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Atmospheric Simulations and their Optimal Control

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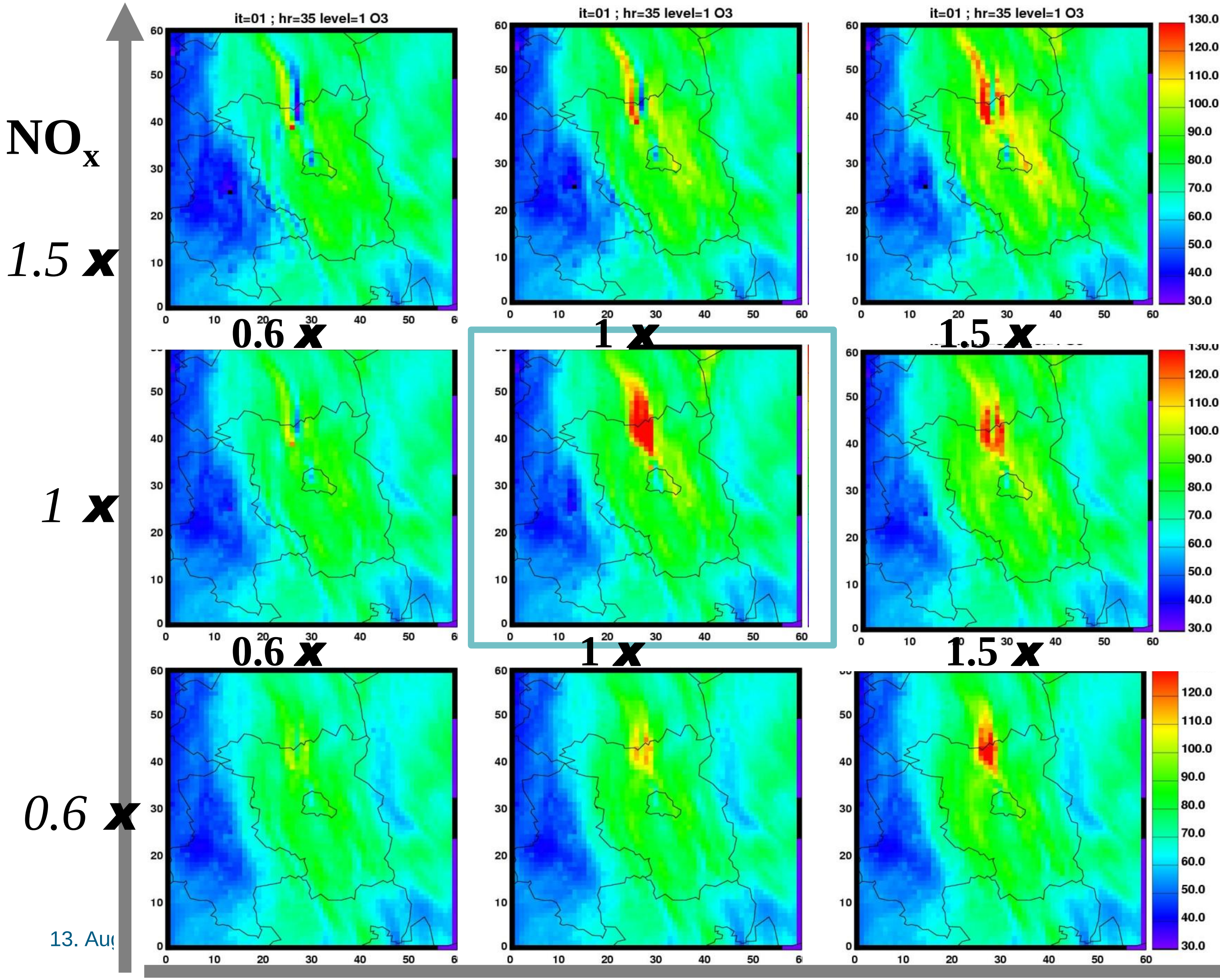
Outline

1. Optimisation: a universal scientific objective
2. Problem: How can we control a system with high degrees of freedom?
3. How can we optimally combine models with observations?
   1. a means to upgrade our knowledge basis
   2. test hypotheses

Specifically in atmospheric sciences:

1. for green house gas inversion
2. for air quality and climate monitoring/reanalyses
3. Extension: “detection and attribution” algorithm for climate change

How can “good”simulations be identified?

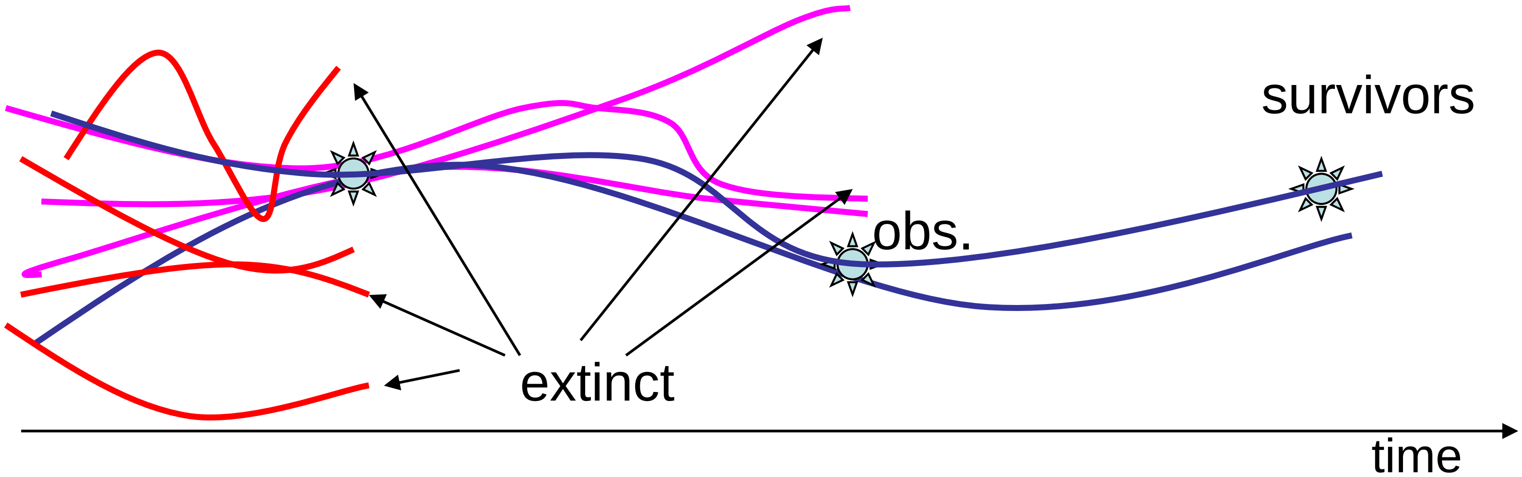


Ozone: NO$_x$-VOC emissions variation ensemble (21.7.1998, 15:00 UTC)

Note:
not **C**-orthogonal, not max. sensitivities aligned

VOCs

How can "good"simulations be identified? Sequential Importance Resampling

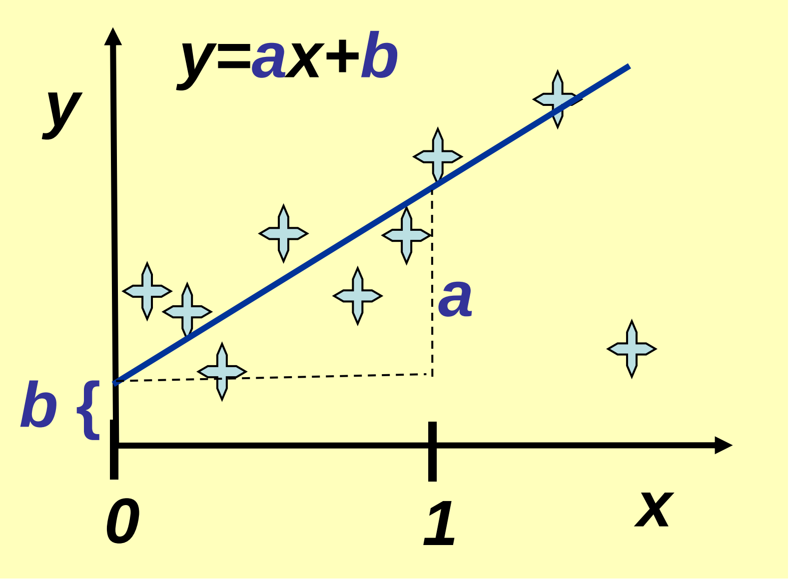


How to select weights w_i?

Other techniques:

- Ensemble modelling
- (Markov Chain) Monte Carlo methods (MCMC)
- and many more versions …..

Are there more focussed approaches? e.g. quadratic optimisation



Given

- the "model" $y = M(x; a, b) := ax + b$, and
- observations $y_i, \quad i = 1, \ldots, K,$

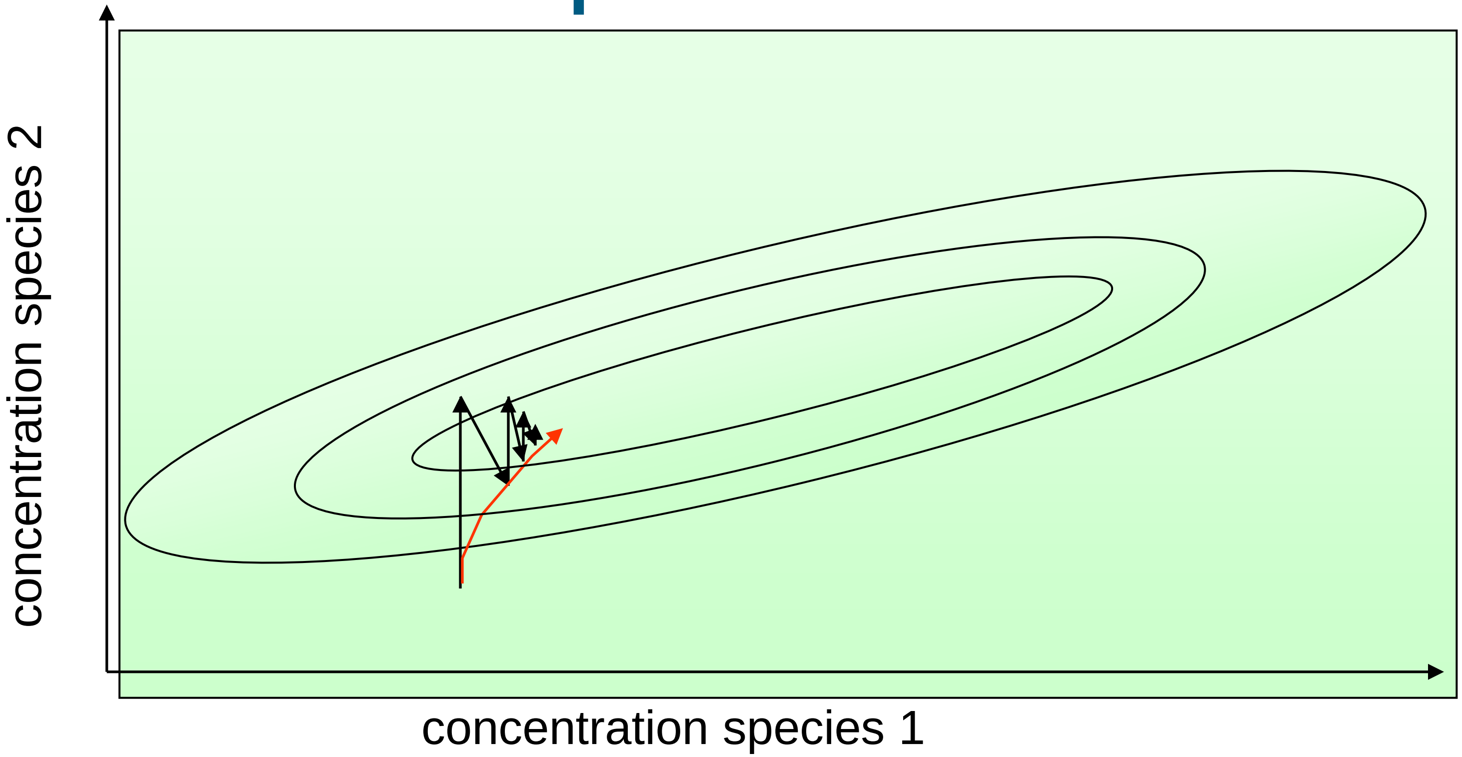
provide a best estimate of model parameters a, b in a sense that

$$\min_{a,b} \left[\sum_i (y_i - (ax_i + b))^2 \,|\forall \text{ observations}(x_i, y_i) \right]$$

Writng the set of observations in column vector notation $\mathbf{y}, \mathbf{x}$, minimise

$$(\mathbf{y} - M(\mathbf{x}; a, b))^T (\mathbf{y} - M(\mathbf{x}; a, b))$$

Isopleths of the cost function and minimisation steps



Minimisation by mere **gradients,** quasi-Newon method **L-BFGS** (Large dimensional Broyden Fletcher Goldfarb Shanno),

Extensions to Generality

1. **very high degree of freedom** of highly nonlinear systems **M**: *"curse of dimensionality" O(10^7-10^8)*
2. underdetermined system: **too few observations**, i.e. less than degrees of freedom
3. observations **scattered in time** and space,
4. different observation techniques:
   errors and representativity of observations **diverse**
5. observations often **indirectly** related to parameters of interest: remote sensing data

Methodology applicable to a wide range of problems:
Consider optimisation problem
with unique optimum

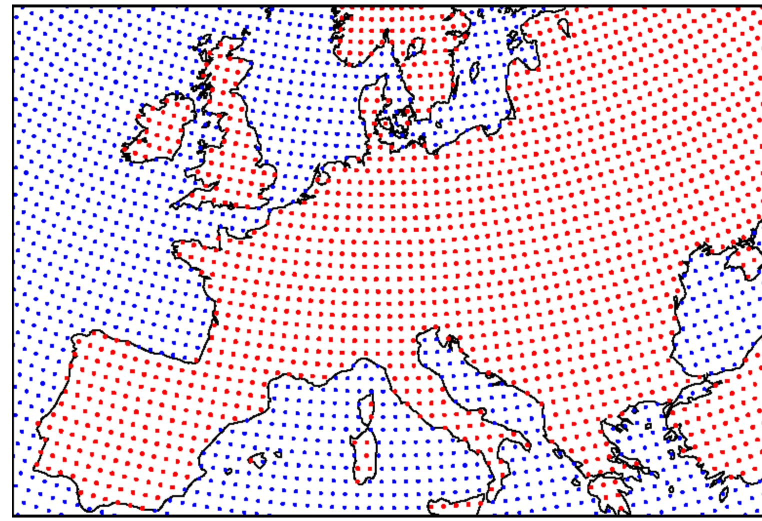
1. Very high degree of freedom:

“curse of dimensionality” $O(10^7\text{-}10^8)$

(grid points x 10-100 variables)

$$\frac{\partial U}{\partial t}+\frac{1}{a\cos^2\theta}\left\{U\frac{\partial U}{\partial\lambda}+v\cos\theta\frac{\partial U}{\partial\theta}\right\}+\dot{\eta}\frac{\partial U}{\partial\eta}$$
$$(-fv)+\frac{1}{a}\left\{\frac{\partial\phi}{\partial\lambda}+R_{\mathrm{dry}}T_v\frac{\partial}{\partial\lambda}(\ln p)\right\} = P_U+K_U$$

$$\frac{\partial V}{\partial t}+\frac{1}{a\cos^2\theta}\left\{U\frac{\partial V}{\partial\lambda}+V\cos\theta\frac{\partial V}{\partial\theta}+\sin\theta(U^2+V^2)\right\}+\dot{\eta}\frac{\partial V}{\partial\eta}$$
$$+fU+\frac{\cos\theta}{a}\left\{\frac{\partial\phi}{\partial\theta}+R_{\mathrm{dry}}T_v\frac{\partial}{\partial\theta}(\ln p)\right\} = P_V+K_V$$

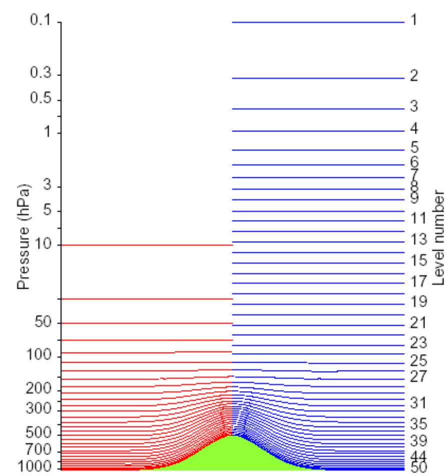


$$\frac{\partial T}{\partial t}+\frac{1}{a\cos^2\theta}\left\{U\frac{\partial T}{\partial\theta}+V\cos\theta\frac{\partial T}{\partial\theta}\right\}+\dot{\eta}\frac{\partial T}{\partial\eta}-\frac{\kappa T_v\omega}{(1+(\delta-1)q)p} = P_T+K_T$$

$$\frac{\partial q}{\partial t} = \frac{1}{a\cos^2\theta}\left\{U\frac{\partial q}{\partial\lambda}+V\cos\theta\frac{\partial q}{\partial\theta}\right\} = \eta\frac{\partial q}{\partial\eta} = P_q+K_q$$

$$\frac{\partial p_{\mathrm{surf}}}{\partial t} = -\int_0^1\nabla\cdot\left(\mathbf{v}_H\frac{\partial p}{\partial\eta}\right)d\eta \qquad \dot{\eta}\frac{\partial p}{\partial\eta} = -\frac{\partial p}{\partial\eta}-\int_0^\eta\nabla\cdot\left(\mathbf{v}_H\frac{\partial p}{\partial\eta}\right)d\eta$$

$$\eta(0,p_{\mathrm{surf}}) = 0$$



now T1299L91 (~16 km)

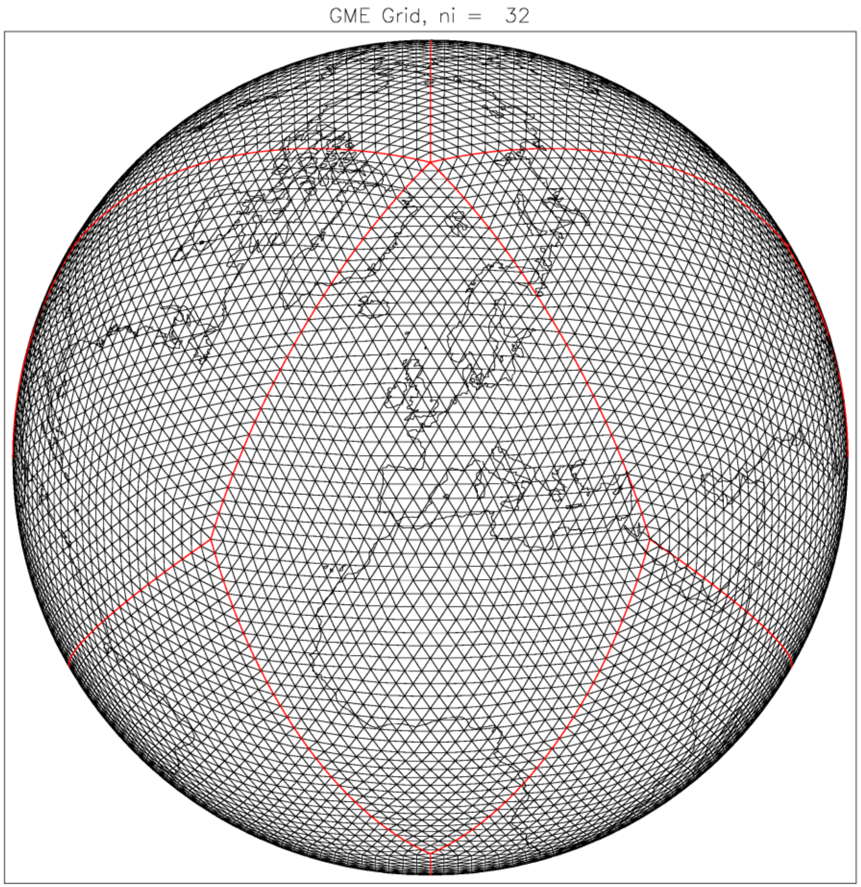
➔

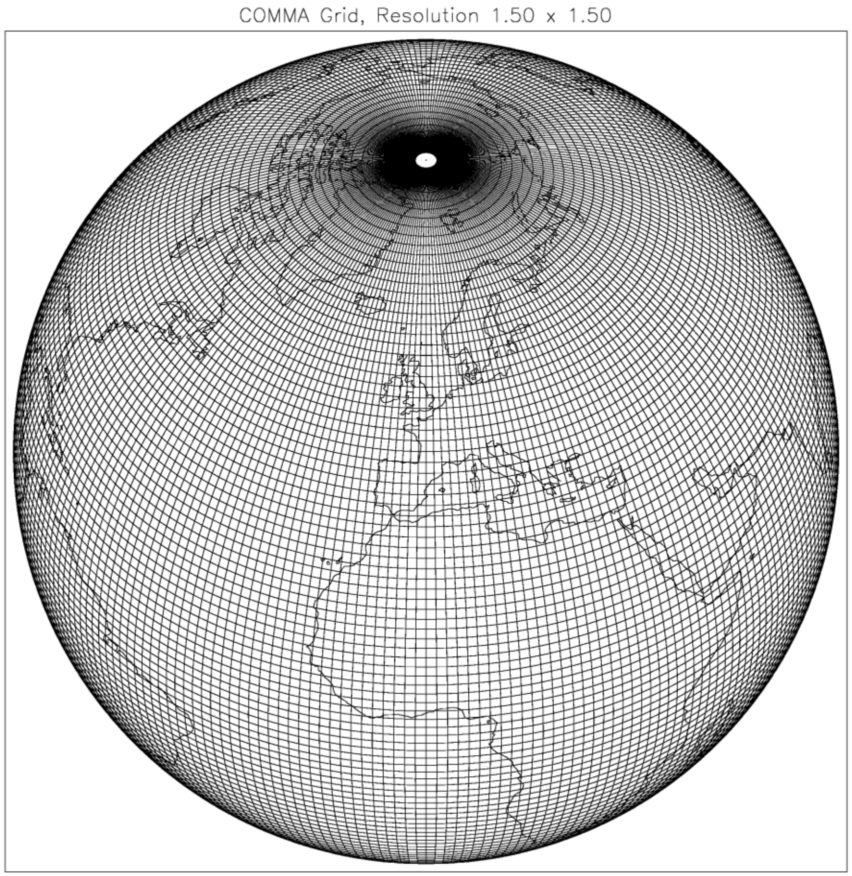
dim **$O(10^8)$**

1. Very high degree of freedom:
"curse of dimensionality" O(10^7-10^{-8})
(grid points x 10-100 variables)

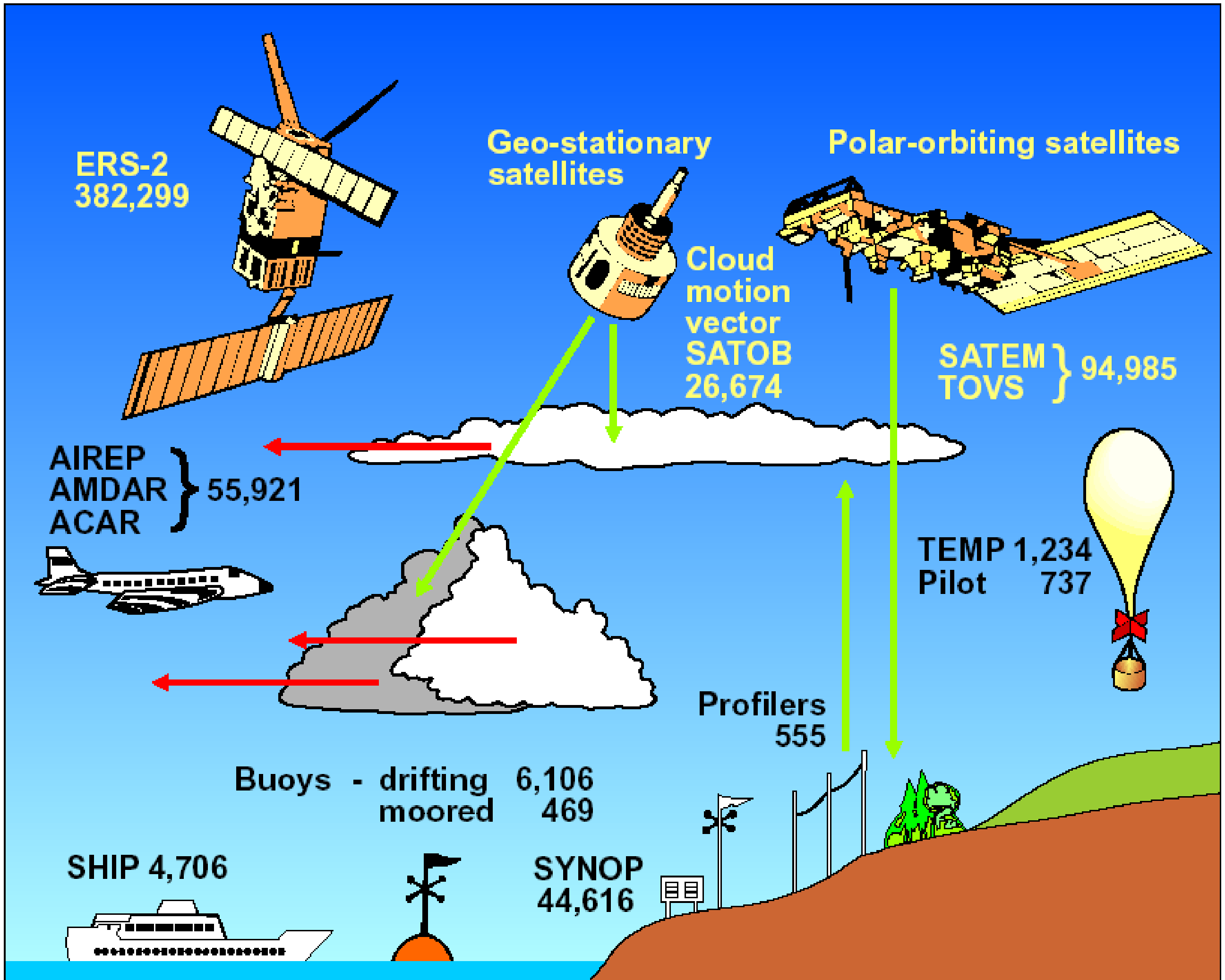
SACADA icosahedral grid
(see presentation K. Kasradze)

3-D models





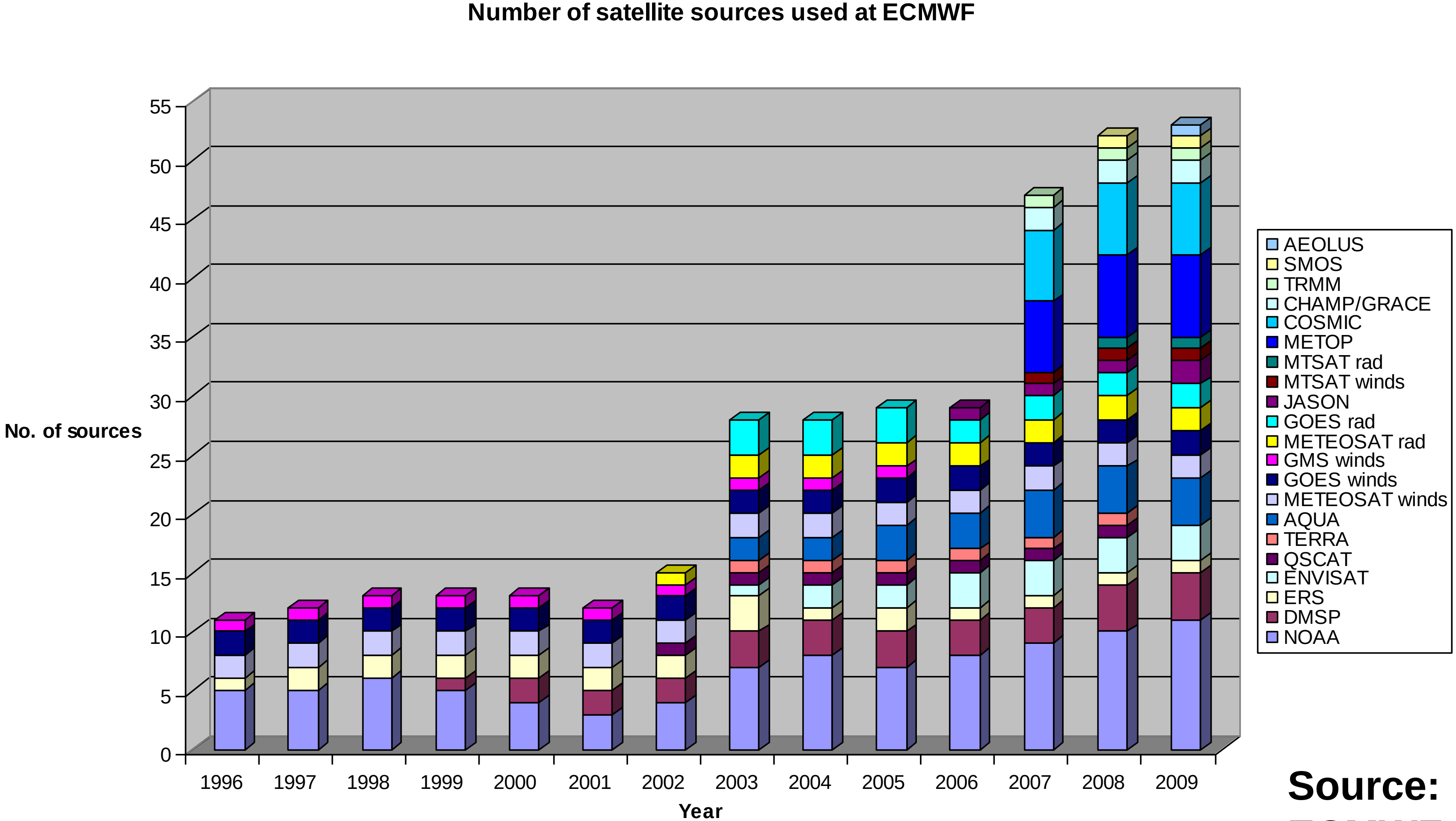
2. Underdetermined system: too few observations, i.e. less than degrees of freedom



$\mathbf{dim}_{\text{observation space}}$
$\mathbf{<< O(10^7)}$

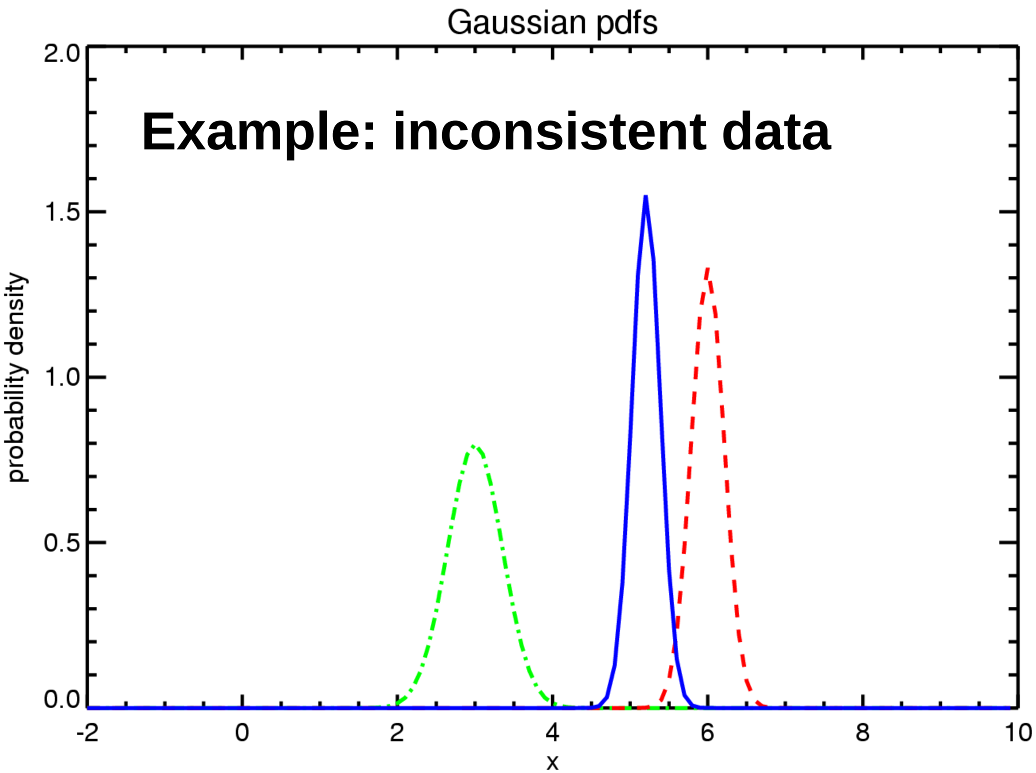
Type and number of observations used to estimate the atmosphere initial conditions during a typical day. (Buizza, 2000)

Satellite data sources in 2007+, but only a fraction can be used



Source: ECMWF

Take the model for over-determination: Synergy of information sources



Bayes' rule:

$$p(x|y_o) \propto p(y_o|x)p(x)$$

Analysis (=estimation) **BLUE**

Best Linear Unbiased Estimate

$$\frac{x_a}{\sigma_a^2} = \frac{y_o}{\sigma_o^2} + \frac{x_b}{\sigma_b^2}$$

$$\frac{1}{\sigma_a^2} = \frac{1}{\sigma_o^2} + \frac{1}{\sigma_b^2}$$

$$p(x|y_o) =: \mathcal{N}(x|x_a, \sigma_a^2)$$

$$= \frac{1}{\sqrt{2\pi}\sigma_a} \exp\left(-\frac{(x_a - x)^2}{2\sigma_a^2}\right)$$

$$p(x) =: \mathcal{N}(x|x_b, \sigma_b^2) := \frac{1}{\sqrt{2\pi}\sigma_b} \exp\left(-\frac{(x - x_b)^2}{2\sigma_b^2}\right)$$

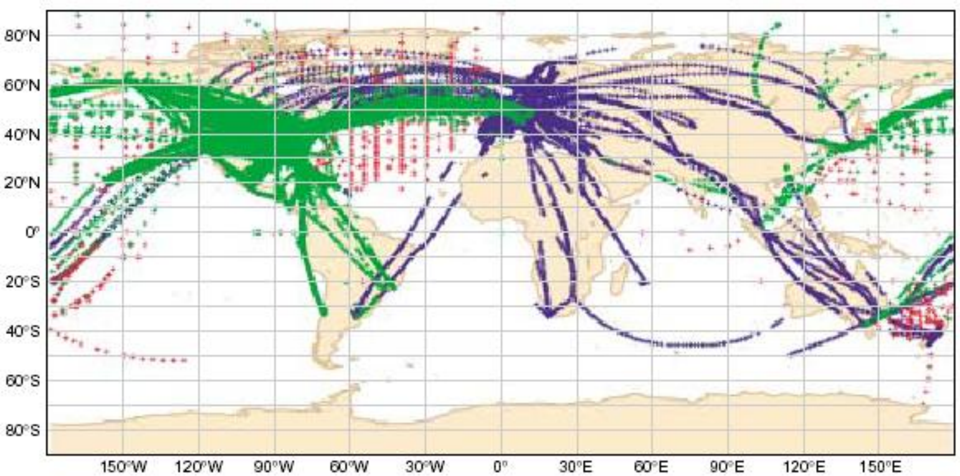
$$p(y_o|x) =: \mathcal{N}(y_o|x, \sigma_o^2) := \frac{1}{\sqrt{2\pi}\sigma_o} \exp\left(-\frac{(y_o - x)^2}{2\sigma_o^2}\right)$$

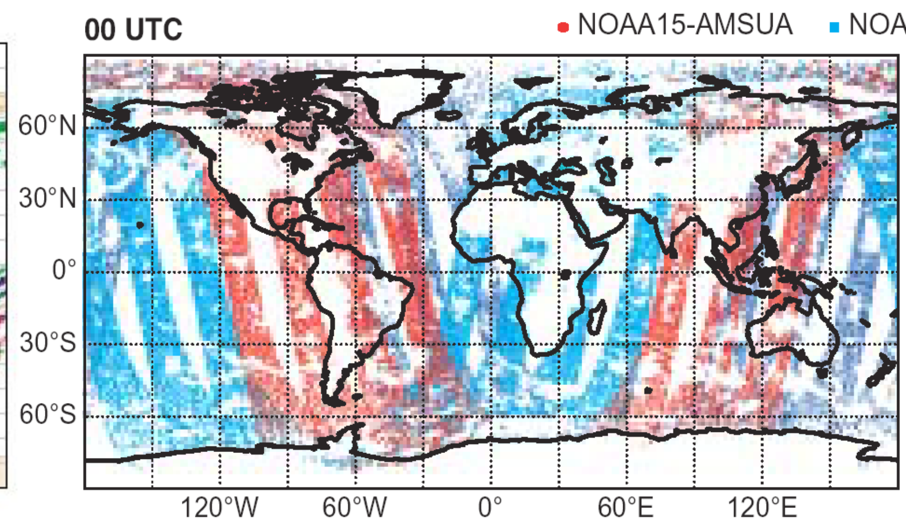
a priori (=prediction or climatology)

observation

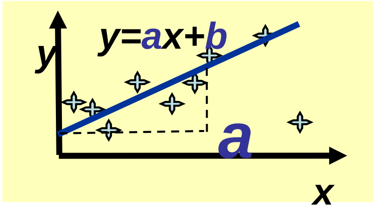
3. Observations scattered in time (and space)

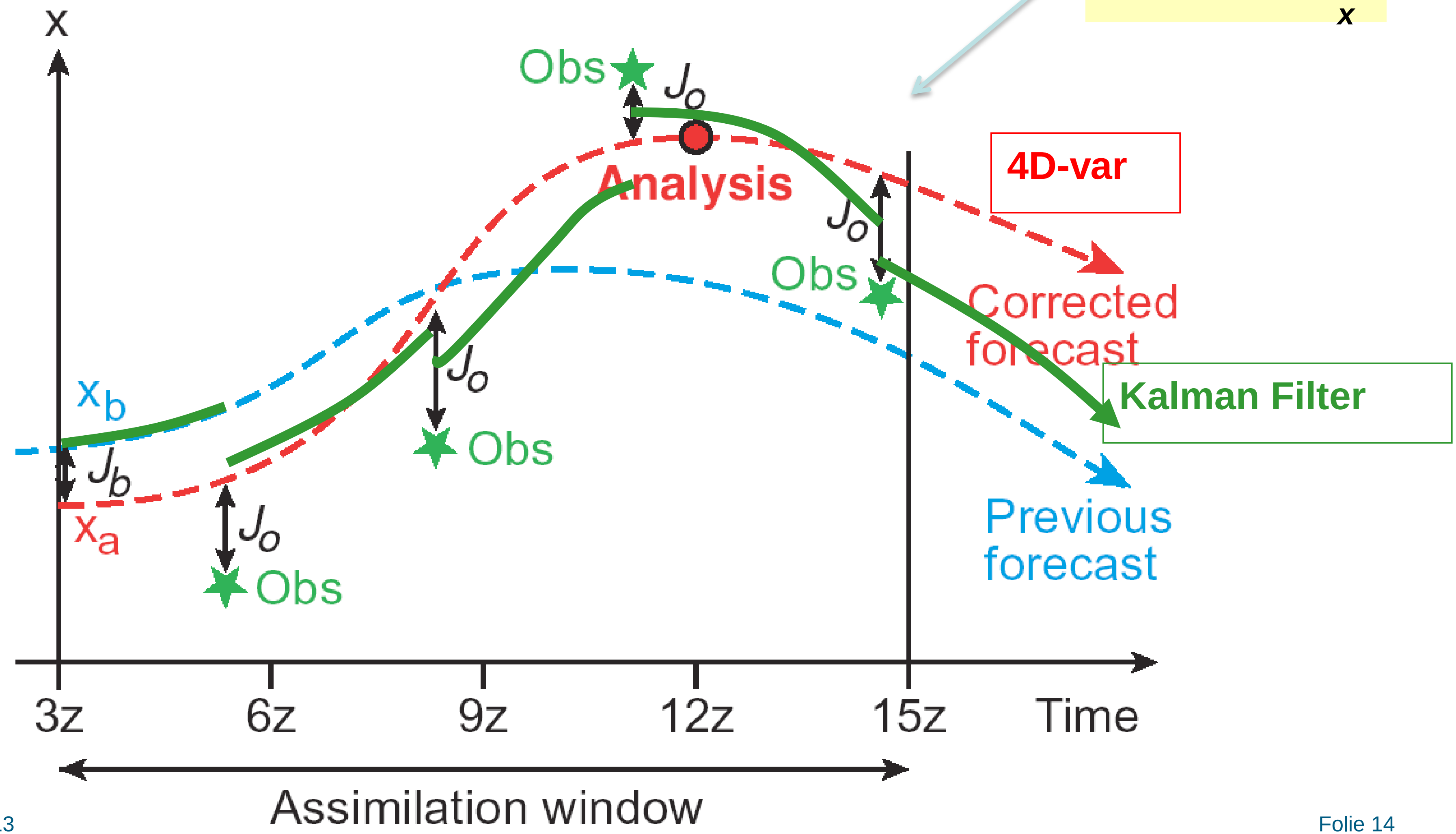
AIREP, AMDAR, ACAR





Types of assimilation algorithms: “smoother” and filter





Tendency Equations

direct chemistry transport equation

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{v} c_i) - \nabla \cdot (\rho \mathbf{K} \nabla \frac{c_i}{\rho}) - \Sigma_{r=1}^{R} \left(k(r) \left(s_i(r_+) - s_i(r_-) \right) \Pi_{j=1}^{U} c_j^{s_j(r_-)} \right) = E_i + D_i$$

c_i	concentration of species i	c_i^*	adjoint of concentration of species i
$\mathbf{v}$	wind velocity	s	stoichiometric coefficient
$k(r)$	reaction rate of reaction r	$\mathbf{K}$	diffusion coefficient
U	number of species in the mechanism	R	number of reactions in the mechanism
E_i	emission rate of species i (source)	D_i	deposition rate of species i (sink)

adjoint chemistry transport equation

$$-\frac{\partial \delta c_i^*}{\partial t} - \mathbf{v} \nabla \delta c_i^* - \frac{1}{\rho} \nabla \cdot (\rho \mathbf{K} \nabla \delta c_i^*) + \Sigma_{r=1}^{R} \left(k(r) \frac{s_i(r_-)}{c_i} \Pi_{j=1}^{U} \bar{c}_j^{\,s_j(r_-)} \Sigma_{n=1}^{U} \left(s_n(r_+) - s_n(r_-) \right) \delta c_n^* \right) = 0$$

Adjoint integration "backward in time"

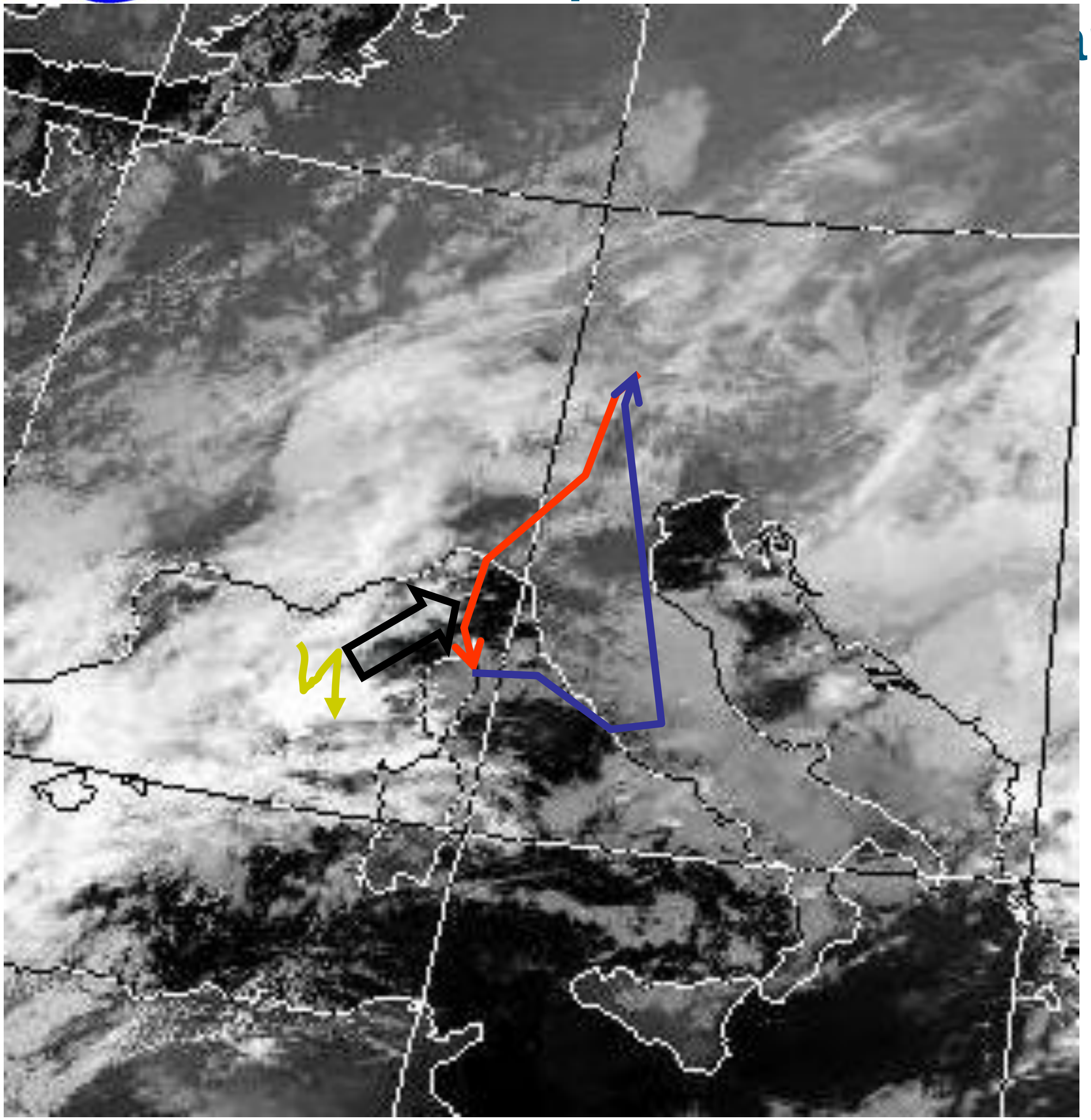
$$
\begin{array}{lll}
\text{direct model} & \frac{d\mathbf{x}}{dt} = \mathcal{M}(\mathbf{x}) + \mathbf{e}(t), \qquad \frac{d\delta\mathbf{x}}{dt} = \mathcal{M}'(\delta\mathbf{x}) + \delta\mathbf{e}(t) & (1) \\
\text{tangent linear model} & \delta\mathbf{x}(t_n) = \mathbf{M}(t_n, t_0)\delta\mathbf{x}(t_0) = \Pi_{i=n}^{1}\,\mathbf{M}(t_i, t_{i-1})\delta\mathbf{x}(t_0) & (2) \\
\text{adjoint model} & -\frac{d\delta\mathbf{x}^*(t)}{dt} - \mathcal{M}'^T(\delta\mathbf{x}^*(t)) = \mathbf{R}^{-1}(\mathbf{y}^0(t) - H[\mathbf{x}(t)]). & (3)
\end{array}
$$

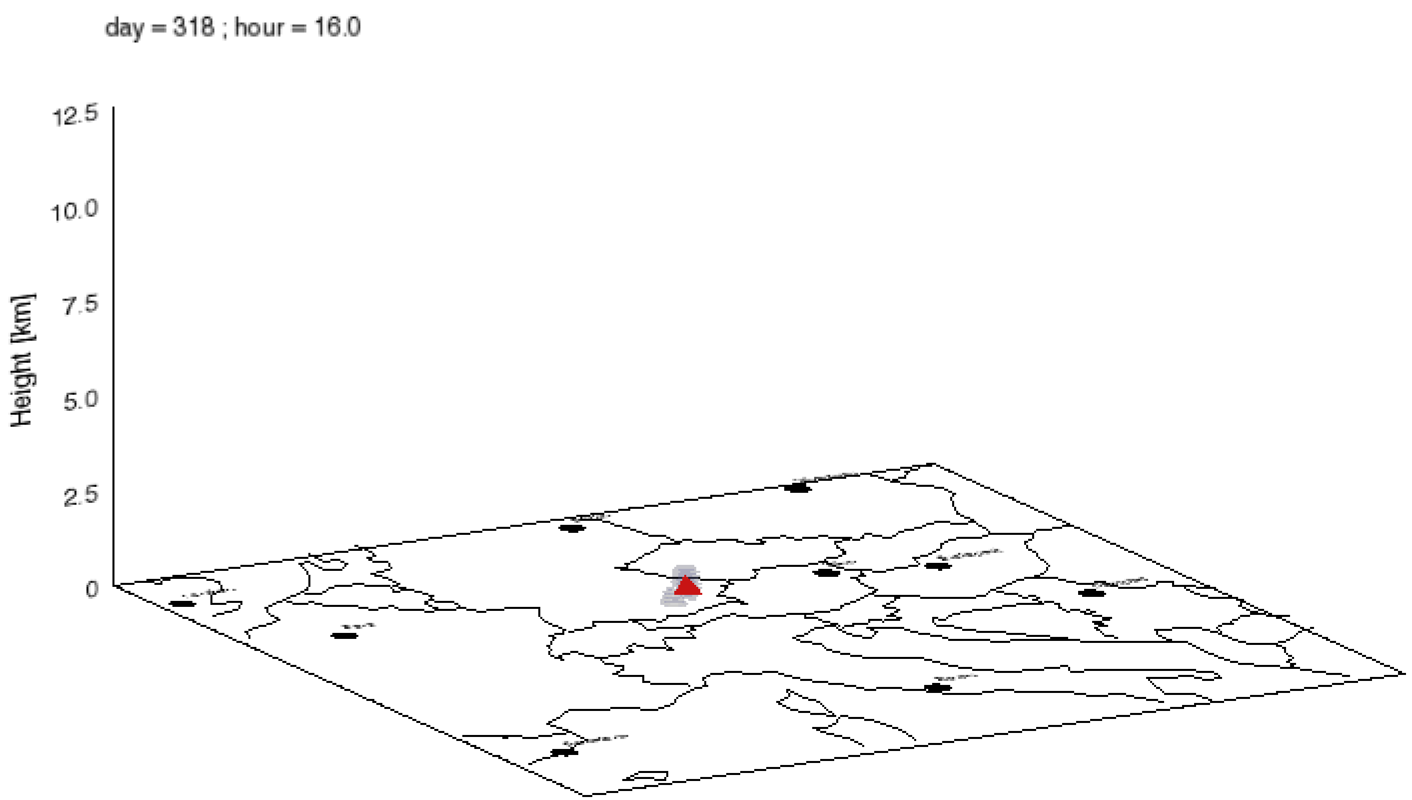
gradient of the cost function

$$\nabla_{[\mathbf{x}(t_0),\mathbf{e}]}J = -\mathbf{B}_0^{-1}(\mathbf{x}^b(t_0) - \mathbf{x}(t_0)) - \mathbf{K}^{-1}(\mathbf{e}^b(t) - \mathbf{e}(t)) - \Sigma_{m=0}^{N}\,\Pi_{i=1}^{m}\,\mathbf{M}^T(t_{i-1}, t_i)\mathbf{R}^{-1}(\mathbf{y}^0(t_m) - H[\mathbf{x}(t_m)])$$

Find minimum of $J(\mathbf{x}(t_0), \mathbf{e})$ with $\nabla_{[\mathbf{x}(t_0),\mathbf{e}]}J$ by use of a minimization routine

CONTRACE
Convective Transport of Trace Gases into the upper ...and Impact of

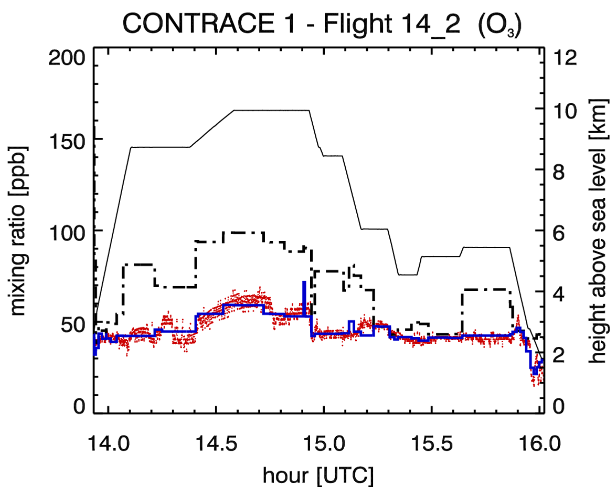



day = 318 ; hour = 16.0
Height [km]
12.5
10.0
7.5
5.0
2.5
0

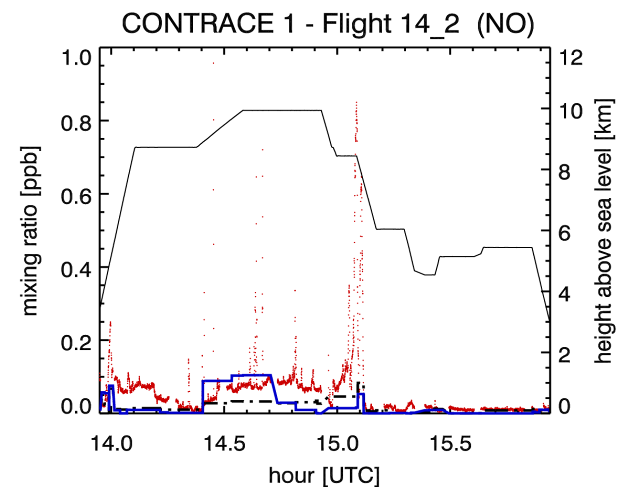
CONTRACE

Nov. 14, 2001 north (= home) bound

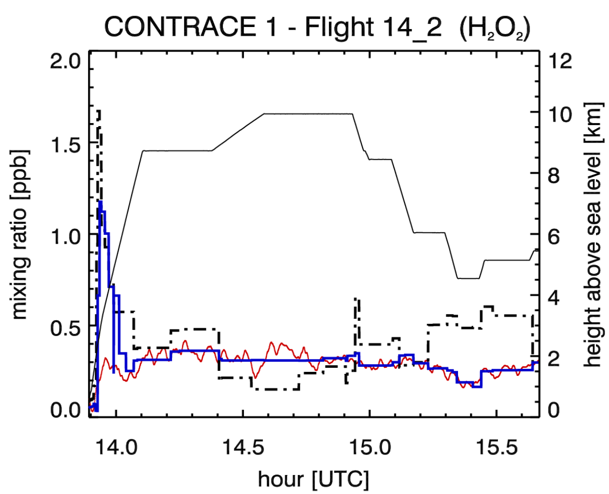
O_3



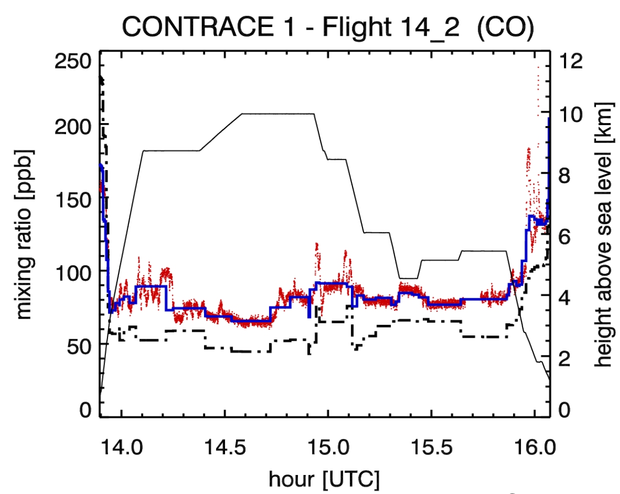
NO



H_2O_2

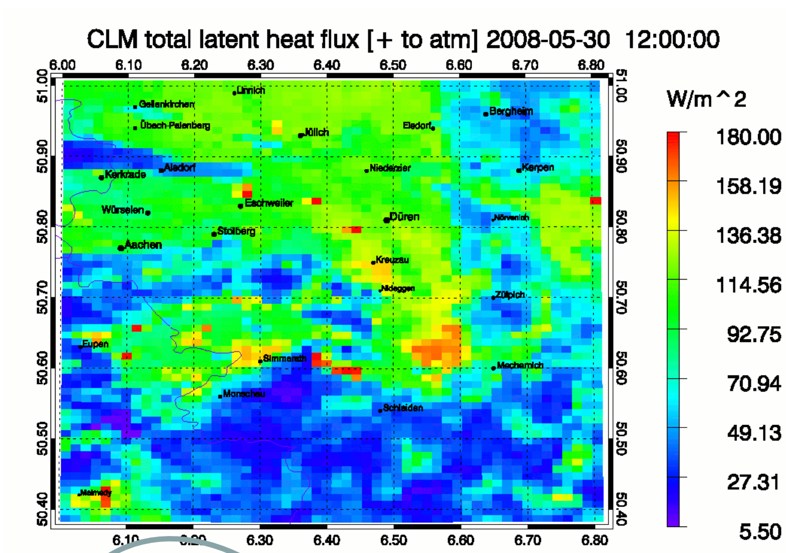


CO

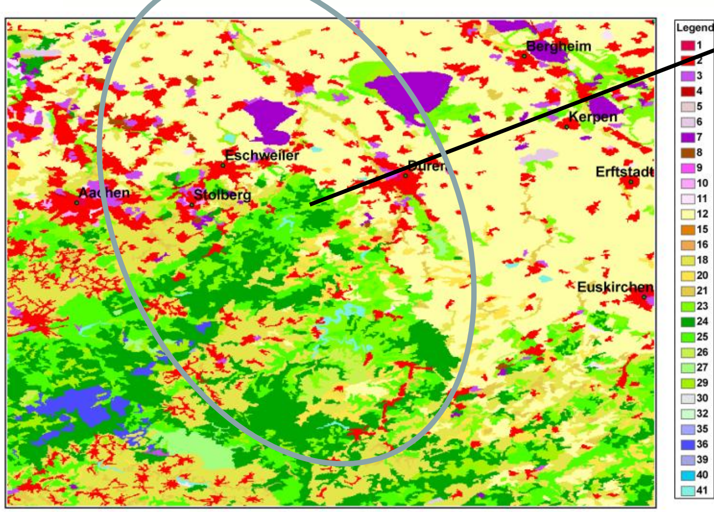


–·–·– 1. guess —— assimilation result ········ observations —— flight height [km]

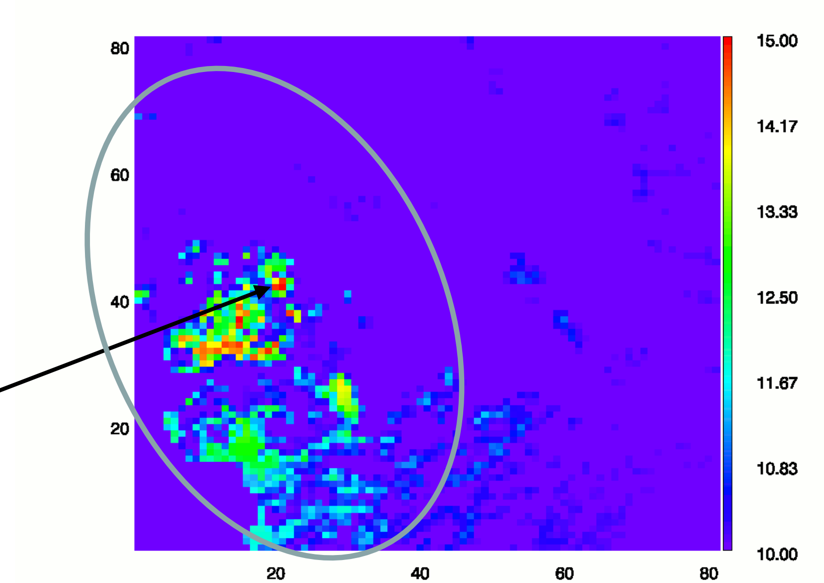
4. Observation errors are varying and representativity of observations are diverse



land use map



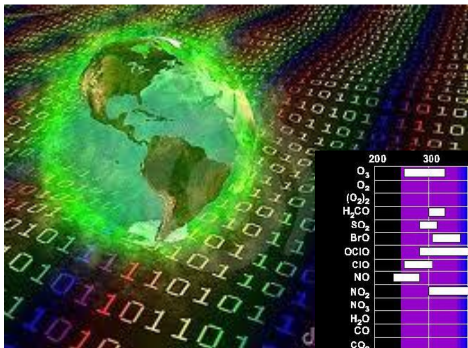
Example: Analysis increments using the novel background error covariance matrix formulation



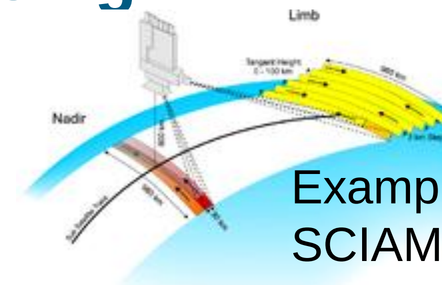
Background (forecast) error correlation can bridge gaps according to subgrid scale land use information:

e.g. **from forest to forest**

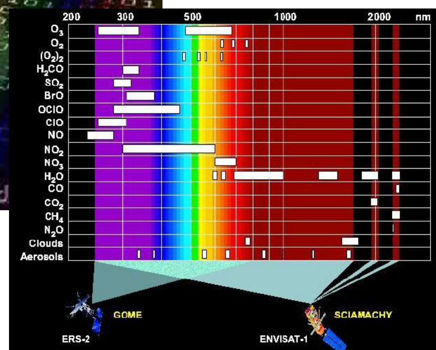
5. Observations often indirectly related to parameters of interest: Remote sensing



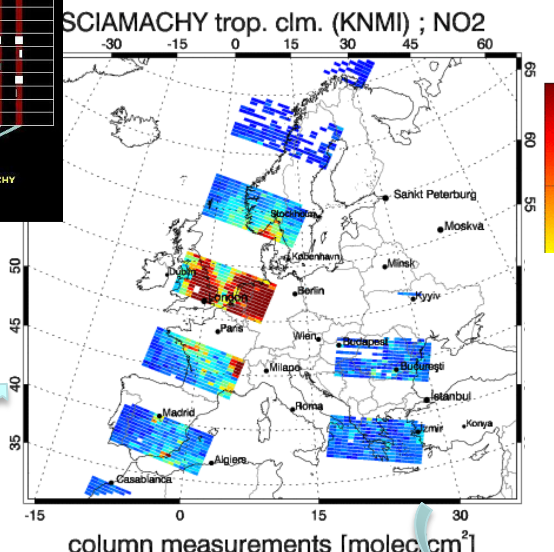
level 0: detector tensions: digital data



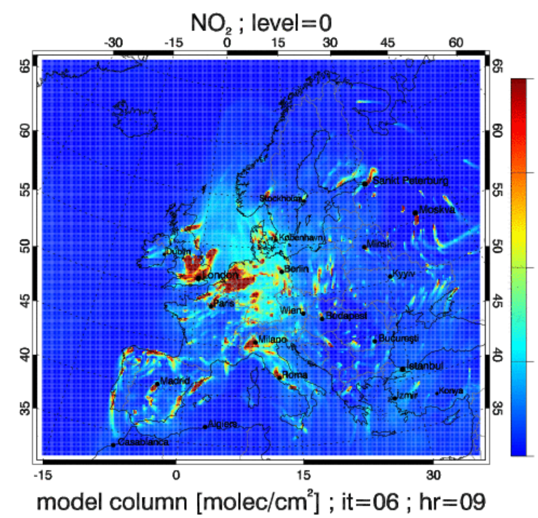
Example: SCIAMACHY



level 1: calculate spectra



level 2: calculate located geo data (say: **y**=[NO_2])



Retrieval:
Solve the model equivalent:
radiative transfer equation **H**(x)

Calculate difference (y – **H**(x)), and assimilate

level 3: "analysis fields" (say NO_2)

Main observational data (spaceborne)

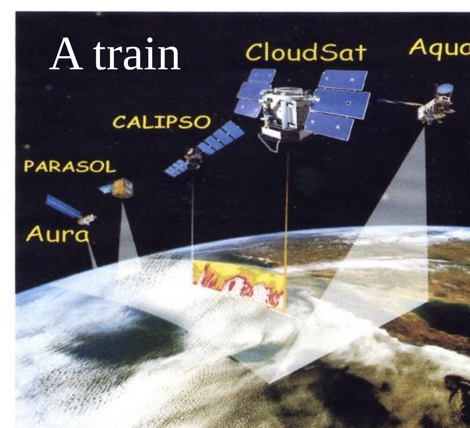
AQUA (2002) AMSR/E: clouds, radiation and precipitation , MODIS: clouds, radiation, aerosol and vegetation parameters , AMSU, AIRS, HSB temperature and humidity, CERES radiation

ENVISAT (2002-2012) MIPAS, SCIAMACHY, GOMOS temperature, ozone, water vapour and other atmospheric constituents (ii) AATSR, MERIS aerosoll, MERIS sea colour , ASAR land and ocean images RA-2 land, ice and ocean monitoring, MWR water vapour column and land surface parameters DORIS cryosphere and land surface parameters

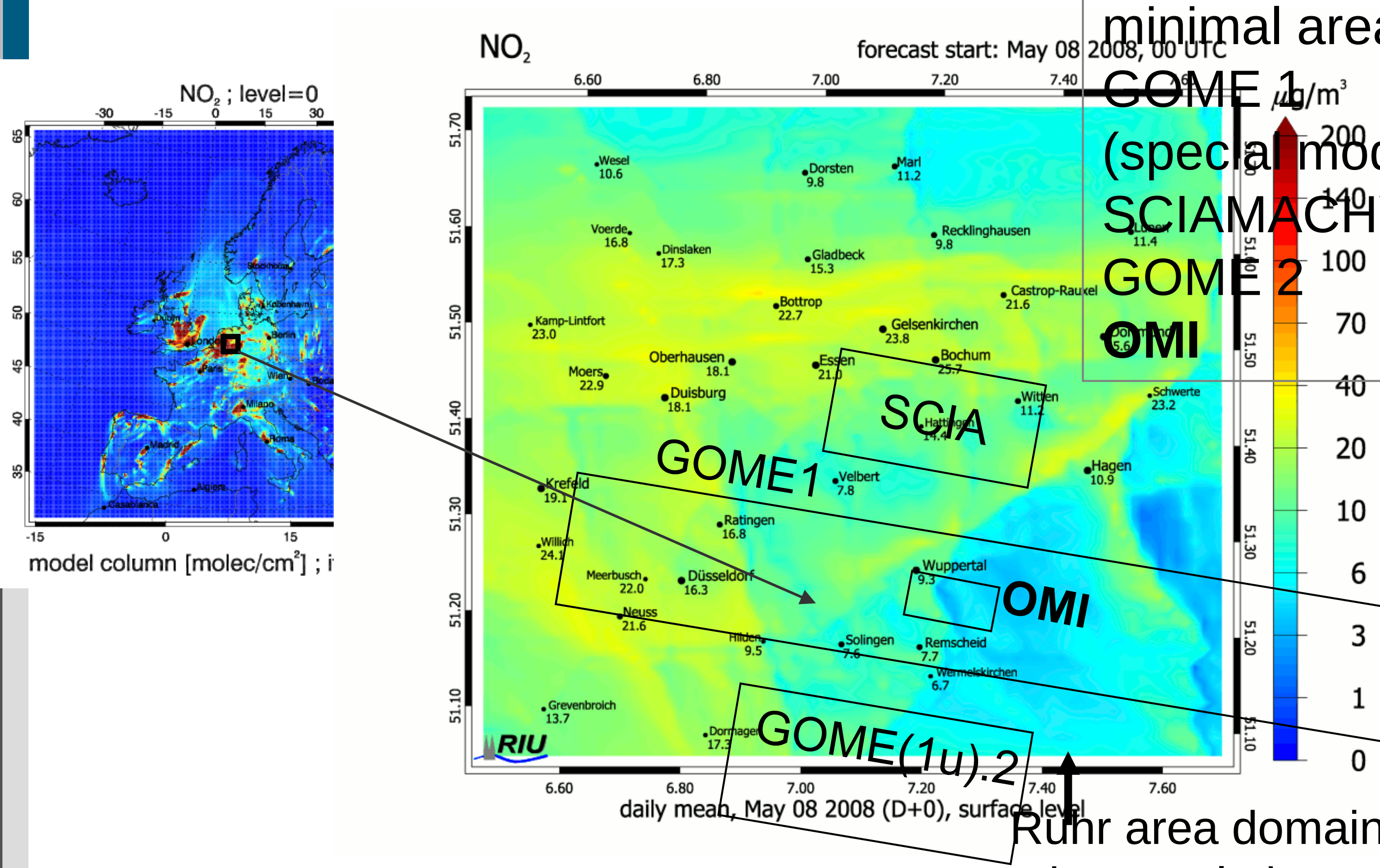
AURA (2004) MLS trace gases of the upper troposphere to upper stratosphere, + water HIRDLS, temperature and trace gases in the upper troposphere, stratosphere and mesosphere TES trop. ozone and some photochemical precursors ; OMI total column ozone and NO2 and UV-B radiation .

TERRA (1999).ASTER,land surface, water and ice, CERES radiation, MISR radiation and biosphere parameters; MODIS biological and physical processes on land and the ocean; MOPITT CO and CH4 in the troposphere, .

MetOp-1 IASI ozone, NO2, GOME-2 ozone SO2 NO2 formaldehde



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



minimal areas:

GOME 1	320 x 40 km²
(special mode)	80 x 40
SCIAMACHY	60 x 30 "
GOME 2	80 x 40 "
OMI	**24 x 13 "**

Ruhr area domain   90 x 80 km²
1 km resolution
(~12 000 000 inhabitants)

We started with: $(\mathbf{y} - M(\mathbf{x}; a, b))^T (\mathbf{y} - M(\mathbf{x}; a, b))$

Generalized cost function to be minimized

Minimize J by variation of $\mathbf{x}(t_0)$:

$$J(\mathbf{x}(t_0)) = \frac{1}{2}(\mathbf{x}^b(t_0) - \mathbf{x}(t_0))^T \mathbf{B}_0^{-1} (\mathbf{x}^b(t_0) - \mathbf{x}(t_0)) +$$

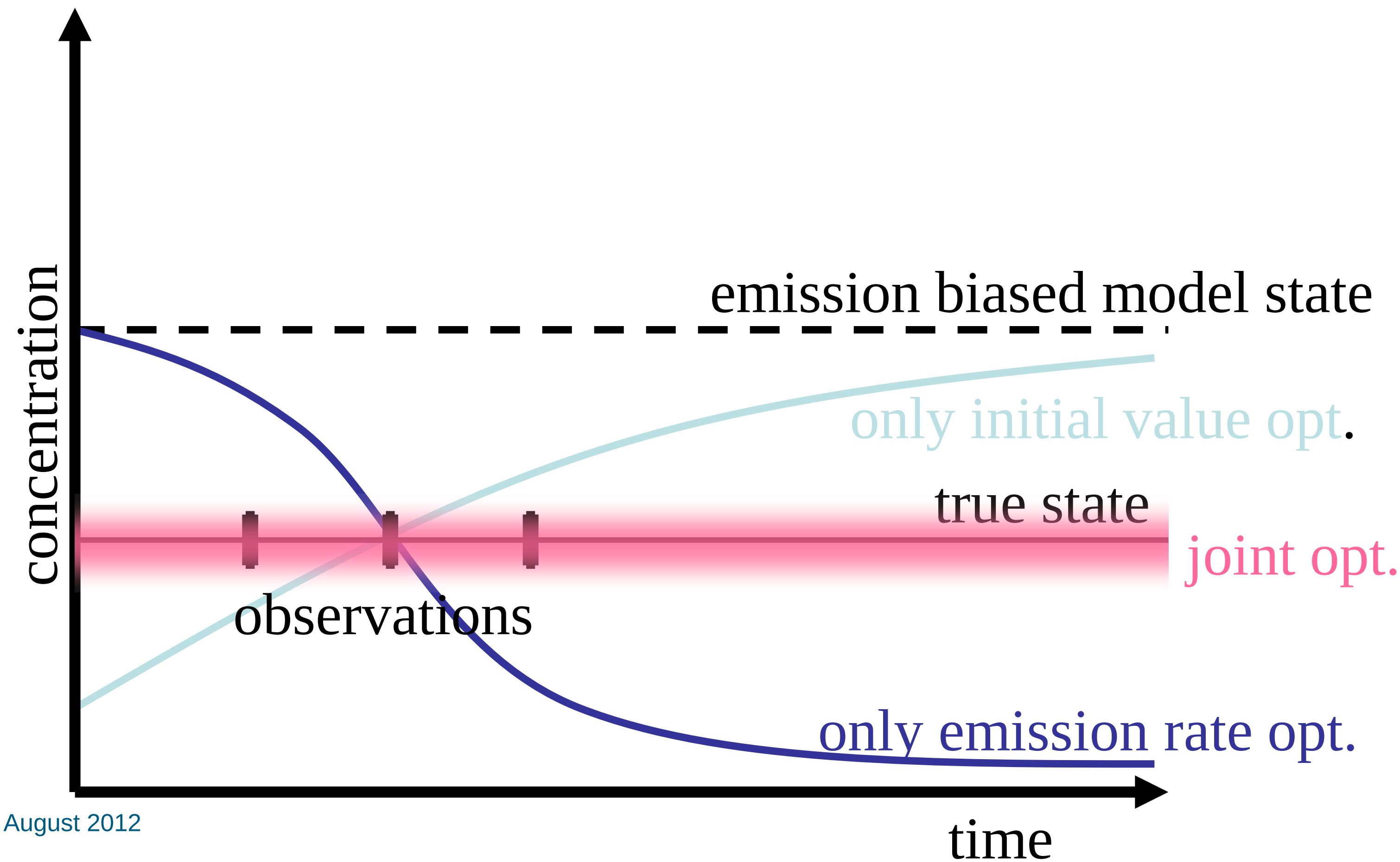
$$\frac{1}{2}\int_{t_0}^{t_N} (\mathbf{y}^0(t) - \mathbf{H}\mathbf{M}[\mathbf{x}(t)])^T \mathbf{R}^{-1} (\mathbf{y}^0(t) - \mathbf{H}\mathbf{M}[\mathbf{x}(t)]) dt$$

1. Model constraint and time propagator (resolvent)
2. Background term for artificial over-determination
3. Forecast errors
4. Observation errors and errors of representativity
5. Observation operator

$\mathbf{x}^b(t_0)$	background state at $t = 0$
$\mathbf{x}(t)$	model state at time t
$\mathbf{e}_b(t_0)$	background emission rate at $t = 0$
$\mathbf{e}(t)$	emission rate field at time t
$\mathbf{K}$	emission rate error covariance matrix
$H[\ \ ]$	forward interpolator
$\mathbf{y}^0(t)$	observation at time t
$\mathbf{B}_0$	background error covariance matrix

Question: Which parameter to be optimized?

Hypothesis:
initial state and emission rates are least known



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)

Data Assimilation in general

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)

Objective of atmospheric data assimilation

"is to produce a regular, **physically consistent four dimensional** representation of the state of the system

from a **heterogeneous** array of in situ and remote instruments

which sample **imperfectly** and **irregularly** in space and time.

Data assimilation

extracts the signal from noisy observations (**filtering**)

interpolates in space and time (**interpolation**) and

reconstructs state variables that are not sampled by the observation network (**completion**)." (Daley, 1997)

Information sources and theories

Information set

***declarative information*:**

•observations/retrievals

•forecasts

•"Climate" statistics,

•error statistics

procedural Information

differential equations

models

•contol theory

•statist. filter theory

•classical numerics

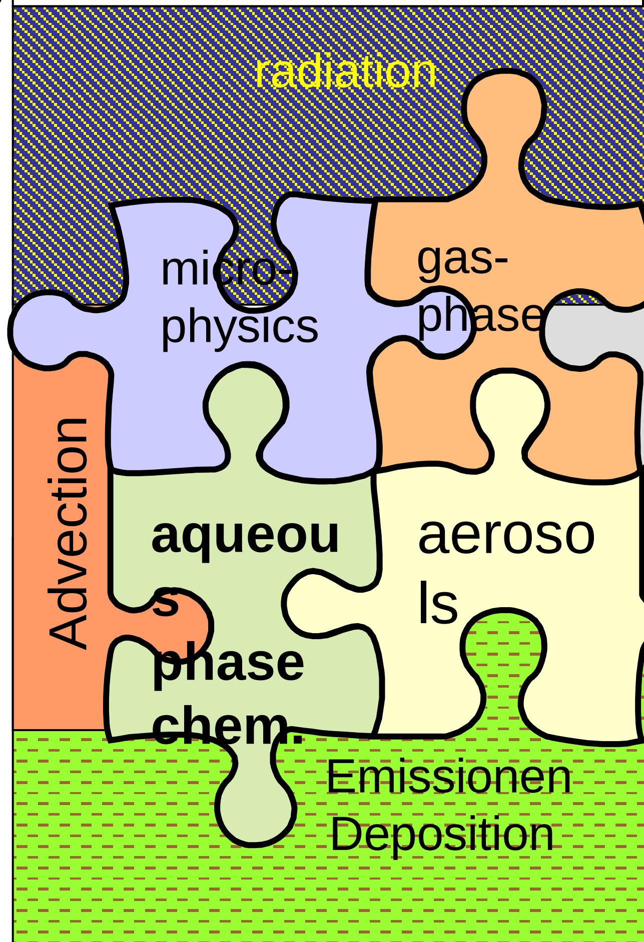
•optimisation algorith.

Interpolation
in space and time

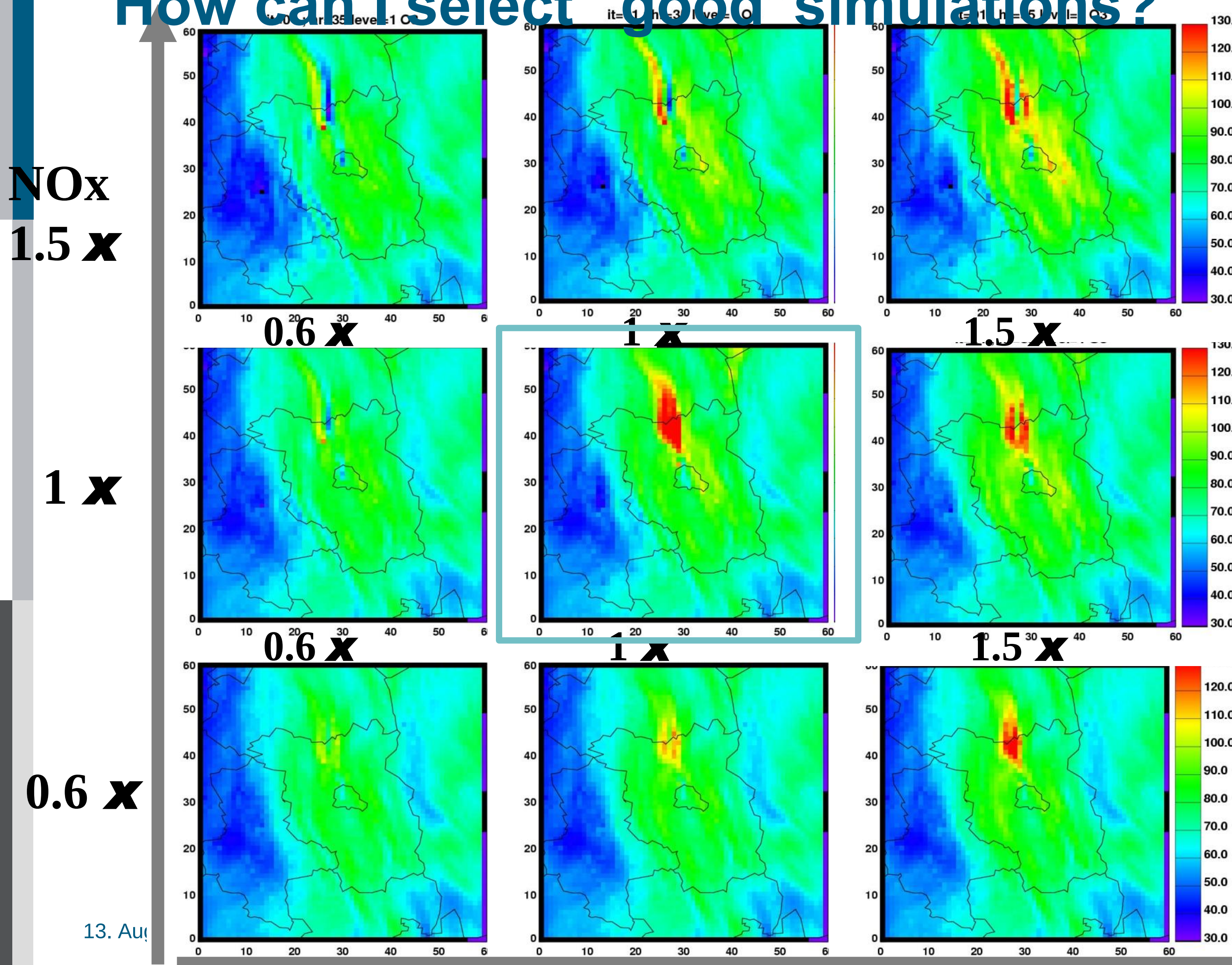
Filter
error affected
data

Completion
non-observed
parameters

4D-consistent
process description



How can I select “good”simulations?



Ozone: NO_x-VOC emissions variation ensemble (21.7.1998, 15:00 UTC)

Note:
not **C**-orthogonal,
not max. sensitivities aligned

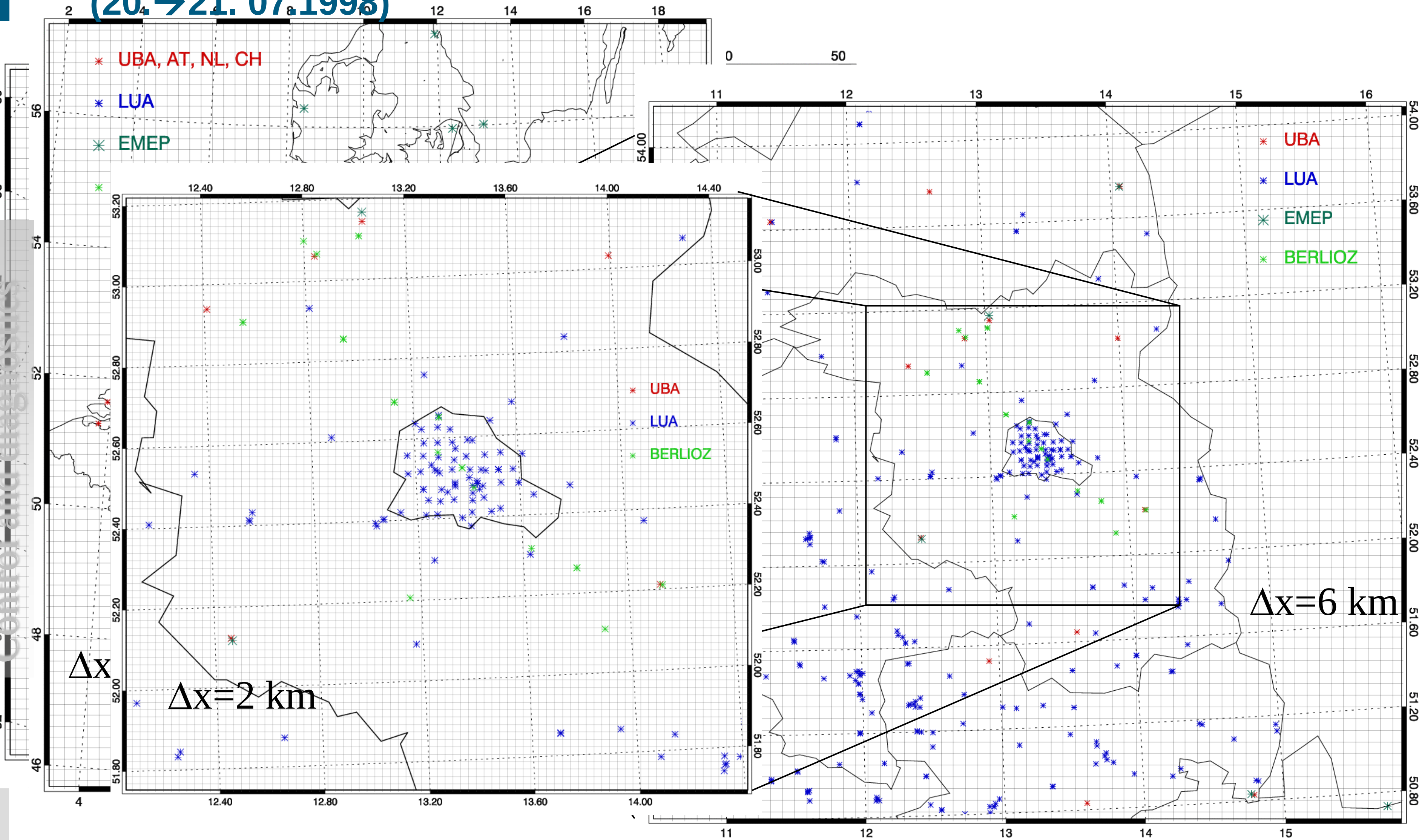
VOCs

RIU

JÜLICH FORSCHUNGSZENTRUM

Which is the requested resolution?

BERLIOZ grid designs and observational sites (20.→21. 07.1998)

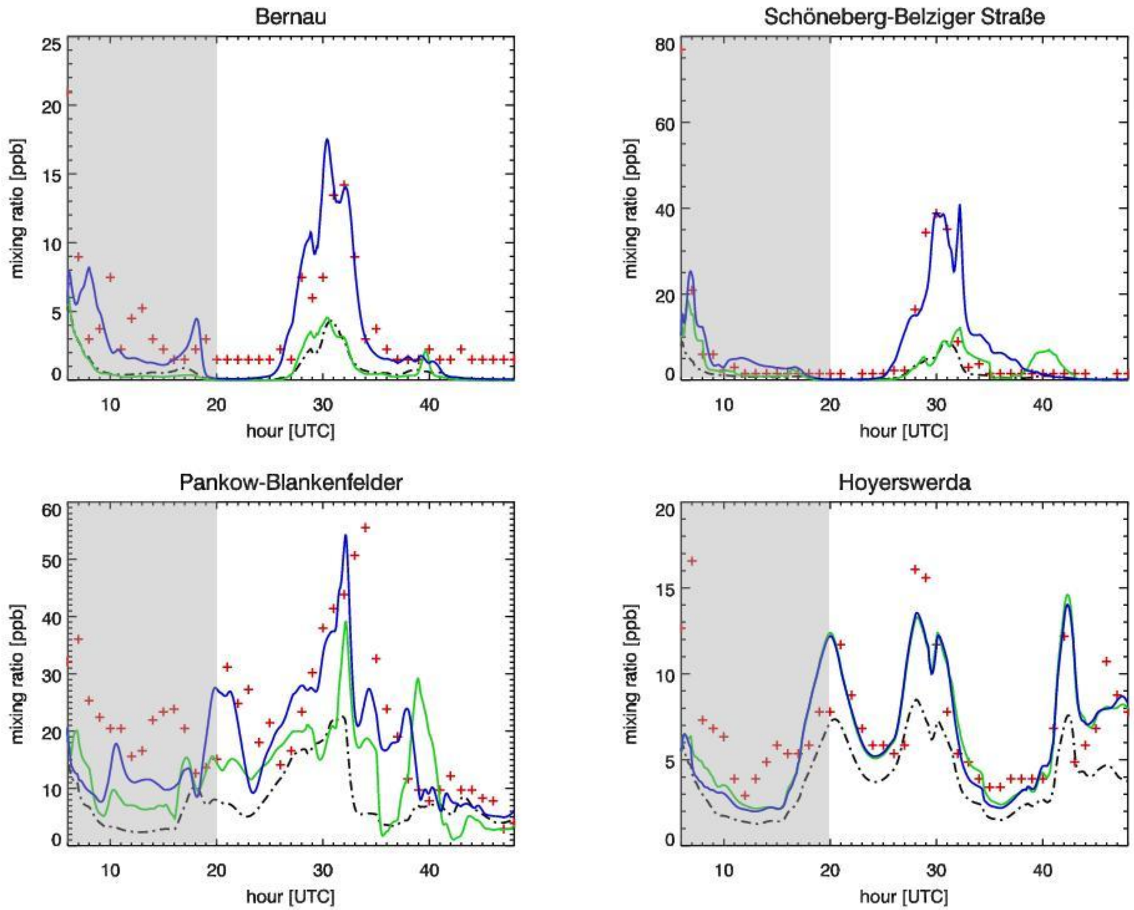


Control and diagnostics

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

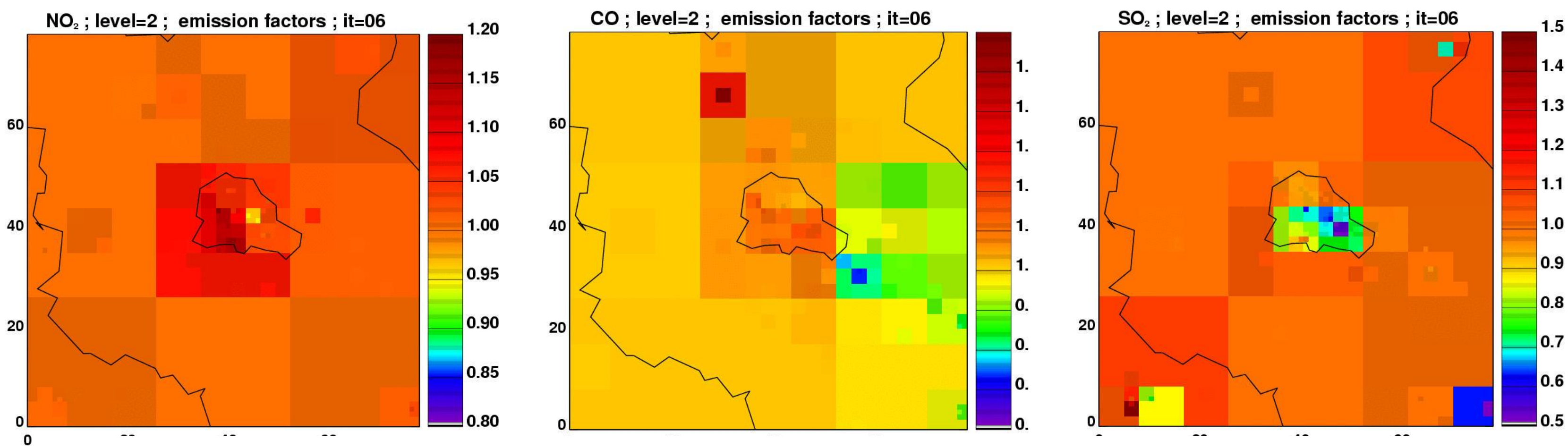
NO

NO_2



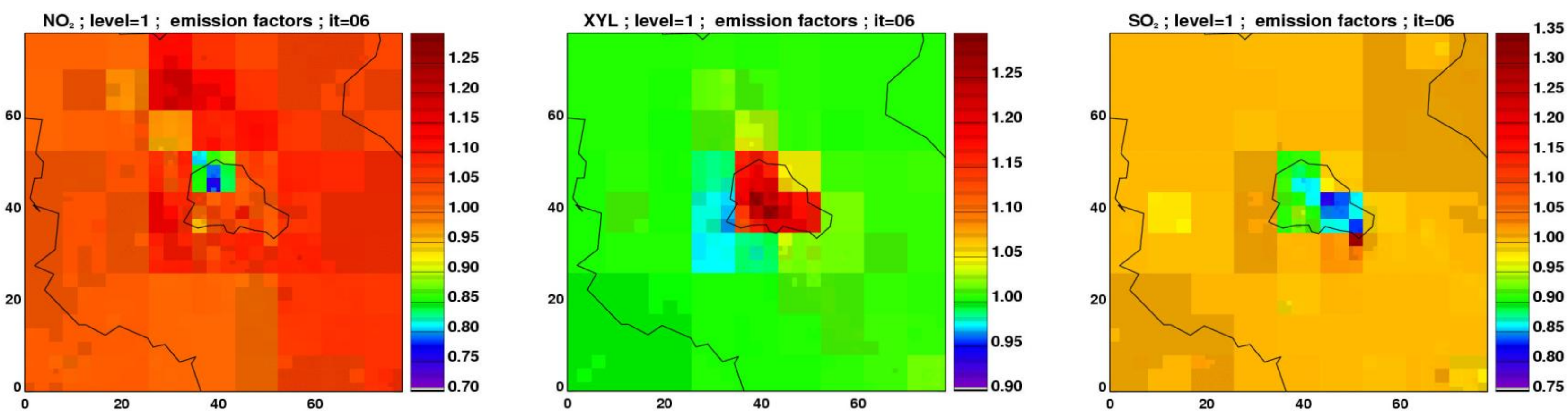
Time series for selected NOx stations on nest 2.
+ observations,
-- - no assimilation,
-_____ N1 assimilation (**18 km**),
-_____N2 assimilation.(**6 km**),
-grey shading: assimilated observations, others forecasted.

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



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

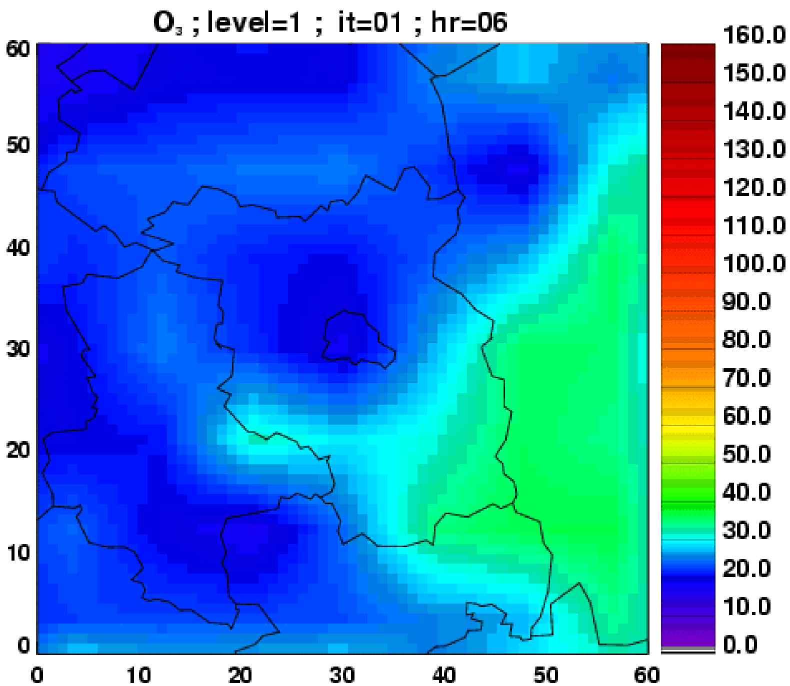
height layer ~32-~70m



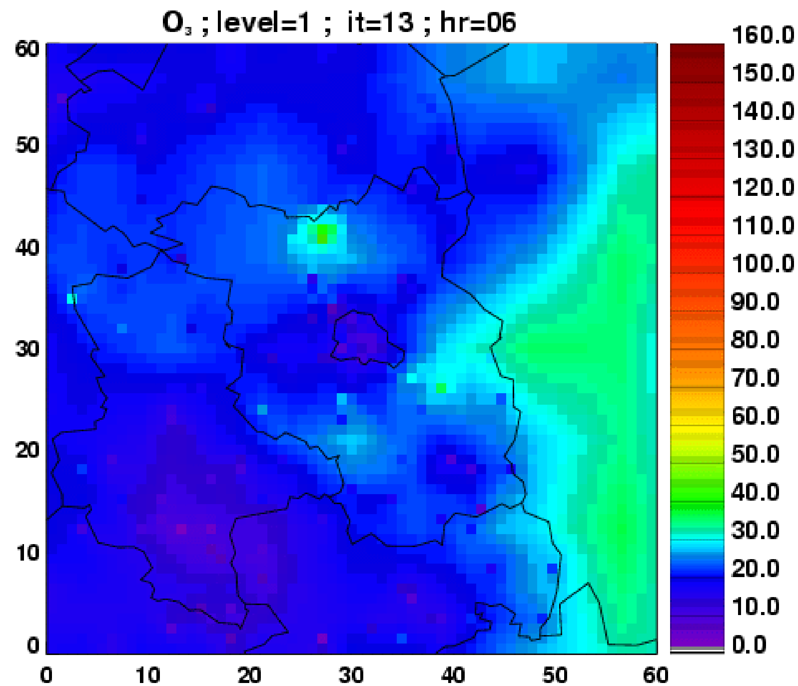
surface

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

without assimilation

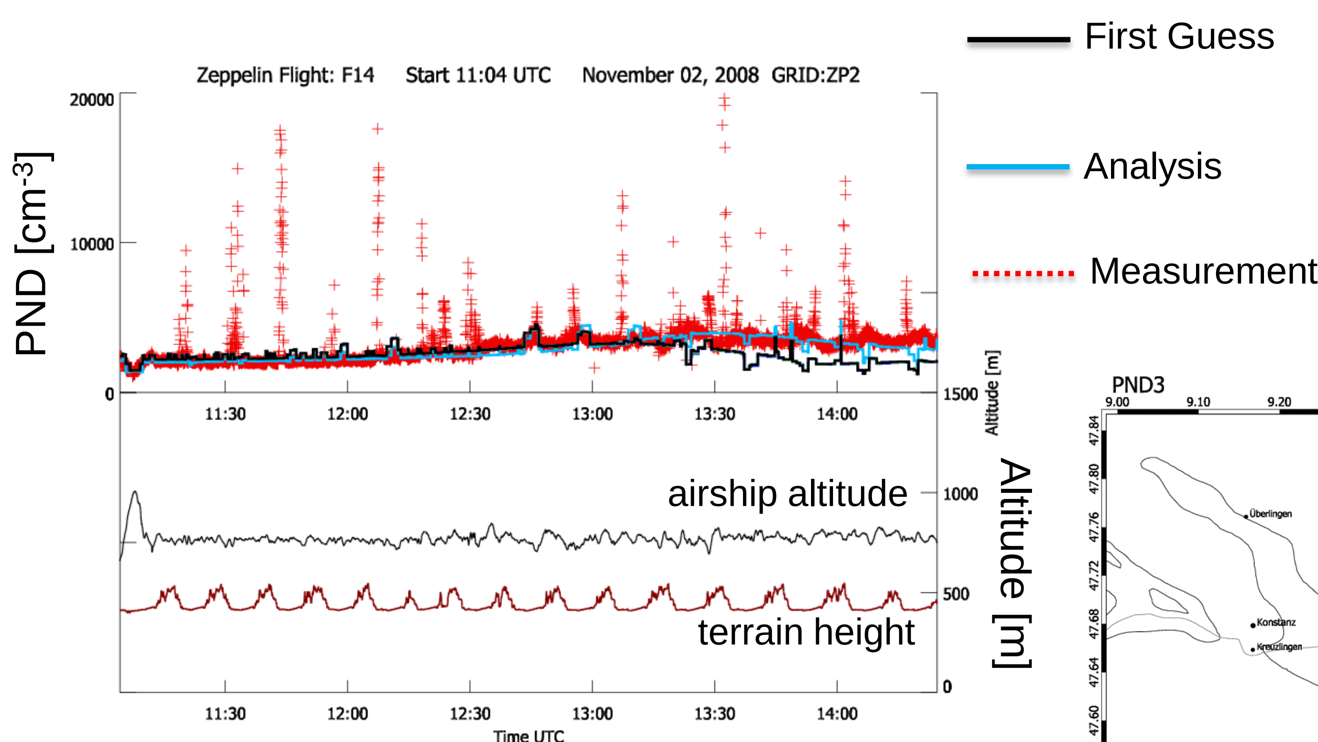


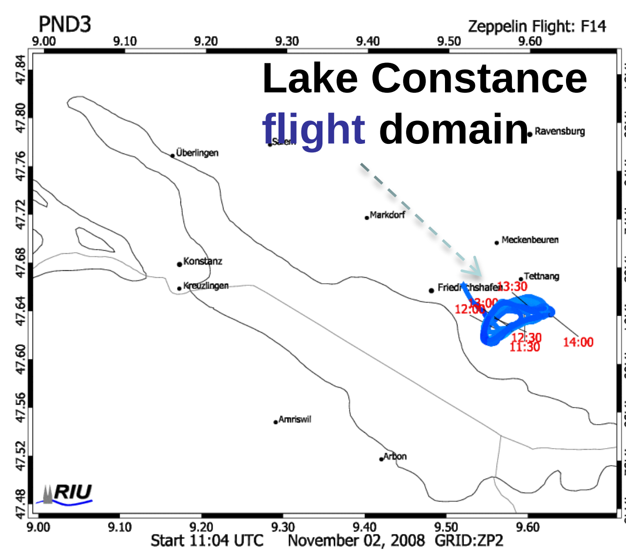
with assimilation



2. Analyses, Example (ii):
Zepter 2: 4D-var assimilation of particle number densities

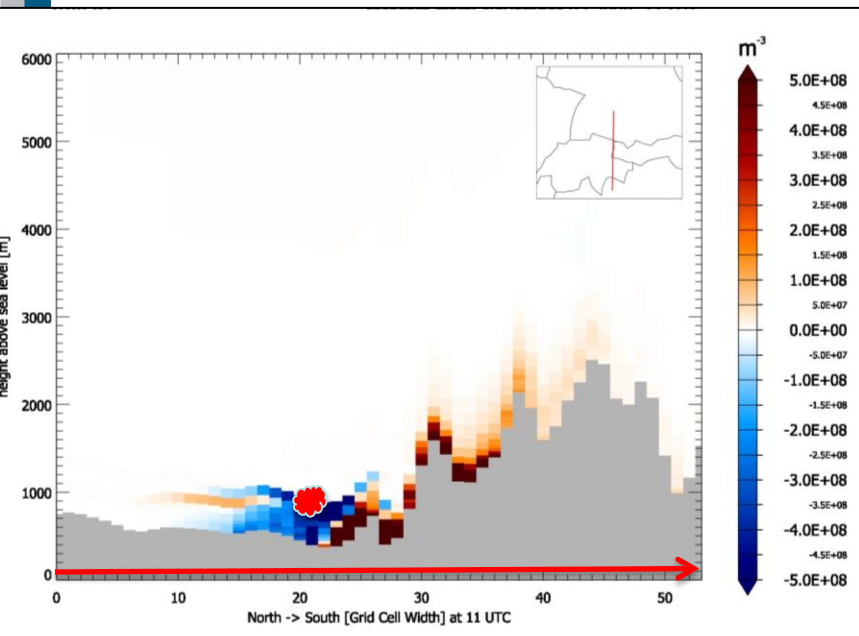
Flight 14 assimilation of PND (0.005-3.0 µm) 02.11.2008 (11-15 UTC)

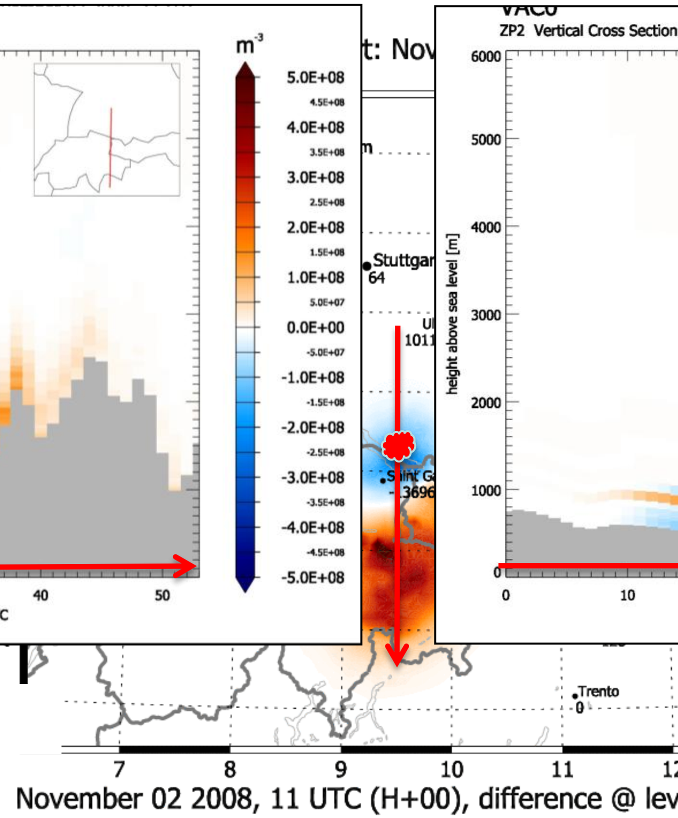


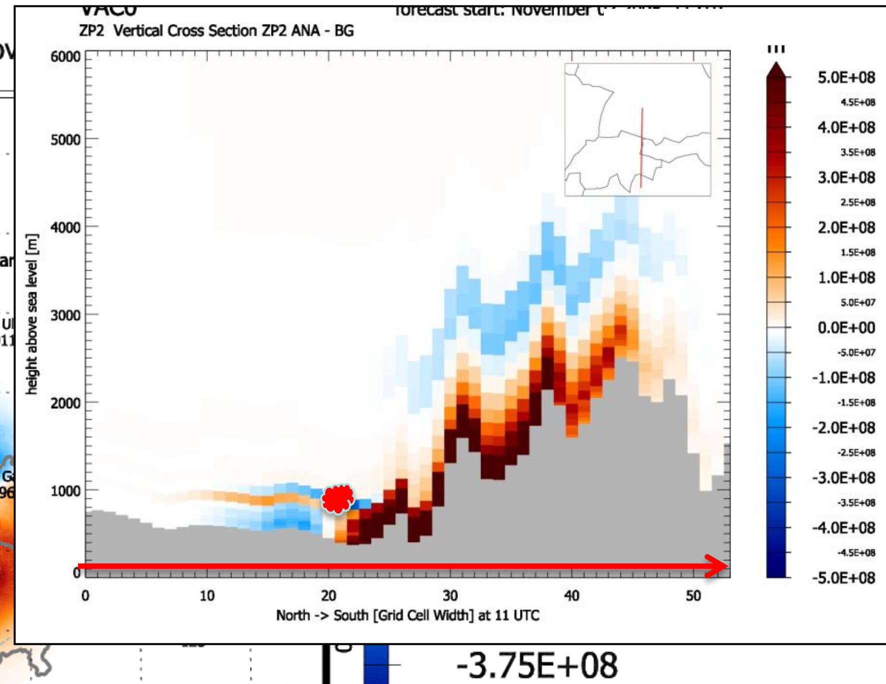


(from Lars Nieradzik, PhD thesis 2011)
water solubles include Friese and Ebel, 2010:
H^+ - NH_4^+ - Na^+ - SO_4^{--} - NO_3^- - Cl^- - H_2O

2. Analyses, Example (ii cntd.):
Flight 14 assimilation of PND (0.005-3.0 µm), Nov. 2
Analysis increment (Analysis – Background)







Aitken mode ΔPND

4 hour assimilation
5 km grid

Acc. mode ΔPND

(~ 450m a.g.)

from Lars Nieradzik, PhD thesis 2011

Thank you for your attention!

Minimize J by variation of $\mathbf{x}(t_0)$:

$$J(\mathbf{x}(t_0)) = \frac{1}{2}(\mathbf{x}^b(t_0) - \mathbf{x}(t_0))^T \mathbf{B}_0^{-1}(\mathbf{x}^b(t_0) - \mathbf{x}(t_0)) +$$

$$\frac{1}{2}\int_{t_0}^{t_N} (\mathbf{y}^0(t) - \mathbf{HM}[\mathbf{x}(t)])^T \mathbf{R}^{-1}(\mathbf{y}^0(t) - \mathbf{HM}[\mathbf{x}(t)])dt$$

$\mathbf{x}^b(t_0)$	background state at $t = 0$
$\mathbf{x}(t)$	model state at time t
$\mathbf{e}_b(t_0)$	background emission rate at $t = 0$
$\mathbf{e}(t)$	emission rate field at time t
$\mathbf{K}$	emission rate error covariance matrix
$H[\ \ ]$	forward interpolator
$\mathbf{y}^0(t)$	observation at time t
$\mathbf{B}_0$	background error covariance matrix

2 Questions:

1. Spatial optimisation only (no time evolution involved): How does a closed formula for the optimum read?

2. Temporal optimisation: How can we integrate “backward in time” with an adjoint model M^T for an optimum at initial time?