CGSWHP'10
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Inverse Modelling and Data Assimilation Atmospheric Chemistry Simulations

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Structure of the presentation

- Introduction: A very special example
- Space-time variational data assimilation
- Results
  - from surface observation assimilation
  - from satellite data assimilation
- Outlook

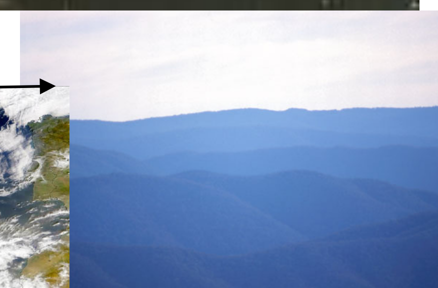
Chemistry-transport model EURAD-IM *(Reaction-advections-diffusion equation)* and further simulated processes

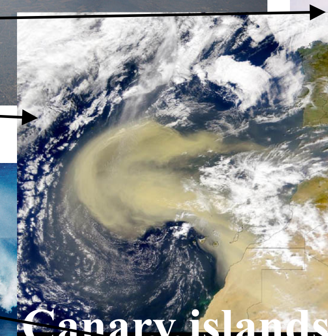
Optionale **Chemiemechanismen,** 0 gas

aqueous phase chemistry
(~5 species)

aerosols (> 50 parameters)

- inorganic
- secondary organic
- mineral dust
- sea salt
- wild fires



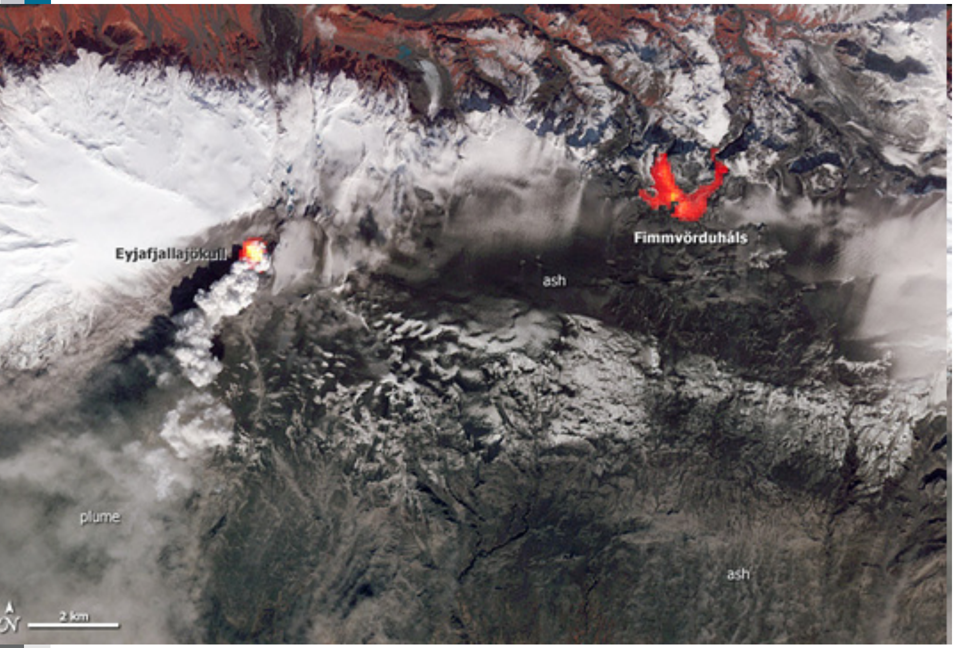


Emissions

- anthropogenic
- biogenic

Deposition
Sedimentation

A current special example for inverse modelling: **Eyjafjallajökull eruption**



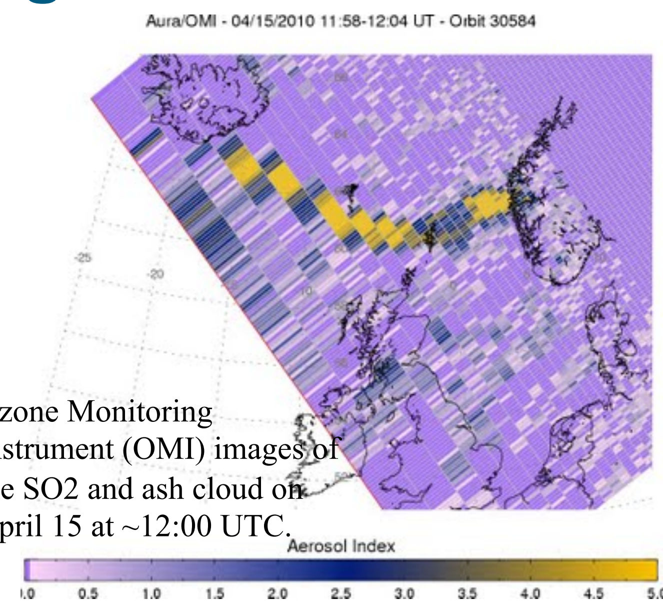
eruption sites Eyjafjallajökull started 14 April, and Fimmvörðuháls 20 March to 12 April. © NASA Earth Observatory.

Flight 27 April 2010 at 12:00, Photo: Sigrún Hreinsdóttir.

We are interested in:

- ash cloud pathway
  - horizontal extension
  - vertical layering
- particle size distribution
- particle composition

We get observations:



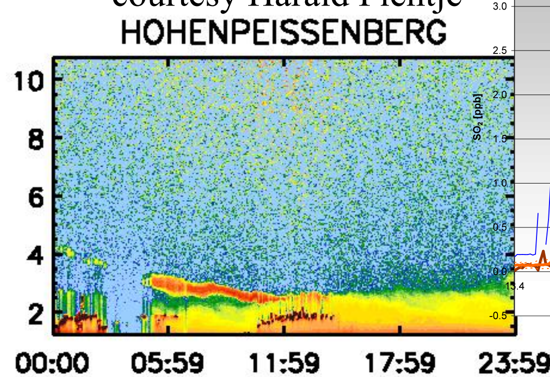
Ozone Monitoring Instrument (OMI) images of the SO2 and ash cloud on April 15 at ~12:00 UTC.

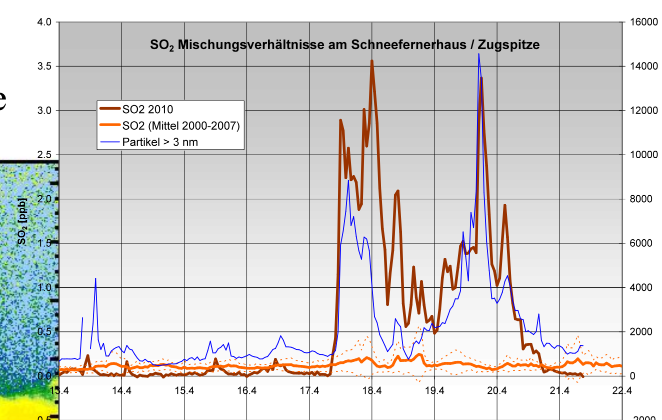
We desperately need, and must invert versus:

eruption characteristics

- injection height profiles
- particle characteristics
- SO2, (fluorines)

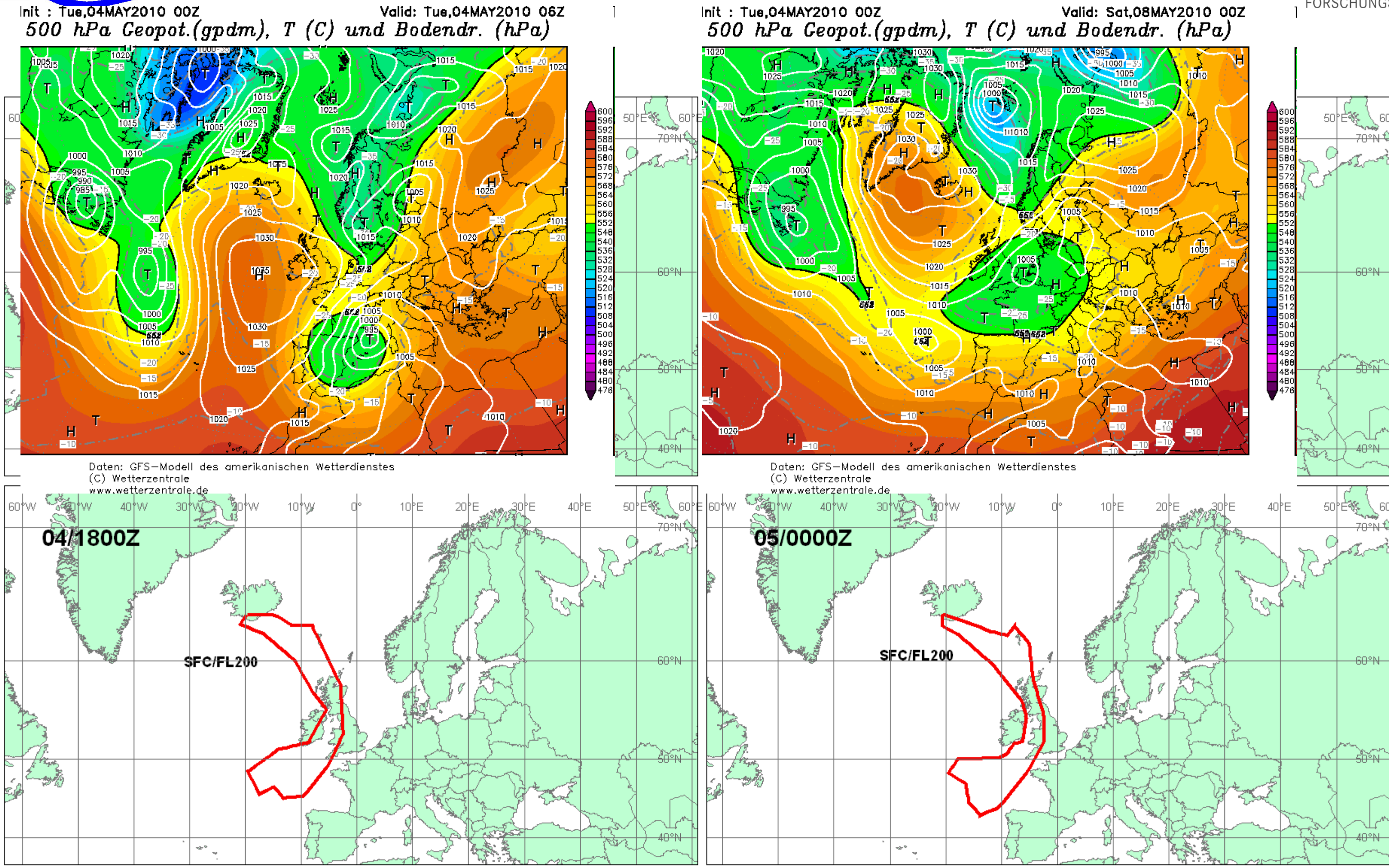
Ceilometer, DWD courtesy Harald Flentje





courtesy Anja Werner, Stefan Gilge, DWD

A short digressing update (for today)



VA ADVISORY
DTG: 20100504/0600Z
VAAC: LONDON
VOLCANO:
EYJAFJALLAJOKULL 1702-02
PSN: N6338 W01937
AREA: ICELAND

SUMMIT ELEV: 1666M
ADVISORY NR: 2010/077
INFO SOURCE: ICELAND MET OFFICE
AVIATION COLOUR CODE: RED
ERUPTION DETAILS: CONTINUING. ESTIMATED
TOPS FL180.

RMK: NO SIG ASH ABOVE FL200
NXT ADVISORY: 20100504/1200Z

Terminology

Inverse Modelling

The inverse modelling problem consists of using the **actual** result of some **measurements** to **infer the values of the parameters** that characterize the system.

A. Tarantola (2005)

Objective of atmospheric data assimilation (1)

The ambitious and elusive goal of data assimilation is to provide a dynamically consistent motion picture of the atmosphere and oceans, in three space dimensions, with known error bars.

M. Ghil and P. Malanotte-Rizzoli (1991)

Information sources and theories

Information set

***declarative information*:**
- **observations/retrievals**
- **forecasts**
- **"Climate" statistics,**
- **error statistics**

procedural Information
differential equations
models

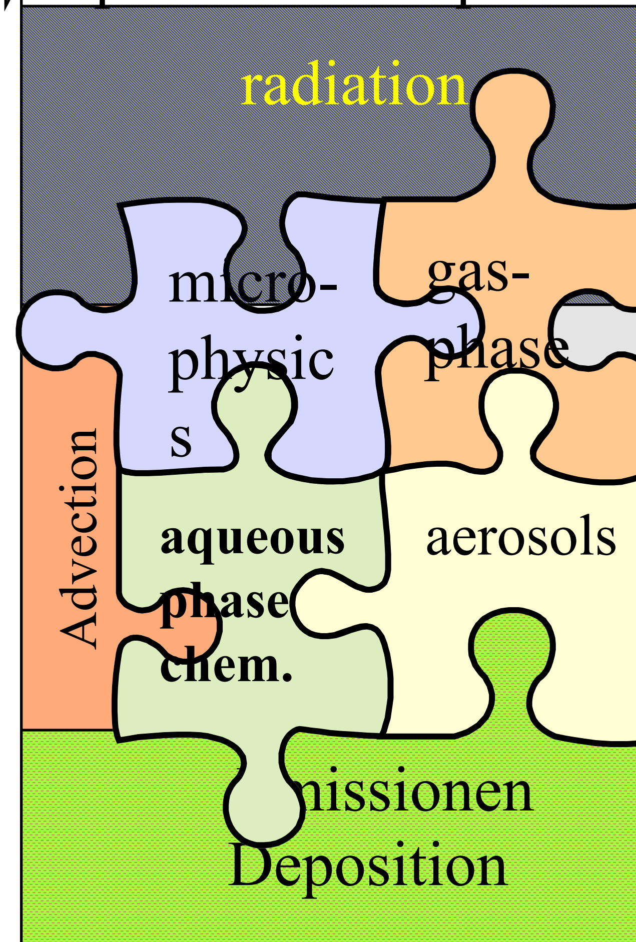
- **control theory**
- **statist. filter theory**
- **classical numerics**
- **optimisation algorith.**

Interpolation
in space and time

Filter
error affected
data

Completion
non-observed
parameters

4D-consistent
process description



Supernational initiatives

Global: "Group on Earth Observations" (GEO) and : **„Global Earth Observing System of Systems“ (GEOSS)**

GROUP ON EARTH OBSERVATIONS

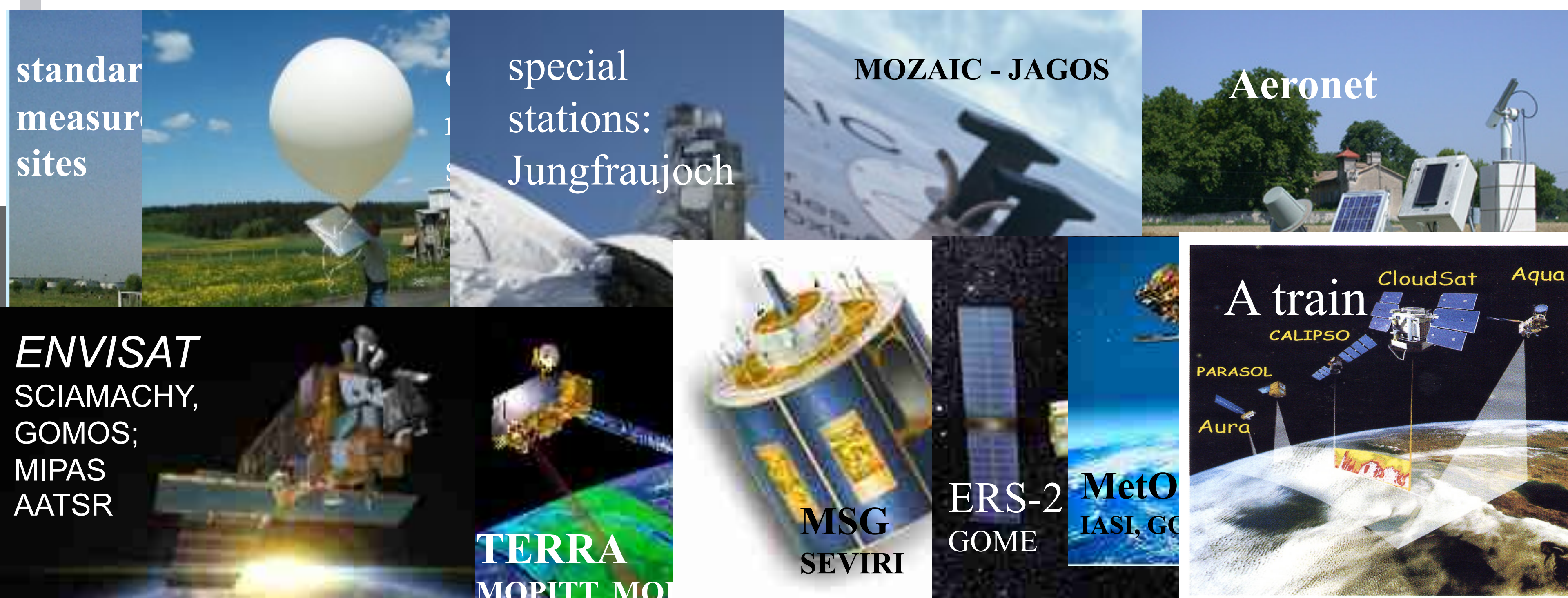
European: Global Monitoring for Environment and Security (GMES)

GMES

Global Monitoring for Environment and Security

“Atmospheric earth observation” for GMES (Global Monitoring and Environmental Security)

EU and ESA-projects for monitoring and short range forecast of air quality



Characteristics of tropospheric chemistry data assimilation (1) physical viewpoint

Main sources of uncertainty:

direct parameters

- Initial values, lateral boundary values
- emission rates,
- deposition and sedimentation velocities
- reaction rates, J-values

indirect parameters

- boundary layer height
- vertical exchange mechanisms: convection

Characteristics of tropospheric chemistry data assimilation (2), mathematical viewpoints

highly underdetermined system - on 2 levels

- variables/gridpoint: ~ 60 -200
- satellite data: scalar column value → profile vector

regionally/locally highly nonlinear chemical dynamics (photo chemistry)

constraints by physical laws/models are insufficient, however central manifolds variable

assimilation or inversion problem to be solved?

The most popular strategy: Linear estimation theory

Provides for a

Best Linear Unbiased Estimate (**BLUE**)

However:

assumes Gaussian error characteristics for positive semi-definite parameters by observations, forecasts, models

Formulation of the background error covariance matrix: Diffusion paradigm
(Weaver and Courtier, 2001)

4D var needs the square root of the background error covariance matrix **B** ($O=10^{12}$):

Basic idea:

1. formulate covariances by Gaussians
2. approximate Gaussians by integration of the diffusion operator over time T
3. calculate $B^{1/2}$ by integration over time T/2 (comp. cheap), and
4. intermittent normalisation (comp. more challenging)

$$\mathcal{C} : \eta(z,0) \longrightarrow (4\pi\kappa T)^{1/2}\eta(z,T)$$

with

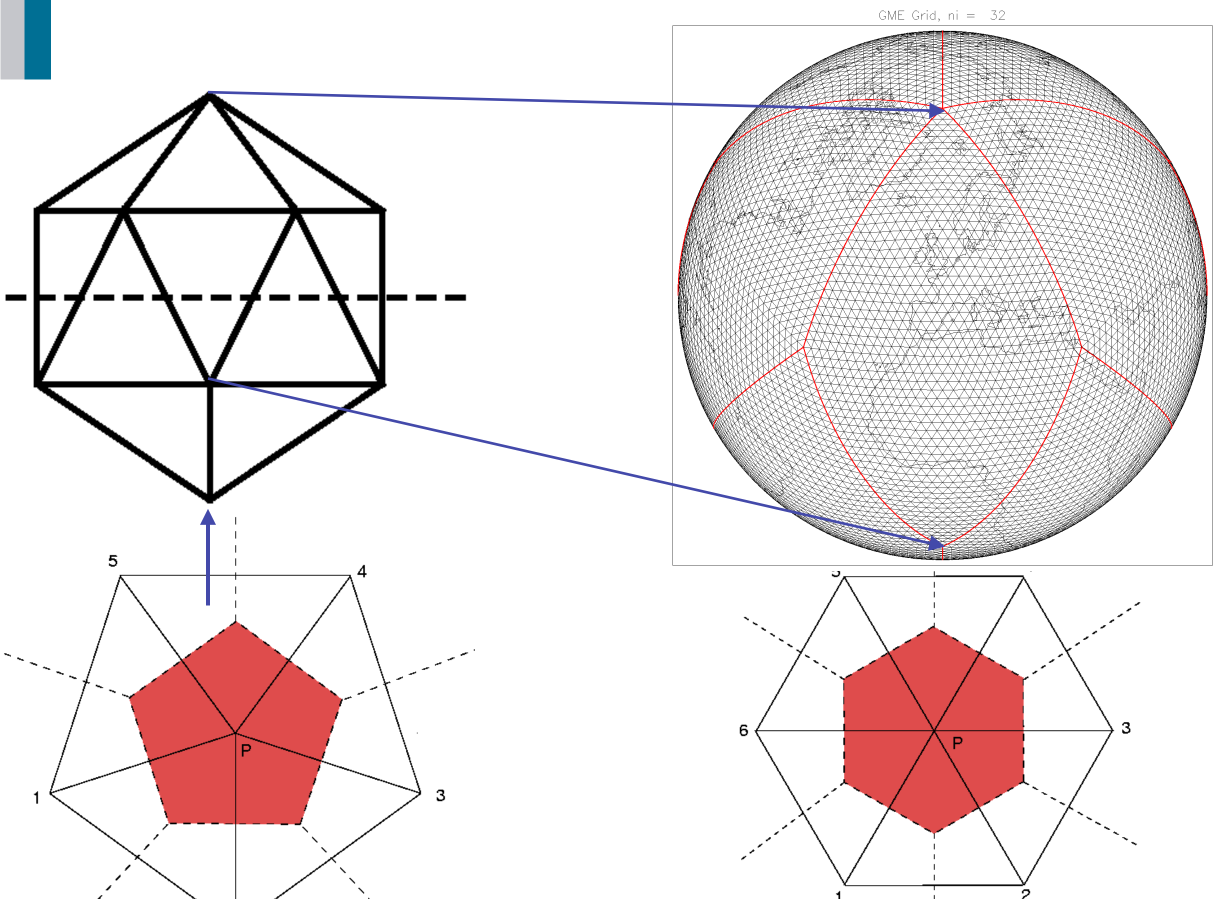
$$\eta(z,T) = (4\pi\kappa T)^{-1/2}\int_{z'} \exp\left(-\frac{(z-z')^2}{4\kappa T}\right)\eta(z',0)dz'$$

and radius of influence

$$L^2 = 4\kappa T$$

SACADA General Chemistry Circulation Model

with GME icosahedral grid structure and met. model



grid cells: 12 pentagons   all other: hexagons

<u>grid:</u>

n_i=32 → Δx~250 km

(~T80, ~ 2.25°)

transport: semi-Lagrange

L42: hybrid, surf→10 Pa

Δz_{strat}~2 km

<u>chemistry:</u>

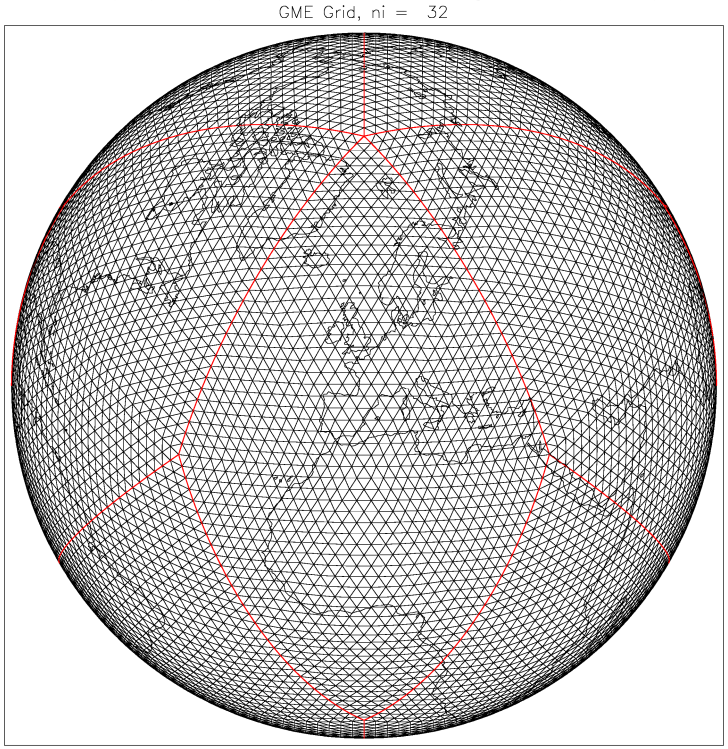
41 species

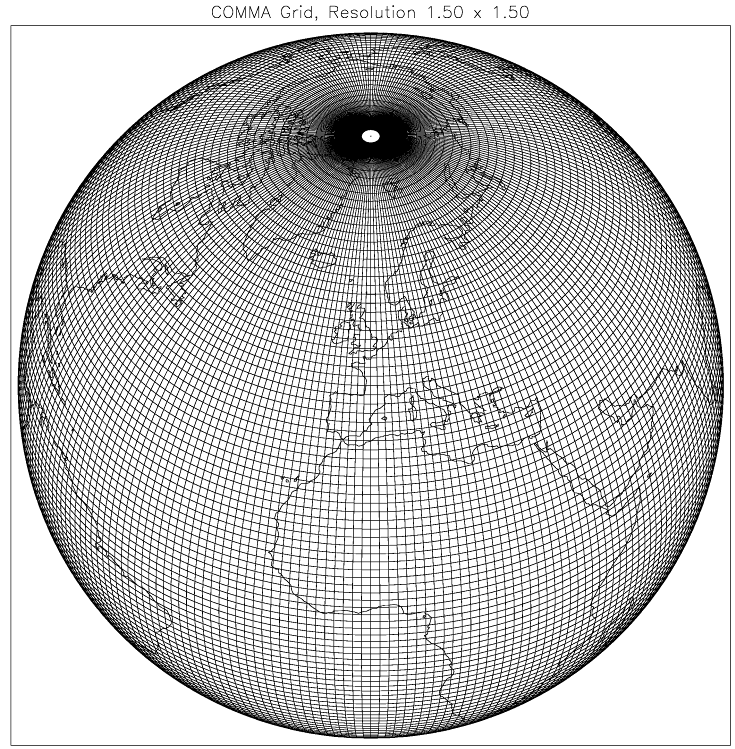
het. chem.:

NAT, ICE, sulf,

(Hendricks et al. 2002)

Icosahedral Grid vs. Conventional lat/lon Grid



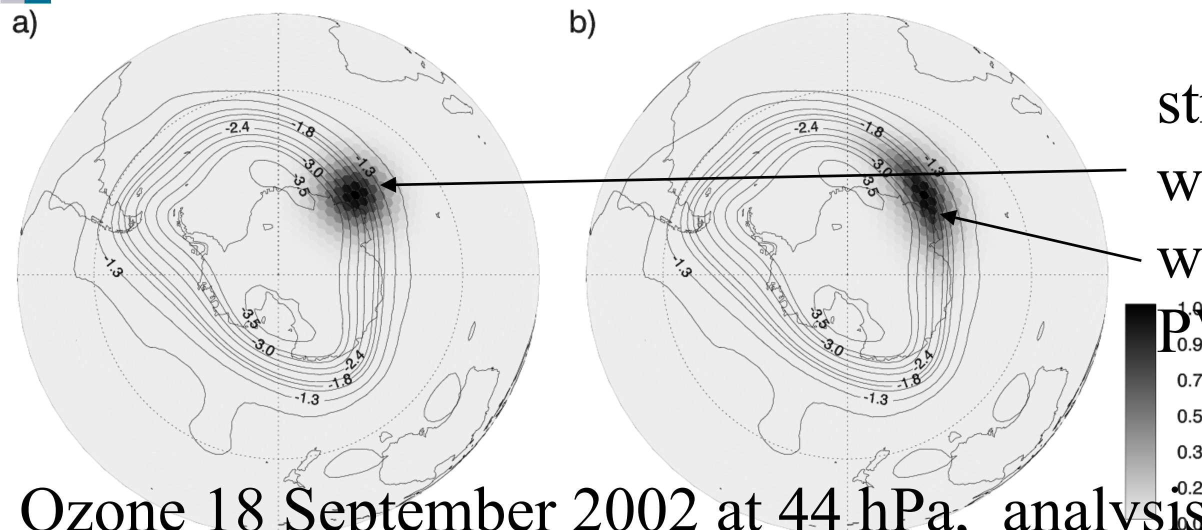


•N_i = 32 → distance between neighbouring grid points ~250 km, nearly homogeneous over the globe

•10242 grid points per level

•Corresponding to 2.25° mesh-size at the equator for lat/lon grid

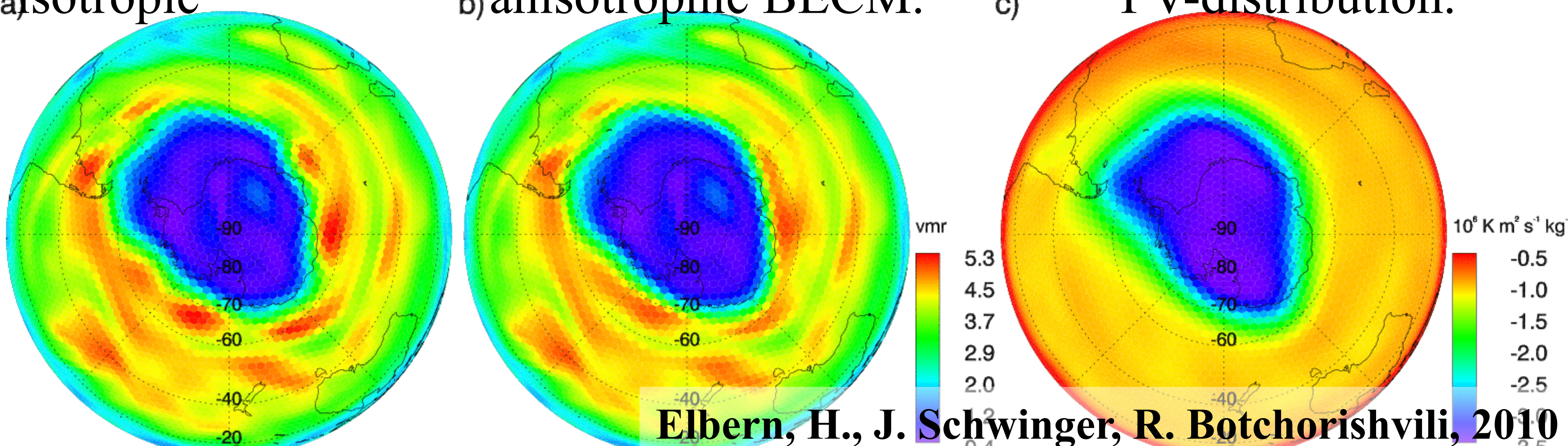
A stratospheric example on diffusion based covariance modelling: PV control in SACADA model



structure functions
without
with
PV gradient control

Ozone 18 September 2002 at 44 hPa, analysis with

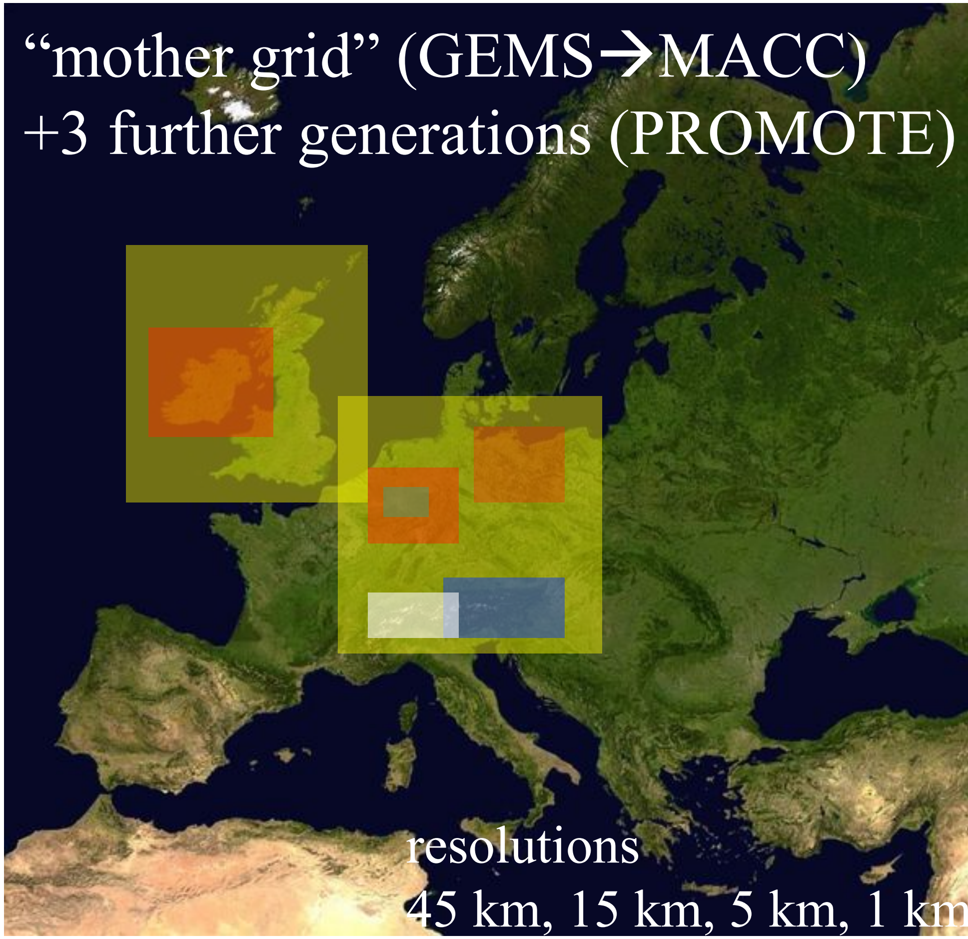
isotropic   anisotrophic BECM.   PV-distribution.



Elbern, H., J. Schwinger, R. Botchorishvili, 2010

EURAD-IM
4D-var system (1)

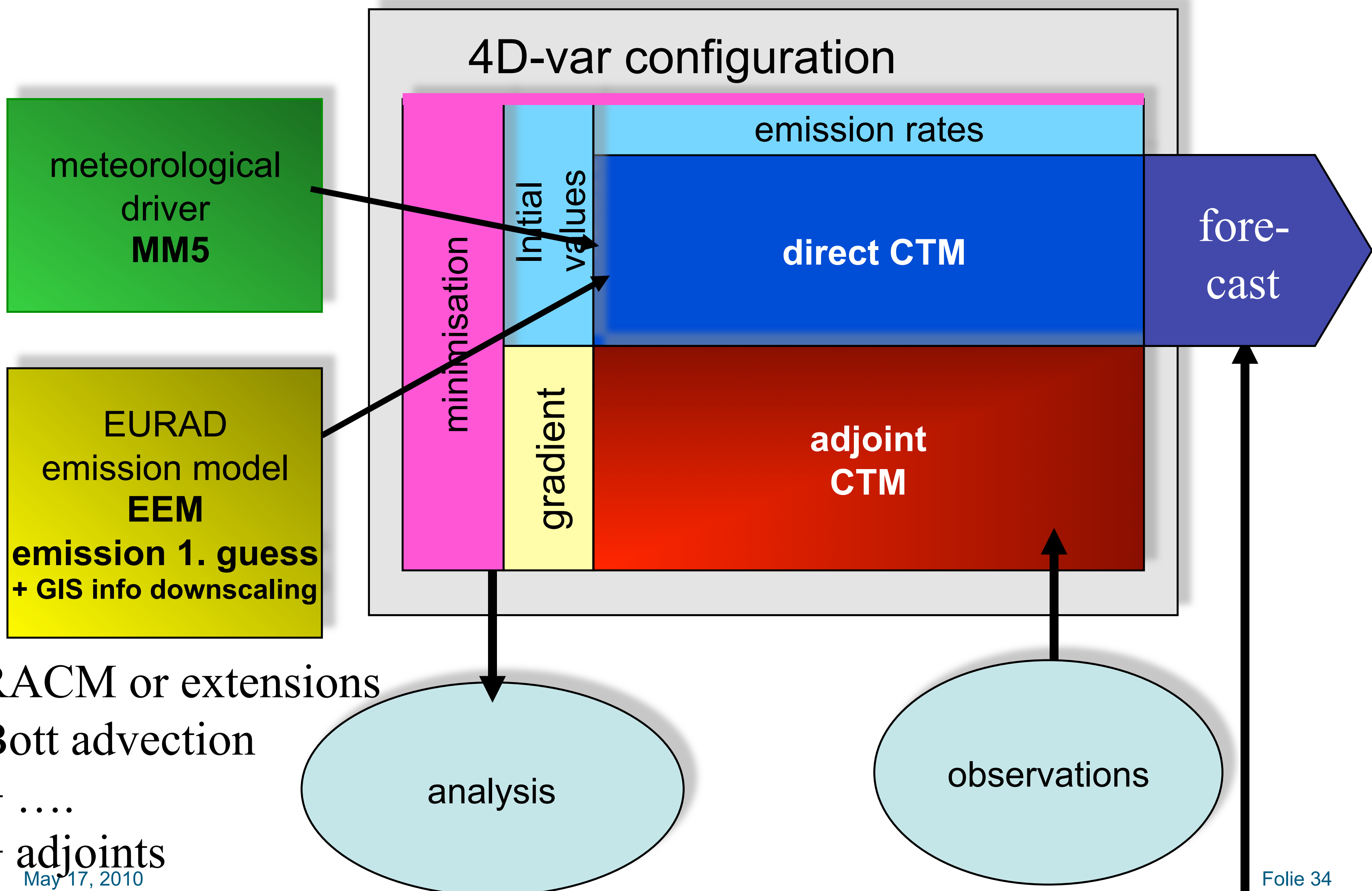
EURAD-IM adjoints
RACM chemistry mechanism
implicit vertical diffusion
explicit horizontal diffusion
Bott 4th order advection
emissions: EMEP, TNO



MADE, SORGAM adjoint version under way

EURAD-IM

(EURopean Air pollution Dispersion-Inverse Model system



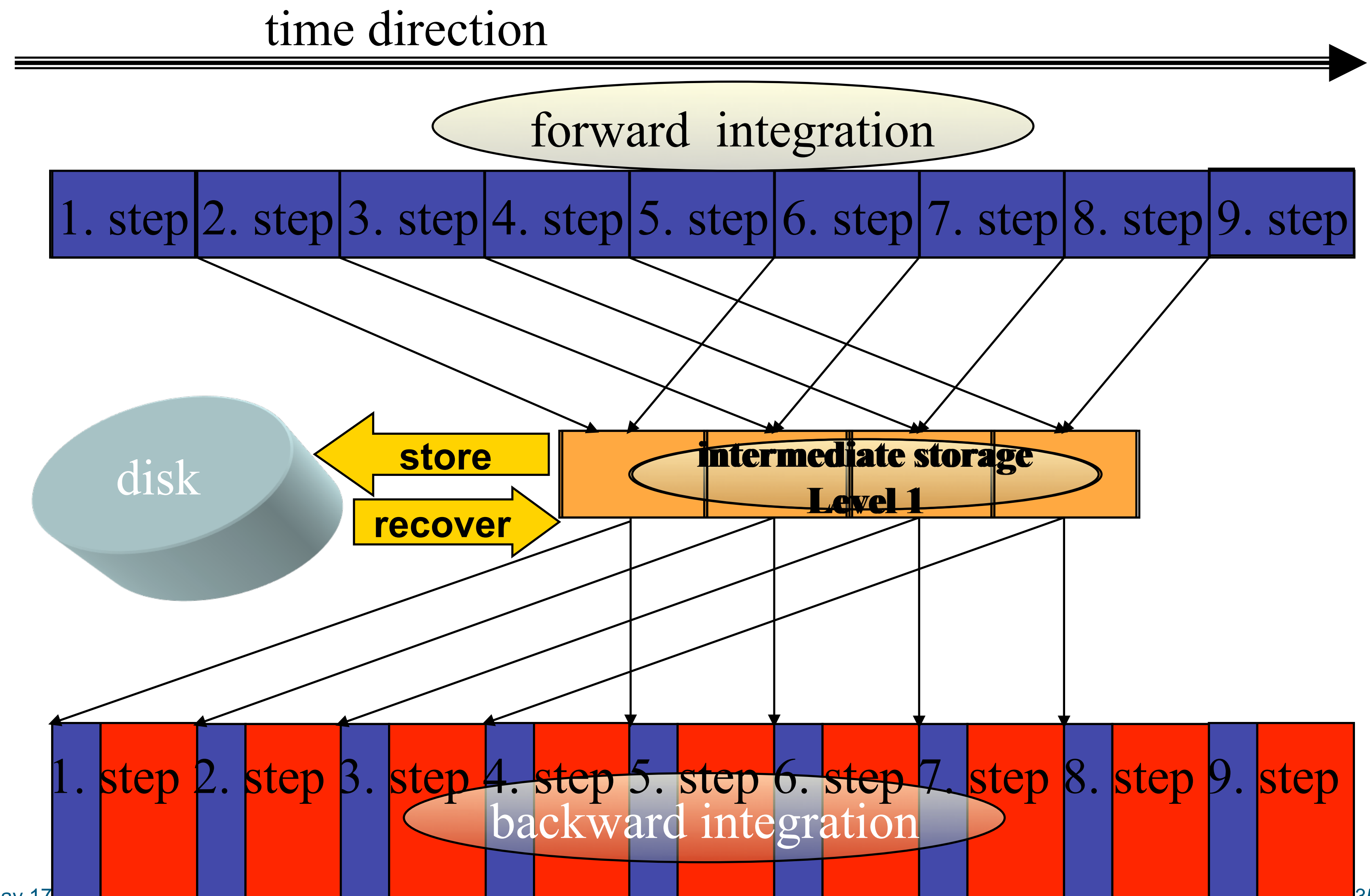
RACM or extensions

Bott advection

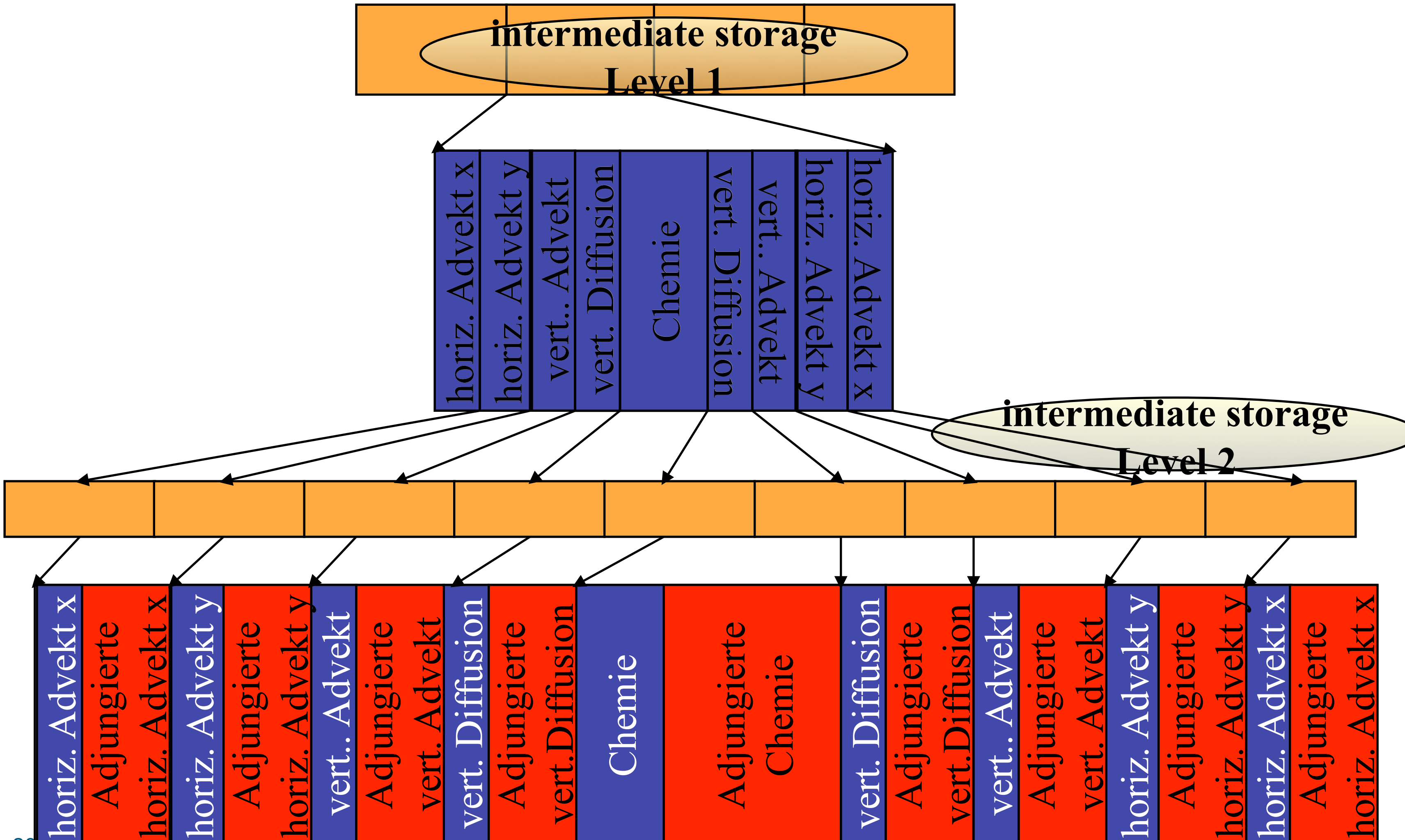
+ ….

+ adjoints

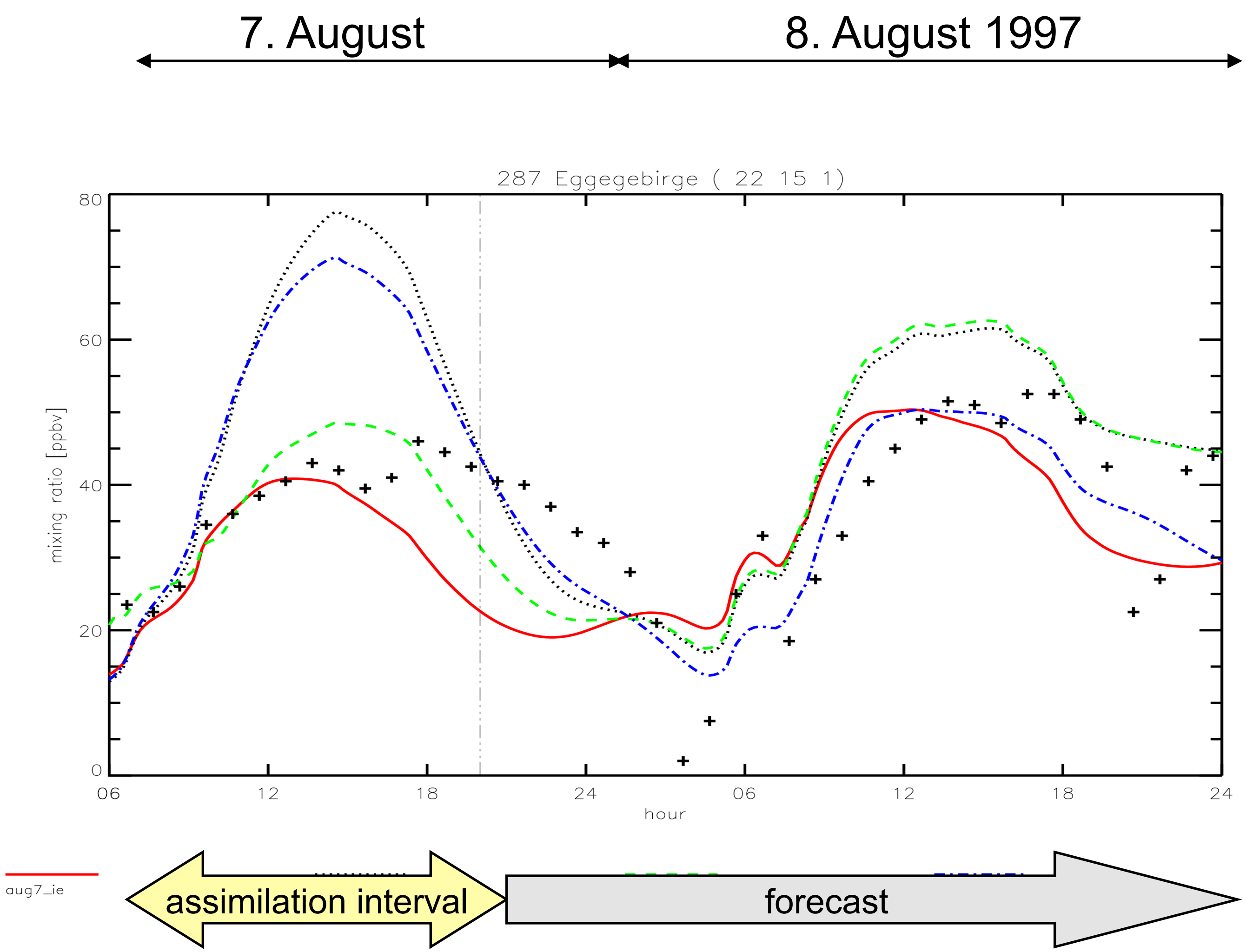
2 level forward and backward integration scheme



storage sequence: level 2, operator split
(each time step)



Semi-rural measurement site Eggegebirge

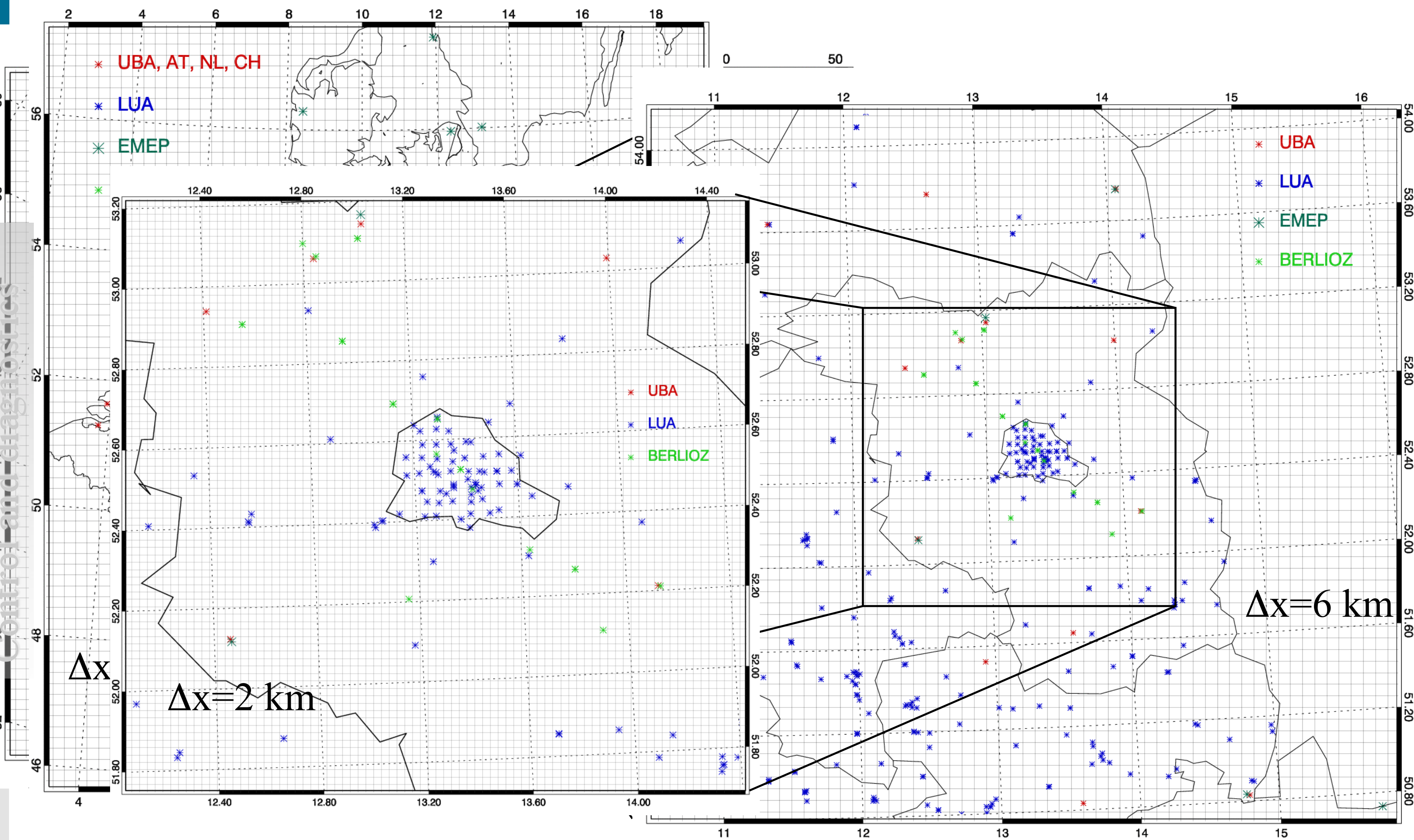


+ observations
no optimisation
initial value opt.
emis. rate opt.
joint emis + ini val opt.

(Elbern, Strunk, Schmidt, Talagrand. 2007)

Which is the requested resolution?

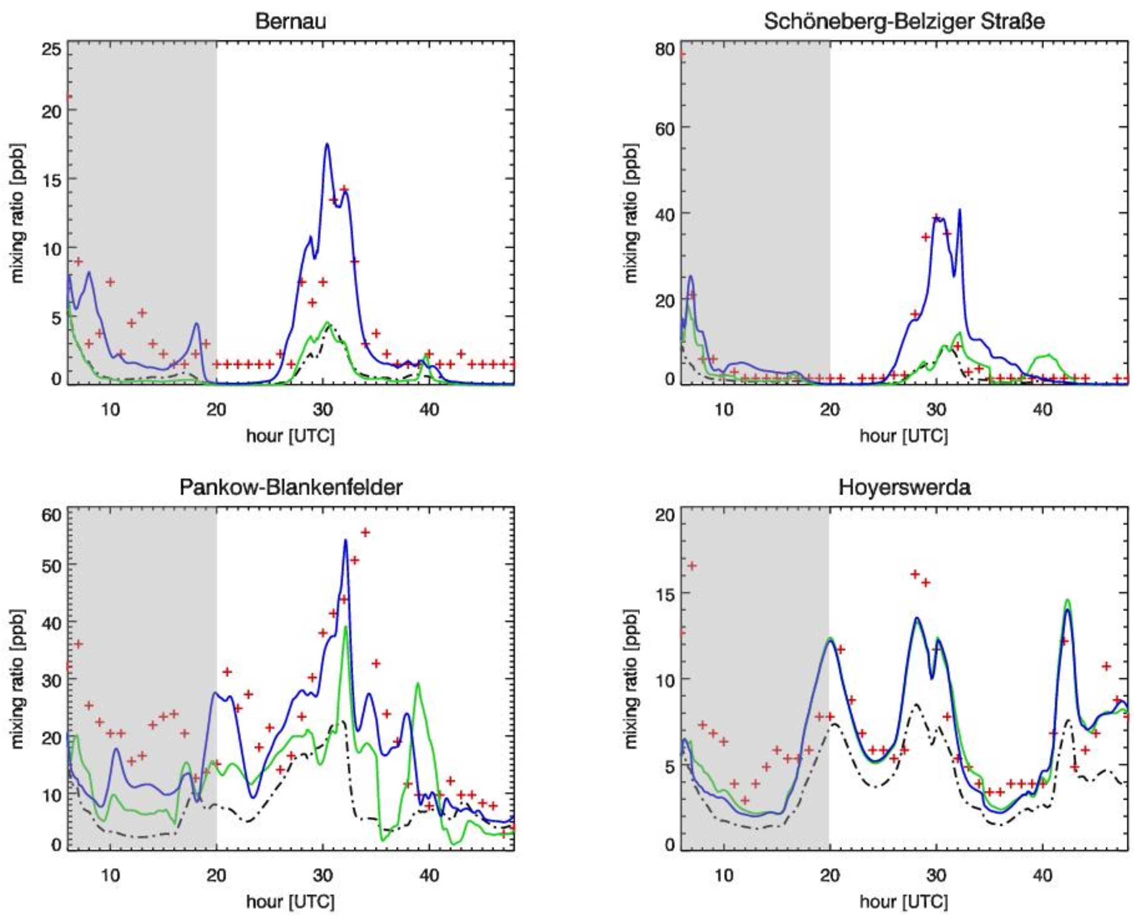
BERLIOZ grid designs and observational sites
(20.→21.07.1998)



Some BERLIOZ examples of NOx assimilation (20.→21. 07.1998)

NO

NO_2



Time series for selected NOx stations on nest 2.

+ observations,

-- - no assimilation,

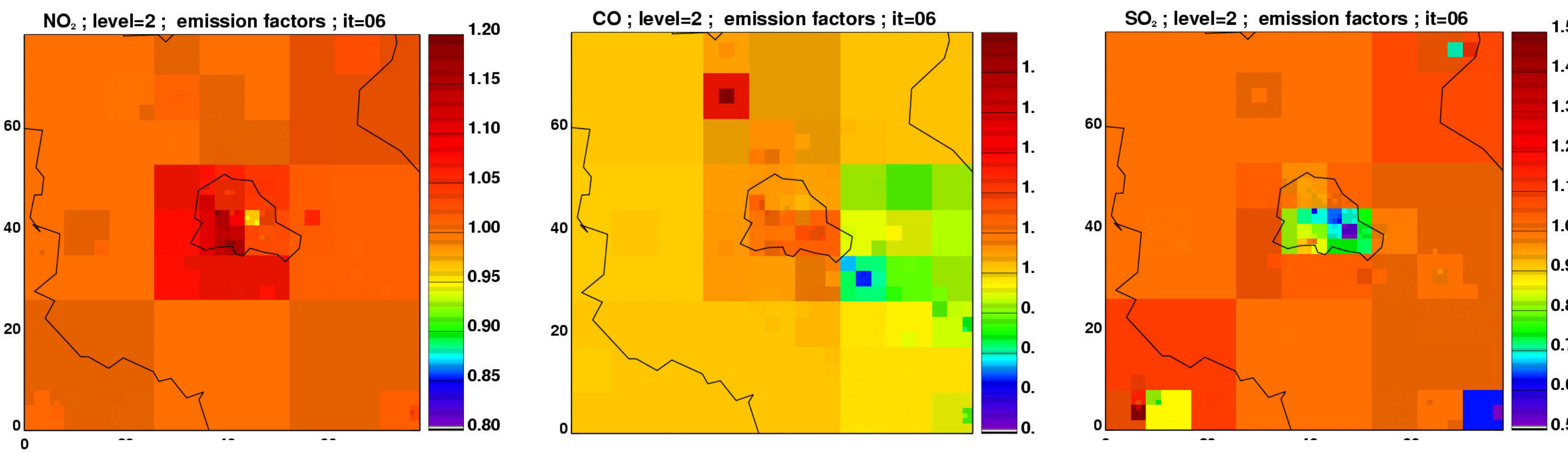
-_____ N1 assimilation (**18 km**),

-_____N2 assimilation.(**6 km**),

-grey shading: assimilated observations, others forecasted.

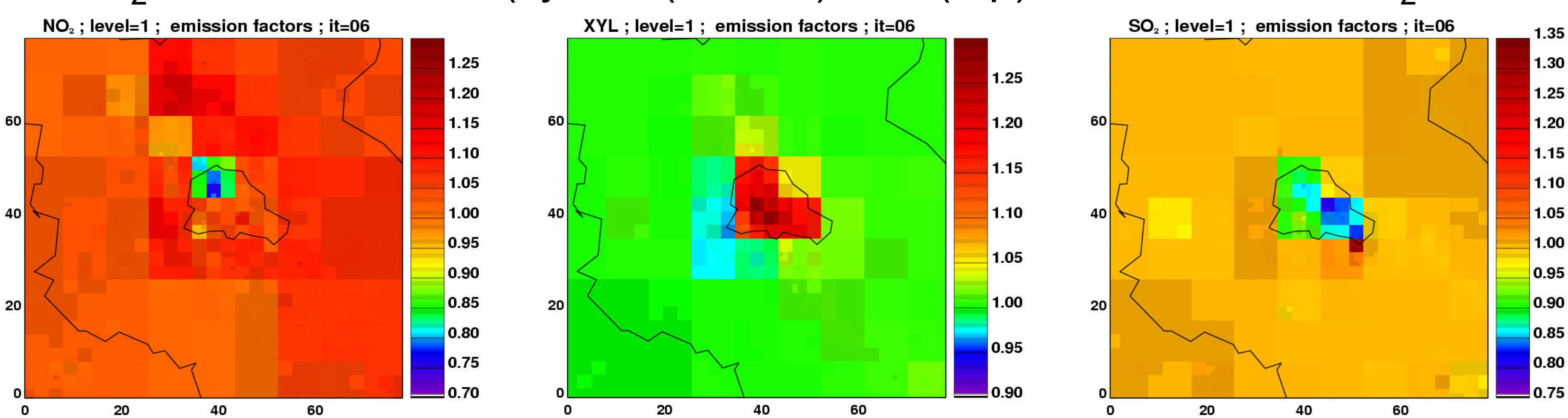
Emission source estimates by inverse modelling
Optimised emission factors for Nest 3

height layer ~32-~70m



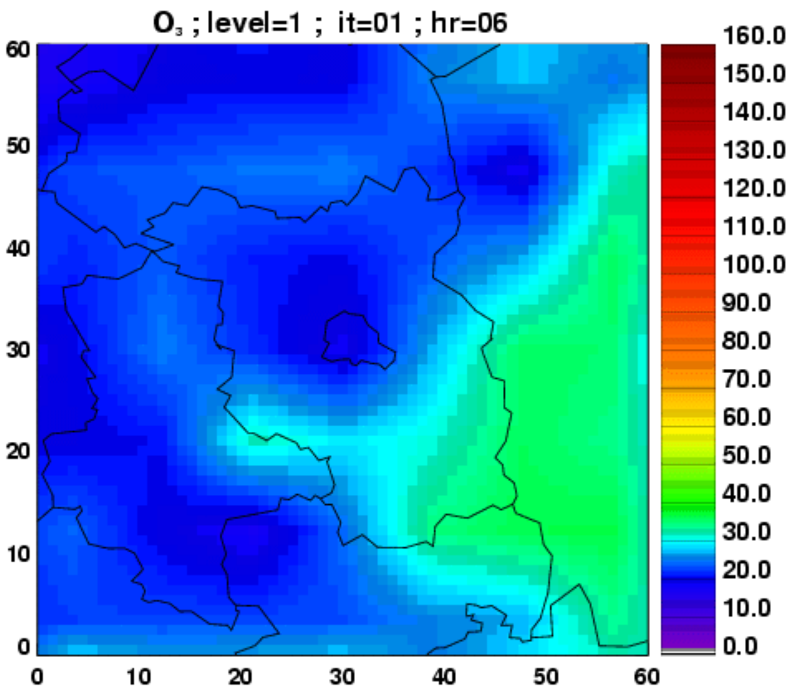
NO_2, (xylene (bottom), CO (top) SO_2 .

surface

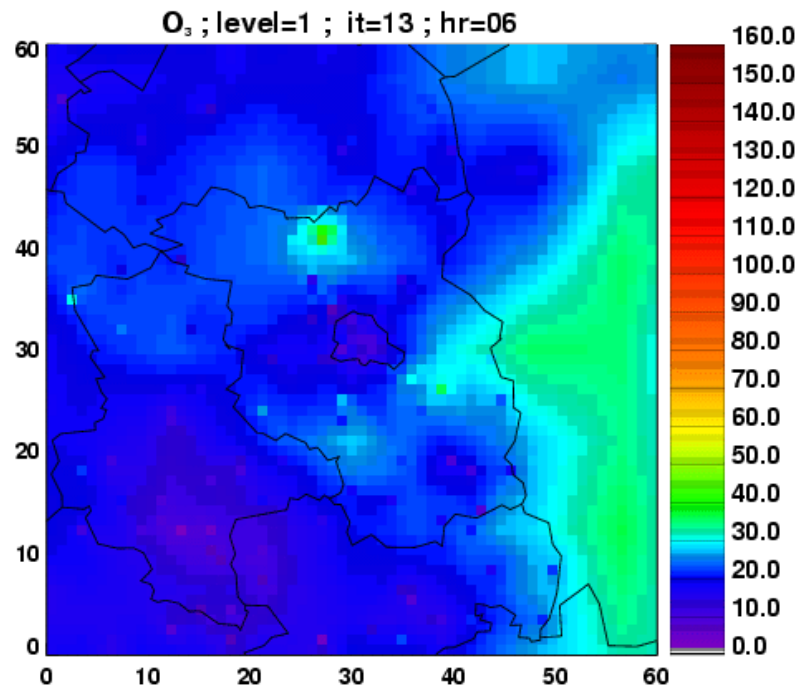


Nest 2: **(surface ozone)**
(20.→21. 07.1998)

without assimilation

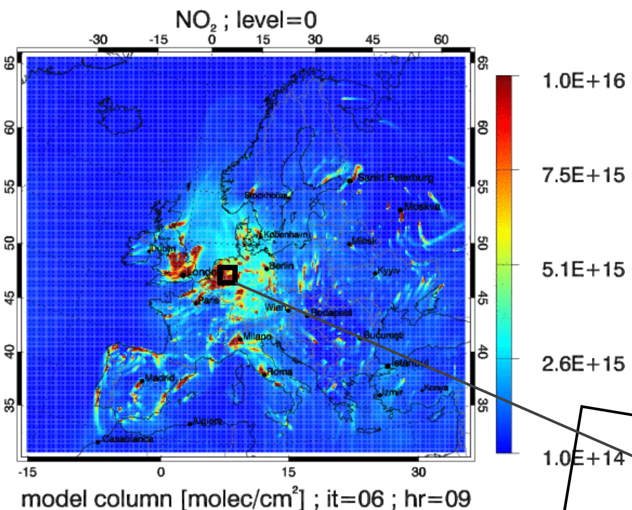


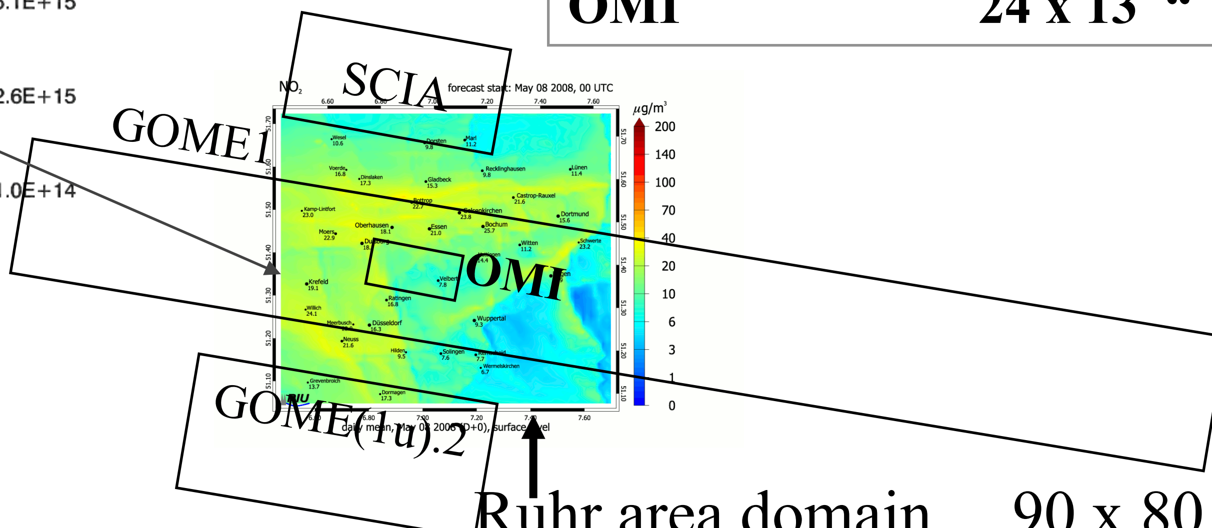
with assimilation



Satellite information:
ESA UV-VIS satellite footprints Ruhr area comparison

minimal areas:	
GOME 1	320 x 40 km^2
(special mode)	80 x 40 “
SCIAMACHY	60 x 30 “
GOME 2	80 x 40 “
OMI	**24 x 13 “**



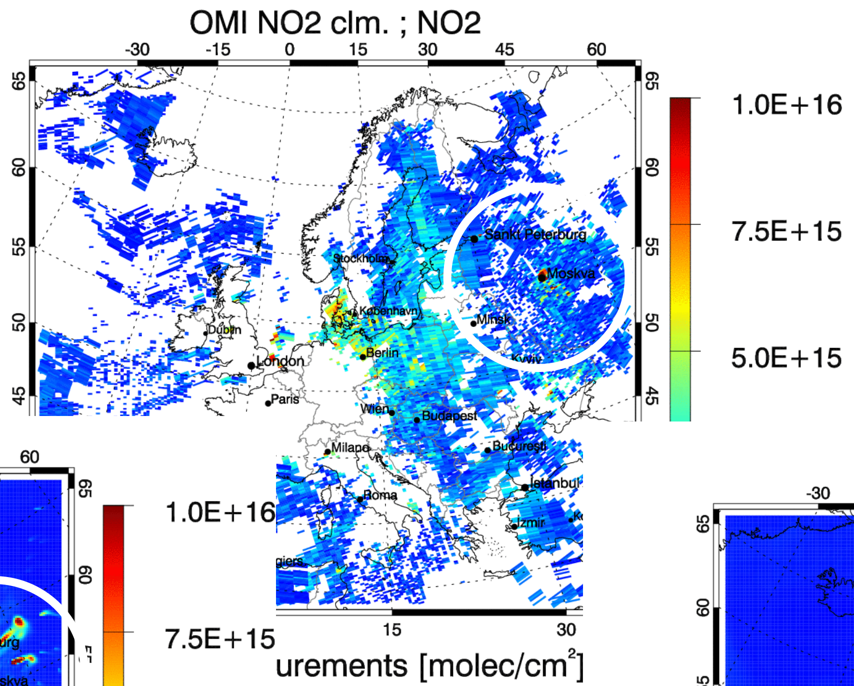


Ruhr area domain   90 x 80 km^2

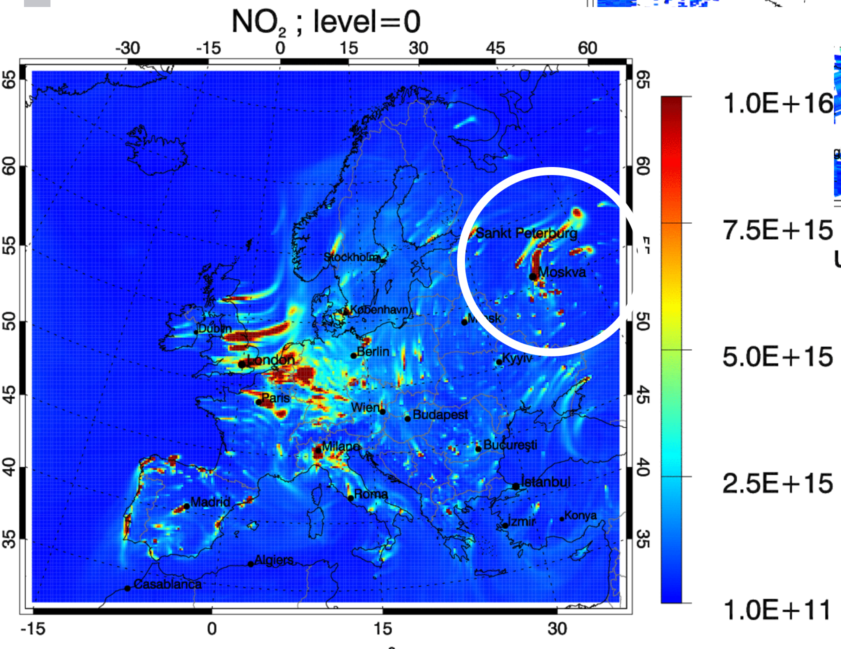
1 km resolution

(~12 000 000 inhabitants)

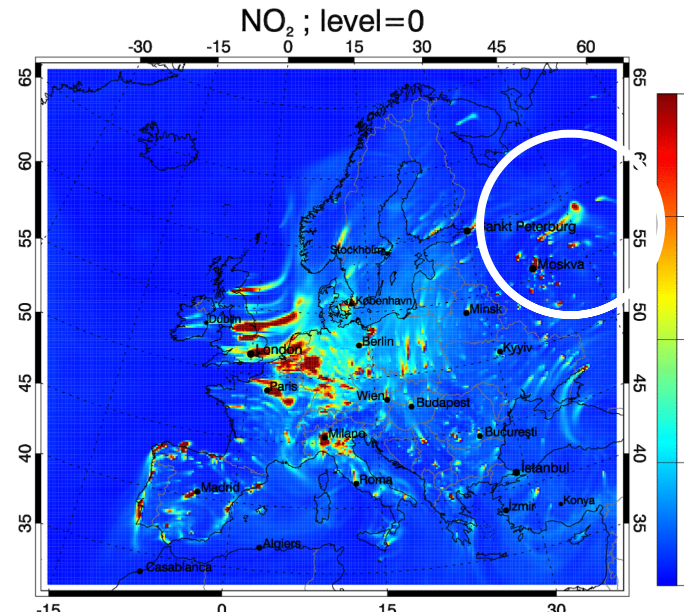
Data assimilation result in terms of tropospheric columns for July 7th, 2006. NO2 model columns based on OMI and SCIAMACHY assimilation within the assimilation interval, 09-12 UTC.



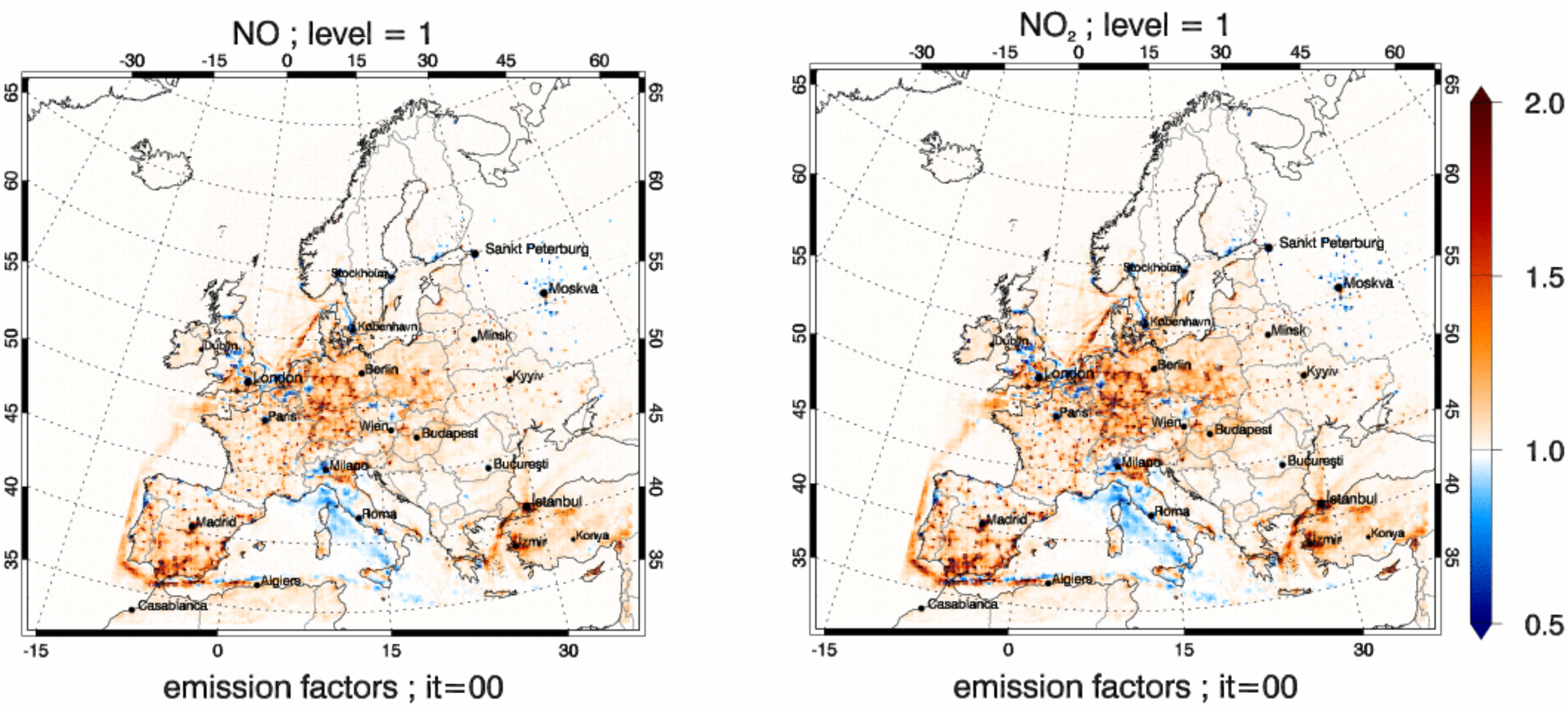
pure forecast



assimilation based forecast



Emission correction factors
for NO and NO2
by OMI NO2 tropospheric column assimilation



Outlook and challenge for the future and invitation to participate

Numerics and scientific computing on

- probabilistic approach in both, (ensemble modelling)
  - forecasting
  - data assimilation
- solution of <u>stochastic</u> reaction-advection-diffusion equation
  →approximation of the related Fokker-Planck equation
- “observability problem”:
  - Given observations, how far can the system be analysed?
- “Targeted observations”:
  - What and where to observe best, given constraints?