Data Assimilation and Synergies for Climate Research

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Outline

1. Introduction and Motivation
2. Theory of data assimilation
3. data assimilation for green house gas inversion
4. data assimilation for climate monitoring/reanalyses
5. Extension: “detection and attribution” algorithm for climate change

1. Introduction

Why data assimilation for climate research?

- The traditional objective of data assimilation is an optimal estimate of the atmospheric state as initial values for better meteorological forecasts.
- But, as the coupled climate system is considered as “nearly ergodic”, that means that initial values of the climate model are of little importance for long enough climate simulations,

then, why data assimilation for climate research?

Two principal objectives, where data assimilation algorithms are applied:

1. Estimate forcing agents of climate change: **greenhouse gases**, by assimilation algorithms/inversion
2. Combine all available information sources synergistically, to **monitor climate** states for better trend analyses:
   – promise signal identification by shorter time series or better signal/noise ratios

2. Theory of data assimilation

General textbook literature for data assimilation

- Daley, R., Atmospheric Data Analysis, Cambridge University Press, pp. 457, 1991.
  - Well established connection between statistics and practical data assimilation
  - Meanwhile behind cutting edge operational data assimilation implementations

- Bennet, A., Inverse Methods in Physical Oceanography, Cambridge University Press, pp. 346, 1992.
- Bennet, A., Inverse Modeling of the Ocean and Atmosphere, Cambridge University Press, pp. 234, 2002.
  - Mathematically very sound, with focus on oceangraphy
  - emphasis on science, rather than operational usage

- Geir Evensen Data Assimilation: The Ensemble Kalman Filter, Springer, 2006

- Kalnay, E., Atmospheric Modeling, Data Assimilation and Predictability, Cambridge University Press, pp. 341, 2003, Chap.
  - Well presented pedagogical introduction to data assimilation theory

- Thiebaux, H.J. and Pedder, M.A. Spatial Objective Analysis with applications in atmospheric science, Academic Press1987.
  - Mathematically rigorous formalism with Optimum Interpolation as central algorithm

Additionally, a collection of overview papers:

- Special Issue: J. Met. Soc. Japan, Vol. 75, No. 1B, pages 1-138, 1997.
- ECMWF tutorials: www.ecmwf.int

Underlying mathematics (advanced level):

- Jazwinski, A., Stochastic Processes and Filtering Theory, Academic Press, San Diego, pp. 376, 1970.
- Marchuk, G., Numerical solutions of the problems of the problems of the dynamics of the atmosphere and ocean, Gidrometeoizadat, Leningrad, 1974.
- Courant, R. and Hilbert, D. Methods of mathematical physics, Volume 1, New York: Interscience, 1953.
- Courant, R. and Hilbert, D. Methods of mathematical physics, Partial differentialequations, Volume 2, New York: Interscience, 1962.
- Lions, J., Optimal control of systems governed by partial differential equations, Spinger Verlag, Berlin, 1971.

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)*

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 (2)

- "is to produce a regular, **physically consistent four dimensional** representation of the state of the atmosphere
- from a **heterogeneous** array of in situ and remote instruments
- which sample **imperfectly** and **irregularly** in space and time.

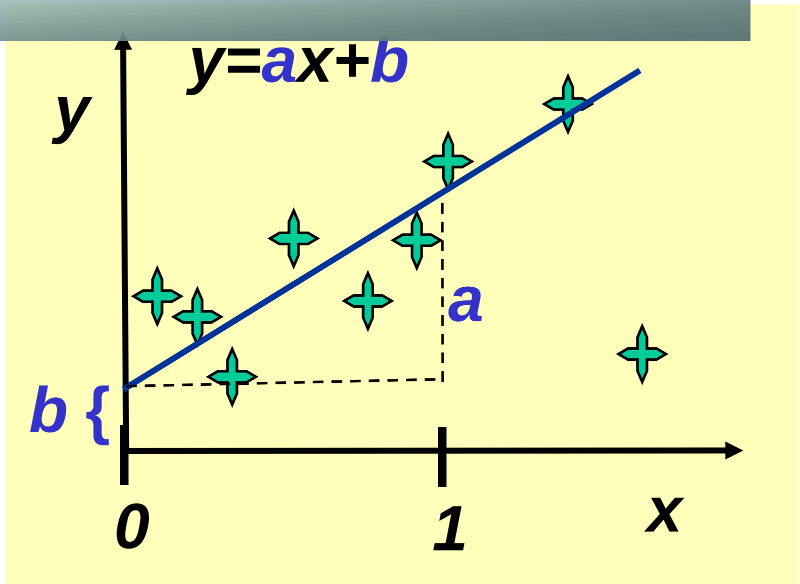
Data assimilation

- 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)

This lecture introduces:
Basic theoretical ideas of data assimilation

1. three basic sources of information
2. combination of information sources
3. the basic ideas of 4D-var and Kalman-filter
4. the limiting assumptions and a look forward

Data assimilation has much of curve fitting: e.g. quadratic optimisation



Given

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

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

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

Characteristics in data assimilation, in contrast to remote sensing retrievals

- high dimensional problem: dim ($\mathbf{x}$) > 10^5
- highly underdetermined system (few observations with respect to model freedom: dim($\mathbf{x}$)>>dim($\mathbf{y}$))
- regionally/locally highly nonlinear dynamics
- constraints by physical laws are insufficient:
  - cloud microphysics
  - dynamics

Advanced data assimilation is an application of the principles of Data Analysis.

(As in satellite retrievals) we strive for estimating a **latent**, not apparent parameter set **x**.

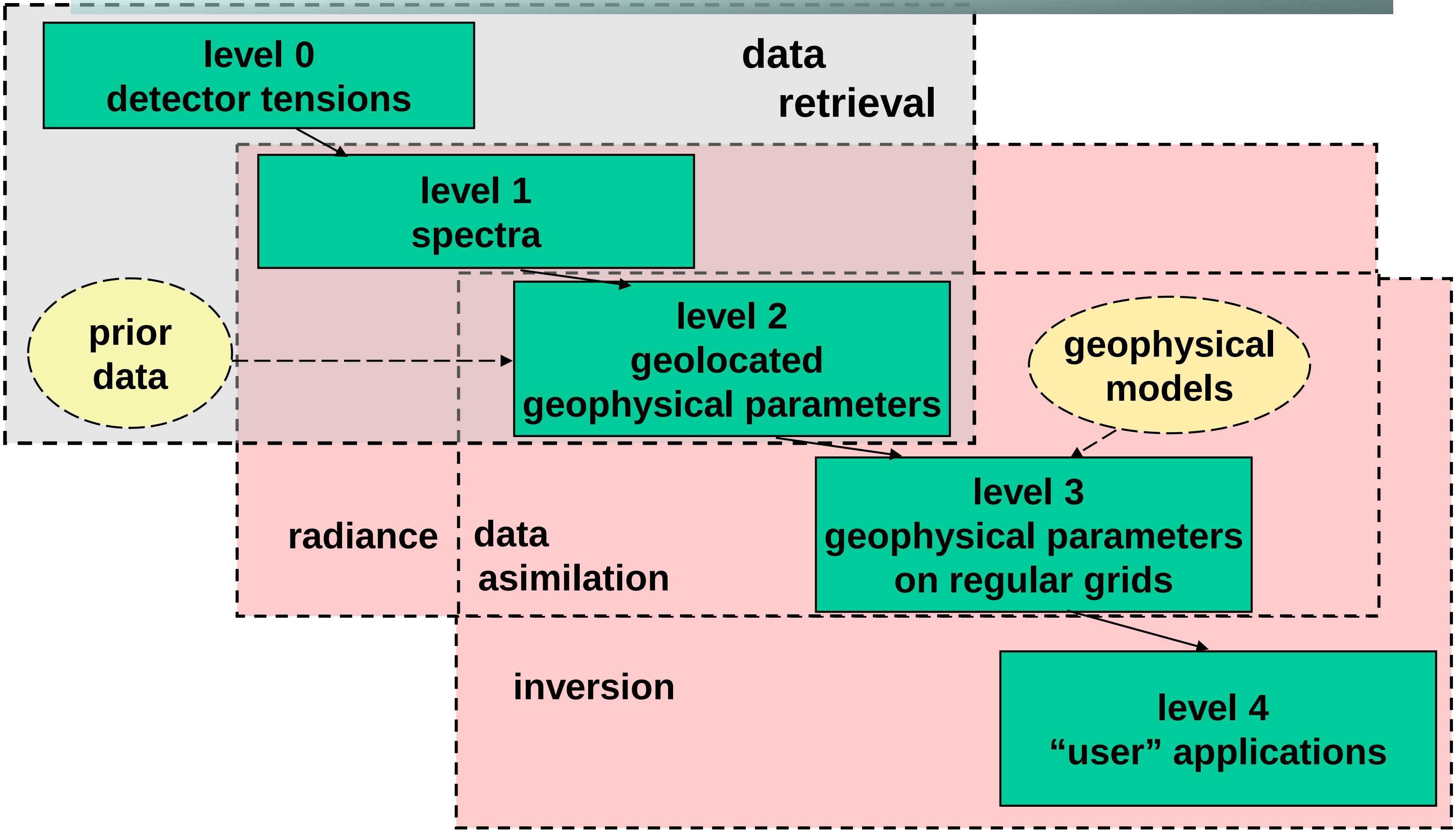
We dispose of

1. indirect information on the state and processes in terms of **manifest**, though insufficient or inappropriate data **y**, and
2. a deterministic model ***M*** connecting **x** and **y**, in some way.

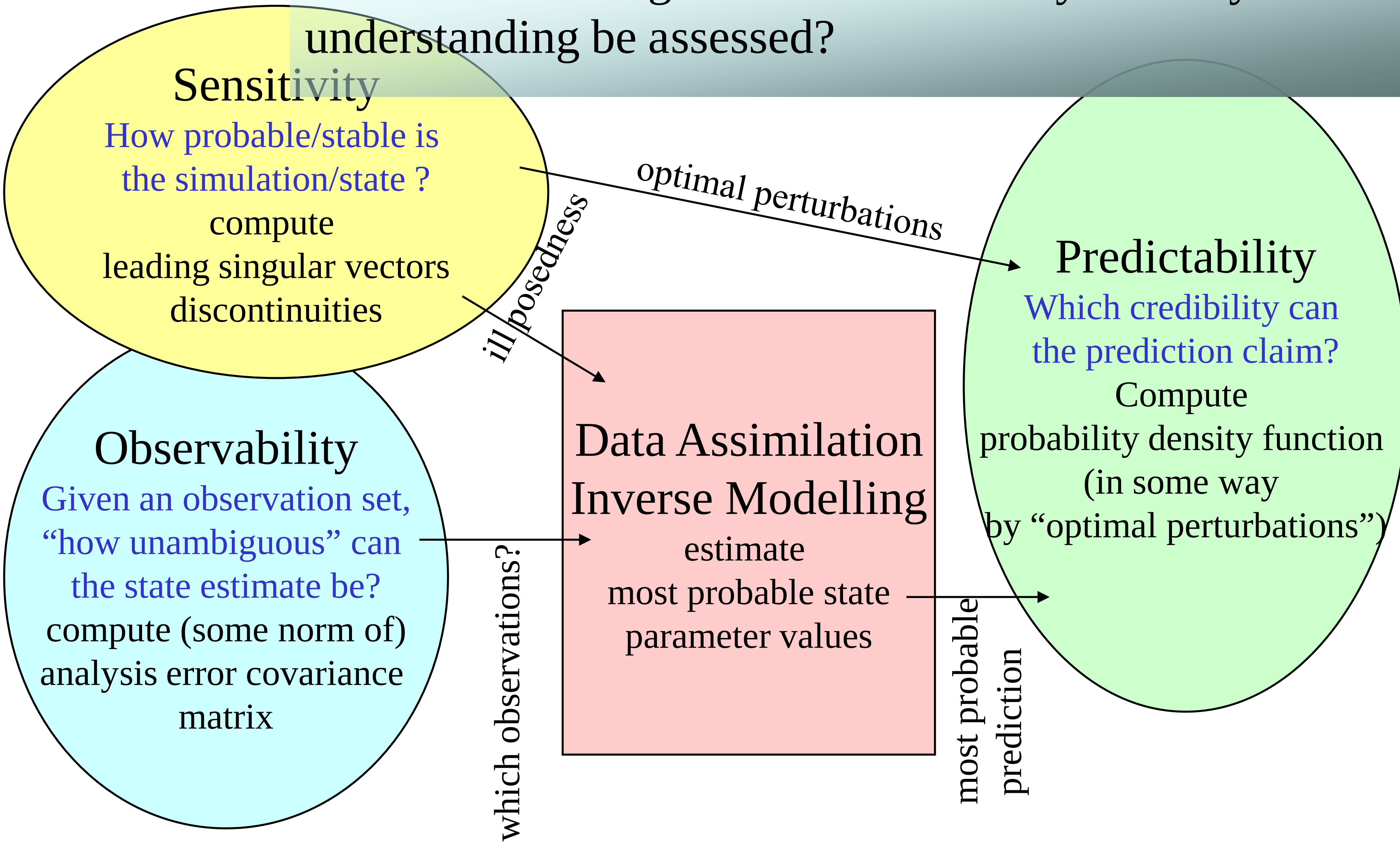
Bayes' rule gives access to the probability of state **x,** given **y** and **M**

$$\mathrm{prob}(\mathbf{x}|\mathbf{y},\mathcal{M}) = \frac{\mathrm{prob}(\mathbf{y}|\mathbf{x},\mathcal{M})\mathrm{prob}(\mathbf{x}|\mathcal{M})}{\mathrm{prob}(\mathbf{y}|\mathcal{M})}$$

DA in the satellite data application chain



DA and related algorithms: How can dynamic system understanding be assessed?



Optimality criteria: Which property can be attributed to our analysis result?

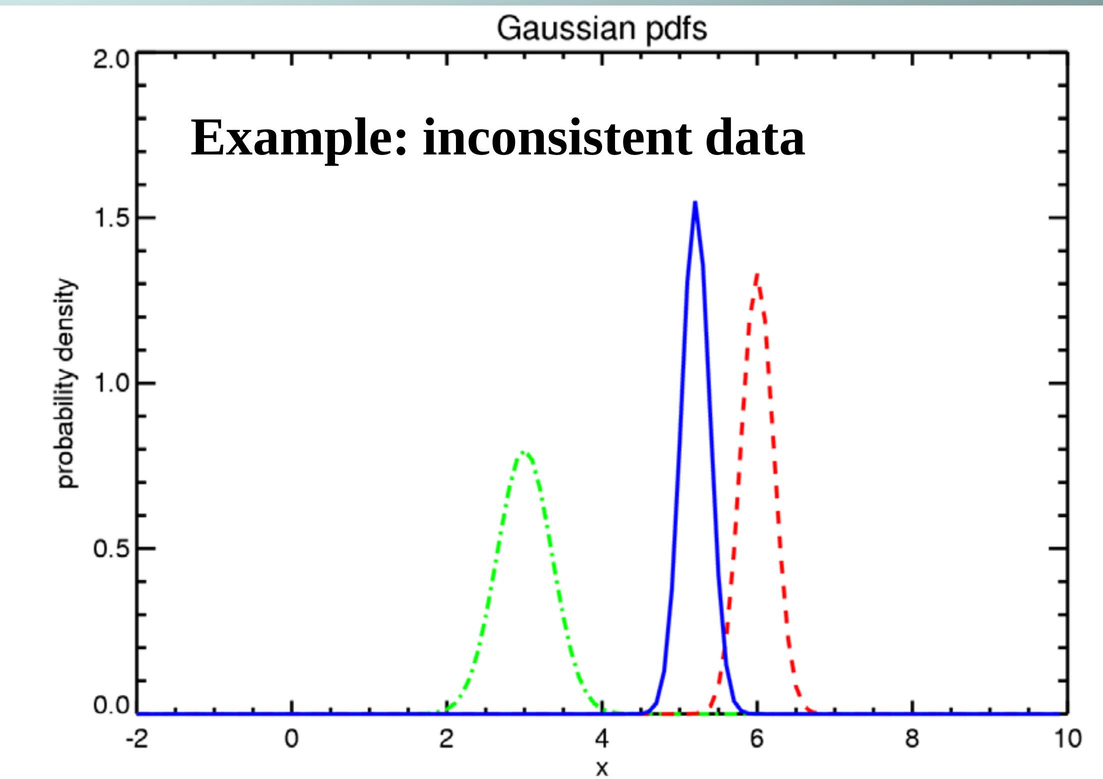
(Need for quantification)

- maximum likelyhood:
  - maximum of probability density function
- minimal variance: l_2 norm
  - parameters optimal, for which analysis error spread is minimal (for Gaussian/normal and log-normal error distributions), Best Linear Unbiased Estimate (**BLUE**)
- minimax norm (discrete cases)
- maximum entropy

Data assimilation: Synergy of Information sources

example: 2 data sets with Gaussian distribution

(here: minimal variance= maximum likelihood)



Bayes' rule:

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

Analysis (=estimation) **BLUE**

Best Linear Unbiased Estimate

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

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

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

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

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

a priori (=prediction or climatology)

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

observation

Optimal Interpolation

$$J(\mathbf{x}) = \frac{1}{2}[\mathbf{x}^b - \mathbf{x}]^T \mathbf{B}_0^{-1}[\mathbf{x}^b - \mathbf{x}] + \frac{1}{2}\{\mathbf{y}^0 - H[\mathbf{x}(t)]\}^T \mathbf{R}^{-1}\{\mathbf{y}^0 - H[\mathbf{x}]\}$$

The gradient then reads

$$\nabla J(\mathbf{x}) = \mathbf{B}_0^{-1}[\mathbf{x}^b - \mathbf{x}] + H^T \mathbf{R}^{-1}\{\mathbf{y}^0 - H[\mathbf{x} + (\mathbf{x}_b - \mathbf{x}_b)]\}$$

where a trivial expanion is introduced for later manipulation.

At the minimum $\mathbf{x} =: \mathbf{x}_a$

$$\mathbf{x}_a - \mathbf{x}_b = (\mathbf{B}_0^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H})^{-1}\mathbf{H}^T\mathbf{R}^{-1}\{\mathbf{y}^0 - H[\mathbf{x}_b]\}$$

$$= \boxed{\mathbf{B}\mathbf{H}^T(\mathbf{R} + \mathbf{H}^T\mathbf{B}\mathbf{H})^{-1}\{\mathbf{y}^0 - H[\mathbf{x}_b]\}}$$

with the latter result obtained after some manipulation.

Notation: Ide, K., P. Courtier, M. Ghil, and A. Lorenc,
Unified notation for data assimilation: operational sequential and variational,
J. Met. Soc. Jap., 75, 181--189, 1997.

Kalman filter: basic equations

$$\mathbf{x}^f(t_i) = \mathbf{M}(t_i, t_{i-1})\mathbf{x}^a(t_{i-1}) + \eta$$

$$\mathbf{P}_i^b = \mathbf{M}(t_i, t_{i-1})\mathbf{P}_{i-1}^a\mathbf{M}^T(t_i, t_{i-1}) + \mathbf{Q}$$

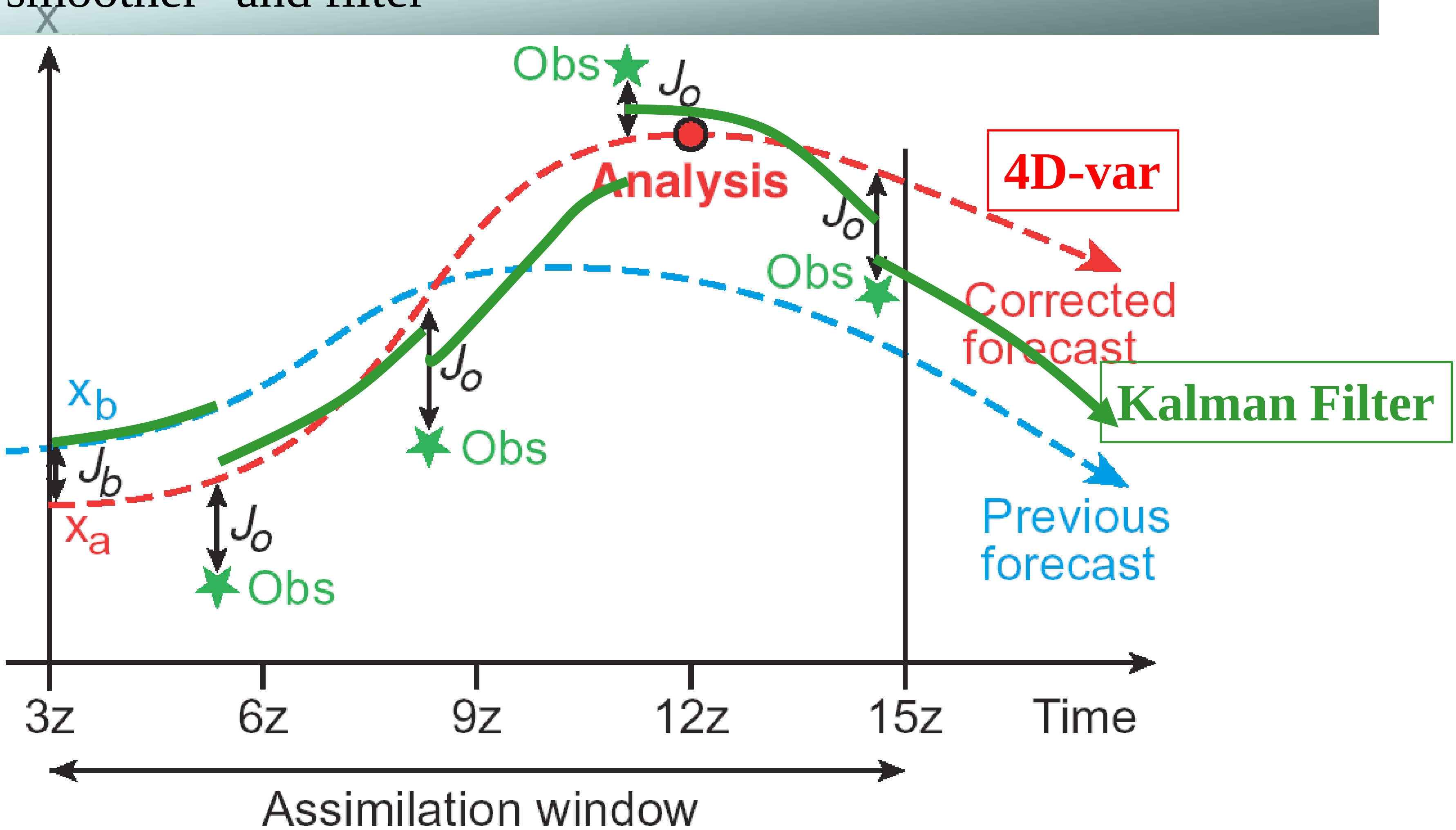
$$\mathbf{x}^a(t_i) = \mathbf{x}^b(t_i) + \mathbf{K}_i\mathbf{d}_i, \qquad (1)$$

$$\mathbf{K}_i := \mathbf{P}_i^b\mathbf{H}_i^T(\mathbf{H}_i\mathbf{P}_i^b\mathbf{H}_i^T + \mathbf{R}_i)^{-1} \quad \in \mathcal{R}^{n\times p_i} \qquad (2)$$

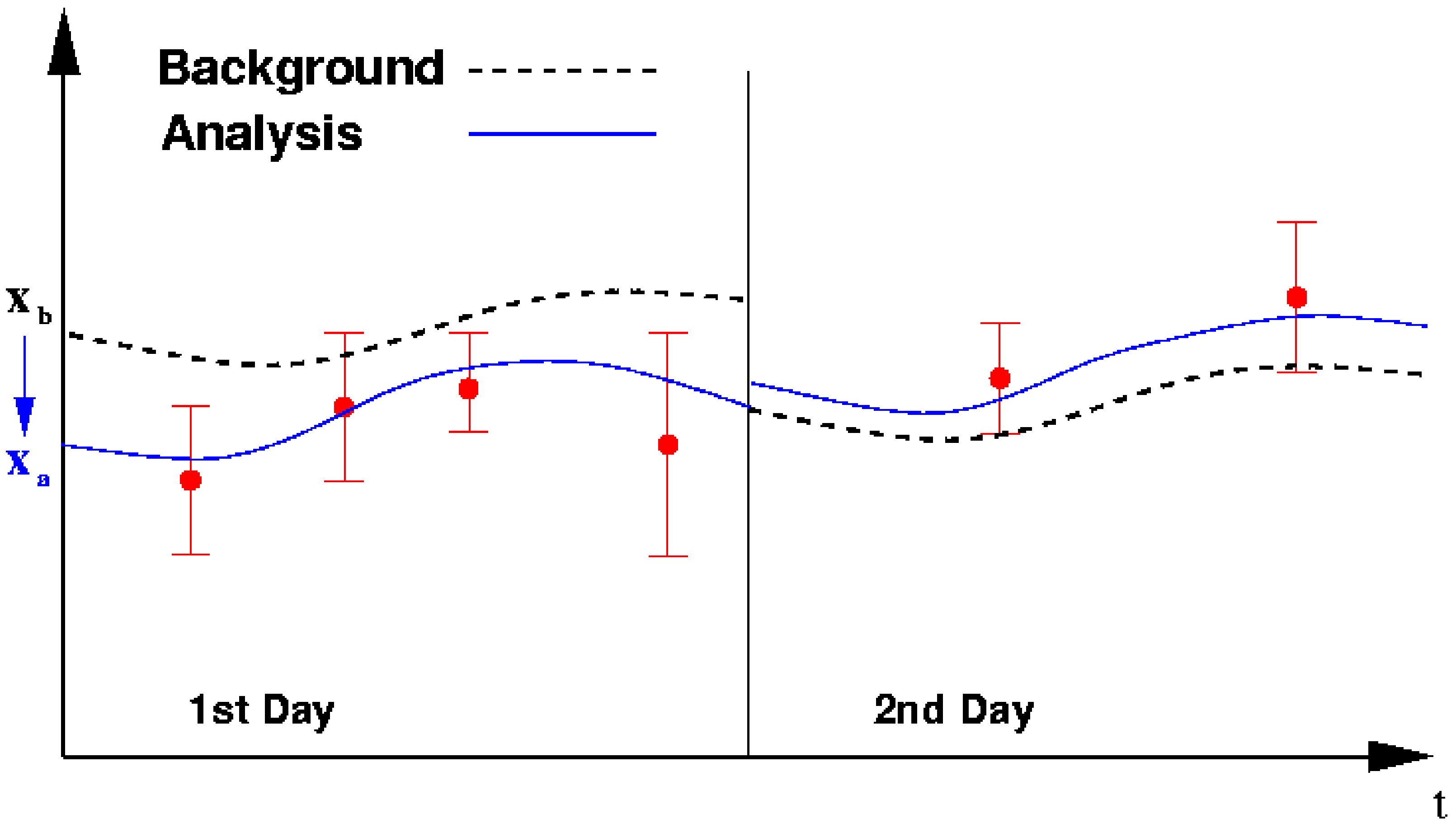
and

$$\mathbf{P}_i^a = (\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\mathbf{P}_i^b. \qquad (3)$$

Types of assimilation algorithms:
"smoother" and filter



How does 4D-var work?



Why is 4D-variational a valuable data assimilation technique?

- provides BLUE (Best Linear Unbiased Estimator).
  Remark: 3D-var → ingested in model does not!
- Potential for "consisteny" within the assimilation intervall (*O* (1 day))
  Remark: fast manifold perturbations (="initialisation problem") mitigated, but not removed. Inconsistencies at the end of the assimilation windows.
- Allows for extensions to estimate analysis error covariance matrix and temporal correlations (red noise)

Derivation of 4D-var (1)

The distance function $\mathcal{J}$ may be defined as follows:

$$\mathcal{J}(\mathbf{x}(t)) = \frac{1}{2}(\mathbf{x}_b - \mathbf{x}(t_0))^T \mathbf{B}^{-1}(\mathbf{x}_b - \mathbf{x}(t_0)) + \frac{1}{2}\int_{t_0}^{t_N} (\hat{\mathbf{x}}(t) - \mathbf{x}(t))^T \mathbf{R}^{-1}(\hat{\mathbf{x}}(t) - \mathbf{x}(t))dt \tag{1}$$

where $\mathcal{J}$ is a scalar functional defined on the time interval $t_0 \leq t \leq t_N$ dependent on the vector valued state variable $\mathbf{x} \in \mathcal{H}$ with $\mathcal{H}$ denoting a Hilbert space. The first guess or background values $\mathbf{x}_b$ are defined at $t = t_0$, and $\mathbf{B}$ is the covariance matrix of the estimated background error. The observations are denoted $\hat{\mathbf{x}}$ and the observation and representativeness errors are included in the covariance matrix $\mathbf{R}$.

Derivation of 4D-var (2)

Let the differential equation of the model $\mathbf{M}$ be given by

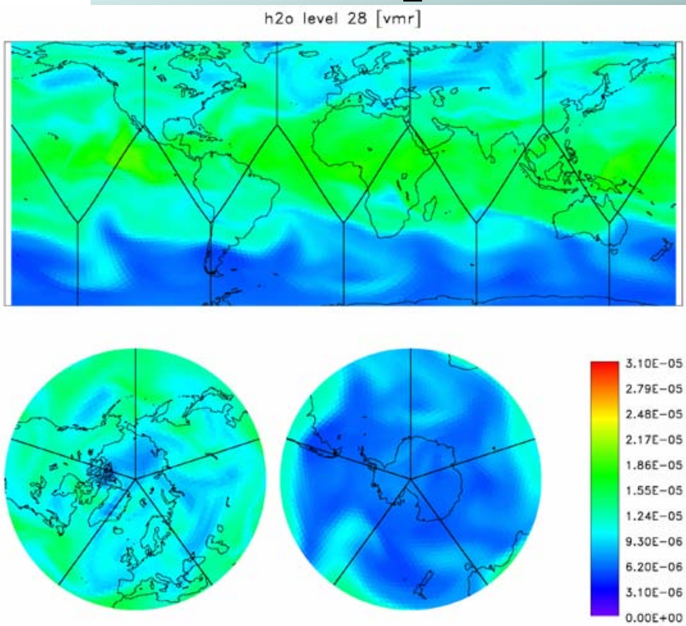
$$\frac{d\mathbf{x}}{dt} = \mathbf{M}(\mathbf{x}), \qquad (1)$$

where $\mathbf{M}$ acts as a generally nonlinear operator defining uniquely the state variable $\mathbf{x}(t)$ at time t, after an initial state $\mathbf{x}(t_0)$ is provided. The linear perturbation equation, giving the evolution of a small deviation $\delta\mathbf{x}(t)$ from a model state $\mathbf{x}(t)$ then reads

$$\frac{d\delta\mathbf{x}}{dt} = \mathbf{M}'\delta\mathbf{x}, \qquad (2)$$

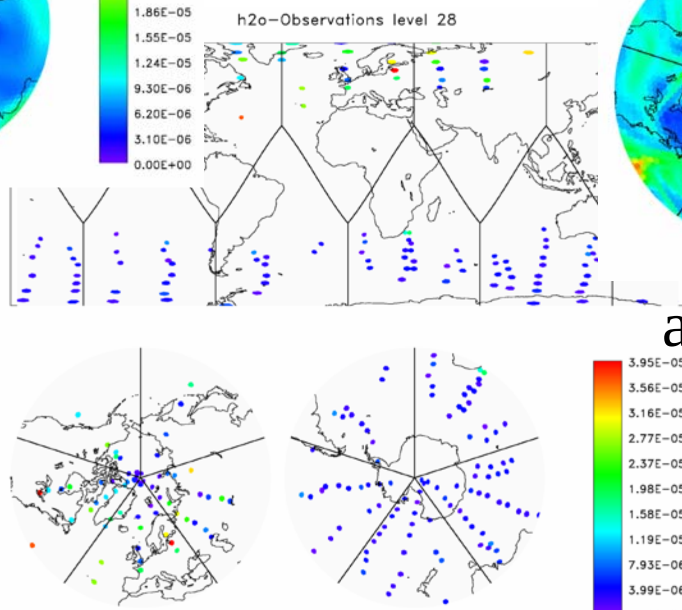
where $\mathbf{M}'$ is the tangent linear model of $\mathbf{M}$.

water vapour assimilation

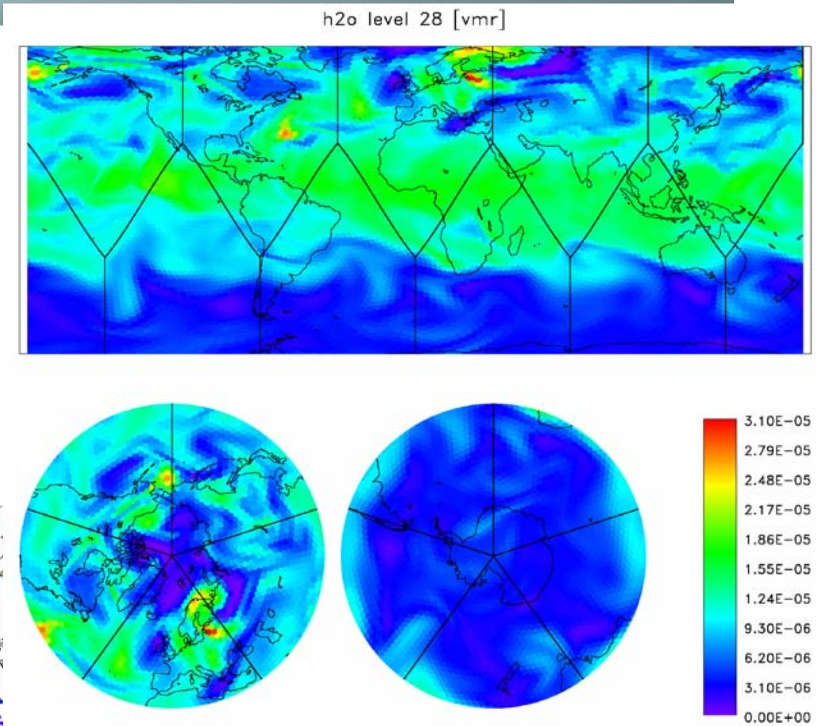


Integration start:
1. July,
no assimilation

20. July 2003
~160 hPa



MIPAS water vapour retrievals



after continuous assimilation

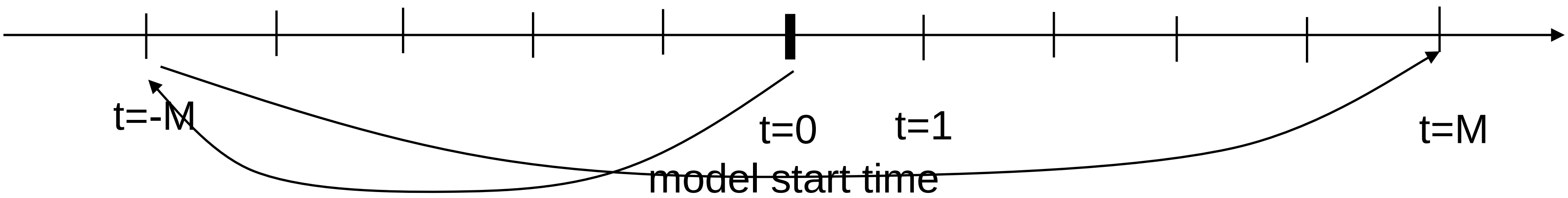
Are contraints by physical laws sufficient? The "Initialisation" / Filtering Problem (1)

- Constraints by physical/chemical equations are insufficient, as they allow for physically/chemically admissible states, but partly very unlikely to occur:
  - high amplitude gravity waves ("fast manifolds")
  - pronounced chemical imbalances
- Legacy procedure: introduce penalty term for fast changes (Normal Mode Initialisation, NMI)

$$J_c(\mathbf{x}) = \mu \left(\frac{d\mathbf{x}}{dt} - \frac{d\mathbf{x}_b}{dt} \right)^2$$

The "Initialisation" / Filtering Problem (2)

- or filter function (Digital Filter Initialisation, DFI, here with Lanczos-filter), x model state:



$$\bar{\mathbf{x}}(0) = \sum_{n=-M}^{M} h_n \mathbf{x}(t_n)$$

where

$$h_n := \frac{\sin(n\theta\Delta t)\sin(n\pi/M)}{(n\pi)^2/M}$$

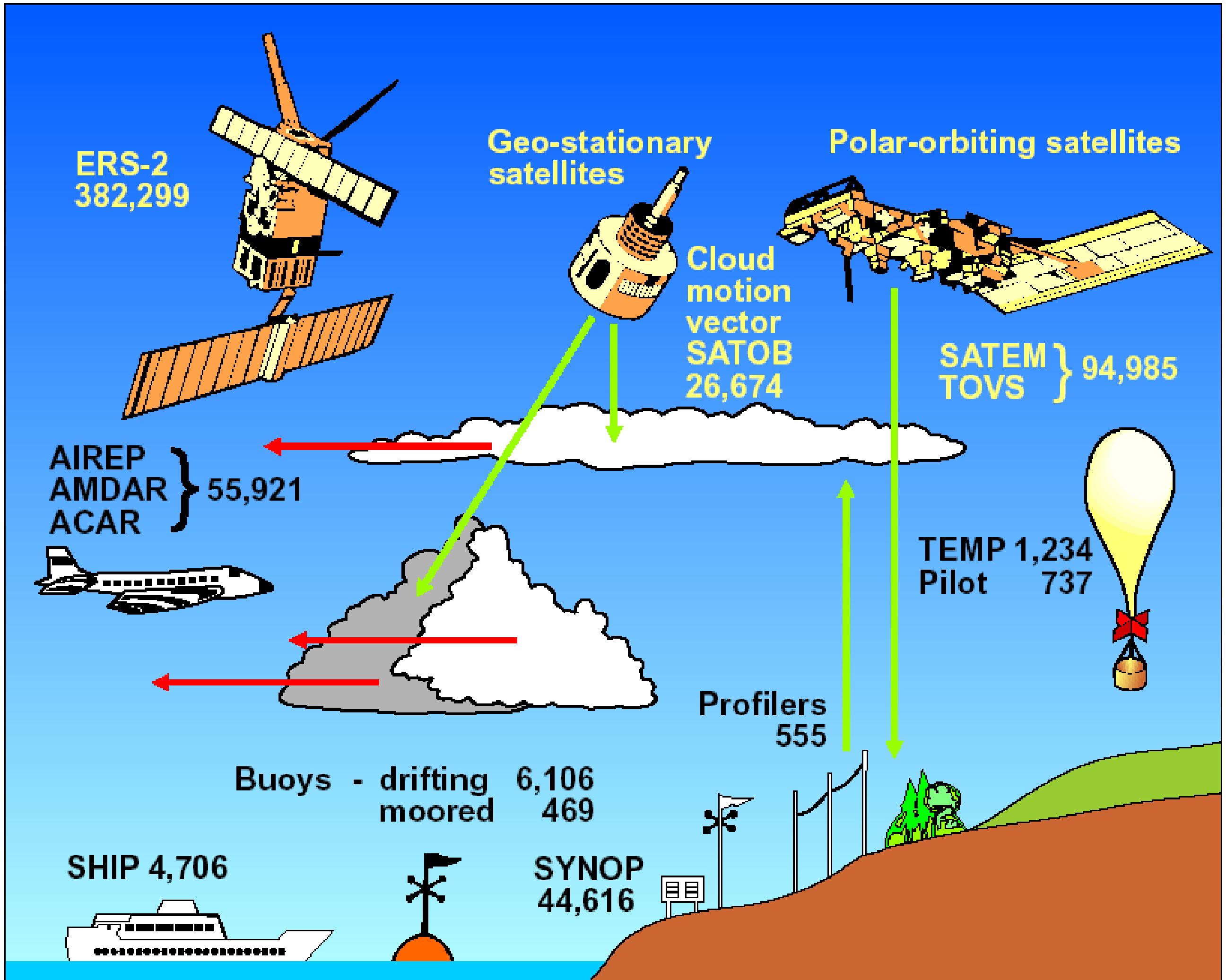
Meteorological remote sensing observation suite (1)

- *Atmospheric* sounding channels from *passive* instruments: atmospheric temperature and humidity (Atmospheric sounding channels from the **HIRS** (High resolution Infrared Sounder) and **AMSU** (Advanced Microwave Sounding Unit) on board NOAA
- *Surface* sensing channels from *passive* instruments "imaging" channels: located in atmospheric "window" regions of the infra-red and microwave spectrum : surface temperature and cloud track information
- Surface sensing channels from active instruments: scatterometer emit microwave radiation for ocean wind retrievals. Some similar-class active instruments such as altimeters and **SARS** (Synthetic Aperture Radars) provide information on wave height and spectra.

Meteorological remote sensing observation suite (2)

- visible (**Lidar**s) or the microwave (**radars**) analyse the signal backscattered
  - molecules, aerosols, water droplets or ice particles.
  - penetration capability allow the derivation of information on cloud base, cloud top, wind profiles (Lidars) or cloud and rain profiles (radars).
- Radio-occulation technique using **GPS** (Global Positioning System). GPS receivers (e.g. METOP/GRAS) measure the Doppler shift of a GPS signal refracted along the atmospheric limb path.

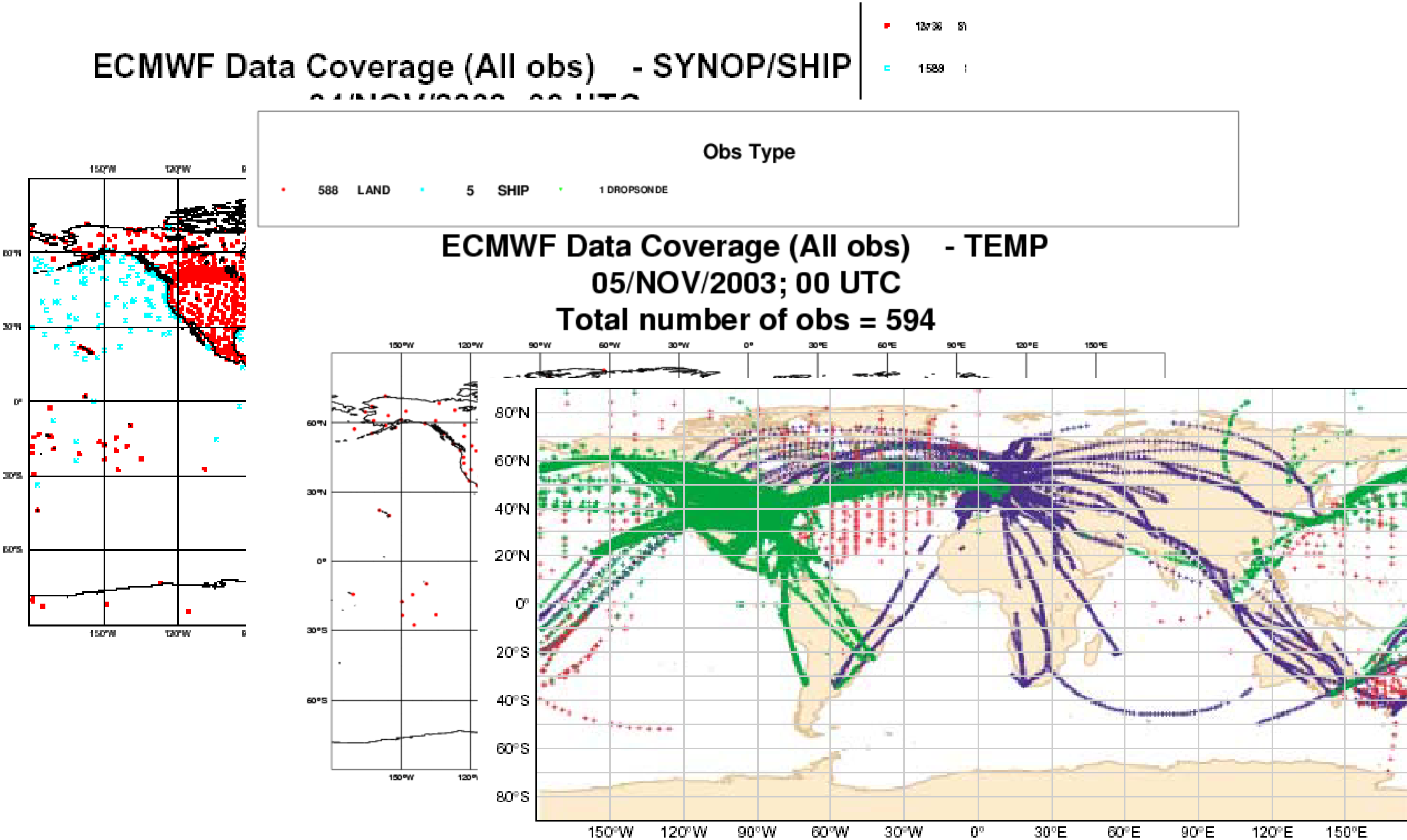
Observation systems (1)



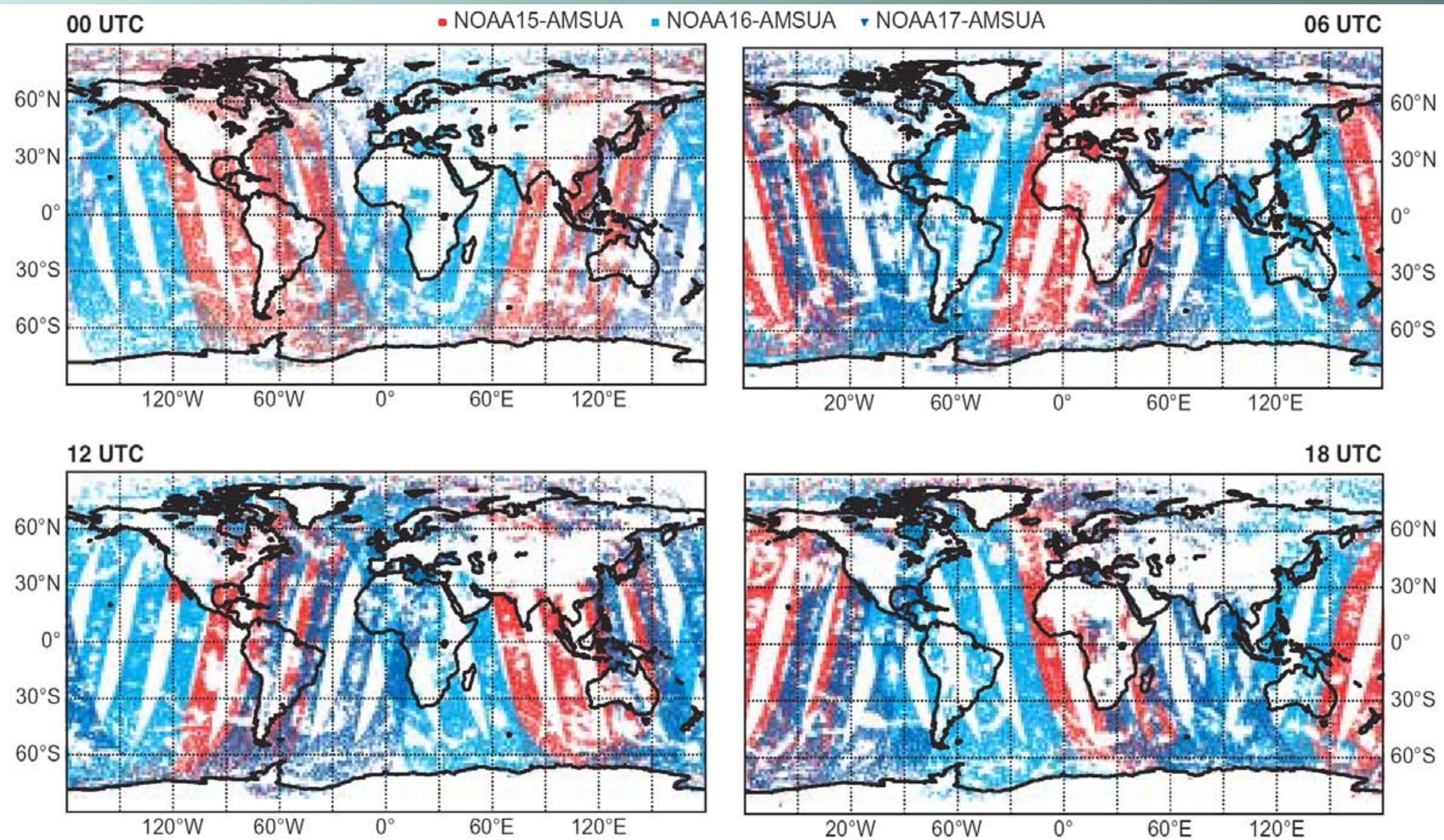
$\mathrm{dim}_{\text{observation space}}$
$= \mathbf{O(10^6)}$

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

Observation systems (2): In-situ observations

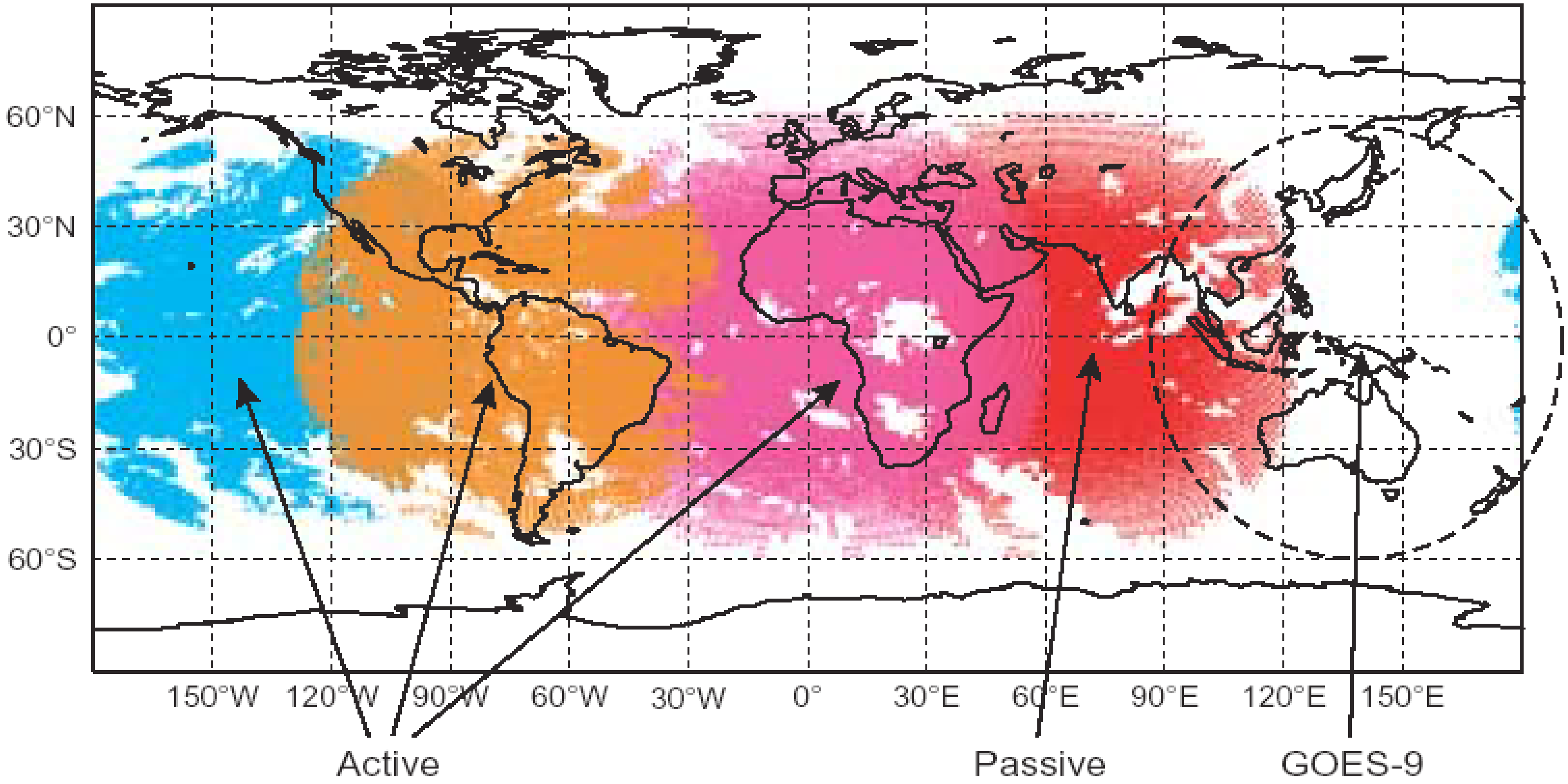


Observation systems (3):
polar orbiting satellites (e.g. AMSU-A)



Data coverage for the NOAA-15 (red), NOAA-16 (cyan) and NOAA-17 (blue) AMSU-A instruments, for the four 6-hour periods centred at 00, 06, 12 and 18 UTC 12 November 2002. The plots show the data used for AMSU-A channel 5, which is a temperature-sounding channel in the mid and lower troposphere.

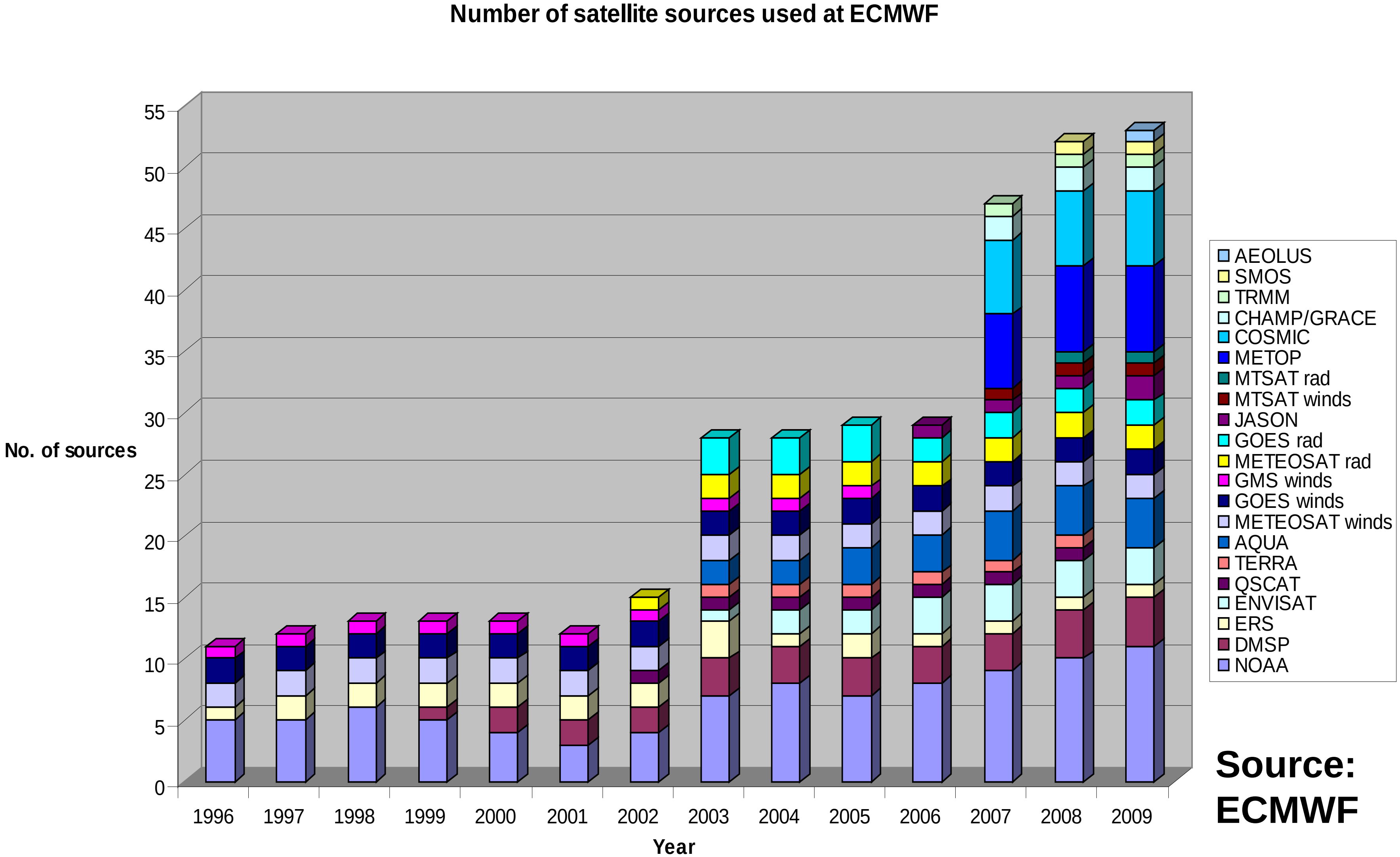
Observation systems (4): geostationary



Data coverage provided by the GOES satellites (cyan and orange) and the METEOSAT satellites (magenta and red) for 00 UTC 10 May 2003. The total number of observations was 266,878.

Source: ECMWF

Satellite data sources in 2007+

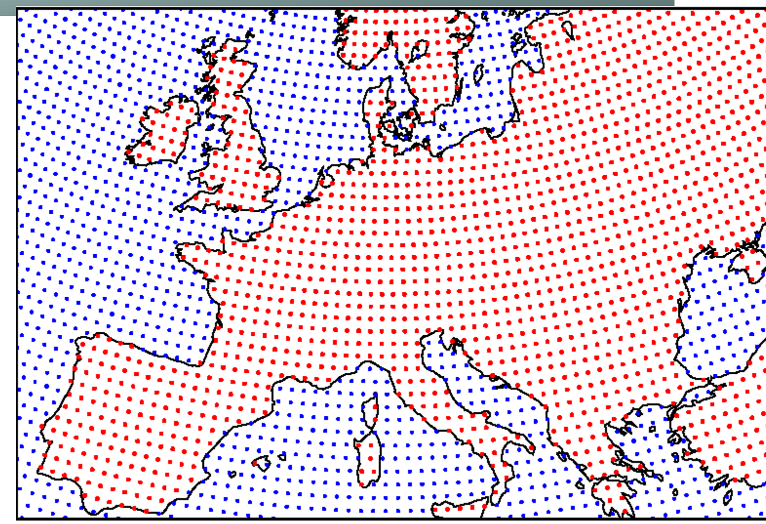


Source: ECMWF

Information source: numerical model

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

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

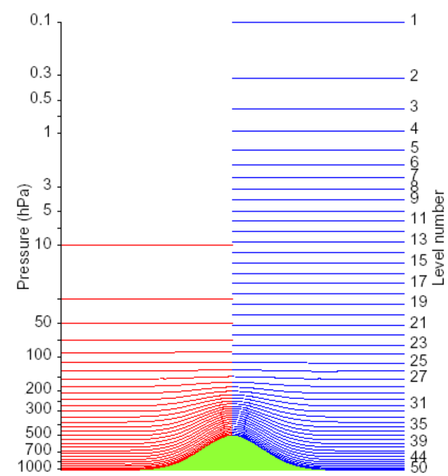


$$\frac{\partial T}{\partial t} + \frac{1}{a\cos^2\theta}\left\{U\frac{\partial T}{\partial \theta} + V\cos\theta\frac{\partial T}{\partial \theta}\right\} + \dot{\eta}\frac{\partial T}{\partial \eta} - \frac{\kappa T_v \omega}{(1 + (\delta - 1)q)p} = P_T + K_T$$

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

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

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



now

T799L91

(~25 km)

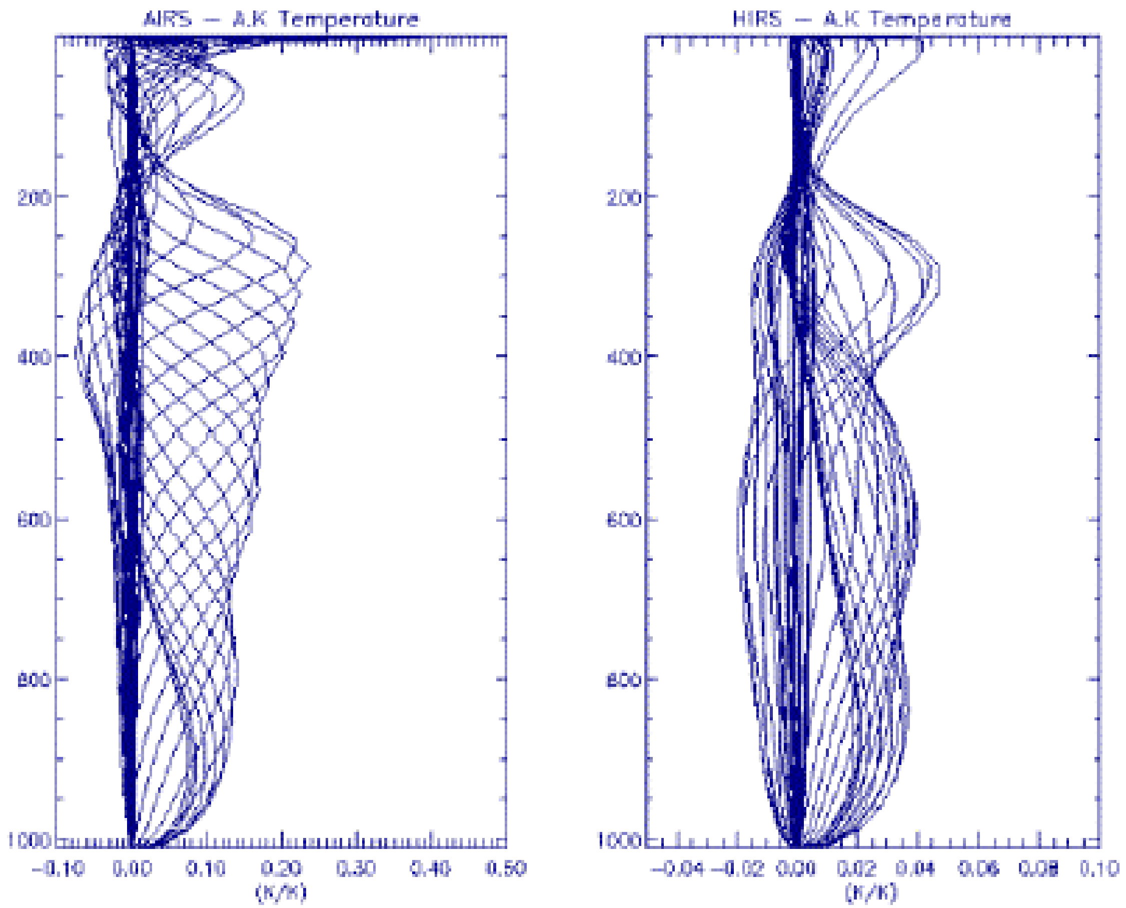
➔

dim **O(10^8)**

At which retrieval level to assimilate remote sensing data ?

- **Assimilation of retrieved products from space agencies or research institutes (“level 2”)**
  - *Pro*: most simple for assimilation (assimilation “like in situ observations”)
  - *Con*: inexact as $\mathbf{x}_b$ and $\mathbf{B}$ are inconsistent, if retrieval and assimilation are independent
- **Locally produced or “1D-Var” or “Averaging Kernel” retrievals**
  - *Pro*: $\mathbf{x}_b$ and $\mathbf{B}$ much better known (e.g. fronts featured and consistent with model)
  - *Con*: $\mathbf{x}_b$ and $\mathbf{B}$ used twice with the subsequent assimilation: $\mathbf{y}$ and $\mathbf{x}_b$ correlated
- **Direct assimilation of radiances (“level 1”)**
  - *Pro*: retrieval step is essentially incorporated within the main analysis by finding the model variables that minimize a cost function measuring the departure between the analysed state and both the background and available observations.
  - *Con*: Fast linearized radiative transfer scheme and its adjoint is needed.

Example for averaging kernels



Averaging kernels (in K/K) for AIRS (left panel) and HIRS (right panel) instruments.

Background Error Covariance Matrix

The design of the BECM is **of utmost importance**, as it

•weights the model error against the competing observation errors

•spreads information from observations to the adjacent area

•influences coupled parameters: temperature ←→ wind field, chemical constituents (i.e. multivariate correlation)

•(serves for preconditioning in the case of variational assimilation)

$$w(r) = \exp(-\frac{r^2}{2L^2})$$

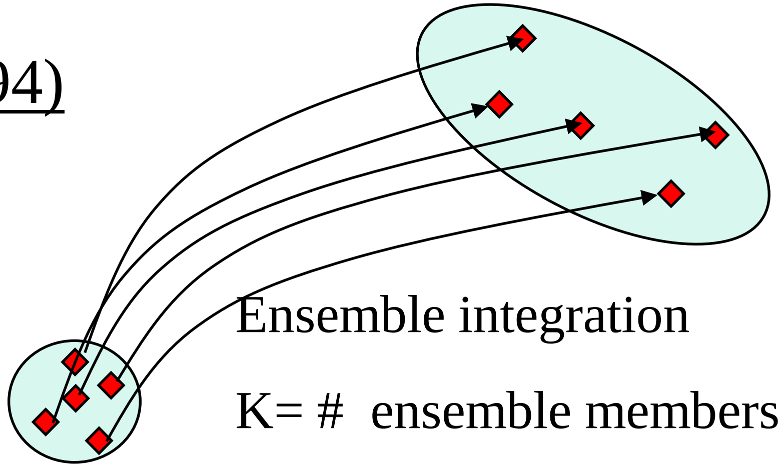
$$w(r) = (1 + \frac{1}{L}) \exp(-\frac{r}{L})$$

2 simple, isotropic and homogeneous covariance models:

Gaussian

Balgovind

Background Error Covariance Matrix **B** (2 pragmatic methods to estimate **B**)



1. Ensemble approach: (e.g. Evensen, 1994)

$$B_{ij} = \frac{1}{K}\sum_{n=1}^{K}\left(x_i^n - \bar{x}_i\right)\left(x_j^n - \bar{x}_j\right)$$

Ensemble integration

K= # ensemble members;

i,j grid cells

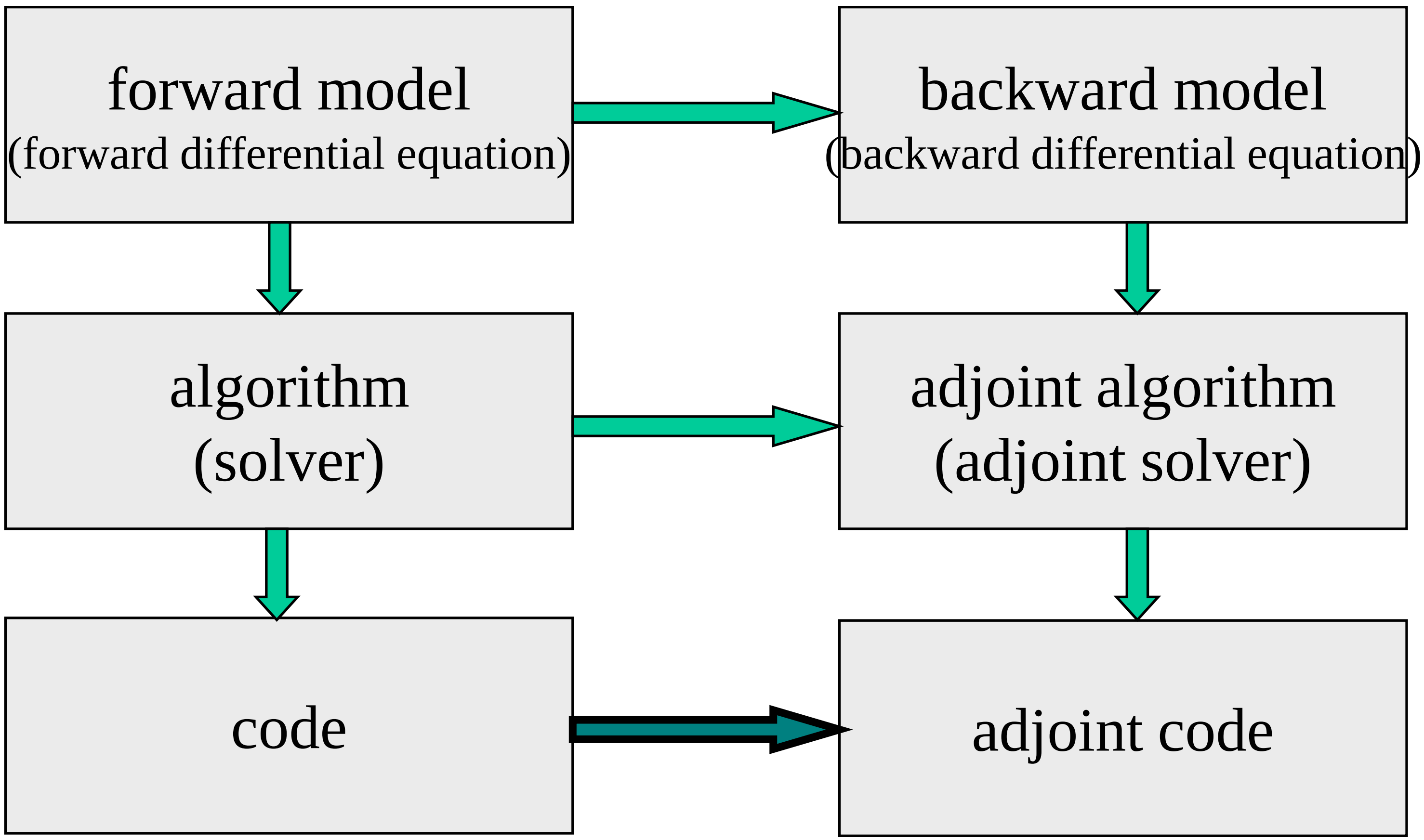
2. NMC method: (e.g. Parrish and Derber, 1992)

$$\delta\mathbf{x}(t_i) = \mathbf{x}^{f48h}(t_i) - \mathbf{x}^{f24h}(t_i)$$

$$\mathbf{B} = \frac{1}{K}\sum_{i=1}^{K}\delta\mathbf{x}(t_i)\,\delta\mathbf{x}^T(t_i)$$

Difference column vector of model states of two forecasts at some absolute time t_i, one starting 24 hours earlier than the other, thus trying to capture the most sensitive errors. Covariances calculated by outer product.

Construction of the adjoint code



Adjoint compiler

Some examples

- Odyssee
- TAMC
- Tapenade
- ADOL-C and ADOL-F (includes ability for higher order derivatives)
- IMAS

For much more comprehensive list see:

www.autodiff.org/?module=Tools&submenu=&language=ALL

Also codes from adjoint compilers must be tested!!

Algorithm and performance bugs occur!

Adjoint integration "backward in time"

How to make the parameters of resolvents *i* **M**(t_{i-1},t_i) available in ***reverse*** order??

direct model

$$\frac{d\mathbf{x}}{dt} = \mathcal{M}(\mathbf{x})$$

tangent linear model

$$\delta\mathbf{x}(t_n) = \mathbf{M}'(t_n, t_0)\delta\mathbf{x}(t_0) = \prod_{i=n}^{1} \mathbf{M}'(t_i, t_{i-1})\delta\mathbf{x}(t_0)$$

adjoint model

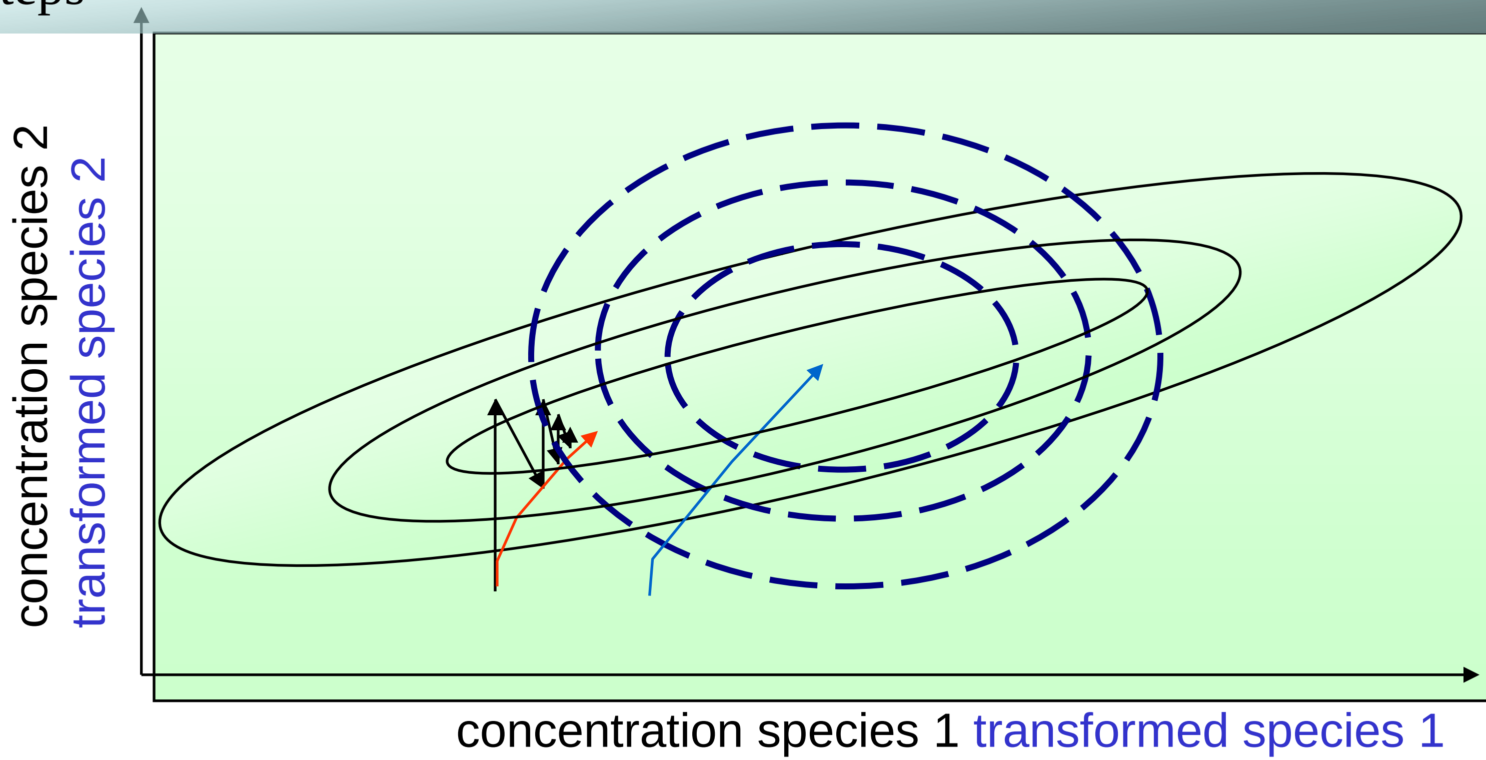
$$-\frac{d\delta\mathbf{x}^*(t)}{dt} - \mathbf{M}'^T\delta\mathbf{x}^*(t) = \mathbf{R}^{-1}(\mathbf{y}^0(t) - H[\mathbf{x}(t)]).$$

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

Isopleths of the cost function and transformed cost function and minimisation steps



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

The Preconditioning Problem

Hessian matrix = (analysis error covariance matrix)$^{-1}$

$$\nabla^2 J = \mathbf{B}_0{}^{-1} + H^T \mathbf{R}^{-1} H$$

the optimum is (linear case)

$$\mathbf{x}_{opt} - \mathbf{x}_b = (\mathbf{B}_0{}^{-1} + H^T \mathbf{R}^{-1} H)^{-1} \nabla J$$

practical problem:
with increasing L, $\mathbf{B}_0$ is increasingly ill–conditioned

Example:
2D grid 25×25
influence radius $L = 6$
gives

$$\mathrm{cond}(\mathbf{B}_0) \sim 10^9$$

Transformed cost function

define $$\mathbf{d}_i := \mathbf{y}_i^o - \mathbf{HM}(t_i, t_0)\mathbf{x}(t_0)$$

$$\delta\mathbf{x}(t_0) := \mathbf{x}^b - \mathbf{x}(t_0)$$

transformation $$\mathbf{v} := \mathbf{B}^{-1/2}\delta\mathbf{x}_b$$

transformed cost function $$J(\mathbf{v}) = 1/2\mathbf{v}^T\mathbf{v} + 1/2\sum_{m=0}^{N}\mathbf{d}_m^T\mathbf{R}^{-1}\mathbf{d}_m$$

transformed gradient of the cost function

$$\nabla_{\mathbf{v}}J(\mathbf{v}) = \mathbf{v} + \mathbf{B}^{1/2}\sum_{m=0}^{N}\mathbf{M}^T(t_m, t_0)\mathbf{H}^{\mathbf{T}}\mathbf{R}^{-1}\mathbf{d}_m$$

Pro transformation:
minimisation problem is better conditioned
Contra:
strictly positive definite approximation to **B** required

Computation of inverse B, square root B, inverse square root B
by (Sca)LAPACK eigenpair decomposition, but better choices available.

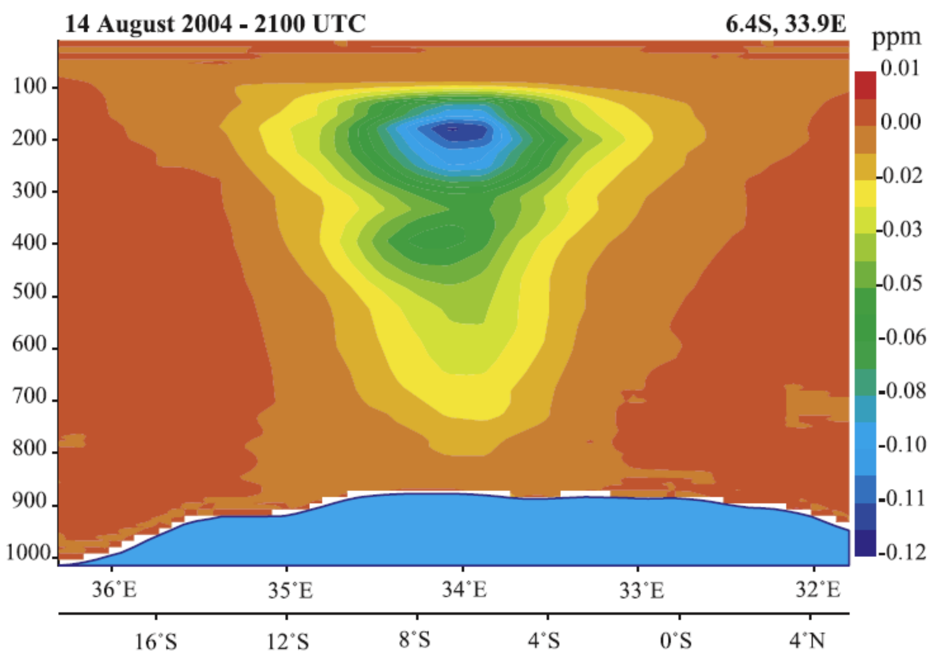
3. Assimilation for Greenhouse Gas Inversion

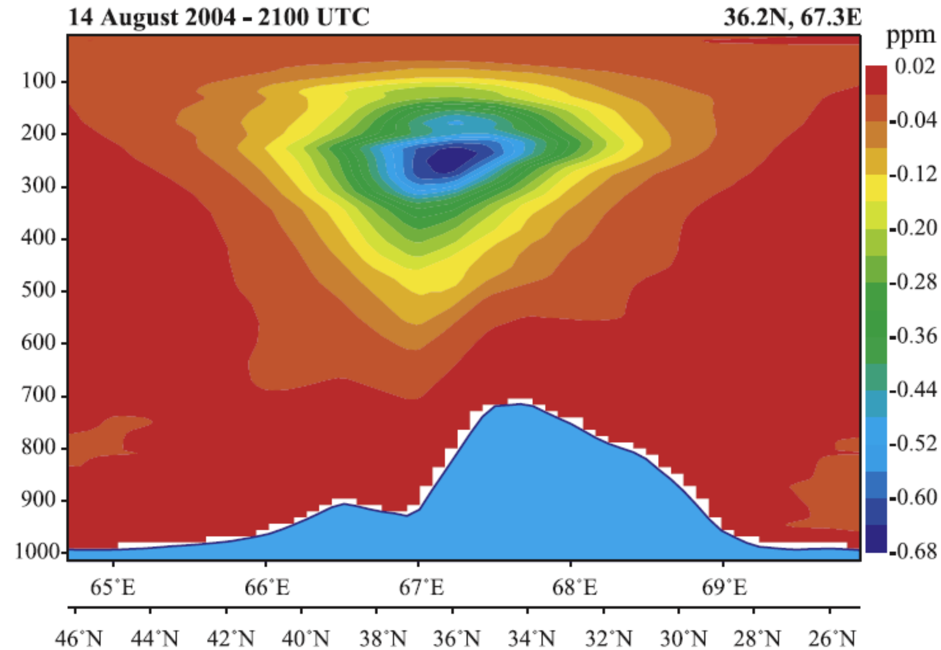
Recent examples

Example 1:Engelen, R. J., et al. (2009), Four-dimensional data assimilation of atmospheric CO2 using AIRS observations, J. Geophys. Res.,

- data: Radiances assimilation from the Atmospheric Infrared Sounder (AIRS)
  - AIRS radiances mainly provides CO2 in the middle and upper troposphere
  - (in readiness for Japanese Greenhouse Gases Observing Satellite (GOSAT))
- model: IFS by ECMWF
  - 125 km resolution, and 60 vertical levels
- method: 4D-var
  - observation operator H: fully nonlinear in the form of the Radiative Transfer for the TIROS Operational Vertical Sounder (RTTOV) radiative transfer model [Matricardi, 2003]

Vertical cross sections of CO2 increments caused by a single AIRS observation (using 24 CO_2sensitive channels)



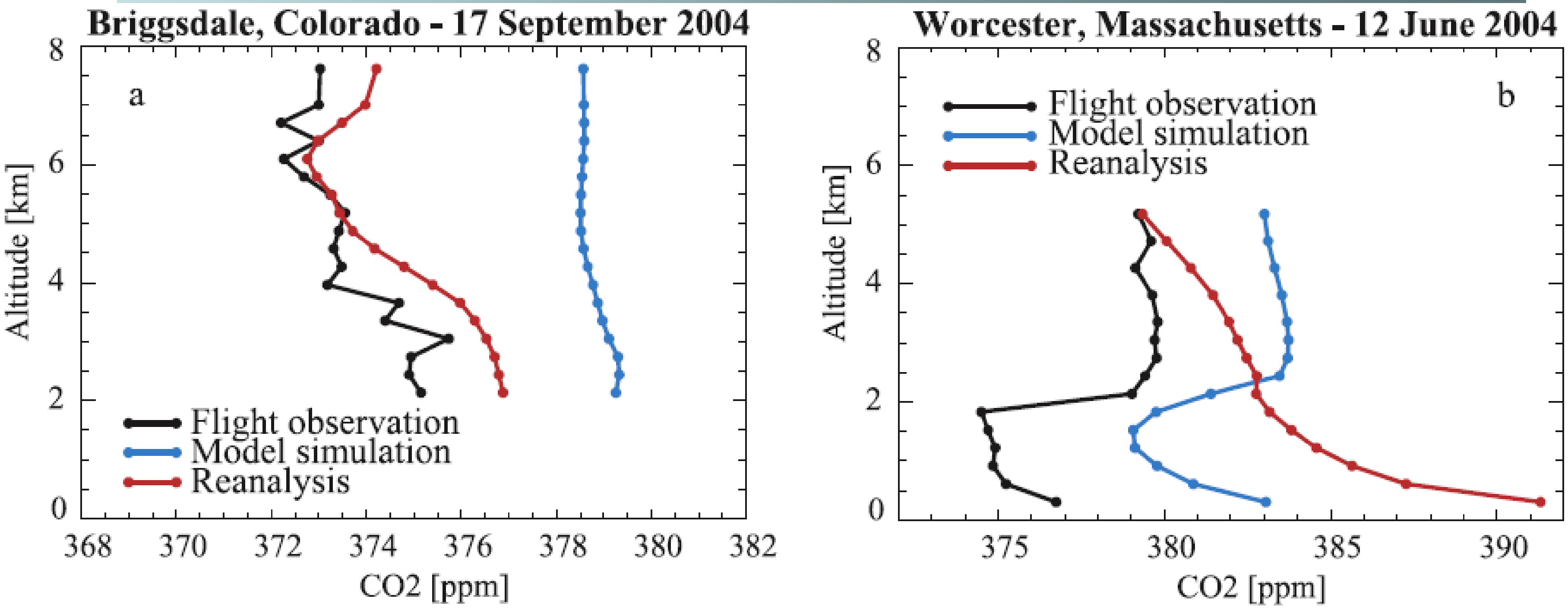


over tropical Africa

over midlatitude Asia.

(Engelen et al., 2009)

Height dependent impact of AIRS sensitivity profiles

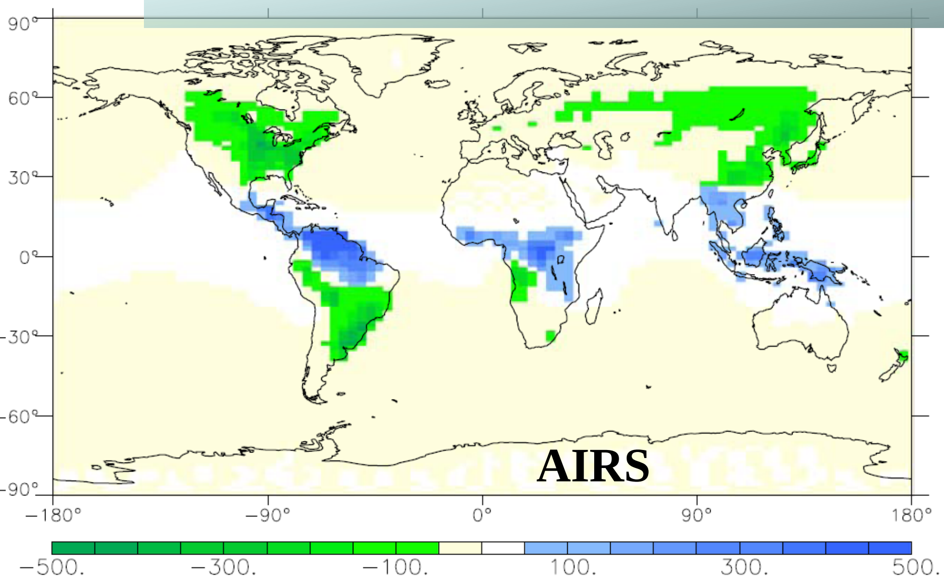


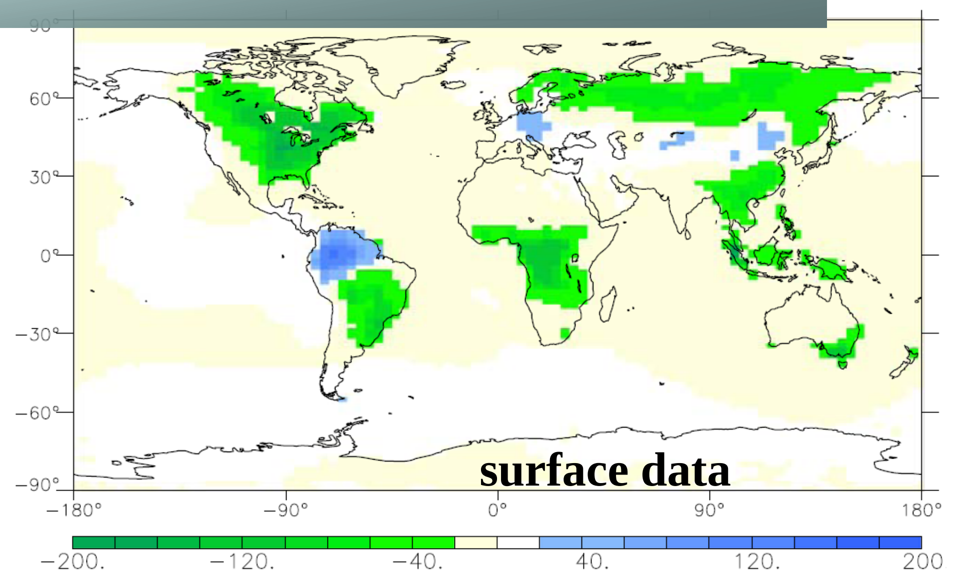
Observed (black), modeled (blue), and reanalyzed (red) profiles of CO2
Flight data were provided by NOAA/ESRL.
(Engelen et al., 2009)

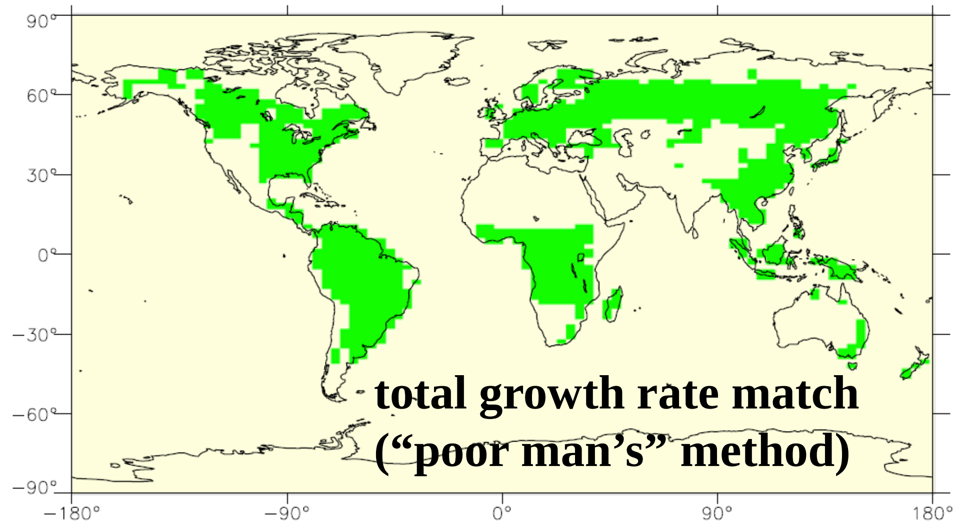
Example 2: Chevallier, F. et al. (2009), AIRS-based versus flask-based estimation of carbon surface fluxes, J. Geophys. Res., 114,

- data: Radiances assimilation from the Atmospheric Infrared Sounder (AIRS)
  - AIRS radiances mainly provides CO2 in the middle and upper troposphere
- model: IFS by ECMWF
  - 125 km resolution, and 60 vertical levels
- method: 4D-var
  - $\mathbf{H}_{LMDZ}(\mathbf{x}_b)$ Jacobian matrix of the transport model of the Laboratoire deMe´te´orologieDynamique (LMDZ) used

Mean flux increments from the three data sources (Chevallier et al., 2009)







Mean flux increment, in gC m^2/year. Positive (blue) values represent increased sources or decreased sinks.

4. Data Assimilation for Reanalyses and Climate Monitoring

Definition **Reanalyses**

- Reanalysis is the assimilation of
  - **long time series** of observations
  - with an **unvarying assimilation system**
  - to produce datasets for **climate variability** studies,
  - (or chemistry-transport, and process studies).

The 1. generation reanalyses

•NCEP/NCAR reanalysis (Kalnay *et al*. 1996),
•European Centre for Medium-Range Weather Forecasts (ECMWF) executed the ERA-15 project (Gibson *et al*. 1997),
•Data Assimilation Office (DAO, now the Global Modeling and Assimilation Office, GMAO): 17-year Goddard Earth Observing System, Version 1 (GEOS-1) reanalysis (Schubert *et al*. 1993).

Reanalysis	Time Period Covered	Horizontal Resolution	Number of Vertical Levels	Assimilation Method	Satellite Data Employed	Primary Sea Ice Determination	Snow Cover
NCEP1	1948–present	T62/ ~209 km	28	3D VAR	retrievals	GISST 1948–1978, SMMR and SSM/I 1979–present	NESDIS
NCEP2	1979–present	T62/ ~209 km	28	3D VAR	retrievals	SMMR and SSM/I	NESDIS
ERA-15	1979–1993	T106/ ~125 km	31	1D VAR	retrievals	SMMR and SSM/I	SYNOP
ERA-40	Sep 1957–Aug 2002	TL159/ ~125 km	60	3D VAR	radiances	HADISST1 1957–1981, then Reynolds OI	SYNOP
JRA-25	1979–2004	T106/ ~125 km	40	3D VAR	radiances	COBE	SSM/I and CPC/NCEP

For sea ice, GISST = Global Sea Ice Cover and Sea Surface Temperature (SST) data; SMMR = Scanning Multichannel Microwave Radiometer; SSM/I =Special Sensor Microwave/Imager;

(from Bromwich et al., 2007)

Lessons learned from 1. gen.: a limited success

- parameters directly constrained by observations agree well across reanalyses
  - temperature ,
  - geopotential → geostrophic winds
- parameters weakly constrained by observations disagree substantially
  - clouds, precipitation, evaporation, surface fluxes,
  - ageostropic winds

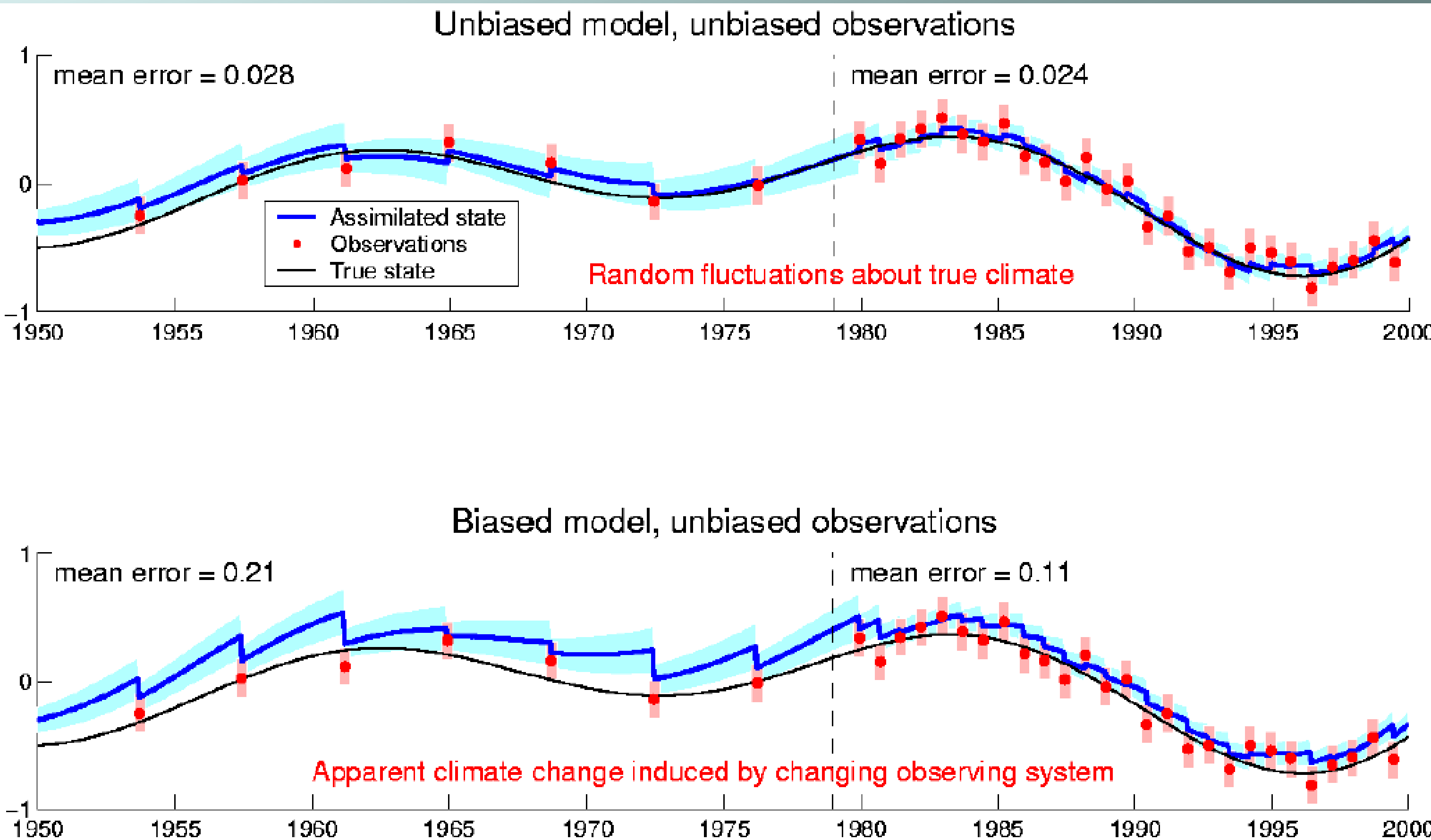
The 2nd generation reanalyses:
better assimilation schemes
better and more satellite retrievals

- incremental evolution of the original NCEP/NCAR reanalysis, Kanamitsu *et al*. (2002)
- ECMWF 40 year reanalysis (Uppala *et al*. 2005)
- JRA-25 Japan Meteorological Agency Onogi *et al*. (2007), emphasis on precipitation,
- NASA Modern Era Retrospective-analysis for Research and Applications (MERRA)
- ECMWF ERA-Interim.

Conceptual problems for reanalyses

- Heterogeneity of the input data stream
- model and data biases
- impact on climate trend determination

The model bias and its treatment



The solid line: known true state of an idealized climate system.

The red dots: observations of the system.

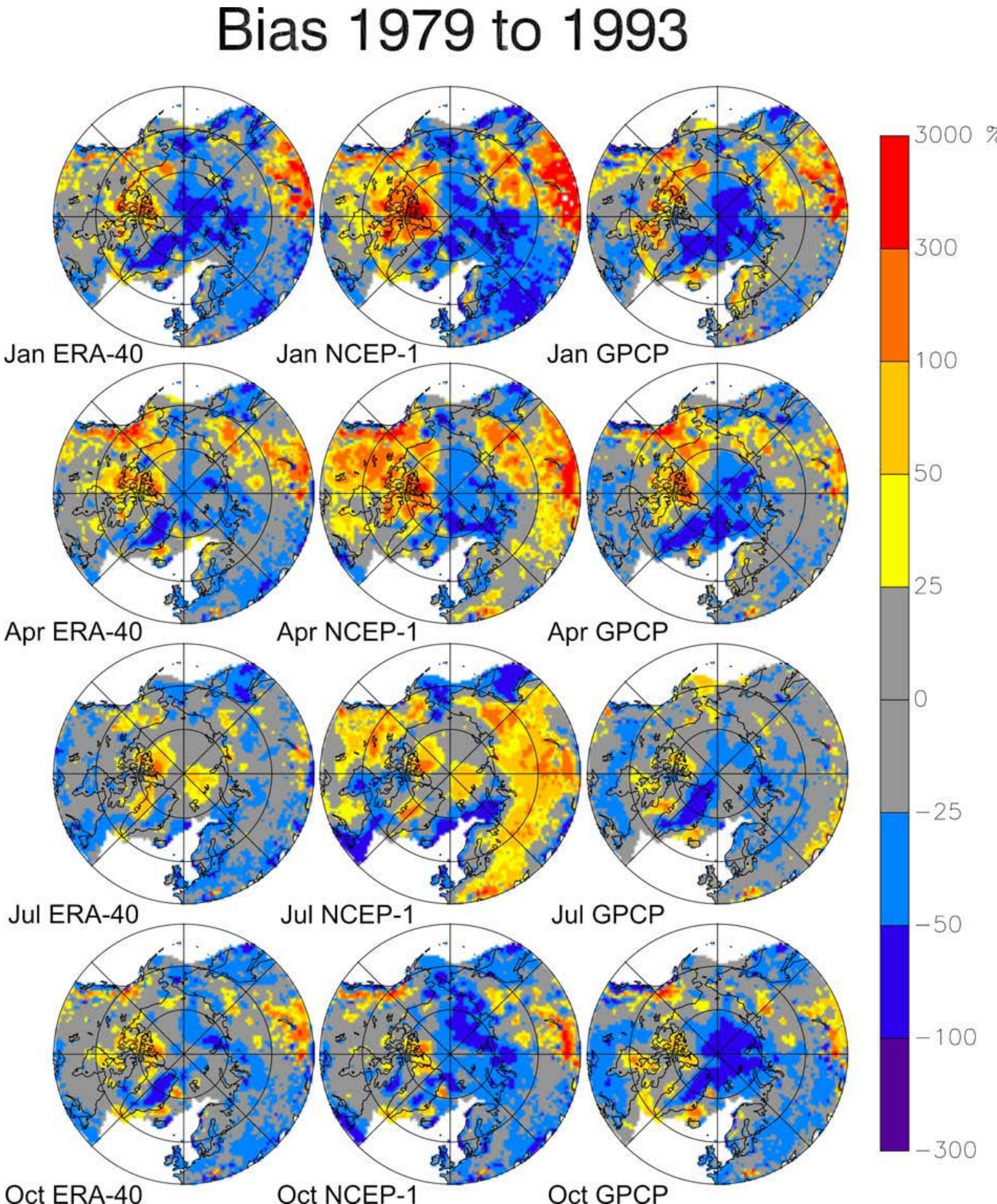
The blue lines: model forecasts of the mean state following assimilation of the observations into the model. (Figure courtesy of D.P. Dee, 2005)

Example application: Grounded Antarctican ice sheet water budget

(Bromwich et al., 2007)

Comparison of the Reanalyses' Trends and 90% Confidence Intervals of Precipitation Minus Evaporation (P E)
Over the Grounded Antarctic Ice Sheet, 1985–2001,
(as by Monaghan et al. [2006])

Reanalysis	Trend, mm yr^{-2}
ERA-40	-0.29 ± 0.62
JRA-25	-0.47 ± 0.88
NCEP2	0.58 ± 0.74



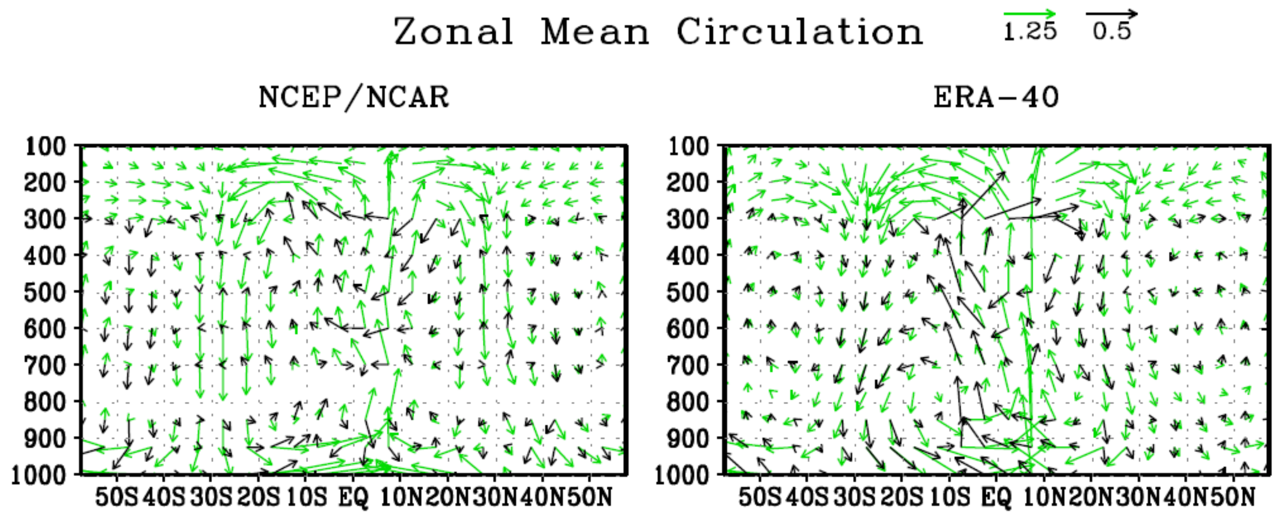
ean bias (1979–1993) of
cumulated precipitation (in %)
mpared against a corrected
dded archive of station observations

ERA-40, NCEP1, and GPCP (NASA Global Precipitation Climatology Project), from Serreze et al. (2005).

Long term trends of

Hadley circulation

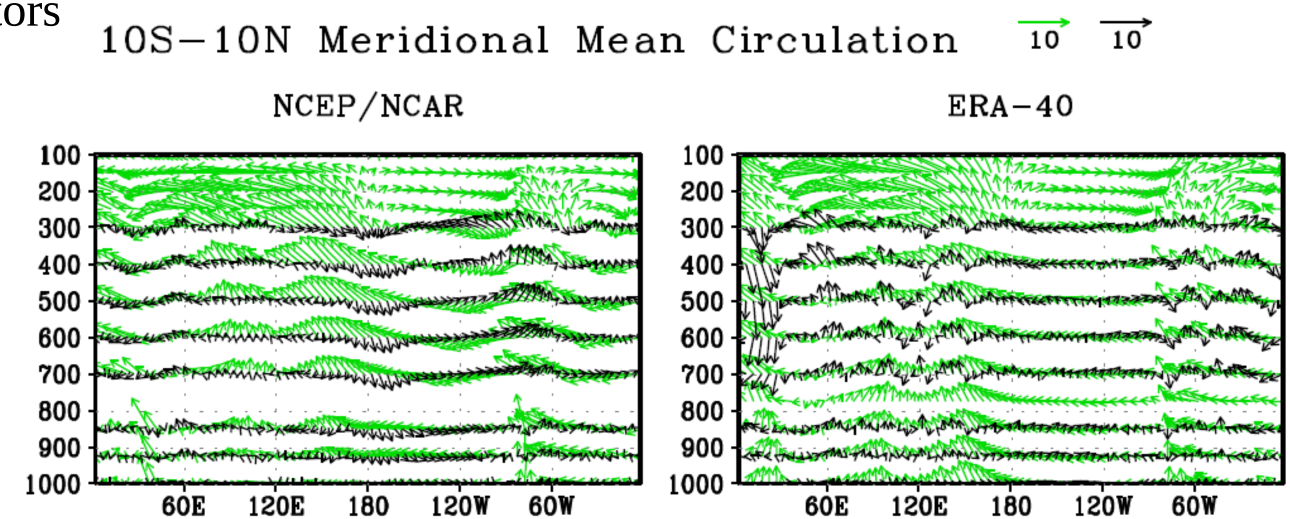
horizontal unit 1(ms-1),
vertical unit –1/60(hPa.s-1).



climatology green vectors
circulation changes black verctors

Walker circulation

horizontal unit 1(ms-1),
vertical unit –1/120(hPa.s-1).



Future challenges for reanalyses:

- physically consistent budgets, especially for
  - hydrological cycles
  - constituent transport
- compliance with conservation laws across data assimilation sequences

4. Detection and attribution problem

Understanding climate change

How can we arrive at a quantitative comprehension?

- Climate models portray effects (***g*** model signal patterns) of climate forcing mechanisms, (say CO2, CO2+aerosols, solar forcing, according to our understanding of mechanisms)
- The differences between model and observations/reanalyses should be small for properly simulated candidate forcings

$$\mathbf{x} - \mathbf{y} \sim N(0, \Sigma_{obs} + \Sigma_M) = N(0, \Sigma), \mathbf{x} \sim N(\mathbf{y}, \Sigma)$$

Detection and attribution

To test the consistency of a detected climate change signal with the signal predicted by a model we need to represent the observed climate change signal in terms of the model signal patterns g_{ν}, $\nu = 1, \ldots, p$

observed climate change signal

amplitude

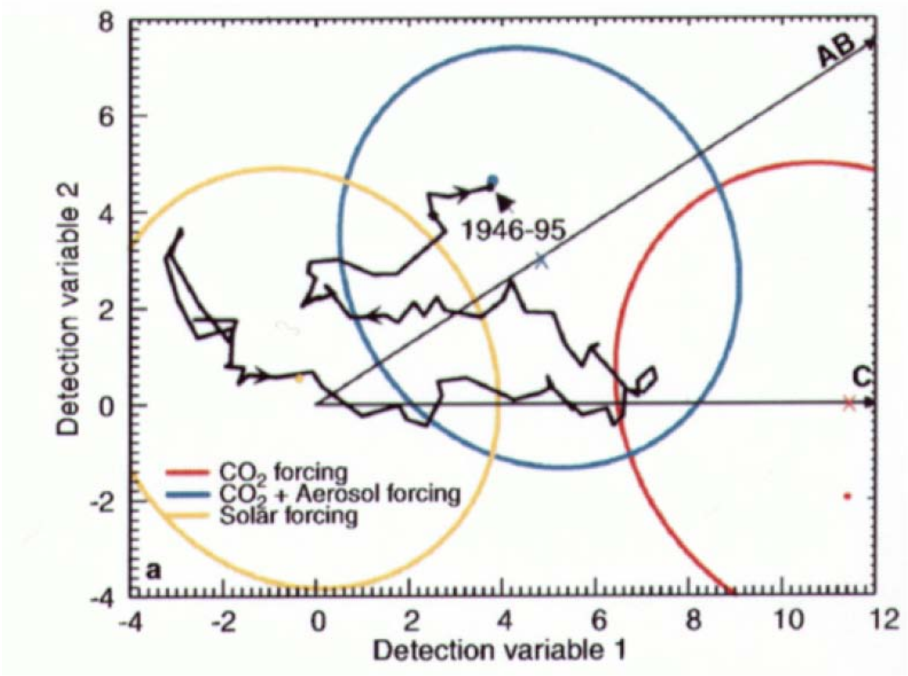
$$\underline{\Psi} = \sum_{\nu=1}^{p} a^{\nu} \underline{g}_{\nu} + \underline{\tilde{\Psi}}_{i}^{r}$$

internal model variability =“residual”, random noise

model signal patterns

Attribution diagram for the observed 50-year northern summer surface temperature trends

Model values for the trend period 1946–1995 indicated by coloured crosses.
90% confidence ellipses for the difference between the observed and predicted detection vectors



(Hegerl et al., 1997)