Satellite data assimilation for Numerical Weather Prediction (NWP)

Sean Healy
European Centre for Medium-range Weather Forecasts (ECMWF)

with contributions from many ECMWF colleagues

Special thanks to: Jean-Noël Thépaut (based on his lecture), Tony McNally, Niels Bormann, Stephen English, Peter Bauer, C. Cardinali …

ECMWF

Outline

1. Introduction to data assimilation for NWP
   - Data assimilation process
   - Observations used
   - Forecast impact of observations
2. Passive atmospheric sounding
   - What do satellite sensors measure?
   - Weighting functions
3. Retrieval algorithms
   - Forward versus inverse problem
   - Solutions to reduced problems
   - Optimal estimation/1DVAR methods with forecast background
4. Direct radiance assimilation and 4DVAR

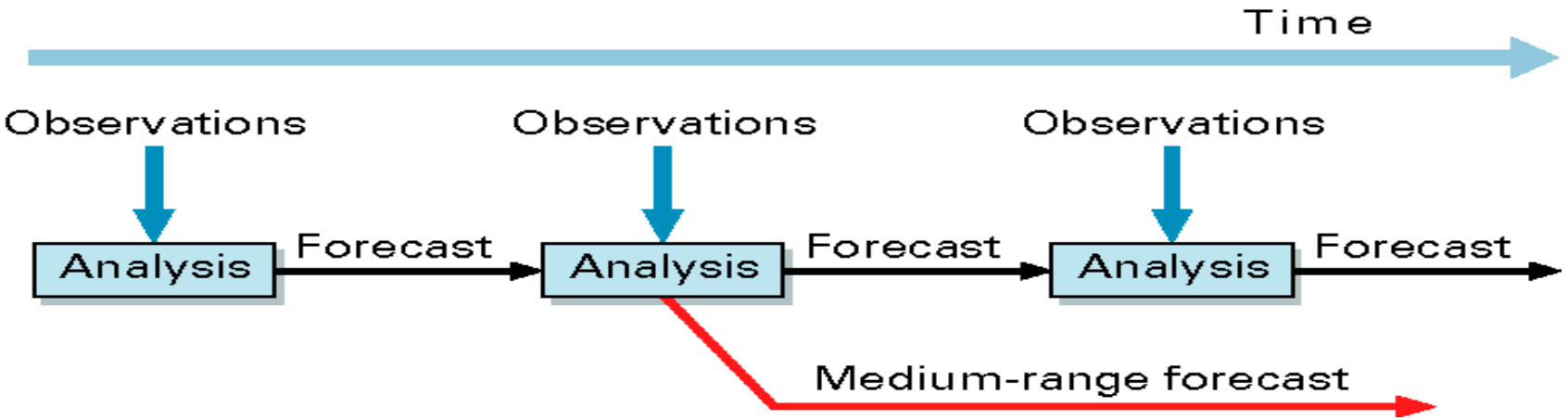
5. Summary

How does NWP use observations?

1.) Introduction to data assimilation for NWP

AIRBUS

Assimilation of measurements in NWP



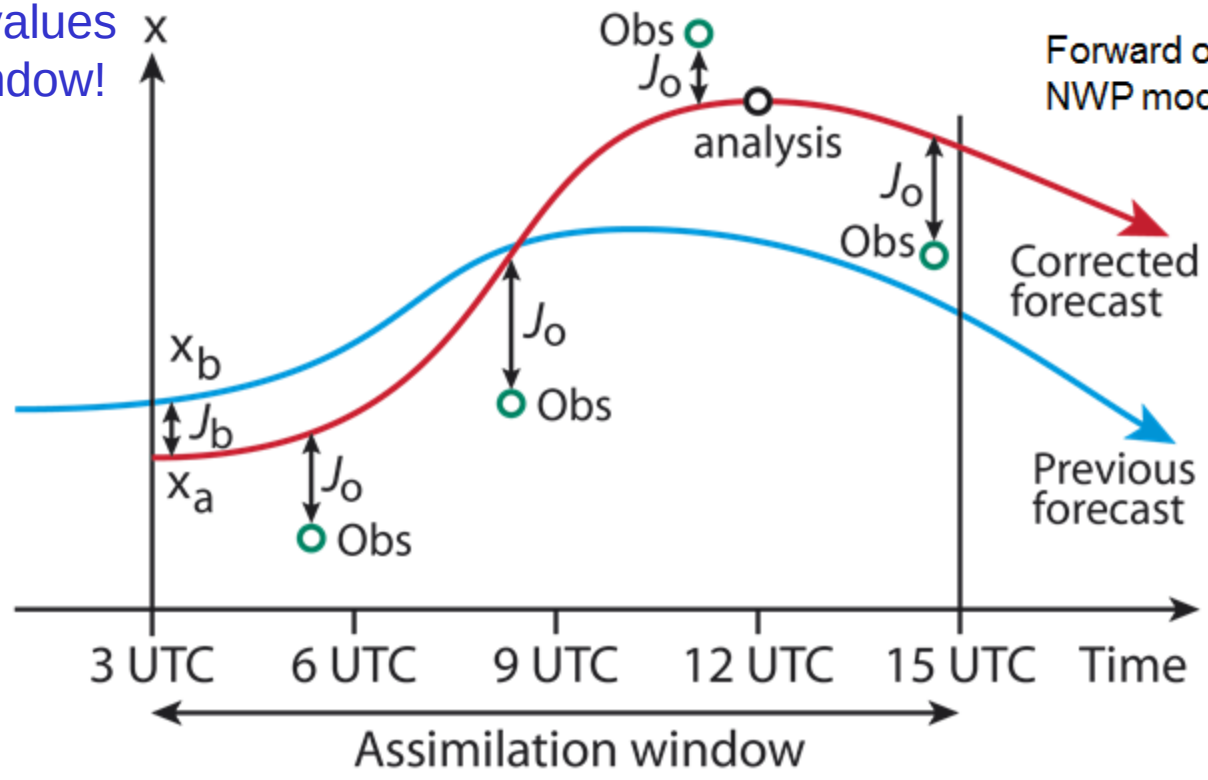
- A cycling data assimilation system.
- A short-range forecast provides us with an 3D estimate of the atmospheric state (P,T, Q, U,V, Ozone).
- We combine the short-range forecast with observations in a statistically optimal way to produce the "**analysis**".
- The analysis provides the initial conditions fore the next forecast.

4D-Var assimilation

Its fancy least squares. Optimal estimation:

$$\mathbf{J(x)} = \left(\mathbf{x} - \mathbf{x_b}\right)^{\mathbf{T}} \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x_b}) + (\mathbf{y_m} - \mathbf{H(x)})^{\mathbf{T}} \mathbf{R}^{-1}(\mathbf{y_m} - \mathbf{H(x)})$$

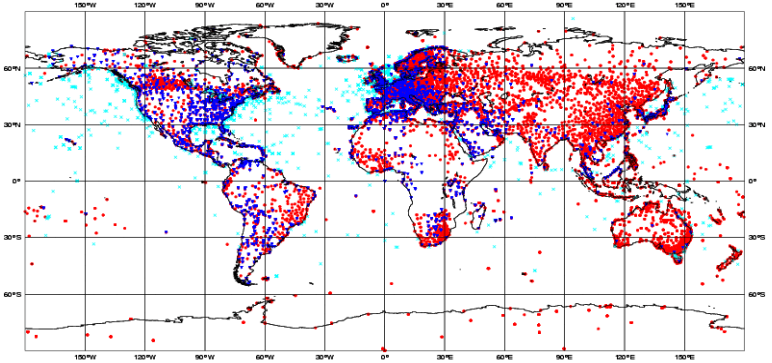
Fit ~10 million values in a 12 hour window!



Example of conventional data coverage

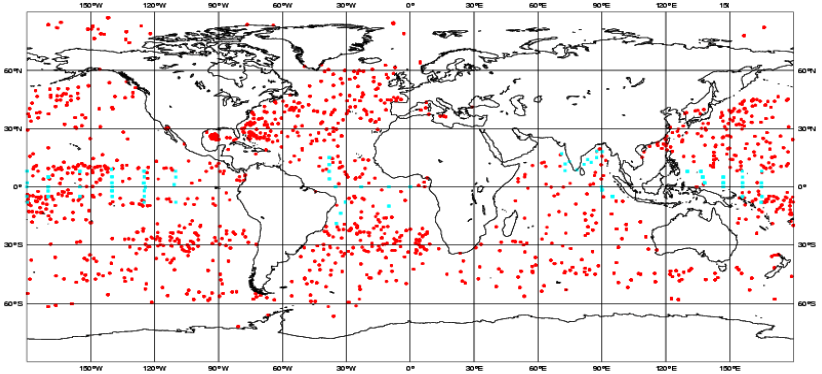
SYNOP/SHIP observations

Total number of obs = 29131



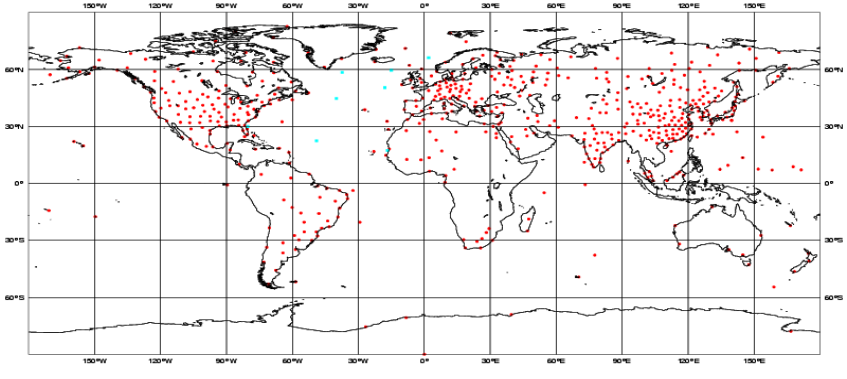
BUOYS

Total number of obs = 5413



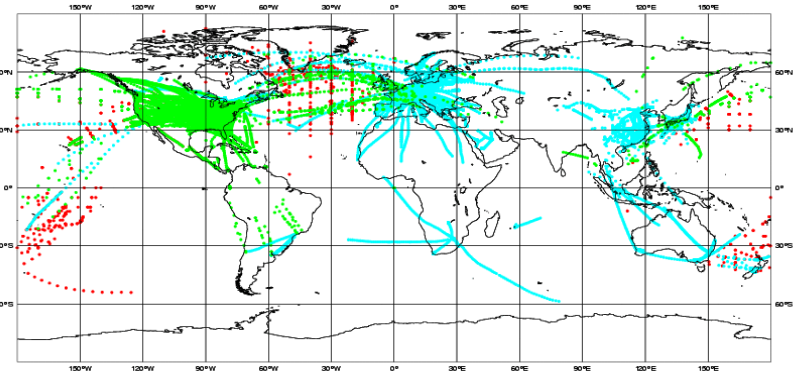
Radiosondes

Total number of obs = 589

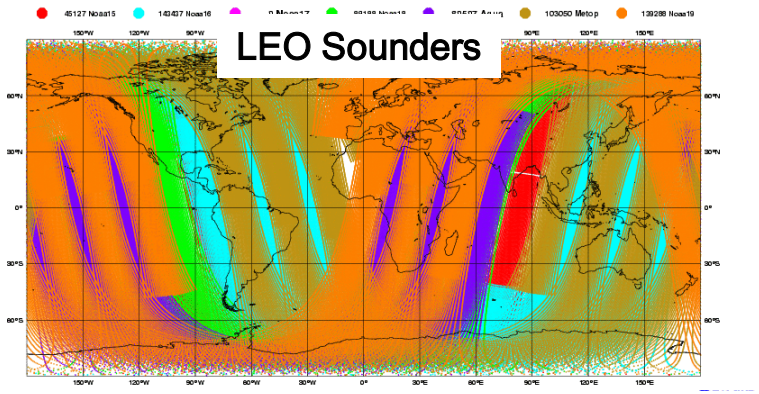


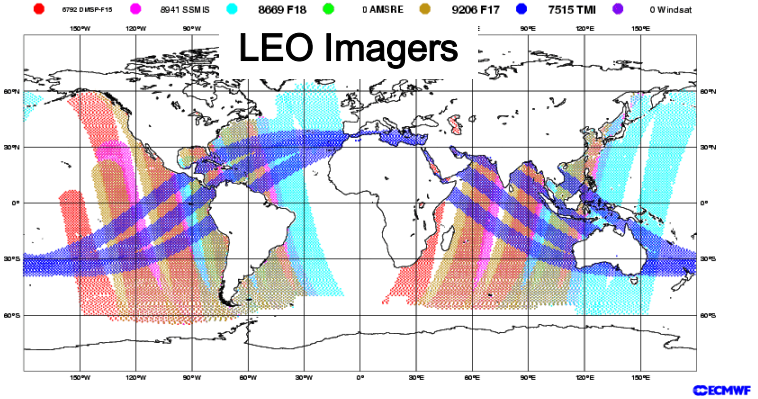
Aircraft data

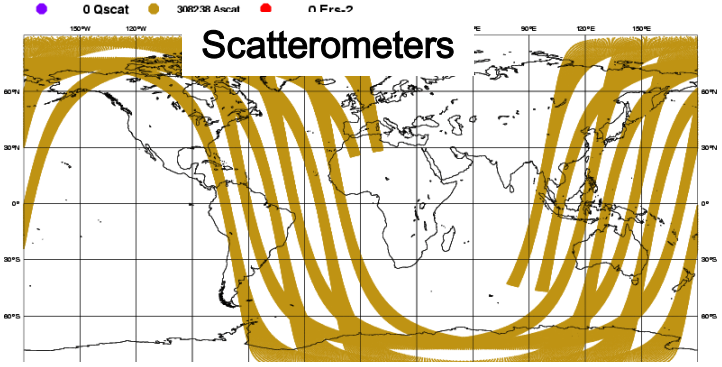
Total number of obs = 40926

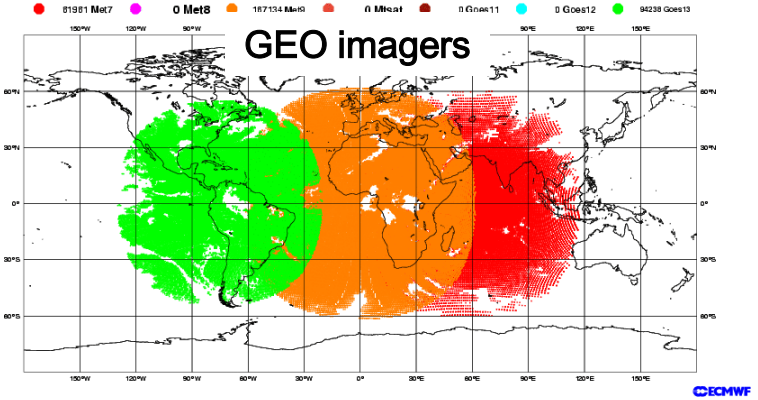


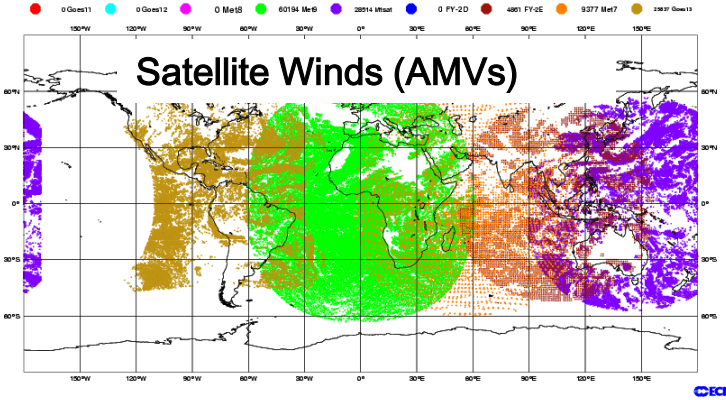
Example of 6-hourly satellite data coverage

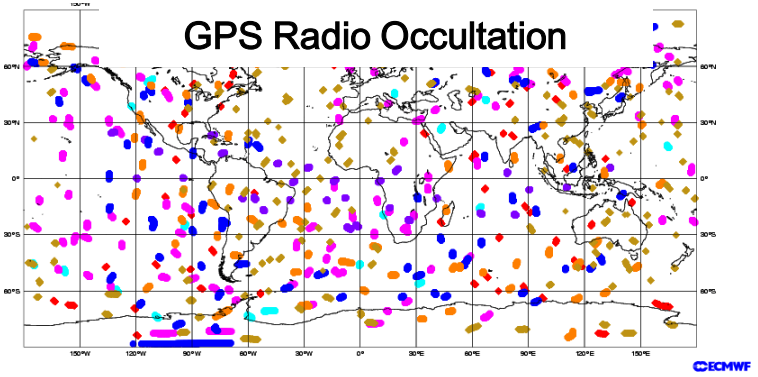


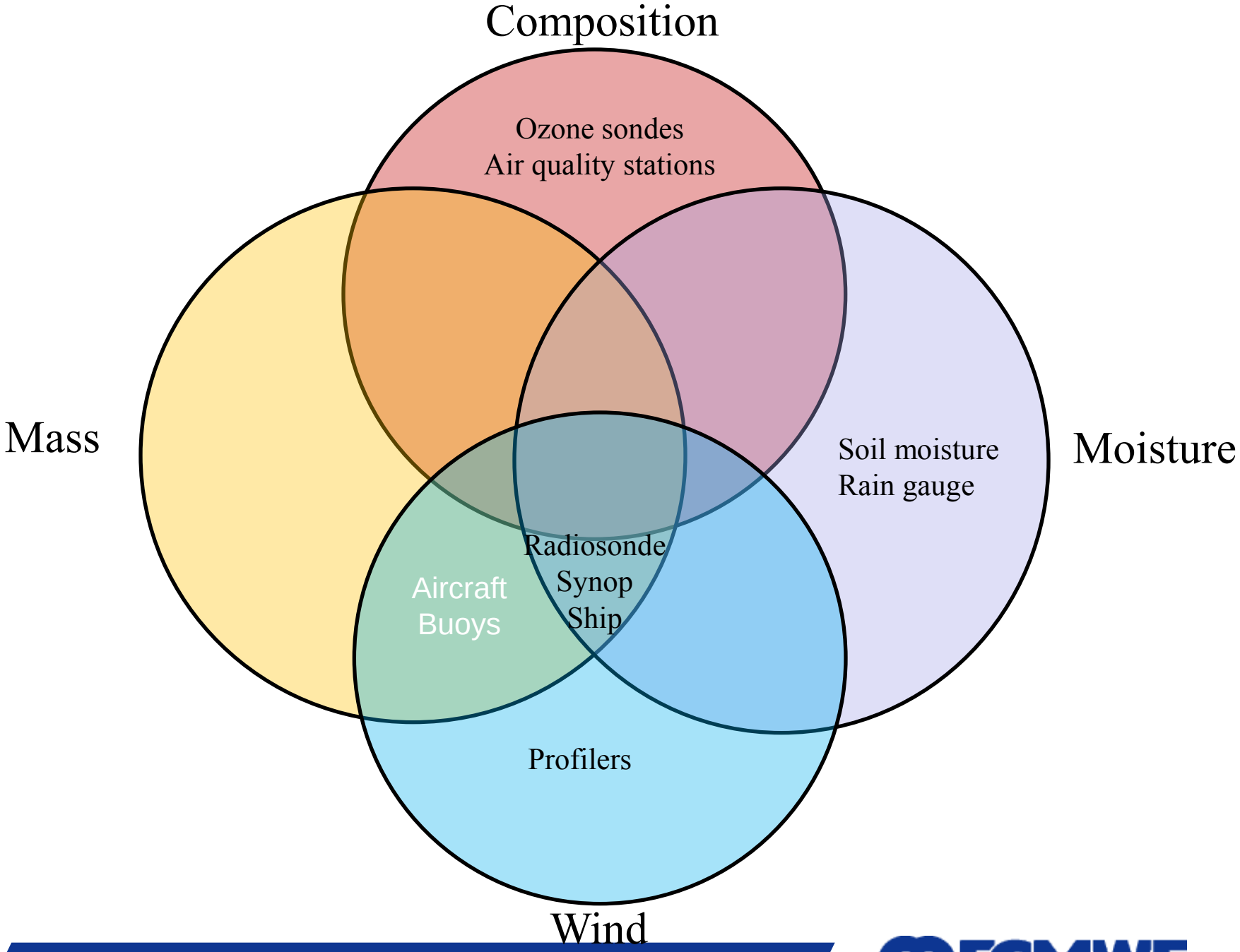


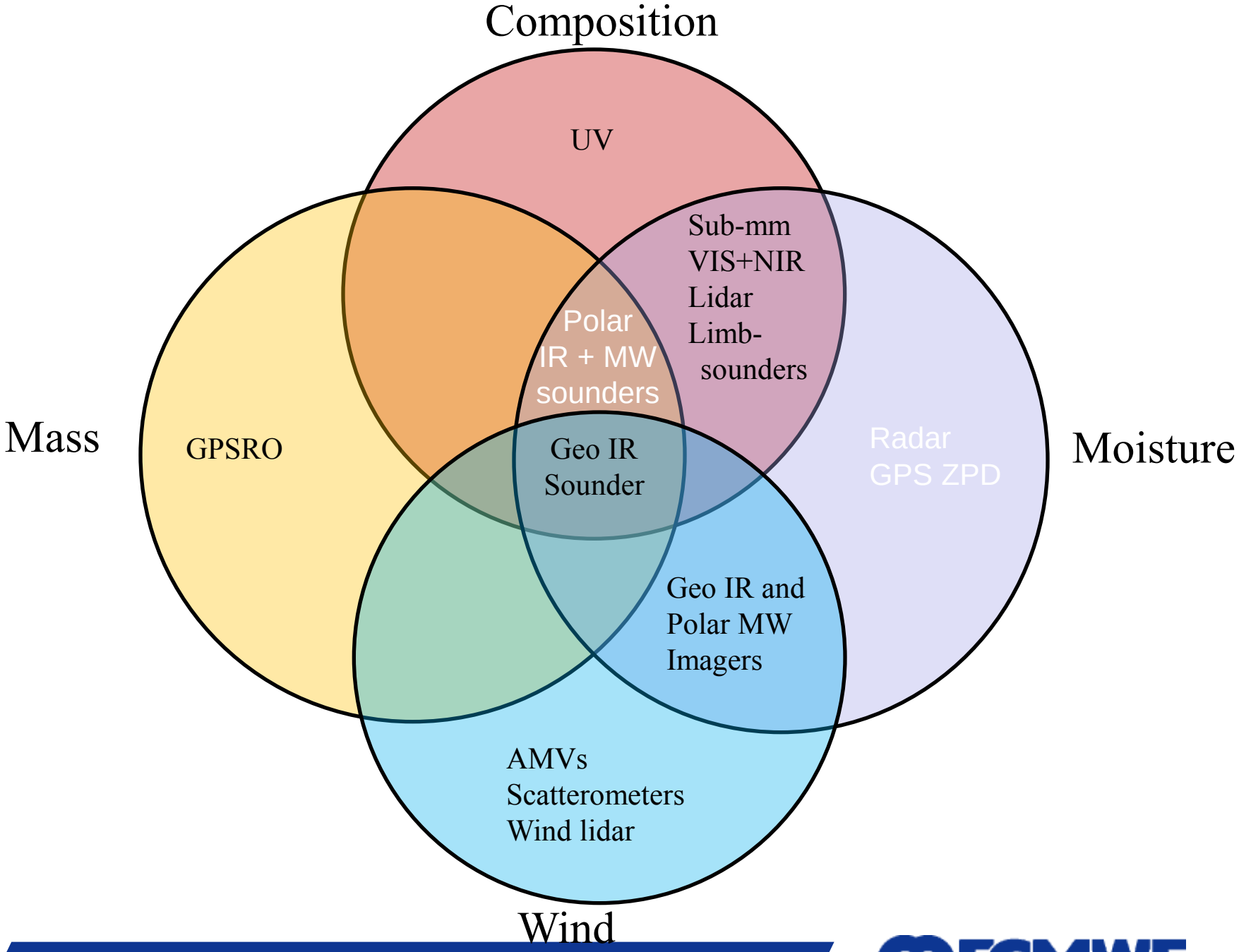


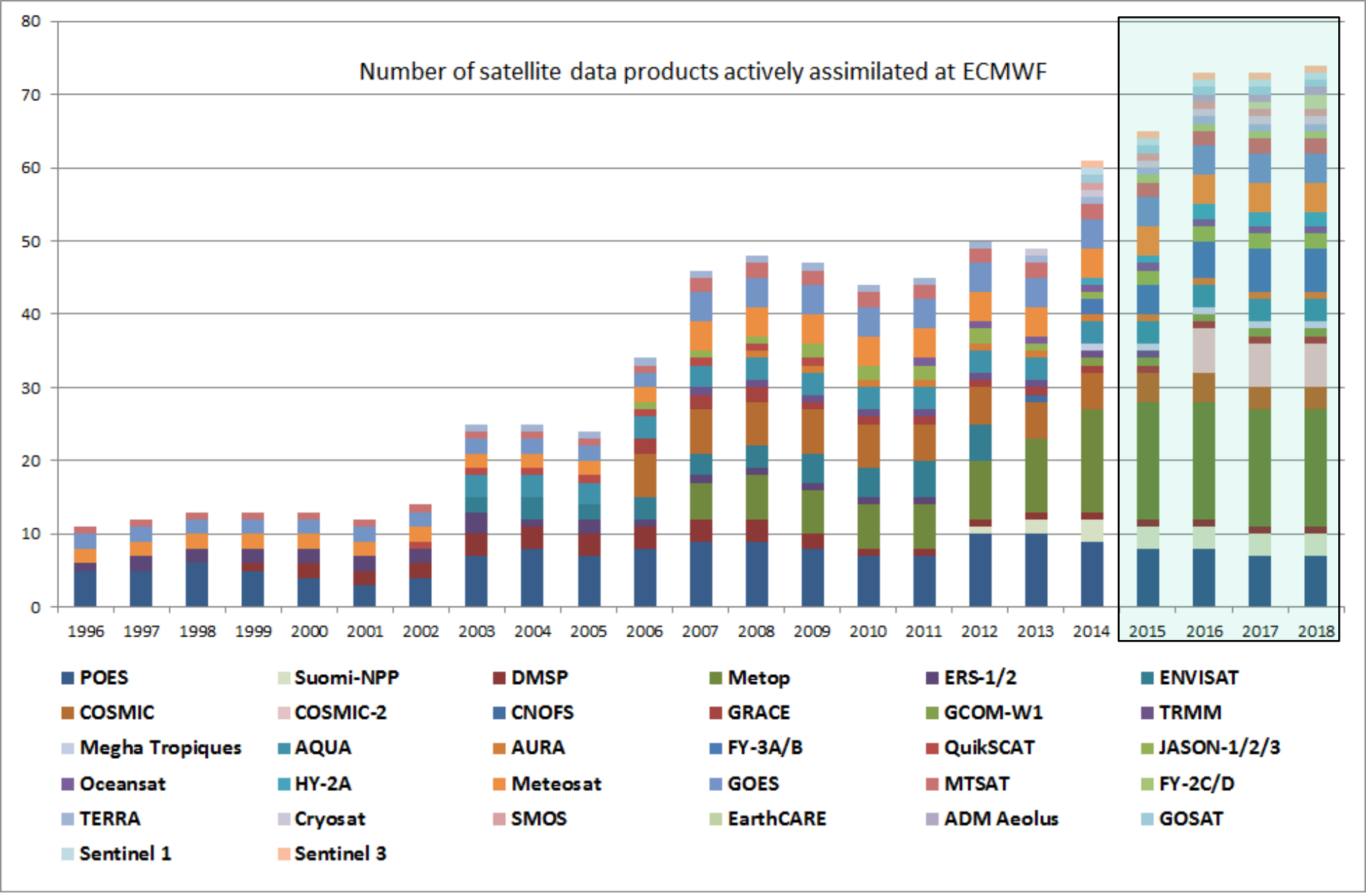


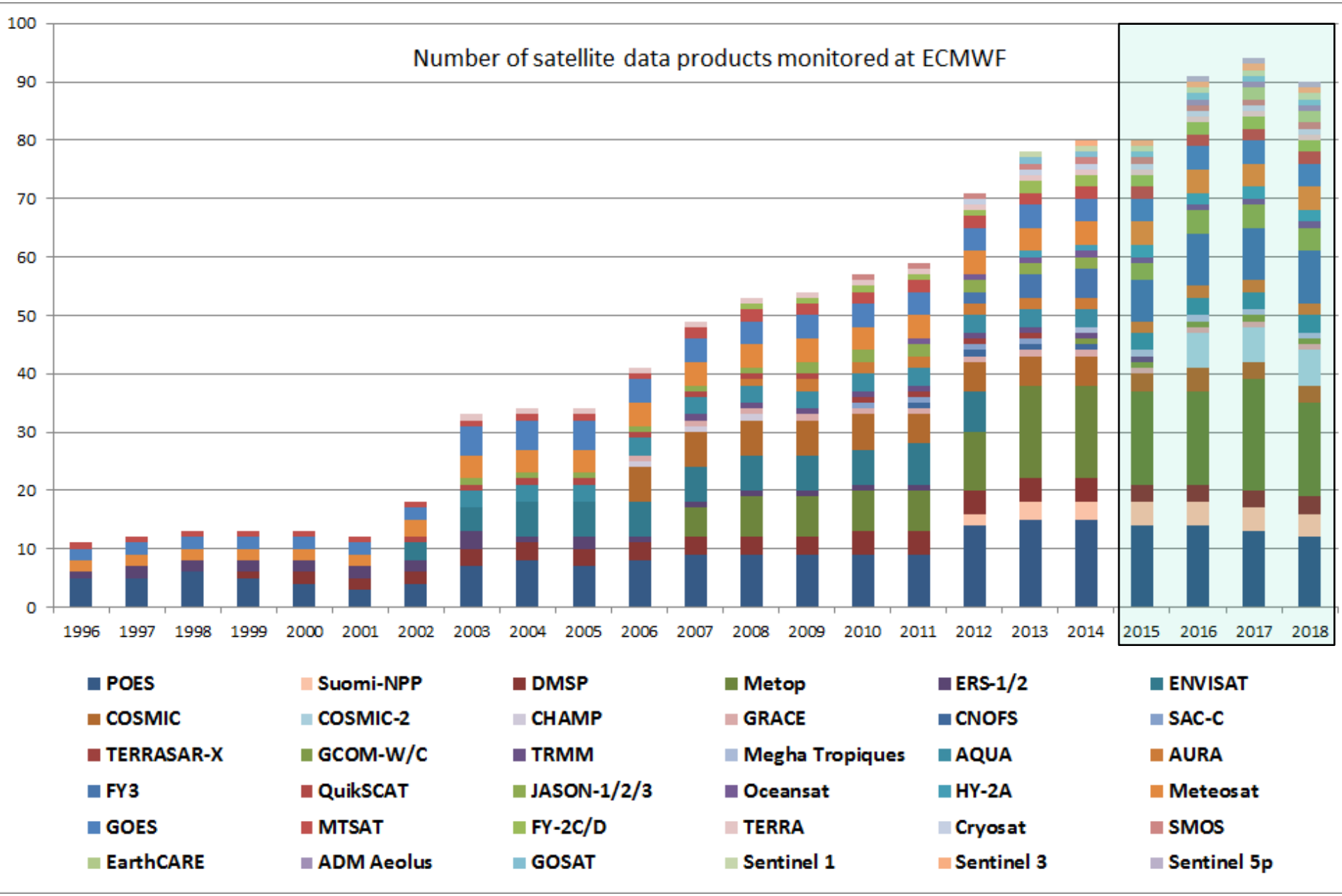




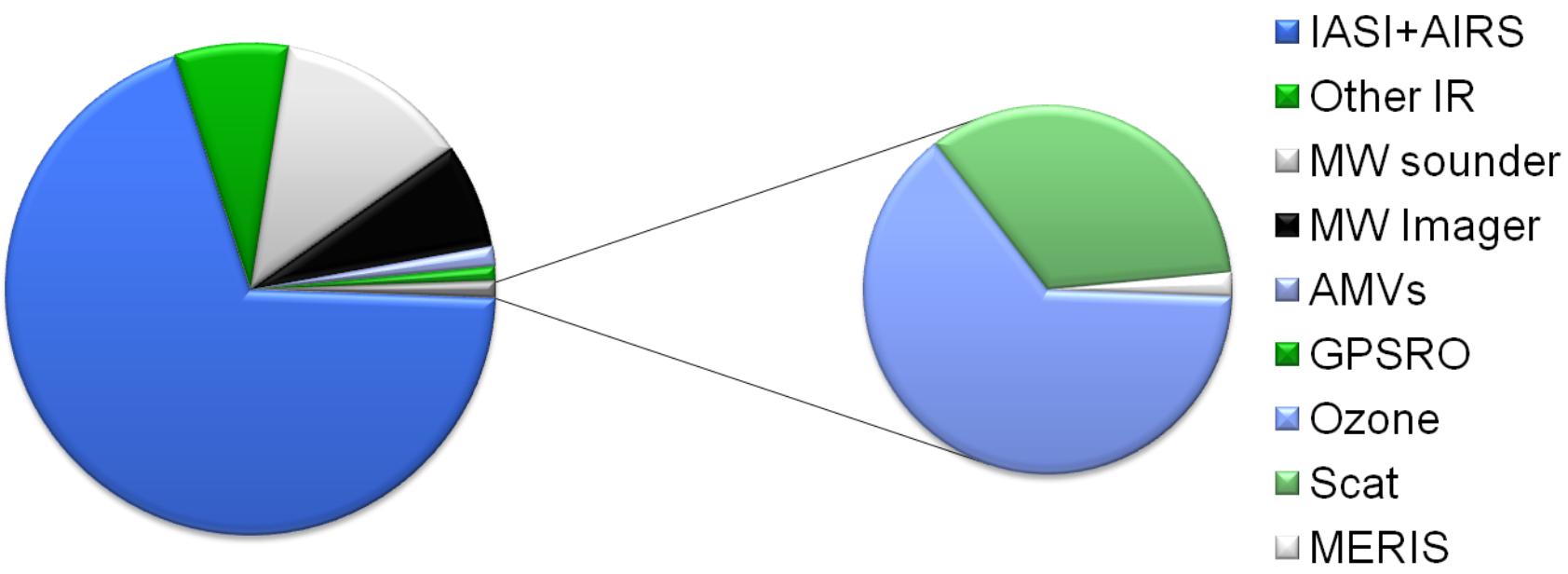

Composition
Ozone sondes
Air quality stations
Mass
Moisture
Soil moisture
Rain gauge
Radiosonde
Synop
Ship
Aircraft
Buoys
Profilers
Wind

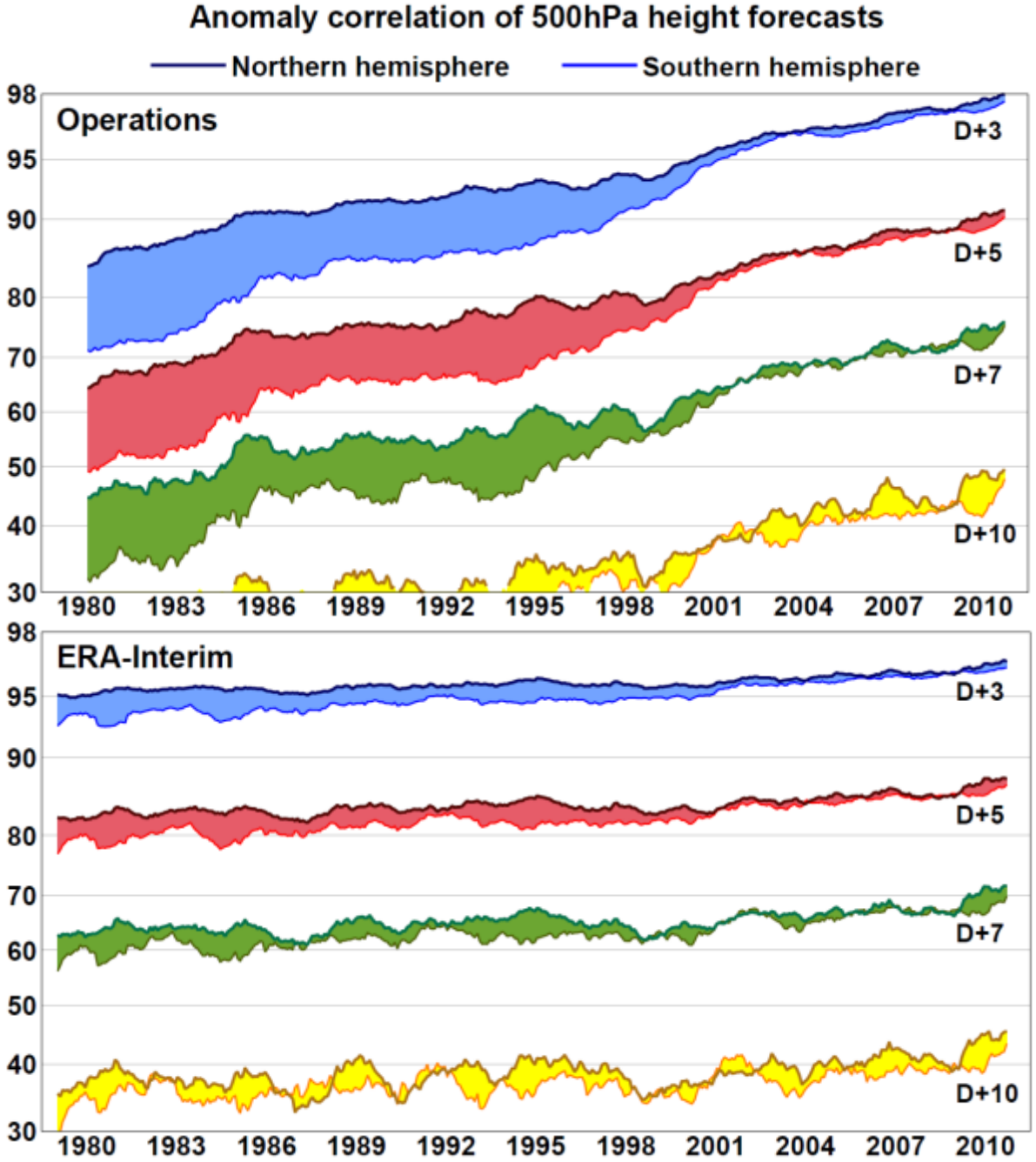

Composition
UV
Sub-mm
VIS+NIR
Lidar
Limb-
sounders
Polar
IR + MW
sounders
Mass
GPSRO
Geo IR
Sounder
Radar
GPS ZPD
Moisture
Geo IR and
Polar MW
Imagers
AMVs
Scatterometers
Wind lidar
Wind


Number of satellite data products actively assimilated at ECMWF
80
70
60
50
40
30
20
10
0
1996
1997
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018
POES
Suomi-NPP
DMSP
Metop
ERS-1/2
ENVISAT
COSMIC
COSMIC-2
CNOFS
GRACE
GCOM-W1
TRMM
Megha Tropiques
AQUA
AURA
FY-3A/B
QuikSCAT
JASON-1/2/3
Oceansat
HY-2A
Meteosat
GOES
MTSAT
FY-2C/D
TERRA
Cryosat
SMOS
EarthCARE
ADM Aeolus
GOSAT
Sentinel 1
Sentinel 3

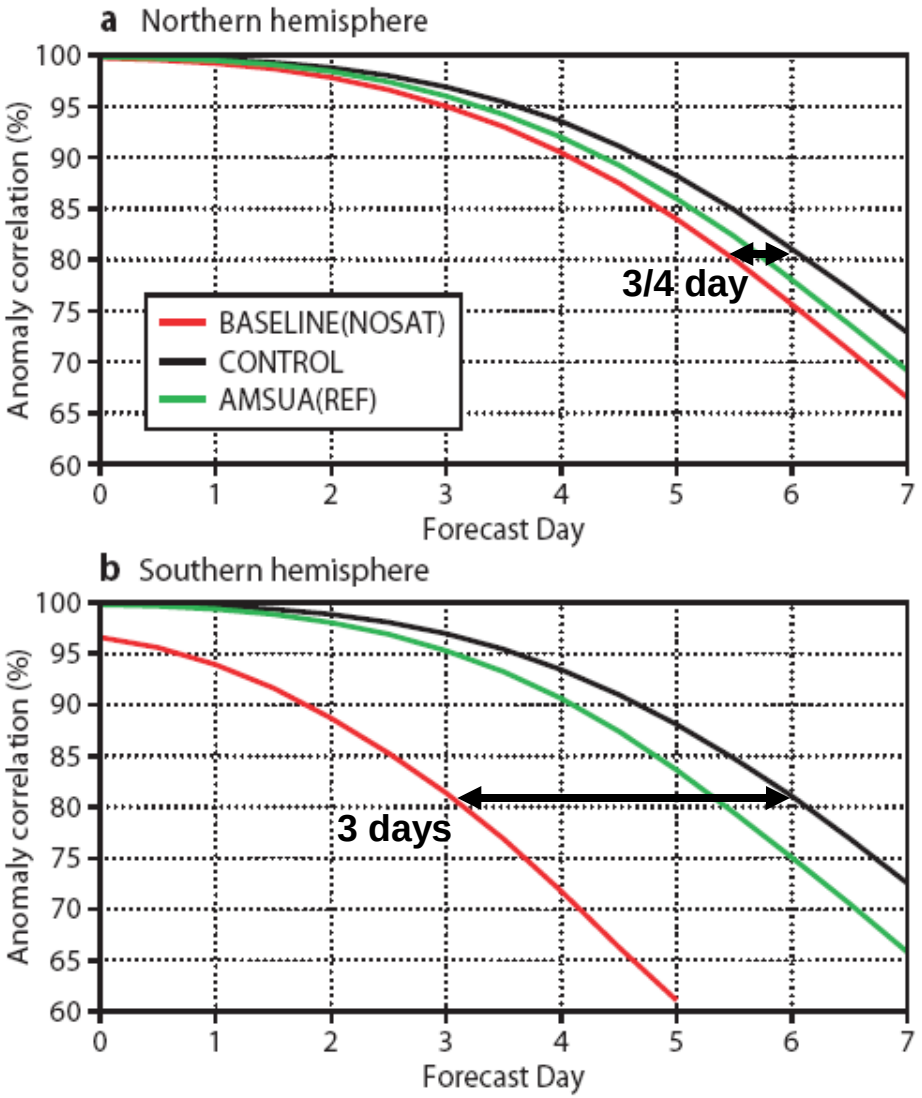

Number of satellite data products monitored at ECMWF
100
90
80
70
60
50
40
30
20
10
0
1996
1997
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018
POES
Suomi-NPP
DMSP
Metop
ERS-1/2
ENVISAT
COSMIC
COSMIC-2
CHAMP
GRACE
CNOFS
SAC-C
TERRASAR-X
GCOM-W/C
TRMM
Megha Tropiques
AQUA
AURA
FY3
QuikSCAT
JASON-1/2/3
Oceansat
HY-2A
Meteosat
GOES
MTSAT
FY-2C/D
TERRA
Cryosat
SMOS
EarthCARE
ADM Aeolus
GOSAT
Sentinel 1
Sentinel 3
Sentinel 5p

Number of observations (1000s)




Anomaly correlation of 500hPa height forecasts
Northern hemisphere
Southern hemisphere
Operations
D+3
D+5
D+7
D+10
ERA-Interim
D+3
D+5
D+7
D+10
98
95
90
80
70
60
50
40
30
1980
1983
1986
1989
1992
1995
1998
2001
2004
2007
2010

Combined impact of all satellite data

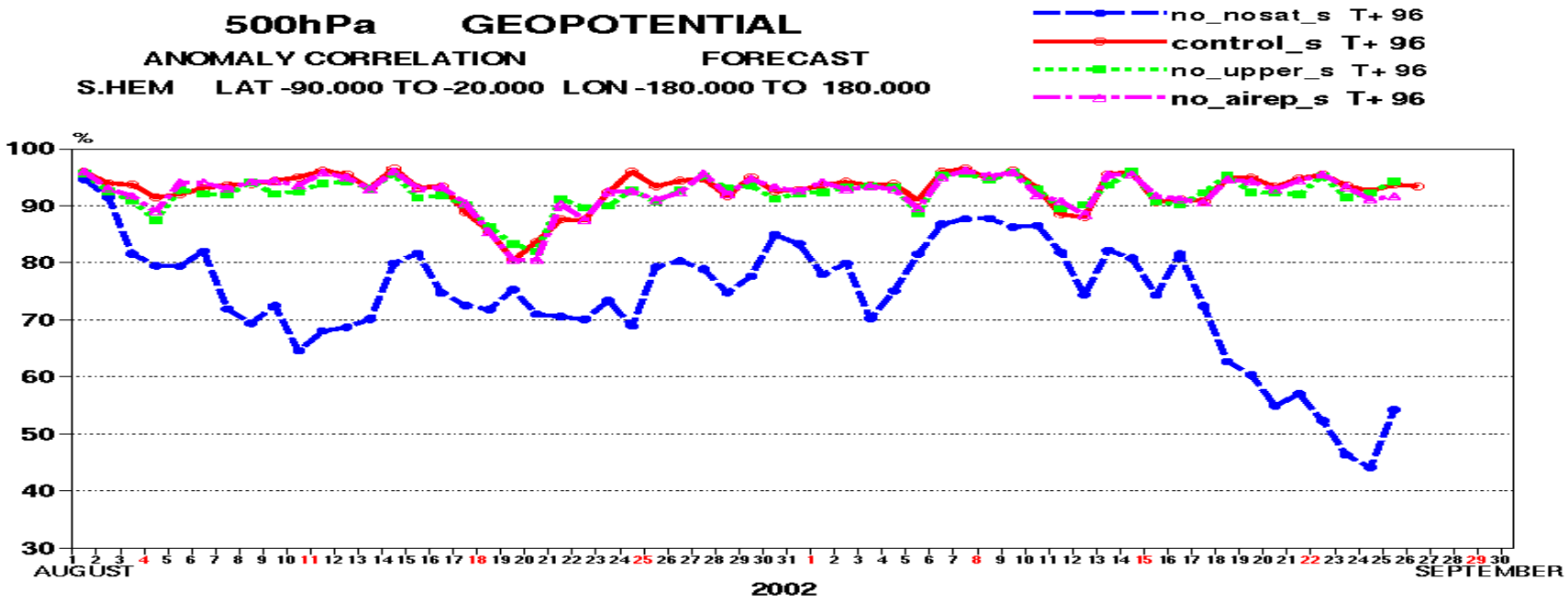


EUCOS Observing System Experiments (OSEs):

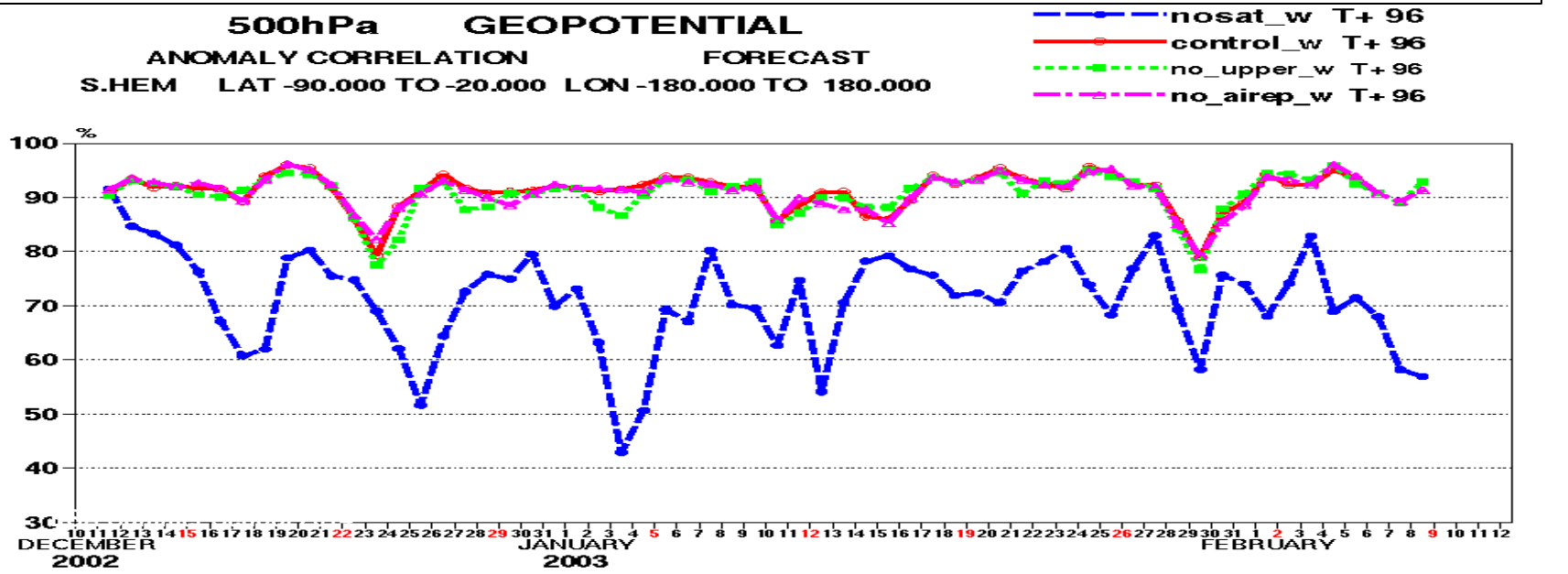
- 2007 ECMWF forecasting system,
- winter & summer season,
- different baseline systems:
  - no satellite data (NOSAT),
  - NOSAT + AMVs,
  - NOSAT + 1 AMSU-A,
- general impact of satellites,
- impact of individual systems,
- all conventional observations.

← 500 hPa *geopotential height* anomaly correlation

ECMWF

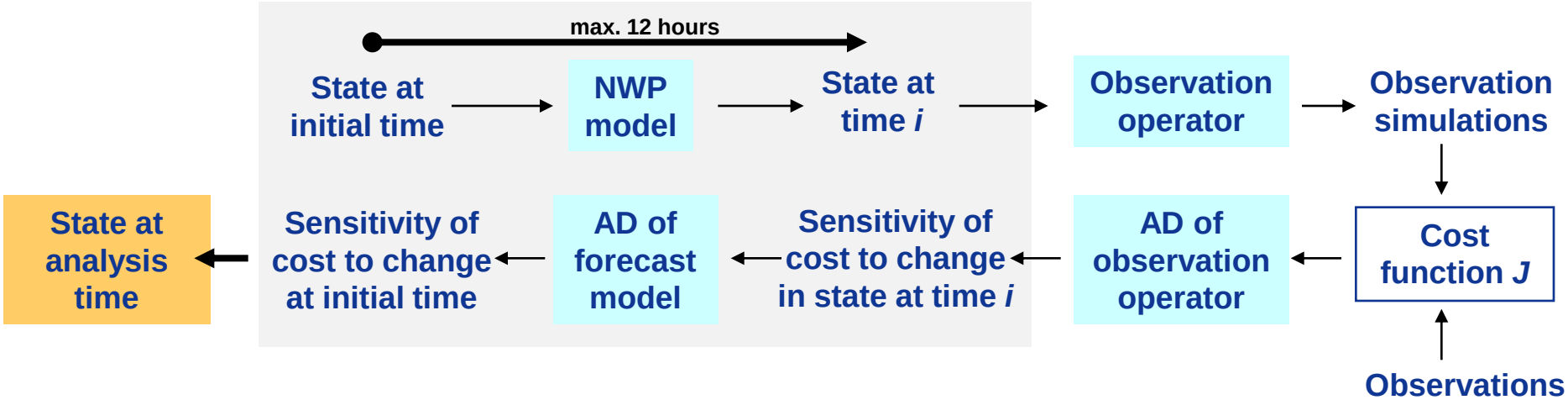


Satellite data provide robustness to the global numerical forecasts

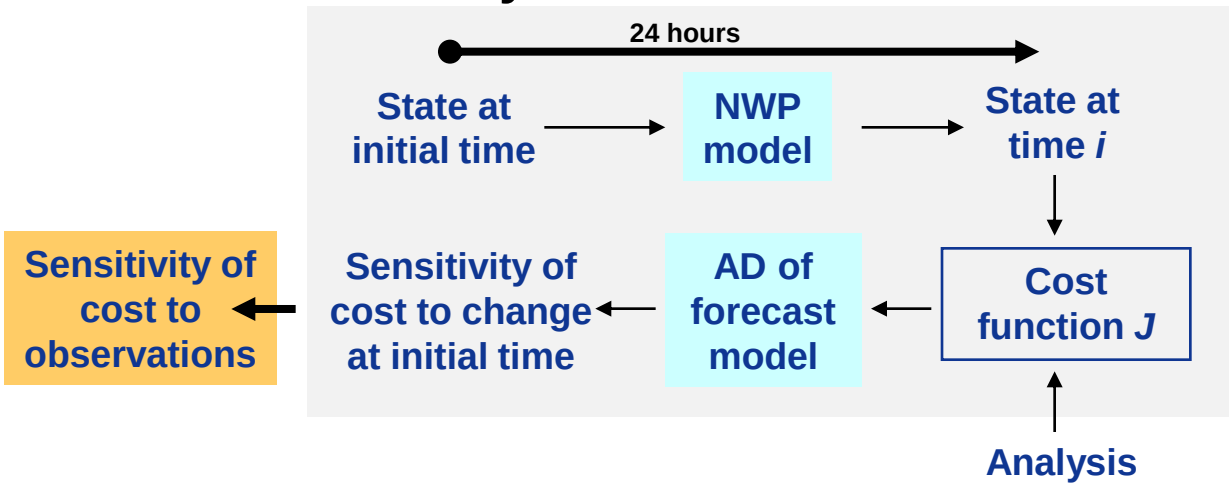


Advanced diagnostics

Data assimilation:



Forecast sensitivity:

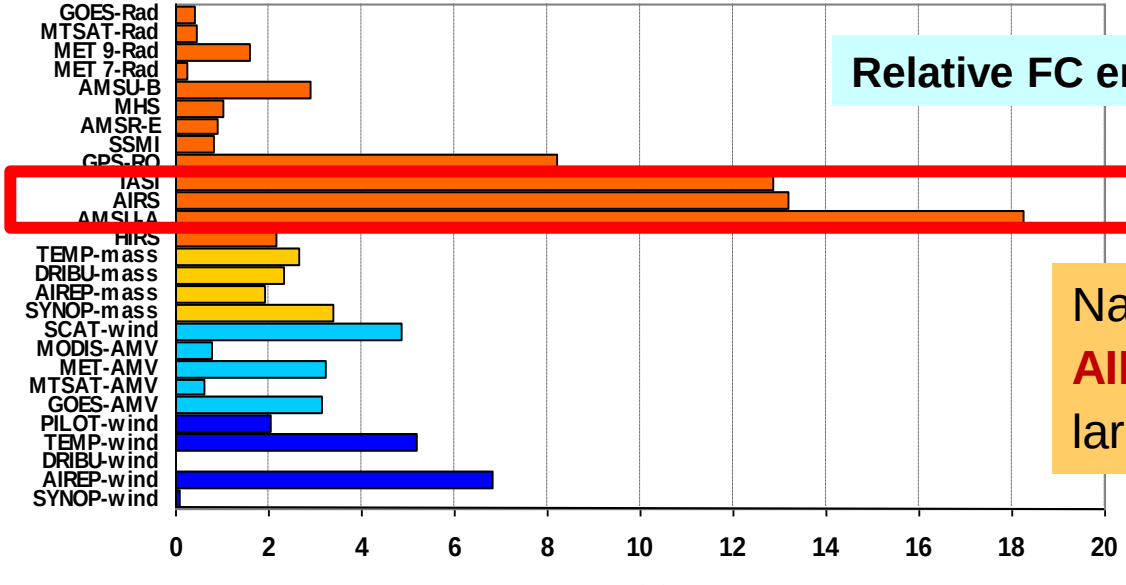


Adjoints come up when minimizing functions

Take the derivative of the model $\frac{\partial \mathbf{M}}{\partial \mathbf{x}}$ to get a matrix and then transpose it. $\left(\frac{\partial \mathbf{M}}{\partial \mathbf{x}}\right)^{\mathbf{T}}$.

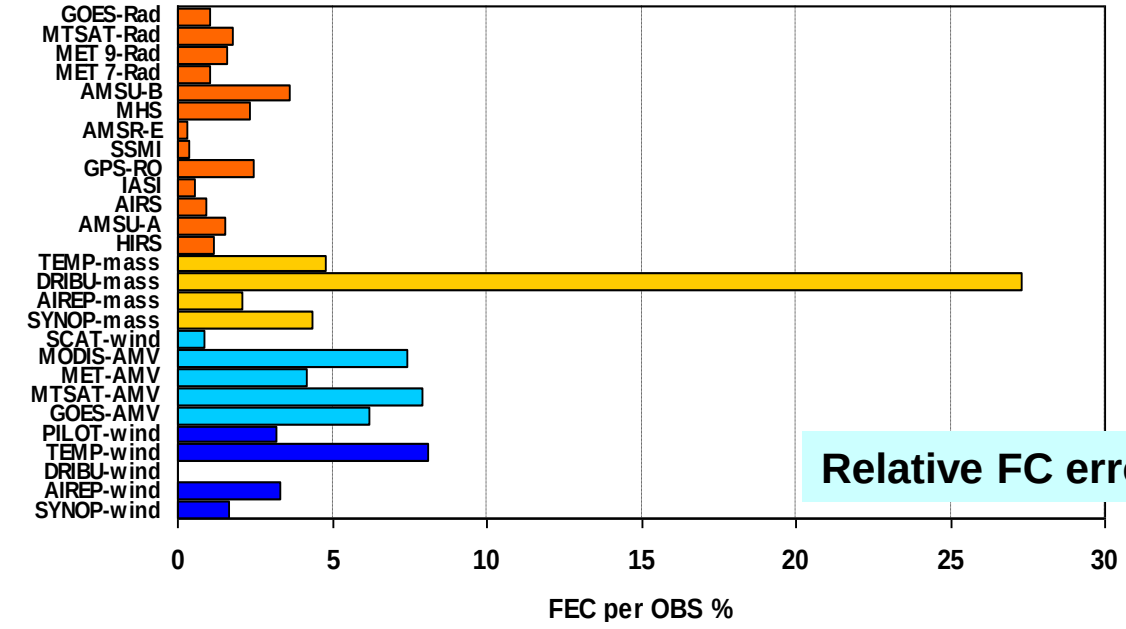
ECMWF

Advanced diagnostics



Relative FC error reduction per system

Nadir sounders **AMSU-A, AIRS, and IASI** provide largest impact



Relative FC error reduction per observation

(From C. Cardinali)

How do passive nadir sounders measure the atmosphere?

2.) Passive atmospheric sounding

What do satellite instruments measure?

They DO NOT measure TEMPERATURE.
They DO NOT measure HUMIDITY or OZONE.
They DO NOT measure WIND.

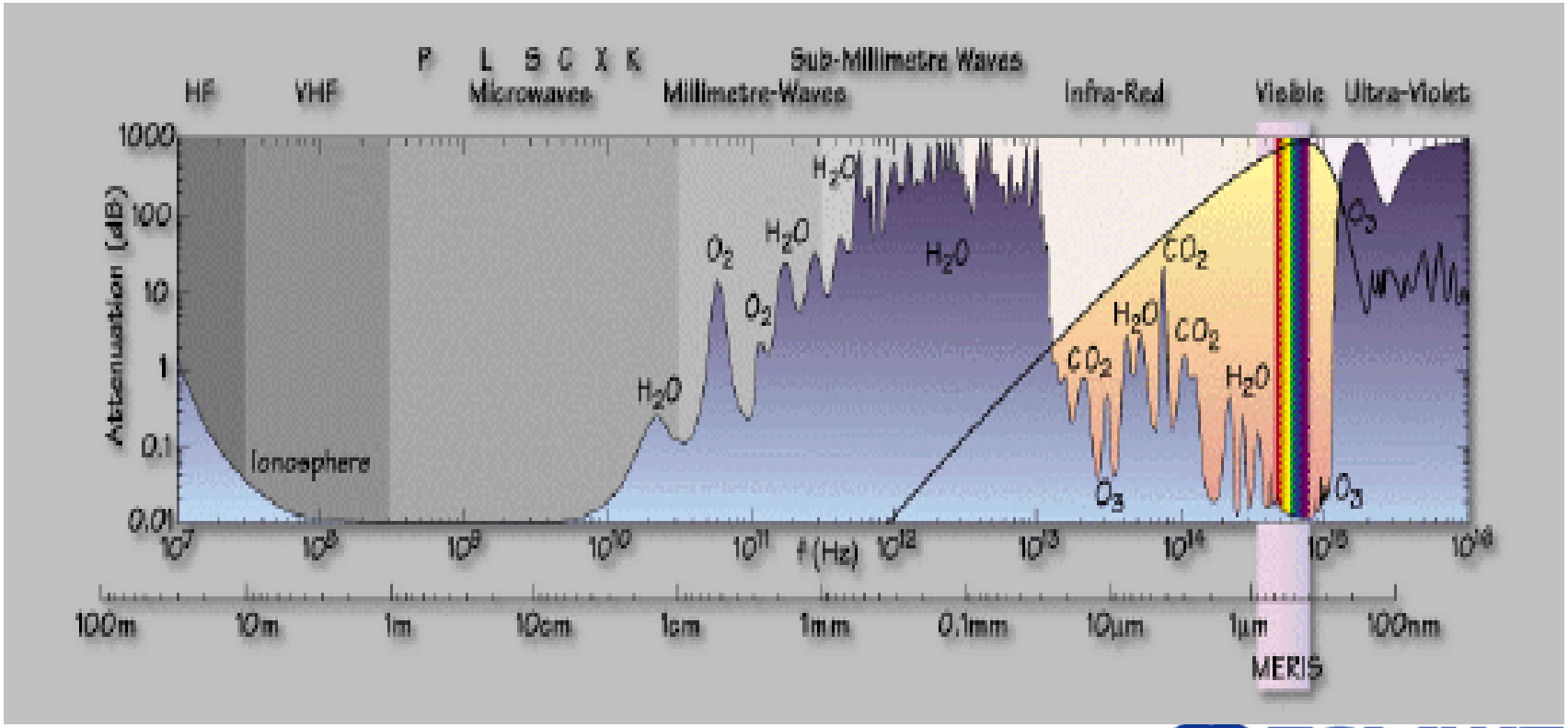
You might retrieve information about these quantities, but you don't measure them directly!

- Satellite instruments measure the radiance *L* that reaches the top of the atmosphere at a given frequency ν .
- The measured radiance is related to geophysical atmospheric variables (T,Q,O_3, clouds etc…) by the radiative transfer equation.

$$L(\nu) = \int_0^{\infty} B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz + \text{Surface emission} + \text{Surface reflection/ scattering} + \text{Cloud/rain contribution} + \ldots$$

Atmospheric spectrum

- Depending on the wavelength, the radiation at the top of the atmosphere is sensitive to different atmospheric constituents



ECMWF

Frequency selection

By selecting radiation at different frequencies or **CHANNELS** a satellite instrument can provide information on a range of geophysical variables.

In general, the channels currently used for NWP applications may be considered as one of two different types:

- Atmospheric sounding channels
- Surface sensing channels

In practice real satellite instruments have a combination of both atmospheric sounding and surface sensing channels.

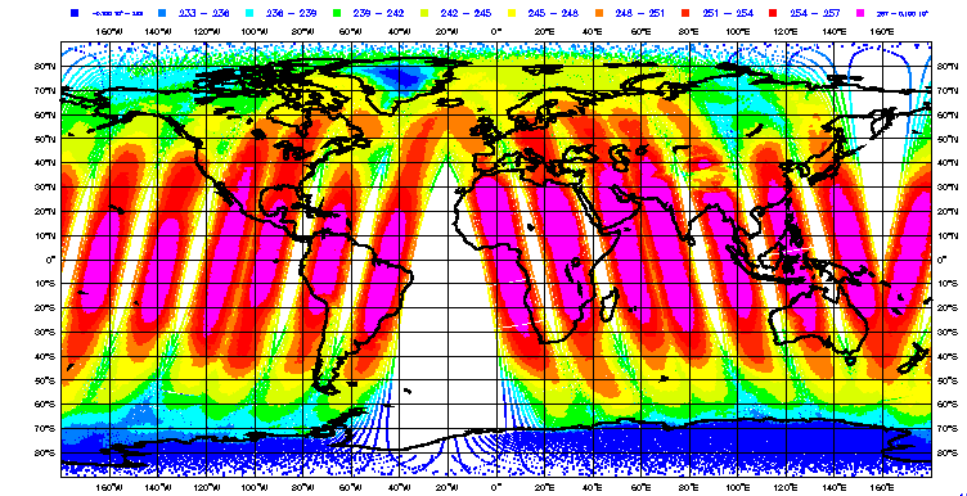
Atmospheric sounding channels

These channels are located in parts of the infra-red and microwave spectrum for which the main contribution to the measured radiance is described by:

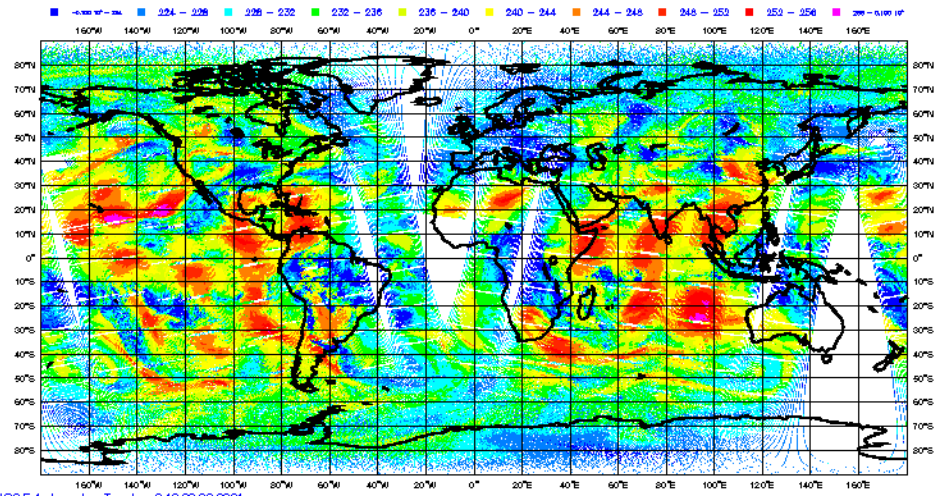
$$L(\nu) = \int_0^{\infty} B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz$$

That is they avoid frequencies for which surface radiation and cloud contributions are important.
They are primarily used to obtain information about atmospheric temperature and humidity.

AMSUA-channel 5 (53GHz)



HIRS-channel 12 (6.7micron)



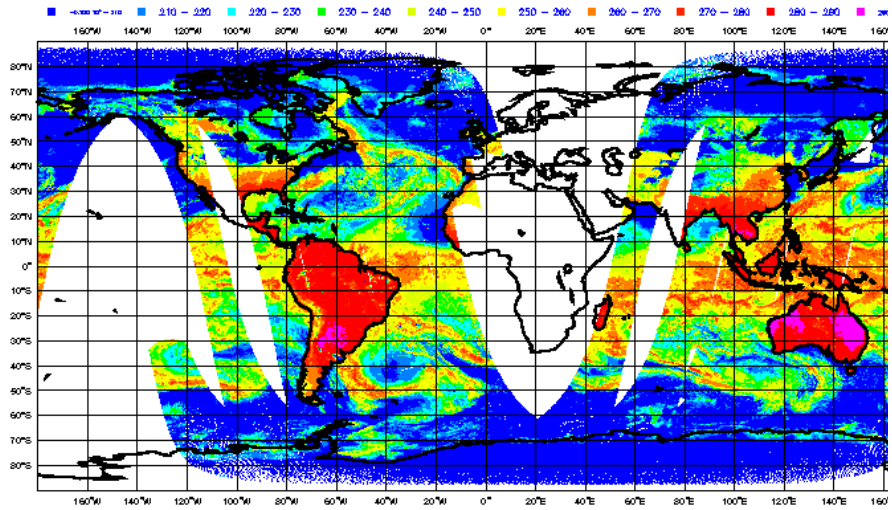
Surface sensing channels

These are located in window regions of the infra-red and microwave spectrum at frequencies where there is very little interaction with the atmosphere and the main contribution to the measured radiance is:

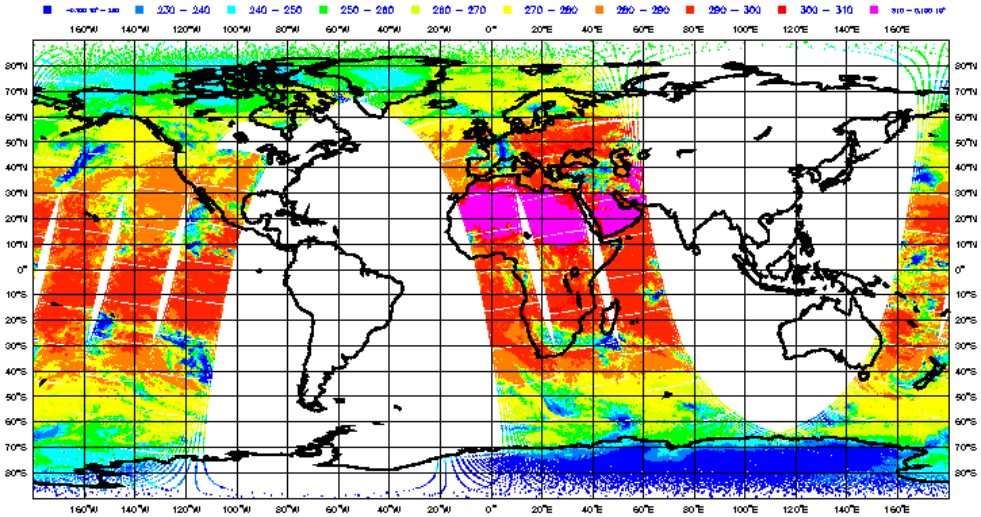
$$L(\nu) = \text{Surface emission } [\, T_{surf} \,,\, \varepsilon(u,v) \,]$$

These are primarily used to obtain information on the surface temperature and quantities that influence the surface emissivity such as wind (ocean) and vegetation (land). They can also be used to obtain information on clouds/rain and cloud movements (to provide wind information) or total-column atmospheric quantities.

SSM/I channel 7 (89GHz)



HIRS channel 8 (11microns)



Atmospheric temperature sounding

Select sounding channels for which

$$L(\nu) = \int_0^\infty B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz$$

and the primary absorber is a **well mixed gas** (e.g. oxygen in MW or CO_2 in IR).

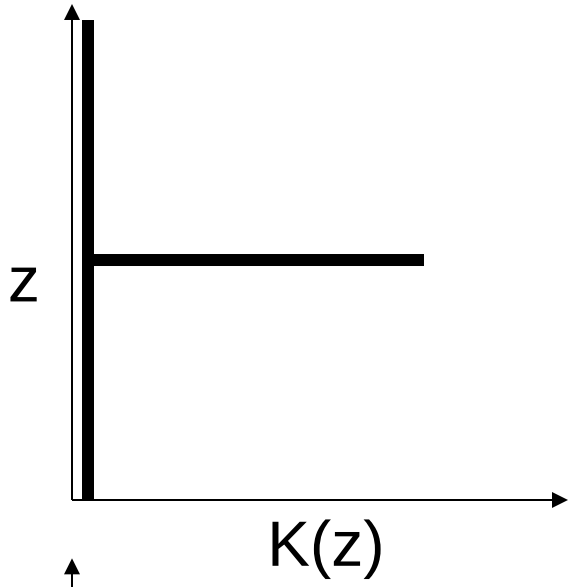
Then the measured radiance is essentially a weighted average of the atmospheric temperature profile:

$$L(\nu) = \int_0^\infty B(\nu, T(z)) K(z) dz$$

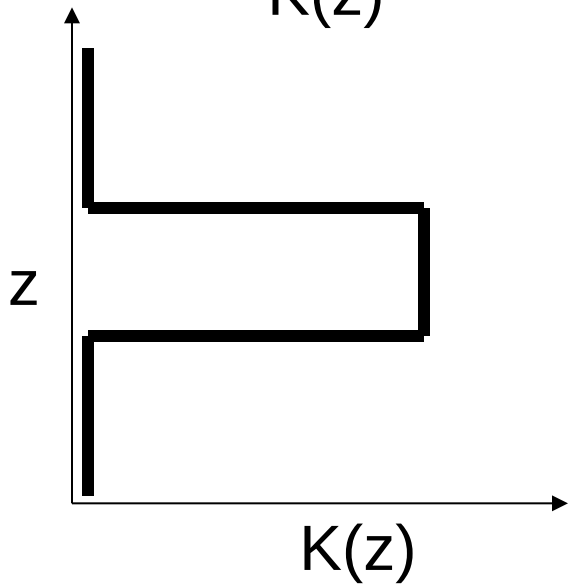
with $K(z) = \left[\frac{d\tau}{dz} \right]$

The function K(z) that defines this vertical average is known as a **weighting function**.

Ideal weighting functions

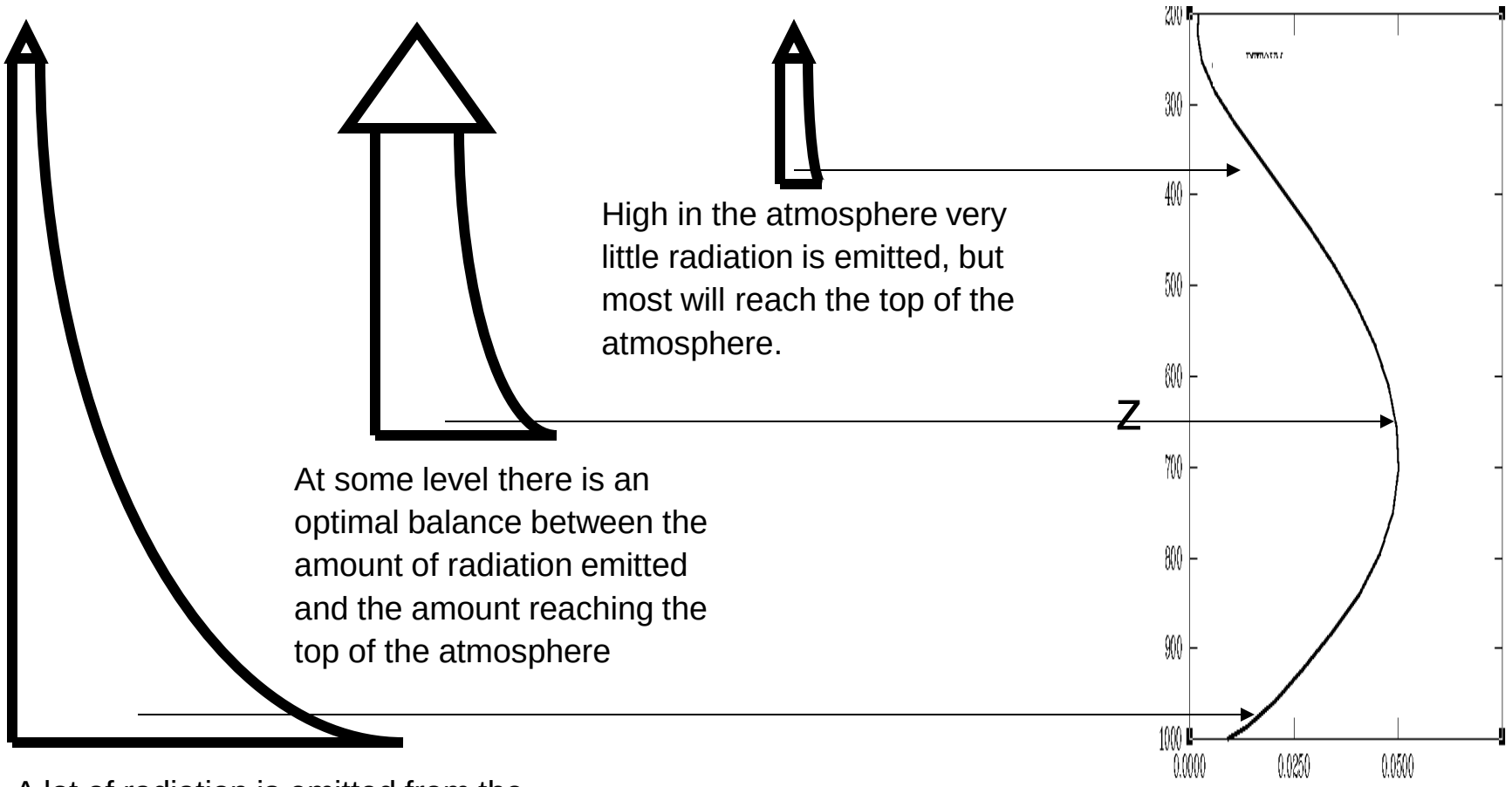


If the weighting function was a delta-function, this would mean that the measured radiance is sensitive to the temperature at a single level in the atmosphere.



If the weighting function was a box-car function, this would mean that the measured radiance was sensitive to the mean temperature between two atmospheric levels

Atmospheric weighting functions



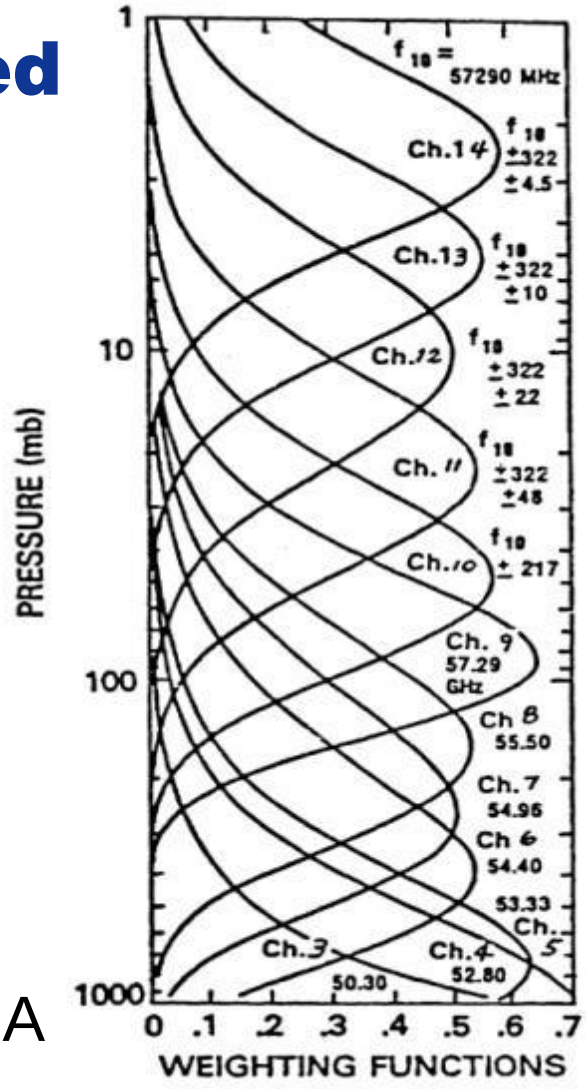
ECMWF

Weighting functions continued

- The altitude at which the peak of the weighting function occurs depends on the strength of absorption for a given channel.

- Channels in parts of the spectrum where the absorption is strong (e.g. near the centre of CO_2 or O_2 lines) peak high in the atmosphere.

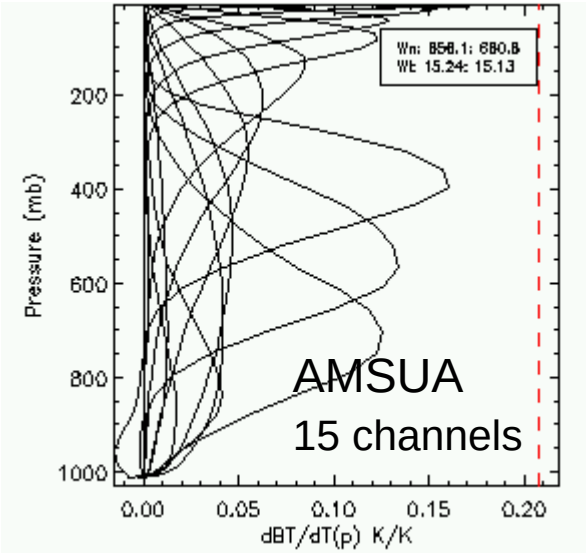
- Channels in parts of the spectrum where the absorption is weak (e.g. in the wings of CO_2 or O_2 lines) peak low in the atmosphere.

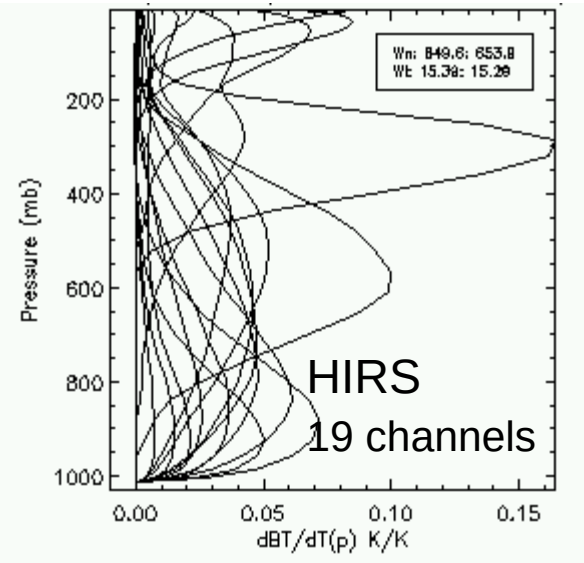


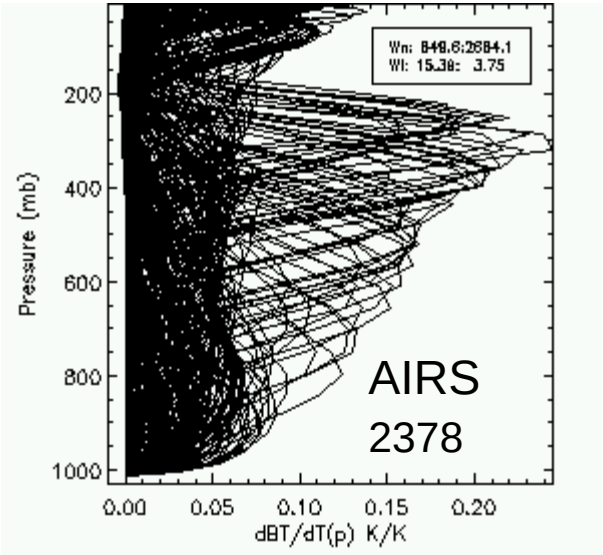
AMSU-A

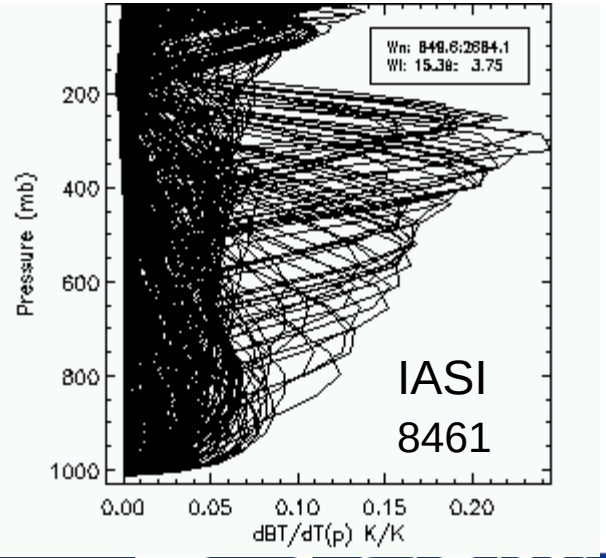
By selecting a number of channels with varying absorption strengths we sample the atmospheric temperature at different altitudes.

More weighting functions





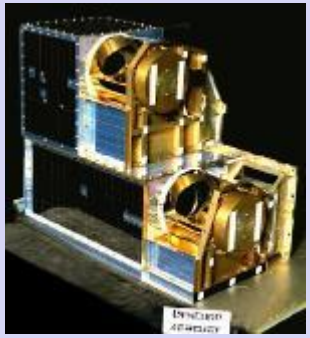


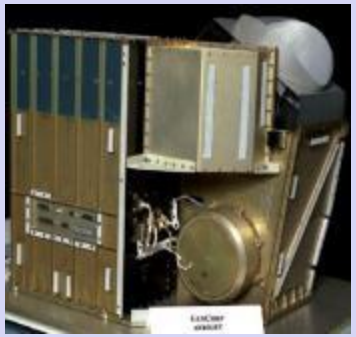


Important satellite instruments for NWP

AMSU-A:

- Advanced **Microwave** Sounding Unit
- **15 channels** (12 in 50-60 GHz region)
- 48 km field-of-view (nadir), 2074 km swath
- Primarily temperature-sounding
- On-board NOAA-15-19, Aqua, METOP-A



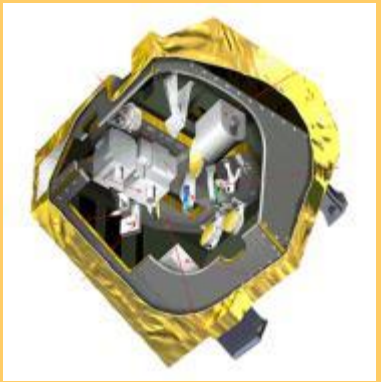


AIRS:

- Atmospheric **Infrared** Sounder
- **2378 channels** covering 650 - 2700 cm^{-1} (3.7-15.4 μm)
- 13.5 km field-of-view (nadir), 2130 km swath
- Primarily temperature/humidity-sounding, trace gases
- On-board Aqua

IASI:

- **Infrared** Atmospheric Sounding Interferometer
- **8461 channels** covering 645 - 2760 cm^{-1} (3.6-15.5 μm)
- 12 km field-of-view (nadir), 2132 km swath
- Primarily temperature/humidity-sounding, trace gases
- On-board METOP-A



How do we extract atmospheric information (e.g. temperature) from satellite radiances?

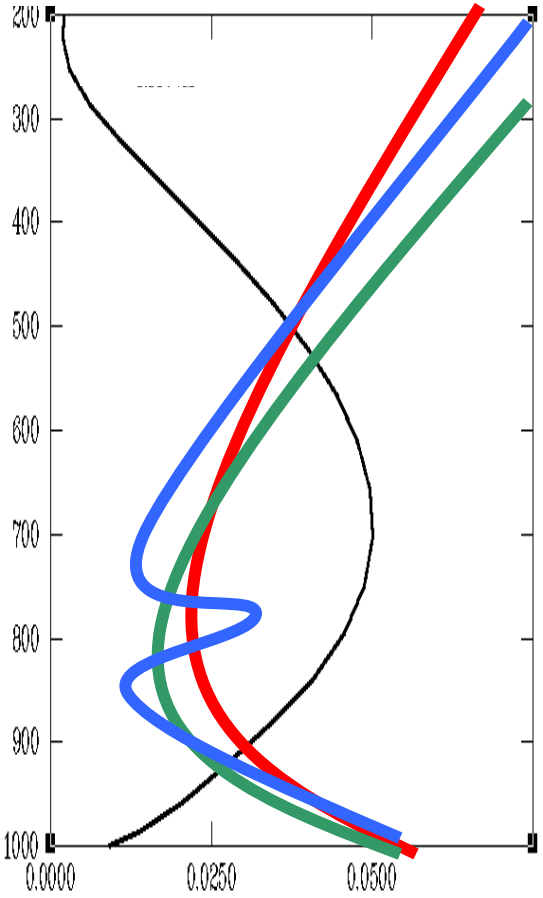
3.) Retrieval algorithms

Extracting atmospheric temperature from radiance measurements

If we know the entire atmospheric temperature profile T(z) then we can compute the radiances a sounding instrument would measure using the *radiative transfer equation*. This is sometimes known as the **forward problem**.

In order to extract or retrieve the atmospheric temperature profile from a set of measured radiances we must solve what is known as the inverse problem.

Unfortunately as the weighting functions are generally broad and we have a finite number of channels, the inverse problem is **formally ill-posed** because an infinite number of different temperature profiles could give the same measured radiances !!!



See paper by Rodgers 1976 Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation. Rev. Geophys.Space. Phys. 14, 609-624

A simple ill-posed problem

- Assume I measure

$$y = x_1 + x_2$$

Ignore any measurement error for the moment.

- But I want to know the individual components of x using y.

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- There are an infinite number of $(x_1 + x_2)$ combinations that are consistent with the measurement.

- We need more, *a-priori,* information to estimate both x_1 and x_2. **The measurement alone cannot provide the solution.**
  A priori: Perhaps I already have an estimate of x_1 and x_2.

Some history … John Eyre (Met Office)

- Satellite data assimilation into NWP models began the 1970's, but by the 1980's it was clear that this was having a –ve impact.

- Early NWP systems designed to make use of sondes. Satellite products made to look like sondes.

- Satellite sounders and sondes have opposite strengths and weaknesses

- Treating satellite soundings as "poor-quality sondes" is flawed.

- Need to really consider the actual information content of the "raw" measurement!

Retrieval schemes for NWP

The **linear data assimilation schemes** used in the past at ECMWF such as Optimal Interpolation (OI) were unable to assimilate radiance observations directly (as they were nonlinearly related to the analysis variables) and the radiances had to be **explicitly converted to temperature products** before the analysis.

This conversion was achieved using a variety of retrieval algorithms that differed in the way they used prior information

All retrieval schemes use some (either explicit of implicit) form of **prior information** to supplement the information of the measured radiances and solve the inverse problem !

Several different types of retrieval have been used in NWP:
Examples:

1. Regression / Neural Net (statistical) methods
2. Forecast background (1DVAR) methods

The difference between (retrievals/products) and observations

- **This is an extremely important point! The retrieval is not the observation.**

- **Retrieval**
  - **= (something **a priori*) +(something_else * observation)**

- **Mathematically, a retrieval can be written as a matrix equation.**

$$\mathbf{x}_a = (\mathbf{I} - \mathbf{KH})\mathbf{x}_b + \mathbf{K}\mathbf{y}_m$$

- **It is crucial to consider the role of the *a-priori* when using retrievals. What information has the observation really provided?**

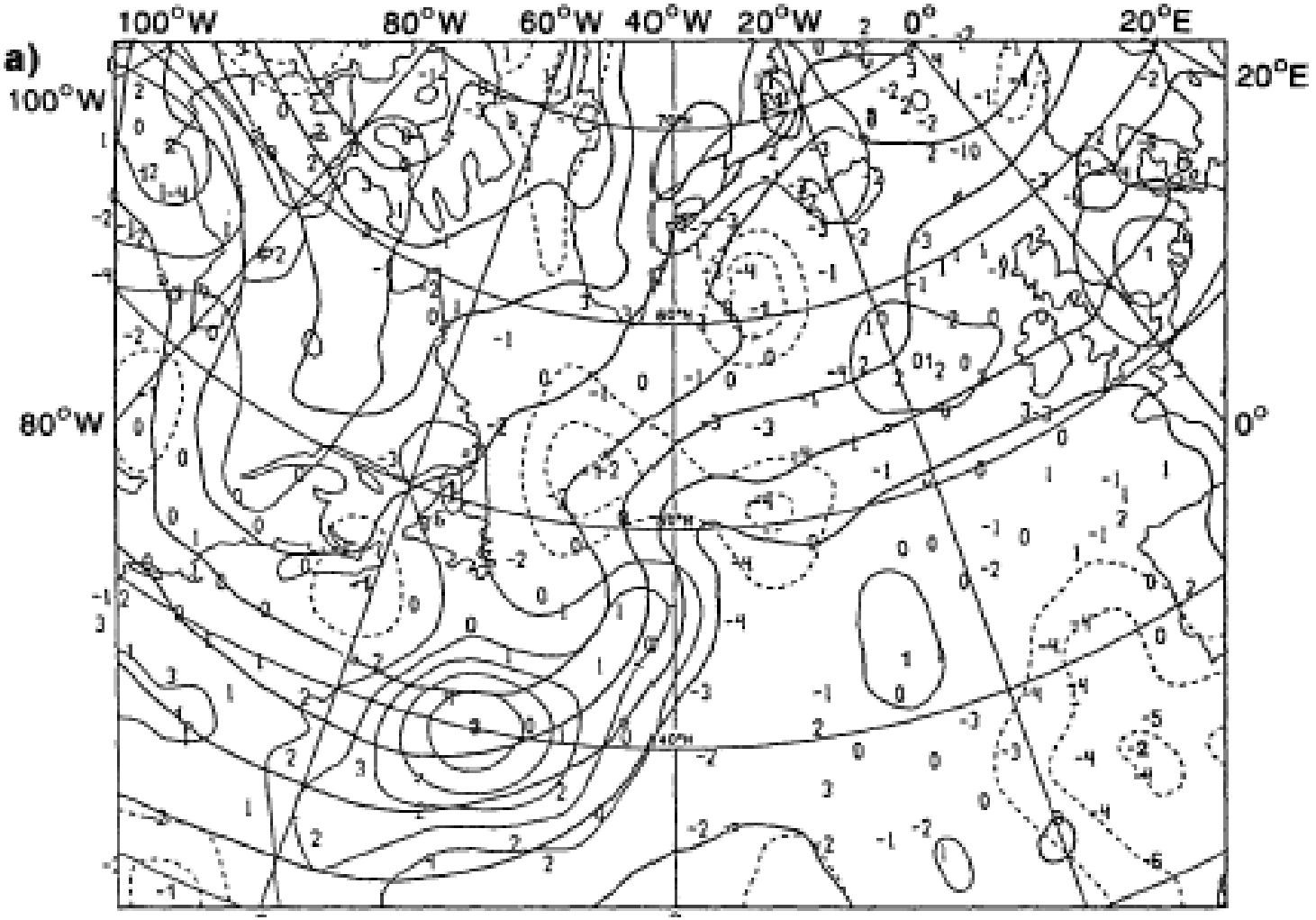
1. Regression and Library search

Using a sample of temperature profiles matched (collocated) with a sample of radiance observations/simulations, a statistical relationship is derived that predicts e.g. atmospheric temperature from the measured radiance.

These tend to be limited by the statistical characteristics of the training sample / profile library and will not produce physically important features if they are statistically rare in the training sample. **Furthermore, their assimilation can destroy sharp physical features in the analysis!**

The climatology used in the retrieval is a poorer estimate of the atmospheric state (the weather) than a short-range forecast!

We do not want to assimilate this information.



From Andersson et al (1991). Analysis increments and background,1000-700 hPa

1DVAR retrievals and the cost function

It can be shown that the maximum likelihood approach to solving the inverse problem requires the minimization of a cost function *J* which is a combination of two distinct terms **(NOTE: The mathematics is the same as 3/4DVAR)**. :

1D state or profile

Radiance vector

RT equation

$$J(\mathbf{x}) = (\mathbf{x}-\mathbf{x_b})^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x_b}) + (\mathbf{y_m}-\mathbf{H}[\mathbf{x}])^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y_m}-\mathbf{H}[\mathbf{x}])$$

Fit of the solution to the background estimate of the atmospheric state weighted inversely by the background error covariance B.

Fit of the solution to the measured radiances (y) weighted inversely by the measurement error covariance R (observation error + error in observation operator H).

***If background and observation errors are Gaussian, unbiased, uncorrelated with each other; all error covariances are correctly specified;

1DVAR retrievals continued …

One simple linear form of the 1D-Var solution obtained by minimization of the cost function is given by the expression:

$$x_a = x_b + [\mathbf{HB}]^T [\mathbf{HBH}^T + \mathbf{R}]^{-1} (y - \mathbf{H}x_b)$$

Correction term, "increment"

The retrieved profile (x_a) is equal to the background profile (x_b) plus a **correction** term applied. Furthermore we can quantify the error covariance $\mathbf{S_a}$ of the 1D-Var retrieval which is needed for subsequent assimilation:

$$\mathbf{S_a} = \mathbf{B} - [\mathbf{HB}]^T [\mathbf{HBH}^T + \mathbf{R}]^{-1} \mathbf{HB}$$

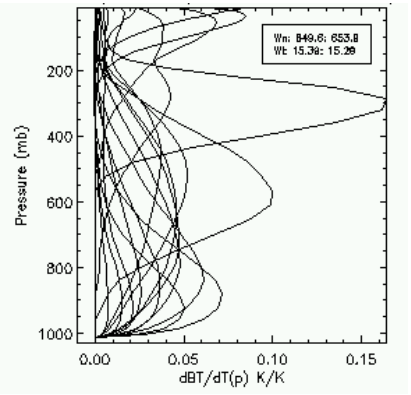
Improvement term

The retrieval being an **improvement** over the background information (assuming all parameters are correctly specified).

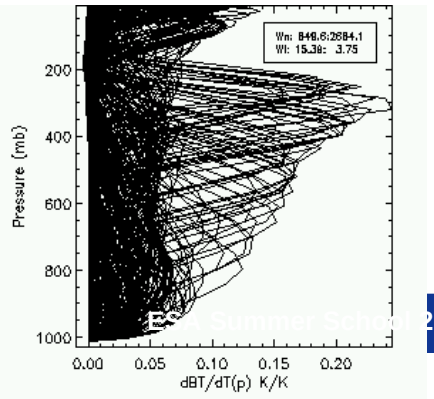
1DVAR retrievals continued…

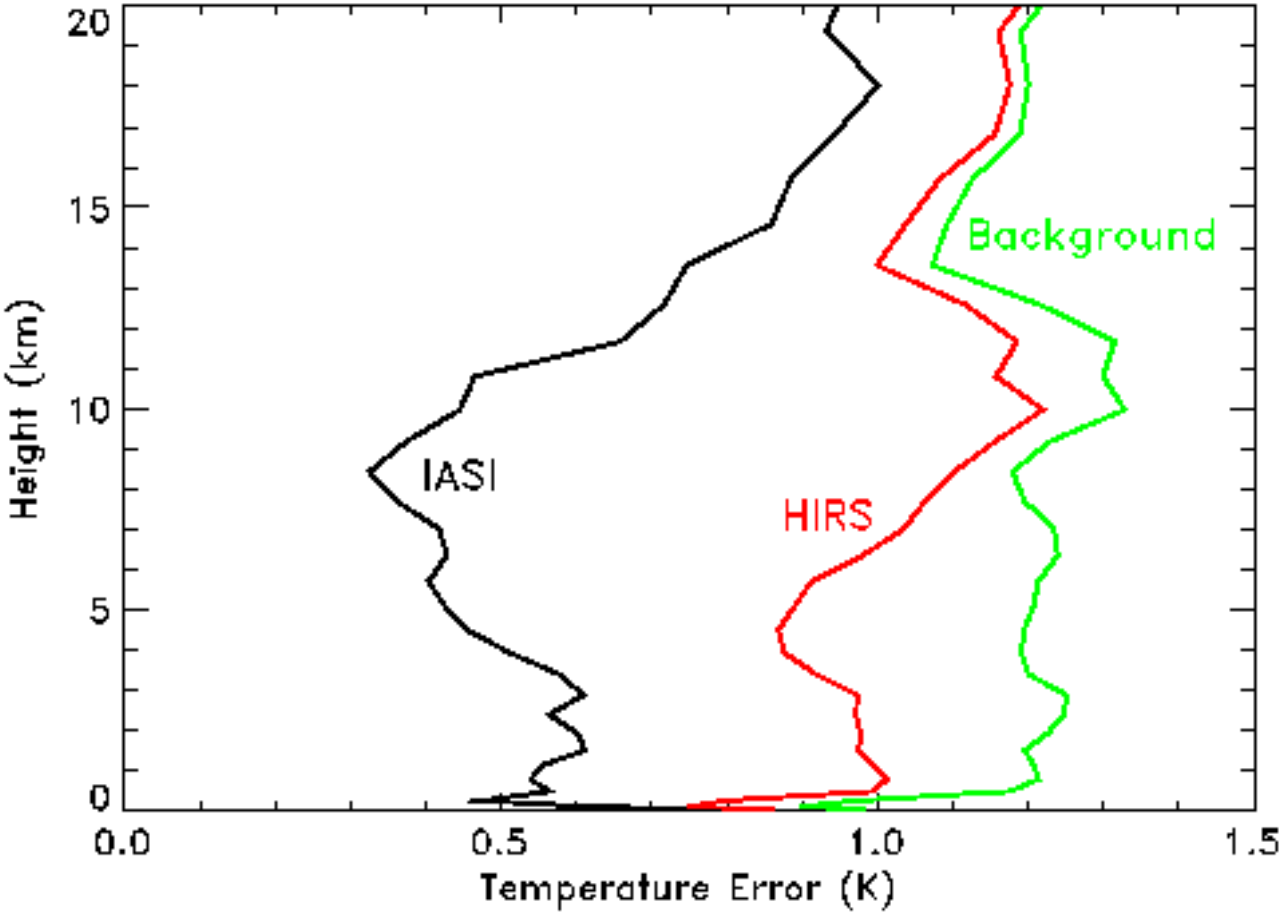
The magnitude of the improvement over the background clearly depends on a number of parameters, but one crucial factor is the number of channels and shape of the weighting functions implied by the radiative transfer operator **H.**

HIRS 19 channels



IASI 8461 channels





Characteristics of 1DVAR retrievals

These have a number of advantages that make them more suitable for NWP assimilation than other retrieval methods:

•The prior information (short-range forecast) is very accurate (more than statistical climatology) which improves retrieval accuracy.

•The prior information contains information about physically important features such as fronts, inversions and the tropopause.

•The error covariance of the prior information and resulting retrieval is better known (crucial for the subsequent assimilation process).

•The 1DVAR may be considered an intermediate step towards the direct assimilation of radiances.

BUT the error characteristics of the 1DVAR retrieval may still be very complicated due to its correlation with the forecast background …

Direct radiance assimilation

But do we really need explicit retrievals for NWP?

4.) Direct radiance assimilation

Direct assimilation of radiances

Variational analysis methods such as 3DVAR and 4DVAR allow the direct assimilation of radiance observations (without the need for an explicit retrieval step).

This is because such methods do **NOT** require a linear relationship between the observed quantity and the analysis variables.

The retrieval is essentially incorporated within the main analysis by finding the 3D or 4D state of the atmosphere that minimizes

$$J(\mathbf{x}) = (\mathbf{x}-\mathbf{x_b})^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x_b}) + (\mathbf{y_m}-\mathbf{H}[\mathbf{x}])^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y_m}-\mathbf{H}[\mathbf{x}])$$

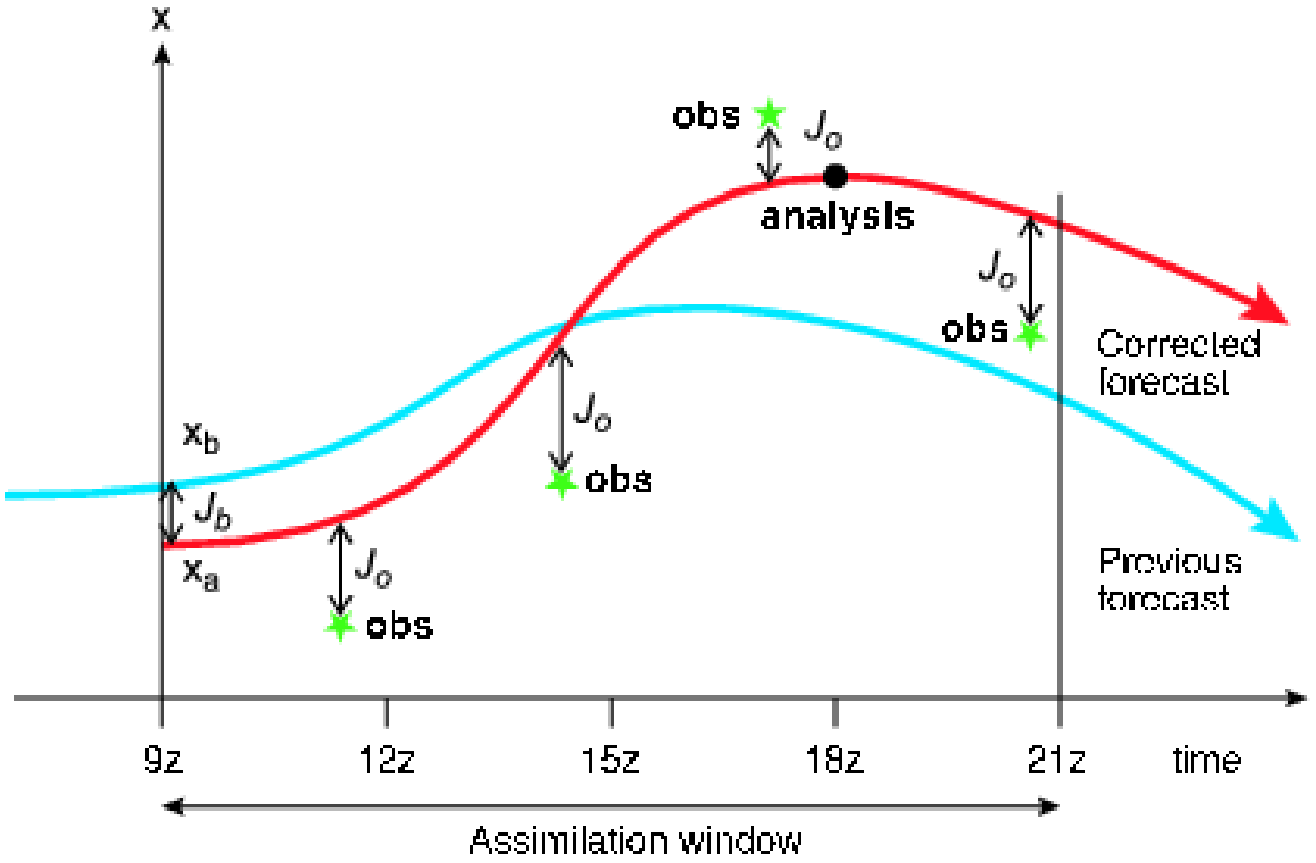
Atmospheric state vector

Vector of all observed data

"Observation operator"
H = radiative transfer equation
(+ NWP model integration in 4DVAR)

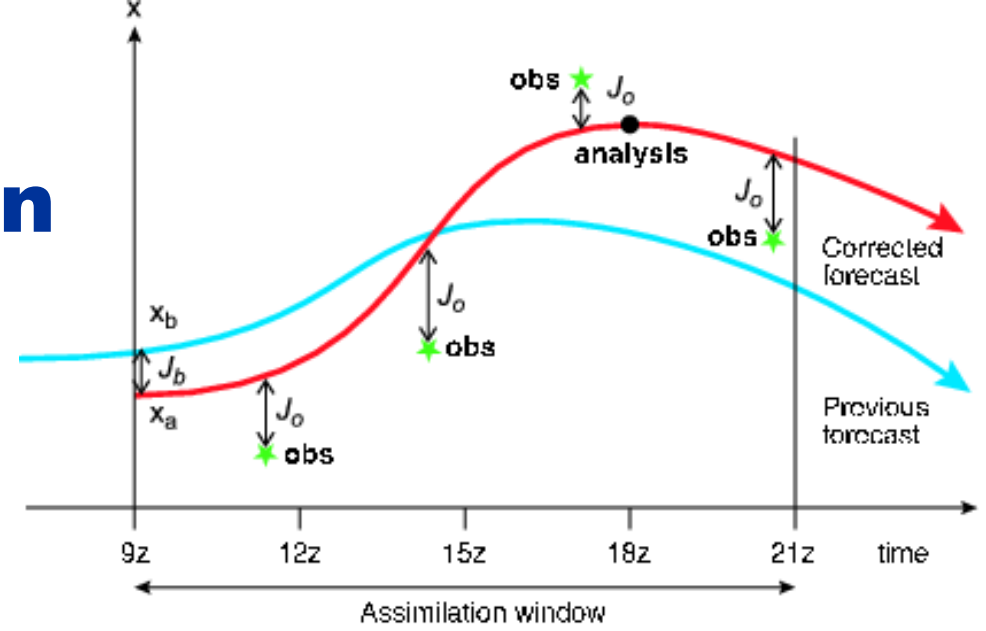
In direct radiance assimilation the forecast background still provides the prior information to supplement the radiances, **but it is not used twice** (as would be the case if 1D-Var retrievals were assimilated).

4DVAR data assimilation

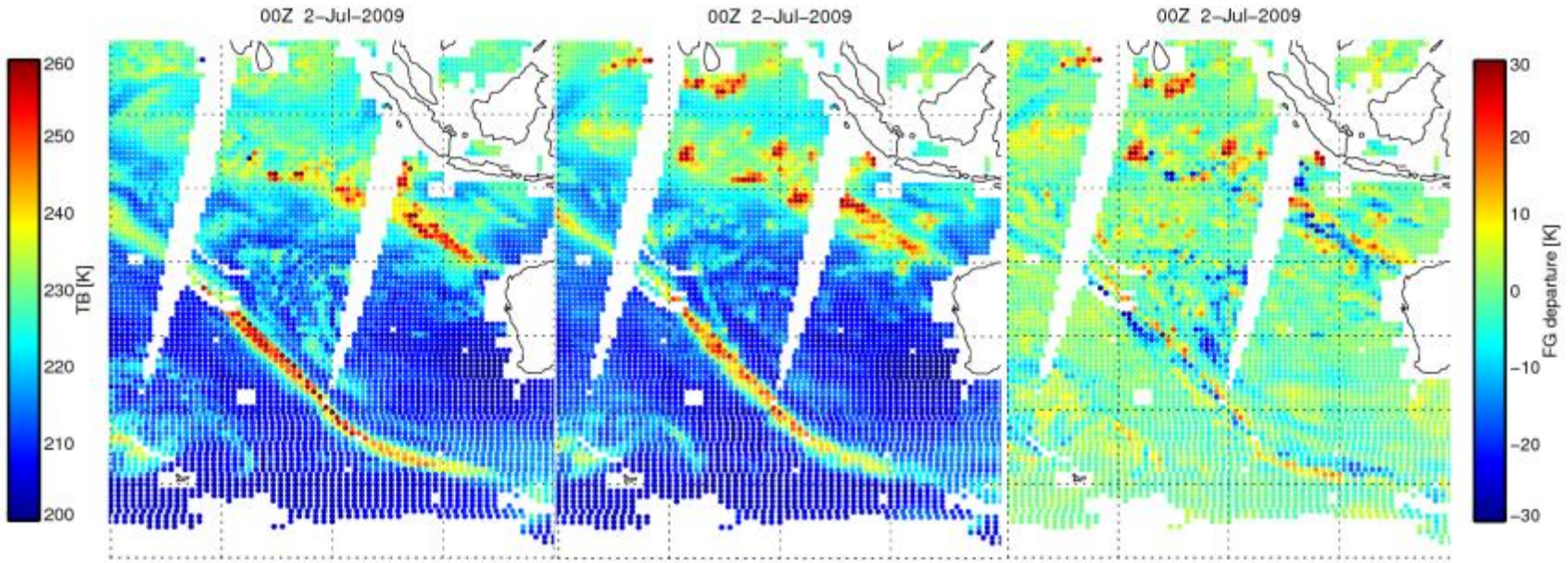


Remember it is least squares! The forecast model is providing a curve that we try to fit through the observations, by adjusting the state at the start of the window.

4DVAR data assimilation



Background **Observation** **Background departure**



ECMWF

Direct assimilation of radiances (II)

By the direct assimilation of radiances we avoid the problem of assimilating retrievals with complicated error structures.

BUT

There are still a number of significant problems that must be handled:

- Specifying the covariance **(B)** of **background error statistics.**
- Specifying the covariance **(R)** of **radiance error statistics.**
- Removing **biases** and **ambiguities** in the radiances / RT model.

→ **Some of these issues are simplified by the direct assimilation of raw (unprocessed) radiance observations.**

Direct assimilation of raw radiances

Further to the move away from retrievals to radiance data, most NWP centres are assimilating **raw radiances** (level-1b/1c).

• Avoid **complicated errors** (random and systematic) introduced by (unnecessary) pre-processing such as cloud clearing, angle (limb) adjustment and surface corrections.

• Avoid having to change (retune) our assimilation system when the **data provider changes the pre-processing**

• Faster **access to data** from new platforms (e.g. new data can be assimilated weeks after launch)

• Allows **consistent treatment of historical data** for re-analysis projects (ERA-40, ERA-interim) and other climate studies

Advantages of 4DVAR (or various flavours of it)

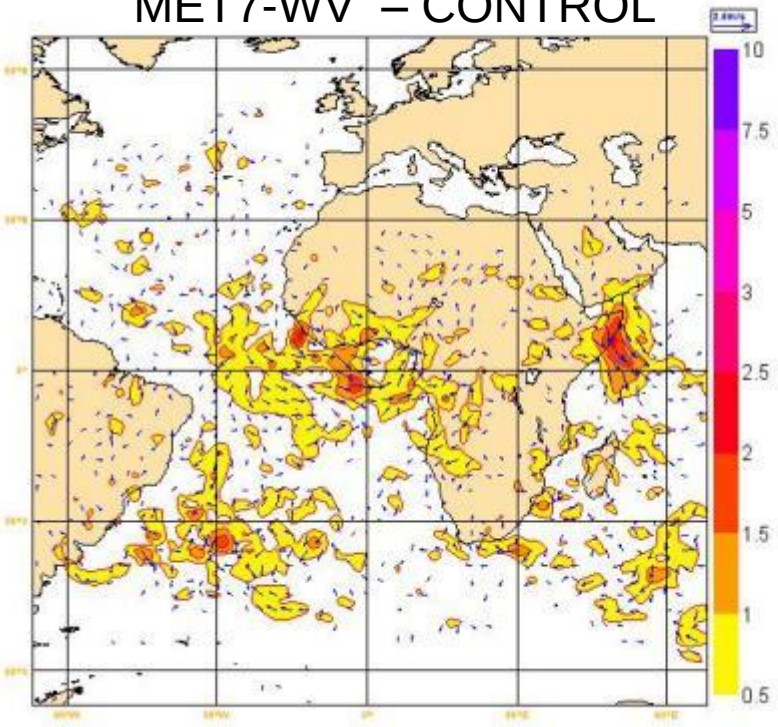
- **Better use is made of observations far from the centre of the assimilation time window (particularly important for satellite data).**
- **The inversion of radiances is constrained by the background and its error covariance, but also by the forecast model's physics and dynamics.**
- **Wind information can be retrieved from radiance data through tracing effects:**
  - **To fit the time and spatial evolution of humidity or ozone signals in the radiance data, the 4DVAR has the choice of creating constituents locally or advecting constituents from other areas. The latter is achieved with wind adjustments.**

Wind adjustments from radiances in 4DVAR

• Assimilation of passive tracer information feeds back on wind field in a single analysis cycle. Small adjustments also visible in mean wind field.

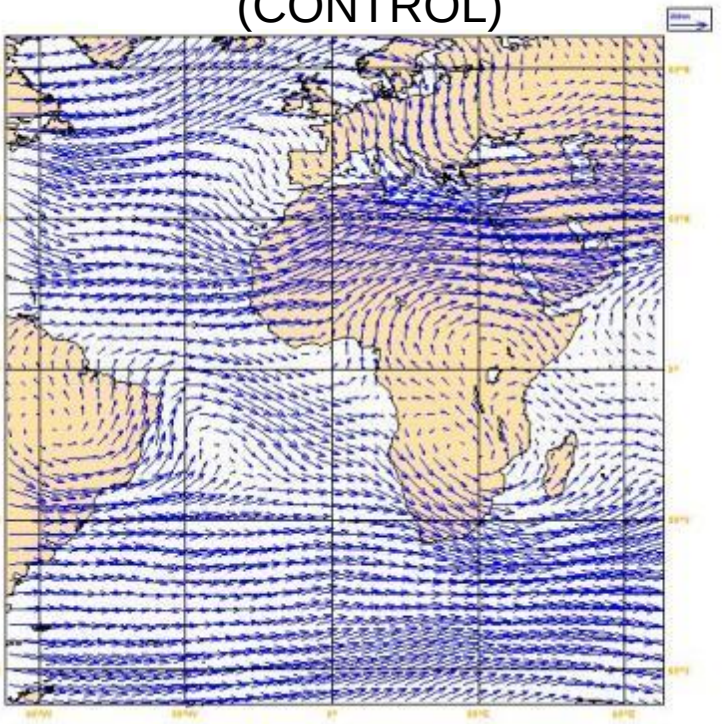
Mean Analysis Difference

MET7-WV – CONTROL



Mean Analysis

(CONTROL)



200 hPa

Summary of key concepts

- **Satellite data are extremely important in NWP.**
- **Data assimilation combines observations and a priori information in an optimal way and is analogous to the retrieval inverse problem.**
- **Passive nadir sounders have the largest impact on NWP forecast skill:**
  - Nadir sounders measure radiance **(not T,Q or wind)**.
  - Sounding radiances are broad vertical averages of the temperature profile (defined by the weighting functions).
  - The retrieval of atmospheric temperature from the radiances is ill-posed and all retrieval algorithms use some sort of prior information.
  - Most NWP centres assimilate raw radiances directly due to their simpler error characteristics. 4DVAR is now widely used (or alternative 4 dimensional techniques).
- **4DVAR is a least squares. Don't be too scared of the maths.**

Key concepts (continued)

- **NWP misused satellite data for many years – problems identified in the 1980's. Don't make the same mistakes!**

- **Always be aware of the difference between a satellite product/retrieval and the actual measurement.**

  - **Satellites do not measure … P,T,Q …**

- **If the retrieval problem is ill-posed (eg, $y=x1+x2$), then the solution must depend on other information or constraints (*a priori*) .**

- **How do errors in the a priori affect your product? Could these error be the dominant error source in your work?**