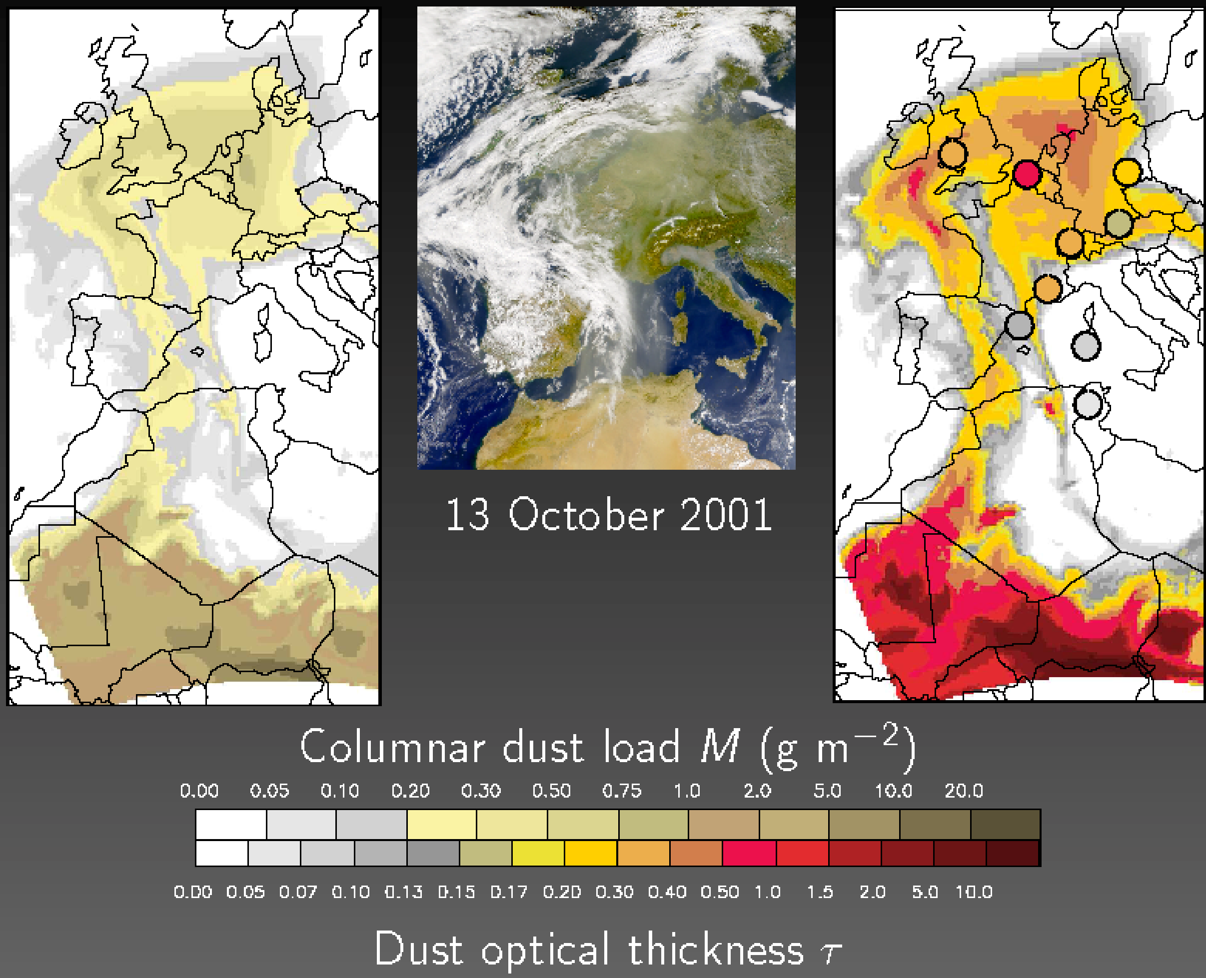
The aim of the project is

- **to develop a physically based predictive model system of the northern African dust cycle by integrating and adapting several existing and newly developed sub-models describing various aspects of dust emission, transport and deposition,**

- **to simulate the spatial and temporary evolution of African dust storms by an Eulerian approach in the mesoscale,**

- **to simulate the influence of long-range transported African dust on atmospheric radiation and cloud microphysics by accompanying Lagrangian process studies.**

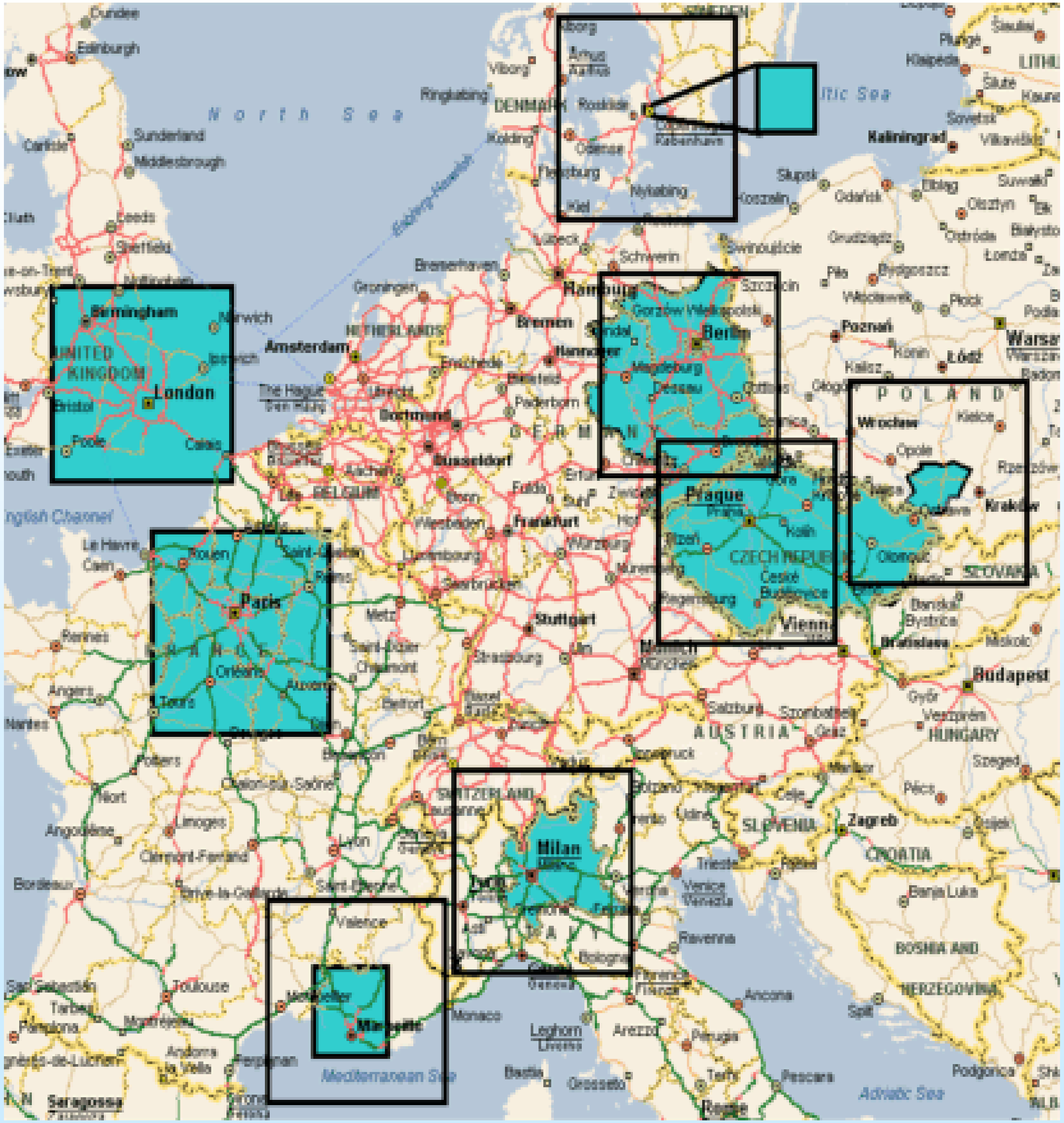
Longrange dust transport



“CityDelta“ Project

- **European Commission program: CAFE - Clean Air for Europe**
  (Initiative: JRC-IES, EMEP, IIASA, EUROTRAC)
- **European modelling intercomparison to predict air quality in 2010 (Ozone, PM)**
- **Sensitivity study (changes in emission scenarios)**
- **Emissions and chemistry boundary data are prepared by Ispra.**
- **Excellent tools (different statistical quantities, graphical interface) for the analysis of simulation results and model intercomparison.**

- **Our focus: “Berlin area“ !!**



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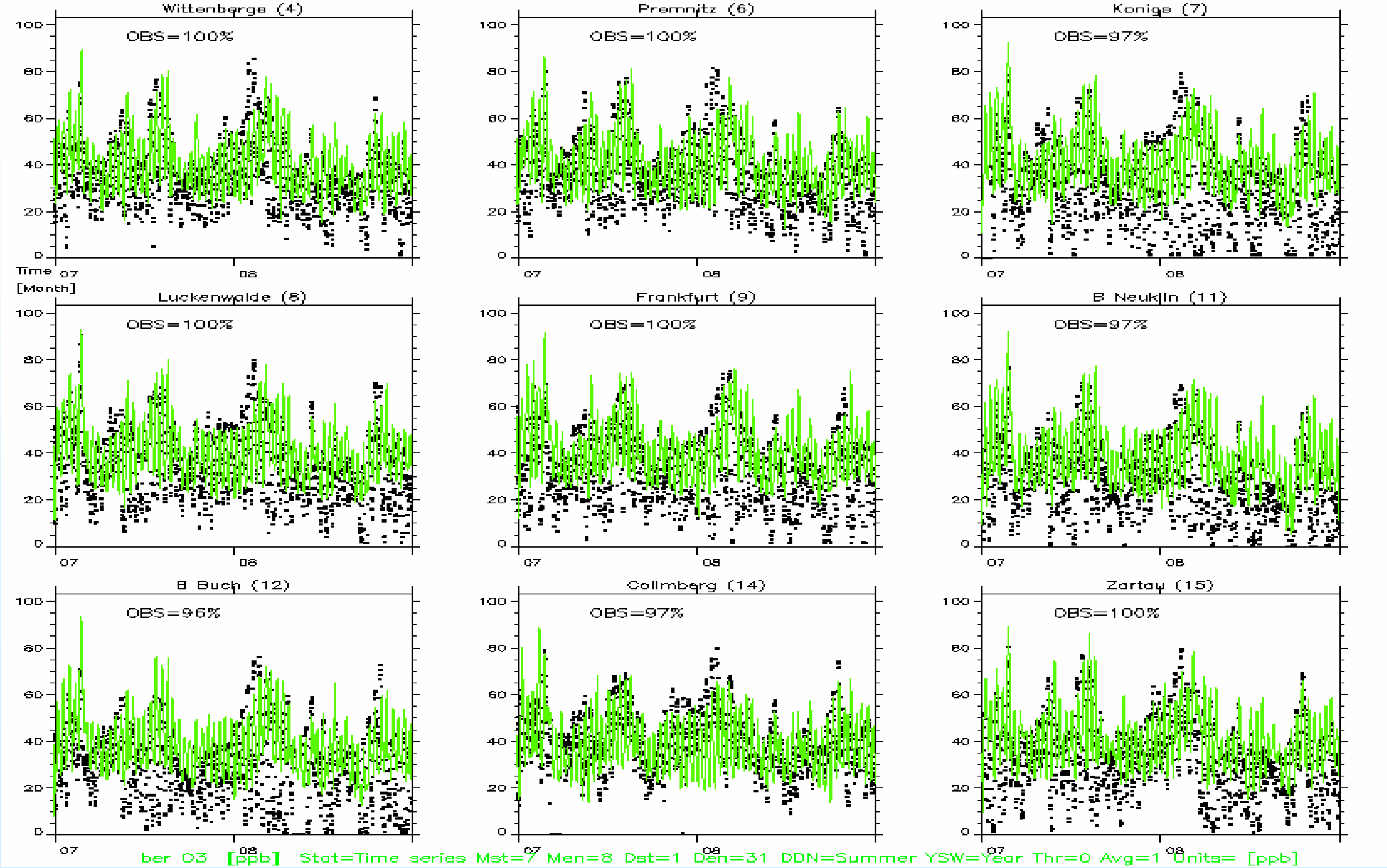
Time series: O3 concentrations (July-August 2000)

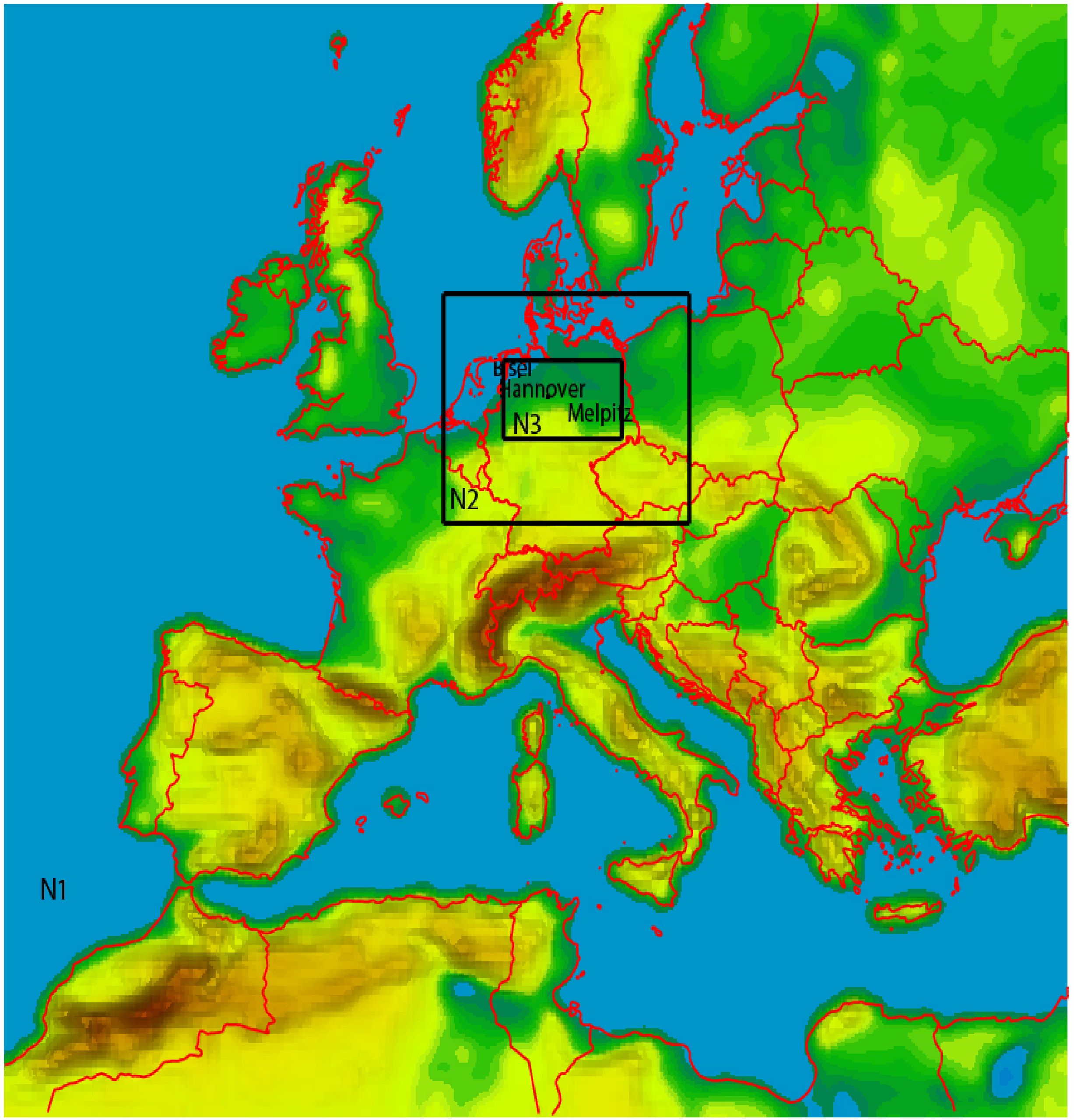


Air quality applications

- LfUG Sachsen
  - *The contribution of two large brown-coal fired power stations in Saxony to the formation of secondary particles (PM10) was examined.*
  - *The highest contribution of PM10 in a narrow plume in the lowest modelling layer on a warm summer day is about 10 µg/m3.*
  - *About 90% of this PM10 are secondary formatted ammonia sulfate.*
- UBA

  Peaks of number concentrations in urban regions
- LA Niedersachsen

  Influence of ammonia emissions on impact of particulate matter.



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Future Work

Dust modelling

1. Land erosion, dust emissions from agriculture activity (together with ZALF Müncheberg)
2. Refinement of the dust emission scheme and dust source areas, convective transport of dust (SAMUM II)
3. Processing of Saharan dust (aging), comparison with EARLINET data

New aerosol module

Extended M7 (cooperation wit MPI Hamburg and ETH Zürich)

+ refined nitrate and ammonia partitioning (ISORROPIA)

+ SOA (z.B. MADRID 2)

Future Work

Multiphase processes in clouds

Implementation in MUSCAT and feedback to LM by use of other ongoing projects:

Spectral Mikrophysics in LM (SPP1167)

Multiphase chemistry (AFO2000 Project MODMEP)

Parcel-Modell SPACCIM: Detailed microphysics and complex multiphase chemistry.

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)