# Modeling and observing the atmosphere: mathematics in atmospheric sciences

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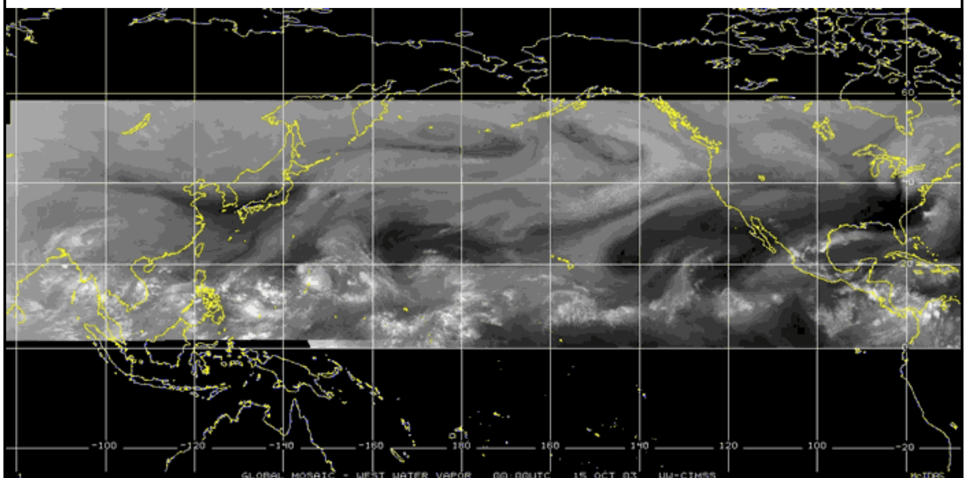
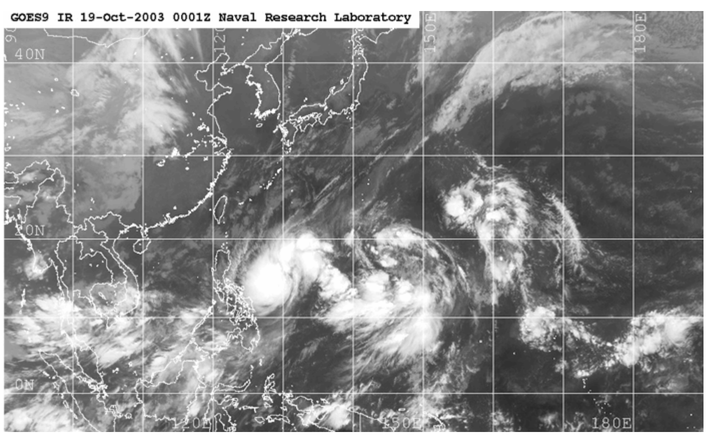
## Outline

- The primitive equations that govern the atmosphere
  - Nonlinearities and scaling issues (spatial and temporal)
- Modeling the atmosphere
  - Discretization of the primitive equations
  - Subgrid scale processes
- Observing the atmosphere
  - Nature of the observations
    - direct and indirect measurements of atmospheric quantities (e.g., temperature, winds, humidity, chemical species)
  - Composition of the Global Observing System
- Data assimilation
  - Merging model forecasts with observations
  - Variational approach: 3D and 4D

# Observed water vapor motion from satellite imagery




# Genesis of Typhoons in Western Pacific



# Northwestern Floods: October 2002

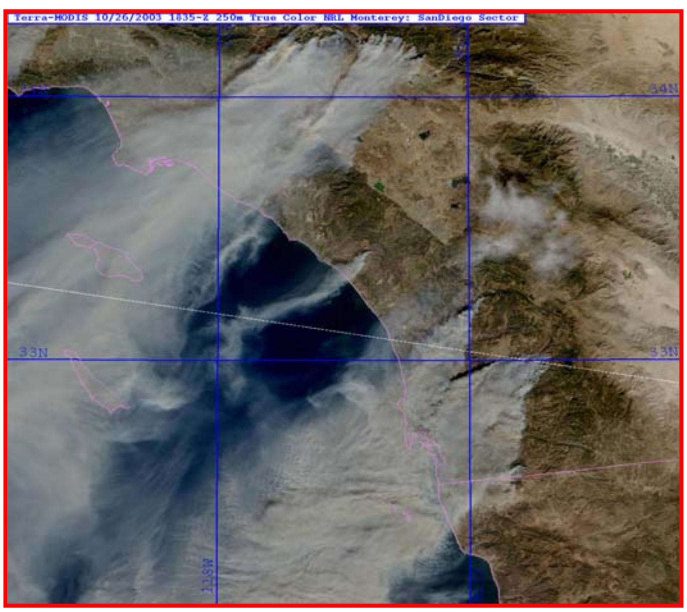

Two sub-tropical weather systems dropped 470 millimetres -- 18.5 inches -- of rain on some parts of coastal B.C. in a six-day period"

British Columbia - Record breaking heavy rain in Vancouver, Abbotsford and Victoria on October 16. Bridge washout cuts access to Pemberton, BC. "It is being called the worst flood of the past century" in British Columbia.

Washington - Skokomish, Nooksack and Skagit rivers overflowed October 17-18. Seattle broke a one-day rainfall record on October 20. Record levels on Skagit River at Concrete. Record levels on Skokomish River on October 21. Entire town of Hamilton under water. Flood damages have exceeded $160 million.

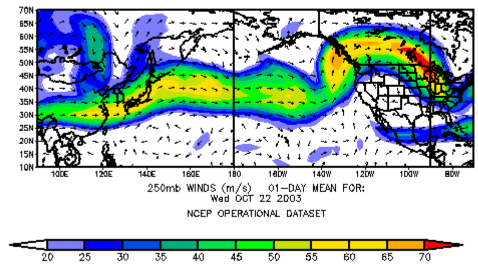
Shapiro, 2004

# Southern California Wild Fires: October 2002



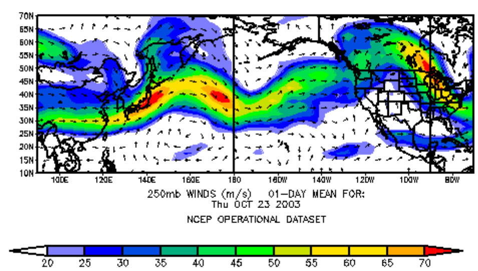

Shapiro, 2004

**22 Oct**

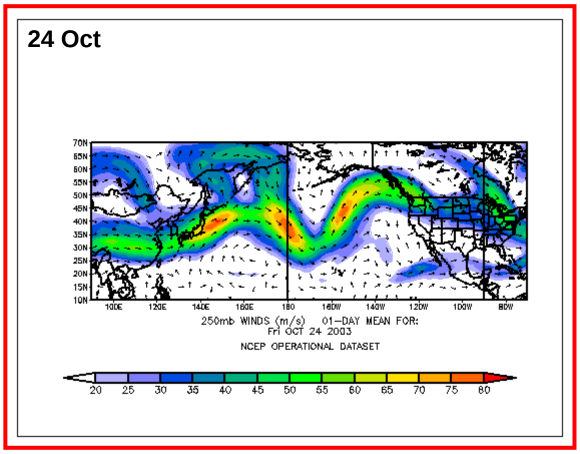



(Shapiro, 2004)

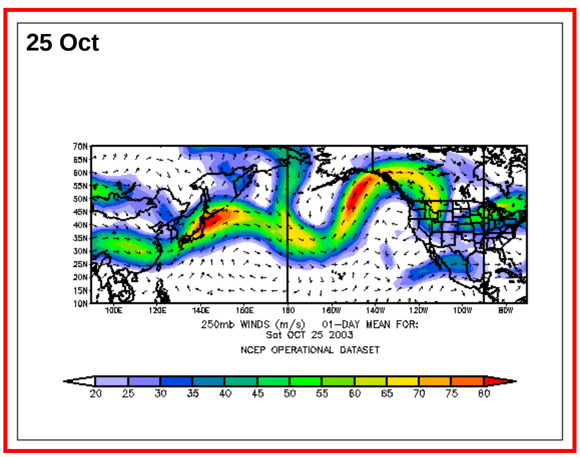
**23 Oct**




(Shapiro, 2004)

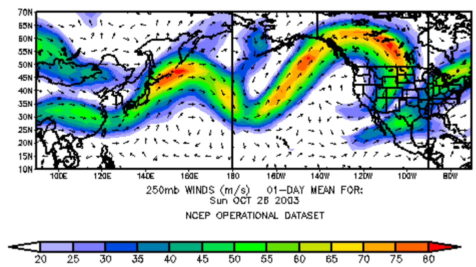



(Shapiro, 2004)



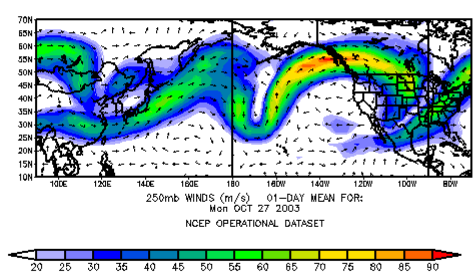

(Shapiro, 2004)

**26 Oct**




(Shapiro, 2004)

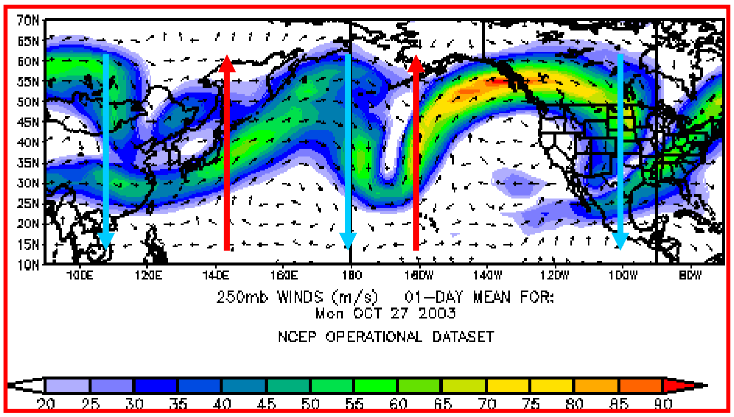
**27 Oct**

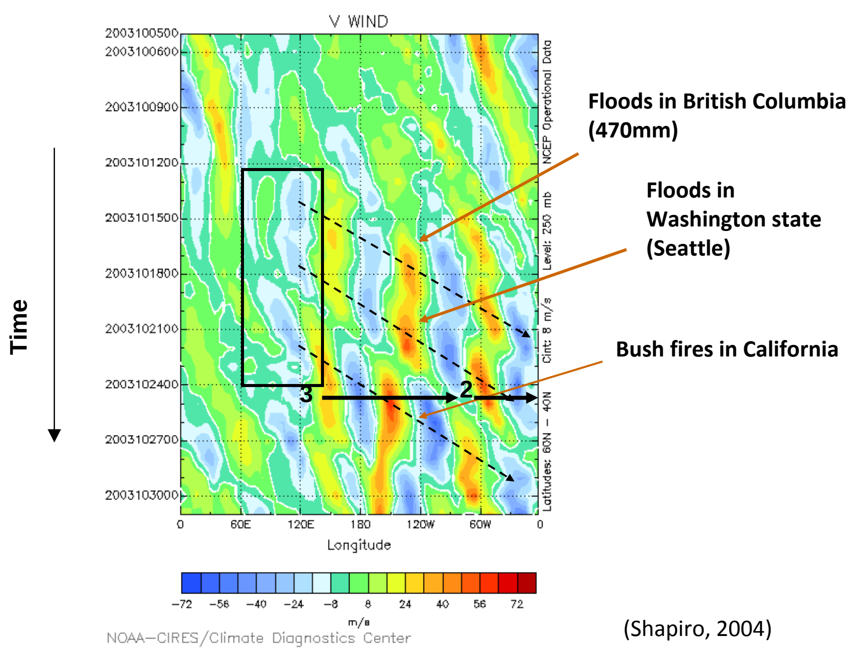



(Shapiro, 2004)

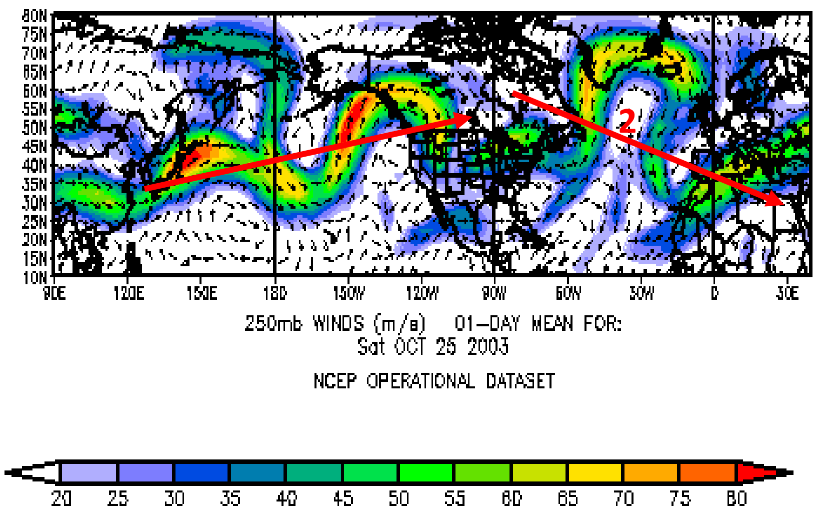
# Hov-Müller diagram

- Average of the north-south (méridional) wind component over a latidudinal band (30N-70N)
  - Indicates the presence of cyclones and anti-cyclones




(Shapiro, 2004)




(Shapiro, 2004)

# Modeling the atmosphere

## Primitive equations

$$\frac{d\mathbf{v}}{dt} + 2\Omega \times v = -\frac{\nabla p}{\rho} + D_{diffusion}$$

- Momentum equations (Navier-Stokes)
  v = (u,v,w): wind
  p : pressure, $\rho$ : air density
  2 $\Omega$ sin $\varphi$ : Coriolis parameter

$$\frac{d\,ln\theta}{dt} = \frac{1}{c_p}\frac{dQ}{dt}$$

$$\theta = T\left(\frac{1000}{p}\right)^{R/c_p}$$

- Thermodynamic equation
  $\theta$ : potential temperature

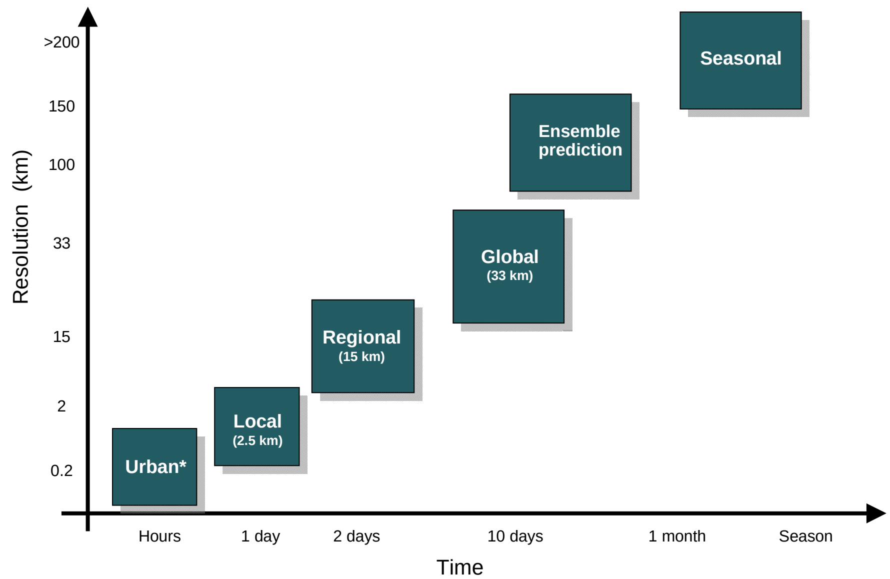
$$\frac{\partial \rho}{\partial t} + \nabla \bullet \rho\mathbf{v} = 0$$

$$p = R\rho T$$

- Continuity equation
- Equation of state for gases

## Modeling the evolution of the atmosphere

- Objective
  - Solve the primitive equations including the dominant mechanisms at the resolved spatial and temporal scales
  - Spatio-temporal discretization of the equations
- Planetary scales: 50-100 km
  - Thermal north-south gradient between poles and the equator
  - Coriolis force
  - Interaction with land and oceans
  - Physical processes at subgridscale (<50-100 km) are parameterized
- Local scales (1-10 km)
  - Cloud processes need to be taken into account
  - Local effects due to detailed topograpy and soil composition (e.g., vegetation, snow, ice, type of soil)
  - Resolve processes associated with cloud formation and fine scale precipitation




# Applications at the global scale

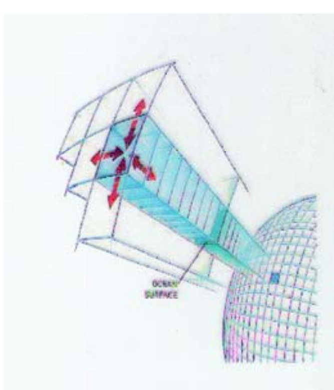
- *Numerical Weather Prediction* (*NWP*)
  - Solve an initial value problem for periods of 1 to 10 days
  - Use available observations to define the initial conditions
  - Detailed evolution (intensity and position) of meteorological systems is important

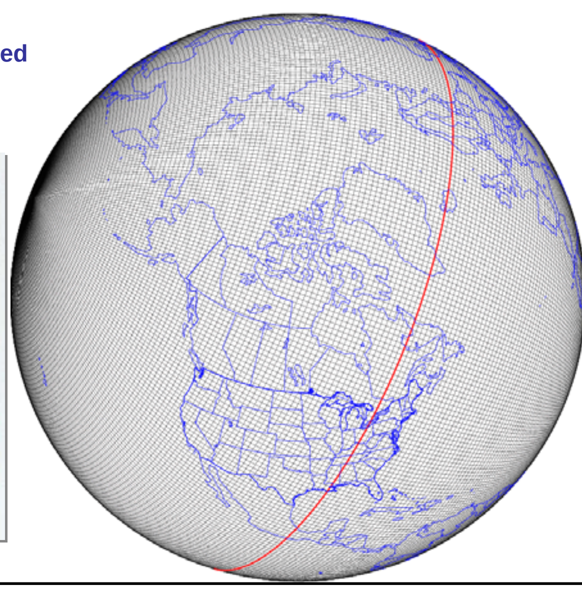
# Applications at the global scale

- Climate simulations
  - Representation of the evolving atmosphere over periods of months to decades
  - Characterization of dynamical and physical forcings that influence the mean behavior of the atmosphere
  - Validation through comparison to observations of the mechanisms the numerical model should be able to resolve
  - Spatial scales are usually larger than those resolved by numerical weather prediction models (100 to 200 km for global climate models)

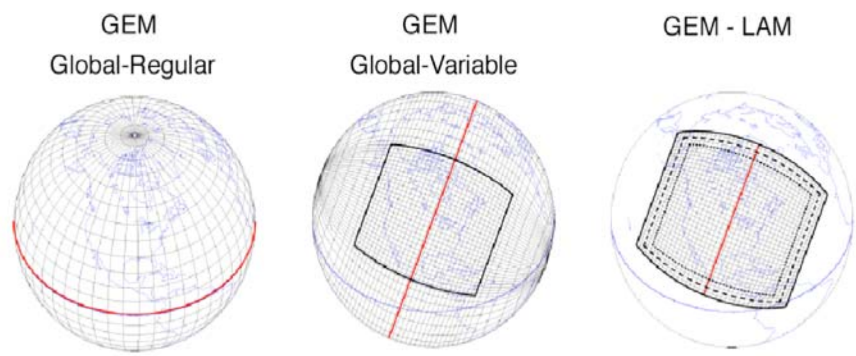
**Numerical grid of the operational global model of Environment Canada (uniform resolution < 40 km)**

**Number of variables associated with this problem: $>10^7$**

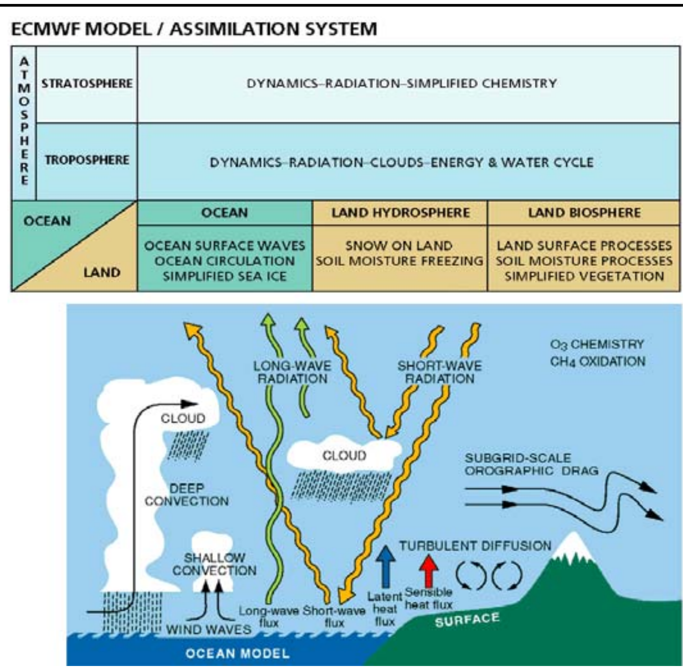




## Global Environmental Model (GEM) possible configurations …




LAM: limited-area model



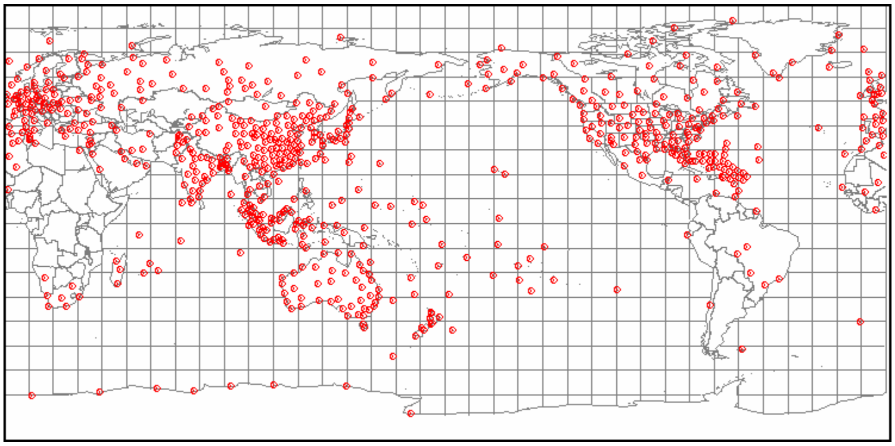

(Hollingsworth , 2004)

## Issues with the development of numerical models

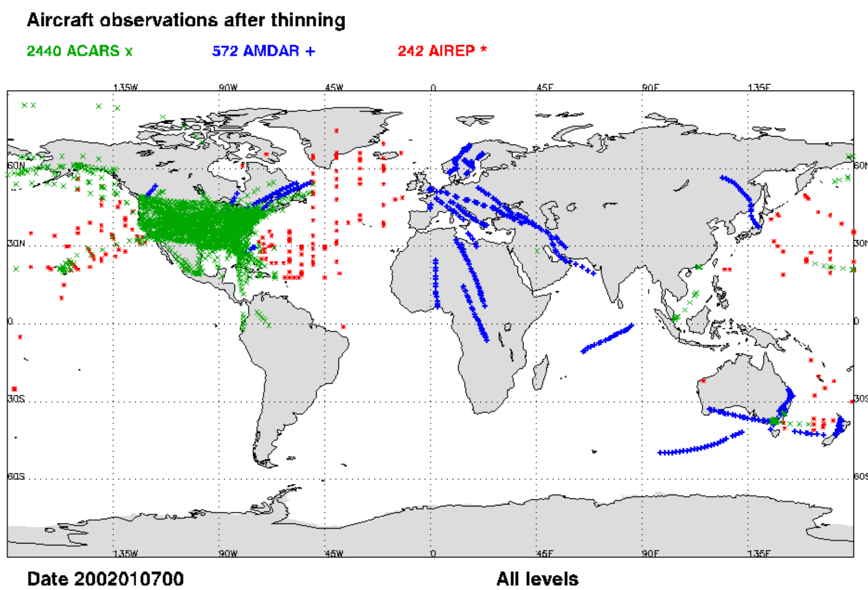
- Formulation of the mathematical equations
  - Discretization
  - Deterministic or stochastic.
- Properties of numerical schemes
  - Structured grids with variable resolution
  - Dynamically adaptive grids
- Interplay of non-resolved scale parameterizations with numerical schemes of dynamical cores.
  - Competition between numerical truncation and subgrid scale closures,
  - Techniques for control of parameterizations in dynamically adaptive models
- Coupling of models for different processes
  - Atmosphere-ocean
  - Atmospheric chemistry (chemical species and aerosols)
  - Land-surface
  - Hydrological models

## Observing the atmosphere

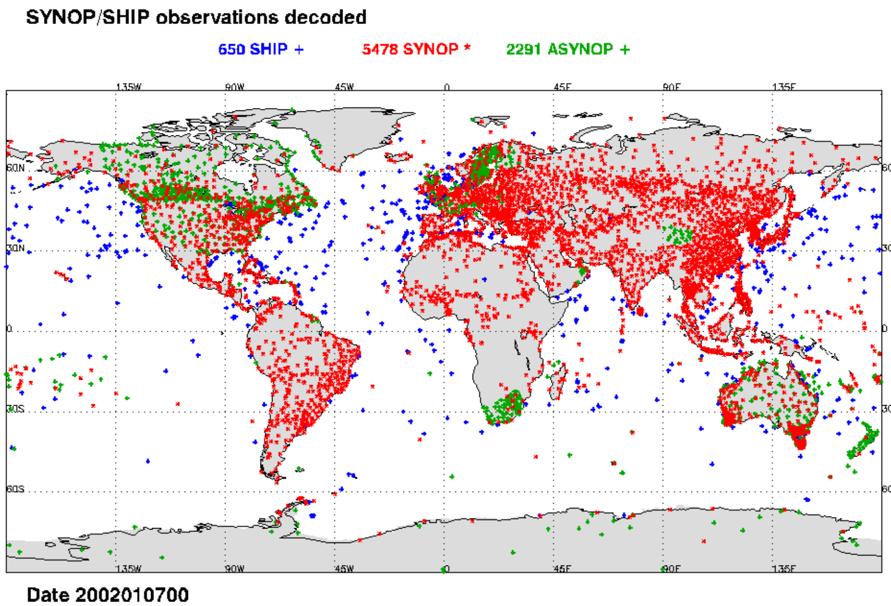
## Radiosondes at  00 UTC and12 UTC

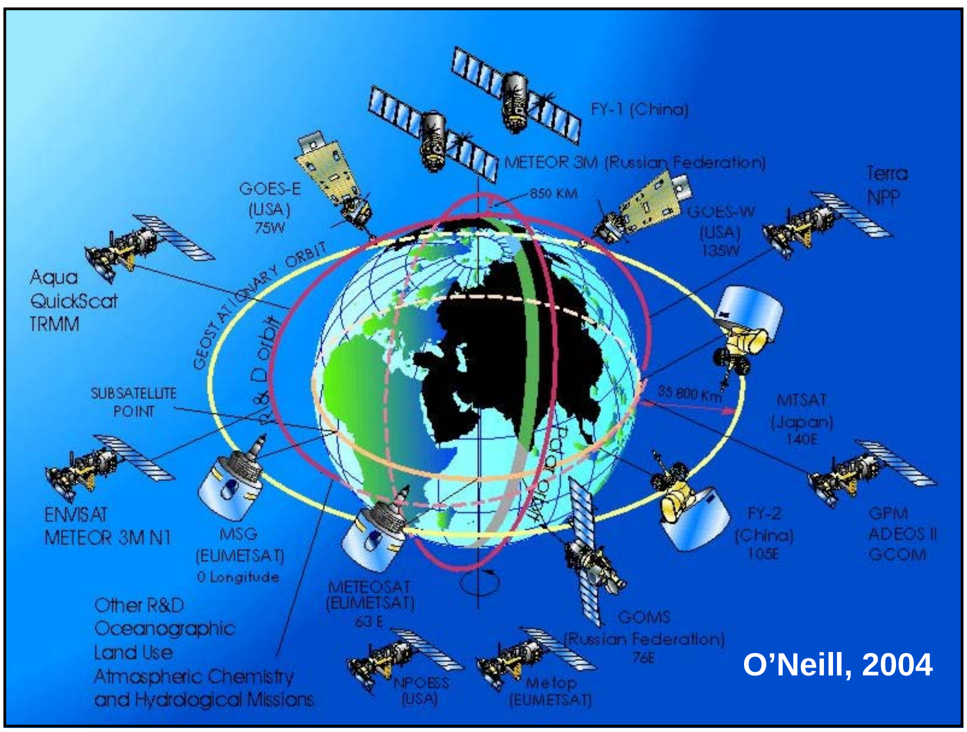


## Aircraft observations(AMDAR)

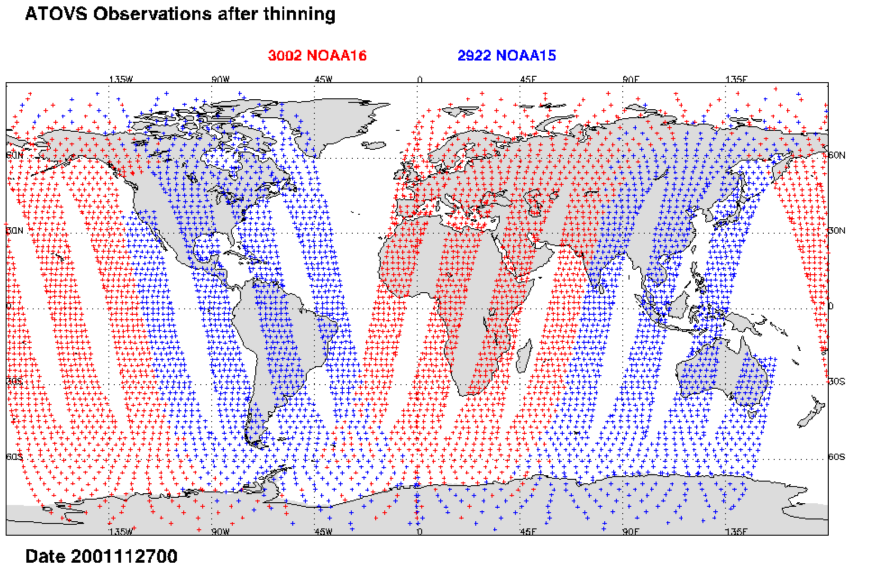


## Surface (SYNOP) and ship (SHIP) observations

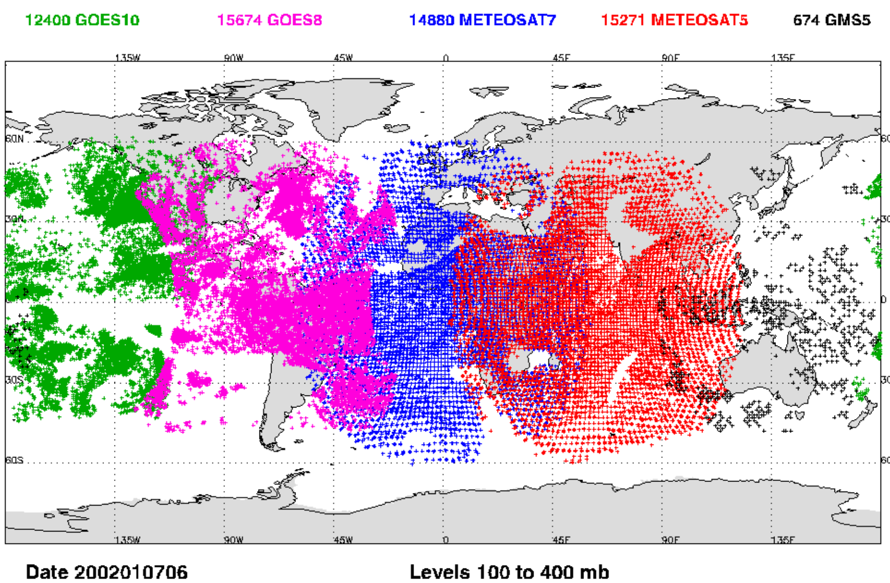


## Horizontal data coverage for ATOVS radiances (over a 6-h period)

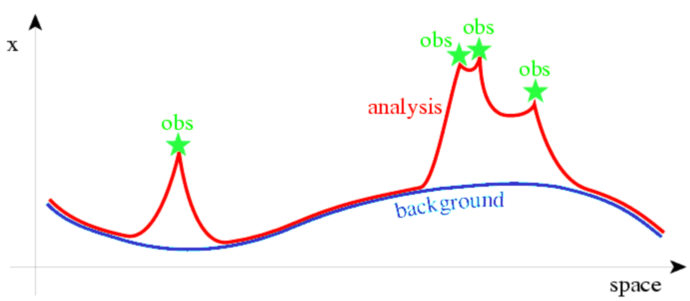



## Atmospheric Motion Vectors derived from cloud motion (SATOB, SATWINDS)



Data assimilation:
merging model forecasts with observations

Schematics of the method of direct insertion



## Difficulties of data assimilation

- **Take into account the relative accuracy of the background field with respect to that of the observations**
  - Observations have different accuracies
  - Background field (model forecast) has a certain accuracy
- **Dynamical balance constraint**
  - Modifications to the background field upsets the internal balance of the fields
  - Generates transients in the first instants of a forecast
- **How to define "optimal" weights**

## Statistical estimation: univariate case

$\mathbf{X}_b$ = forecast (or background field)

$\mathbf{y}$ = observation

$\mathbf{X}_a$ = analysis

and $\mathbf{X}_t$ = true state

| | |
|---|---|
| $\varepsilon_b = (\mathbf{X}_b - \mathbf{X}_t)$: | forecast error |
| $\varepsilon_o = (\mathbf{y} - \mathbf{H}(\mathbf{X}_t))$: | observation error |
| $\varepsilon_a = (\mathbf{X}_a - \mathbf{X}_t)$: | analysis error |
| $\mathbf{H}$: | observation operator |

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Underlying hypotheses to statistical interpolation

– Observation and forecast error is unbiased

$\langle \varepsilon_b \rangle = \langle \varepsilon_o \rangle = 0$

## Statistical interpolation (or *Gauss-Markov* method)

(Gandin, 1963; Rutherford, 1973; Schlatter,1977; Daley, 1991)

**Definitions**

$\mathbf{y} \in R^m$: observation vector ($m \sim 10^5$)

$\mathbf{X} \in R^n$: model state vector ($n \sim 10^7$)

$\mathbf{H}: R^n \to R^m$: observation operator

$\mathbf{B} = \langle \varepsilon_b \varepsilon_b^T \rangle$: background (forecast) error covariances

$\mathbf{R} = \langle \varepsilon_o \varepsilon_o^T \rangle$: observational error covariances

## The variational problem

**Bayes' Theorem:** $$p(\mathbf{x} \mid \mathbf{y}) = \frac{p(\mathbf{y} \mid \mathbf{x}) P(\mathbf{x})}{P(\mathbf{y})}$$

- **Example:**
  - Observation and background error have Gaussian distributions

$$p(\mathbf{y} \mid \mathbf{x}) = \frac{1}{C_3} \exp\left\{ -\frac{1}{2} (\mathbf{y} - \mathbf{H}(\mathbf{x}))^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{H}(\mathbf{x})) \right\}$$

$$P(\mathbf{x}) = \frac{1}{C} \exp\left\{ -\tfrac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) \right\}$$

  - $p(\mathbf{y}|\mathbf{x})$ is Gaussian only if **H** is linear
  - Maximum likelihood estimate (mode of the distribution):

$$J(\mathbf{x}) = -\ln p(\mathbf{x} \mid \mathbf{y})$$
$$= \tfrac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + \tfrac{1}{2} (\mathbf{H}(\mathbf{x}) - \mathbf{y})^T \mathbf{R}^{-1} (\mathbf{H}(\mathbf{x}) - \mathbf{y})$$

- Reducing $J(\mathbf{x})$ implies an increase in the probability of **x** being the true value

Analysis: $\mathbf{X_a} = \mathbf{X}_b + \mathbf{K}(\mathbf{y} - \mathbf{HX_b})$

Weights that lead to the minimum variance estimate

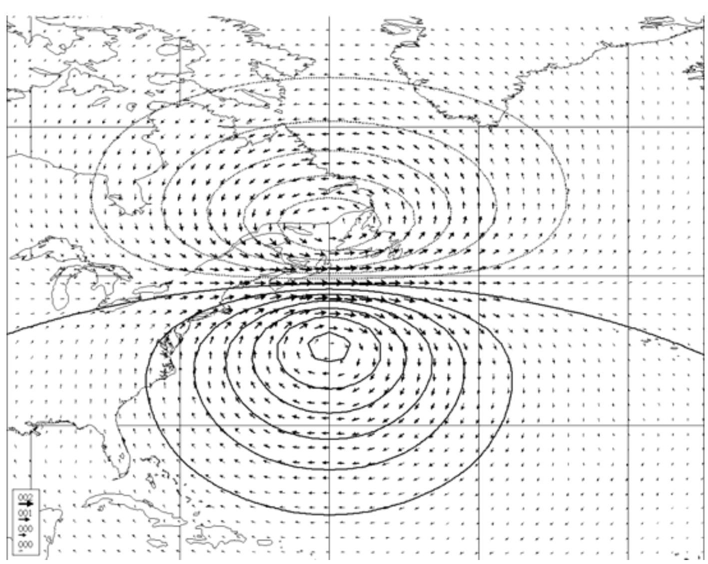
$$\mathbf{K} = \mathbf{BH}^T(\mathbf{R} + \mathbf{HBH}^T)^{-1}$$

- Response to the assimilation of a single observation of *u*

$$\mathbf{BH}^T = \begin{pmatrix} \langle \mathbf{uu}^t \rangle & \langle \mathbf{uv}^t \rangle & \langle \mathbf{u}T^t \rangle & \langle \mathbf{u}p_s{}^t \rangle \\ \langle \mathbf{vu}^t \rangle & \langle \mathbf{vv}^t \rangle & \langle \mathbf{v}T^t \rangle & \langle \mathbf{v}p_s{}^t \rangle \\ \langle T\mathbf{u}^t \rangle & \langle T\mathbf{v}^t \rangle & \langle TT^t \rangle & \langle Tp_s{}^t \rangle \\ \langle p_s\mathbf{u}^t \rangle & \langle p_s\mathbf{v}^t \rangle & \langle p_sT^t \rangle & \langle p_s p_s{}^t \rangle \end{pmatrix} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

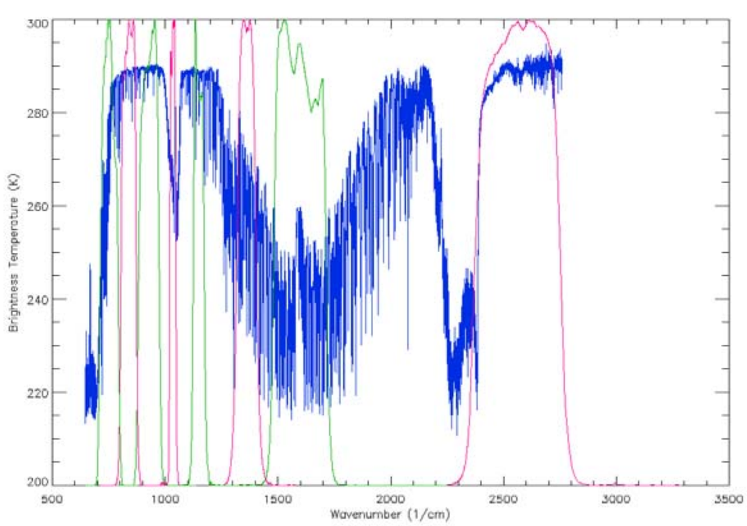
- Dynamical couplings exist between those variables

Wind and geopotential analysis corrections obtained in response to a single observation of the zonal wind component located at 265 hPa in the Northern extra-Tropics (45N-60W) (Gauthier *et al.,* 1998)



# Observation operator **H**

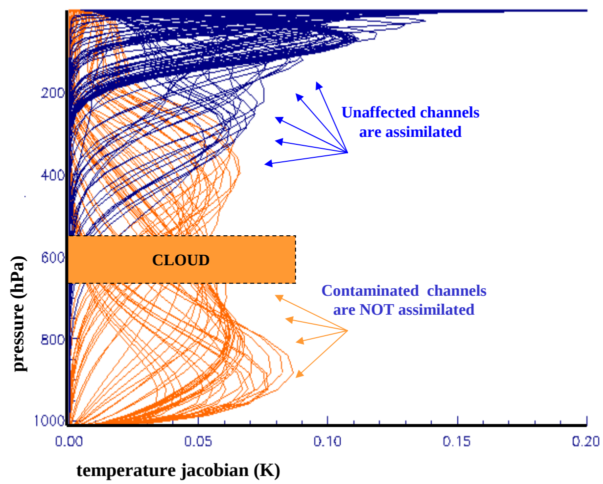
- Link between
  - model variable
    (e.g., Temperature, humidity, ozone) and the
  - observed quantity
    (e.g, radiance emitted at a given wavelength $\lambda$)




Spectrum showing IASI brightness temperature measured by IASI (in blue) and spectral response functions from several SEVIRI channels (red and green). If expressed in wavelengths, the range corresponds to 36 to 167 mm. (from Hewison and König, 2008)

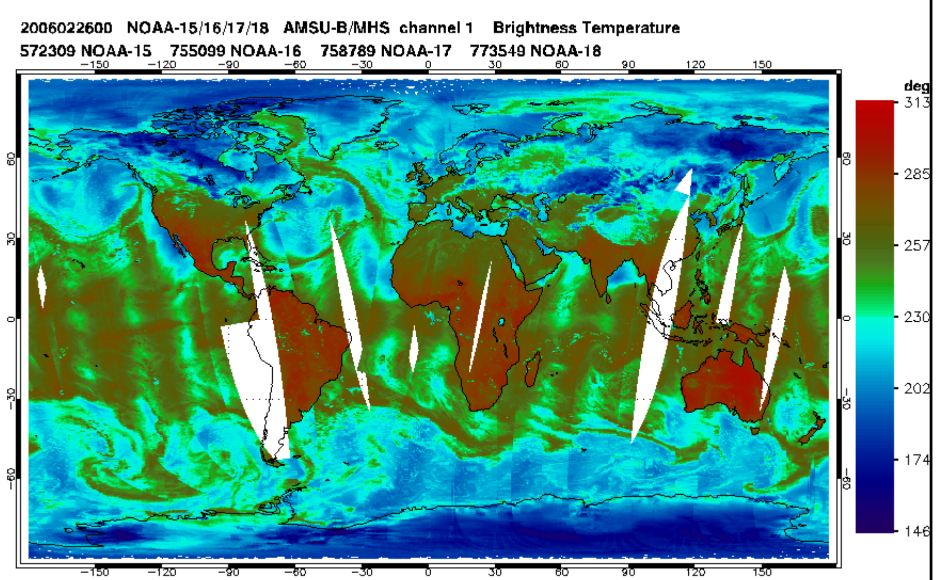
# Cloud detection

ECMWF scheme
(McNally & Watts, 2001)

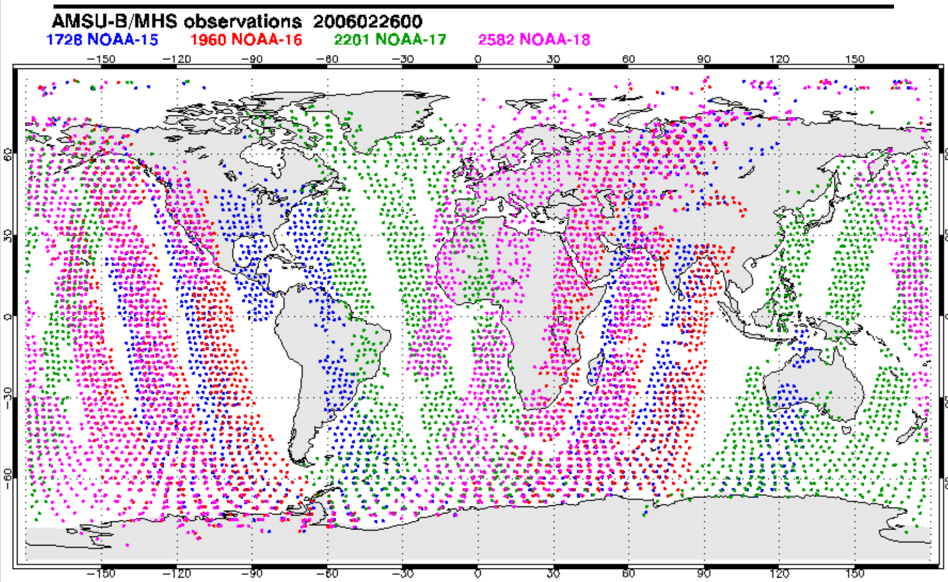



Credits to T. McNally, ECMWF

# AMSU-B Data received – February 2006, 00Z



## Distribution of ATOVS (AMSU-b) satellite data assimilated over a 6h period




## Selection of IASI channels in sensitive areas (Fourrié and Rabier, 2003)

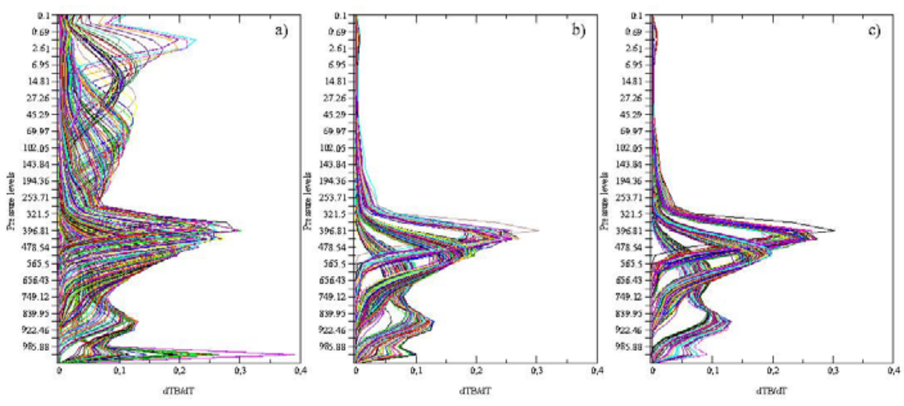
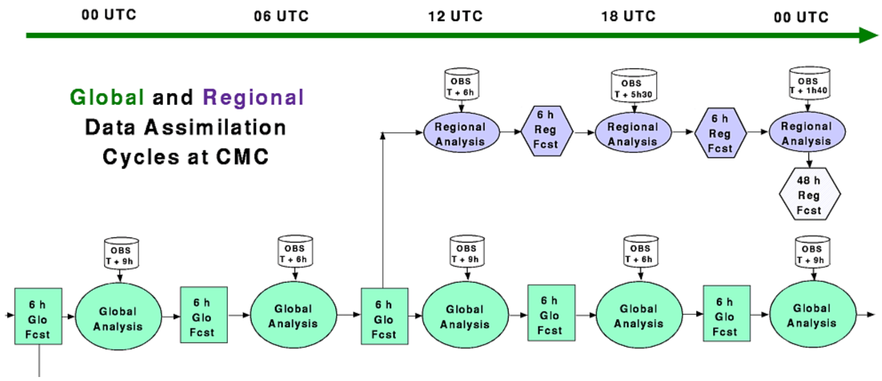



Figure 6. Jacobians (i.e. derivative of the brightness temperature with respect to the temperature at the different levels of the radiative transfer model) of the 300 channels selected by the channel selection methods based on different criteria: Entropy Reduction (a), sensitivity to observations (b) and Kalman Filter Sensitivity (c). The y-axis varies from 1013.15 hPa to 0.1 hPa.

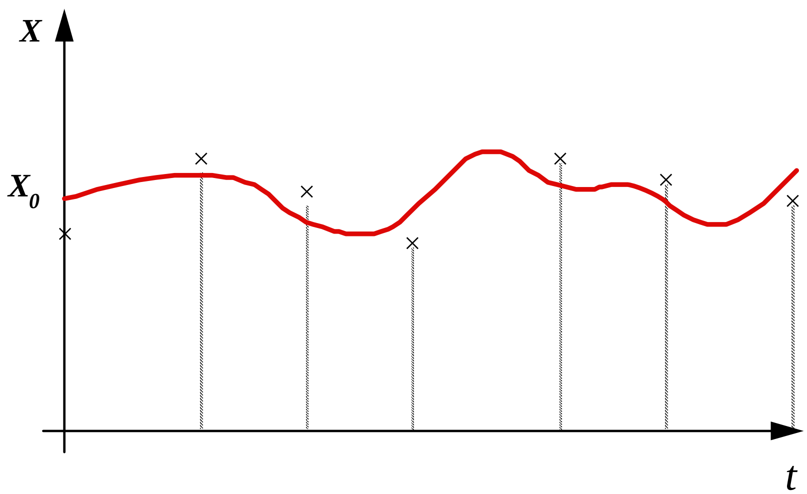
# Data assimilation cycle




# Data assimilation cycle

- Analysis contains the information gained from the observations used
- Forecast uses this analysis as initial conditions
  - Transport of information in both time and space
- Background field (model forecast)
  - cumulates our prior knowledge of the atmospheric state gained from the assimilation of past information

4D variational data assimilation (4D-Var)




## Preconditioning through change of variable

Definition:

$$\xi = \mathbf{B}^{-1/2}\delta\mathbf{x} = \mathbf{B}^{-1/2}(\mathbf{X} - \mathbf{X}_b)$$

$$\delta\mathbf{x} = \mathbf{B}^{1/2}\xi \equiv \mathbf{G}\,\xi$$

Cost Function: $\boxed{J(\xi) = \frac{1}{2}\xi^T\xi + \frac{1}{2}(\mathbf{H}'\mathbf{G}\xi - y')^T\mathbf{R}^{-1}(\mathbf{H}'\mathbf{G}\xi - y')}$

- **Extension to 4D**: observation operator now includes a model integration from time $t_0$ to $t_i$, the observation time: **H** $\rightarrow$ **H** M

**Propagator**: $\delta\mathbf{x}(t_i) = M(t_0,t_i)\,\delta\mathbf{x}(t_0)$

(Gauthier *et al., 2007*)

## 4D Variational Data Assimilation

- Definition of a measure of observation departure

$$J(\mathbf{X}_0) = \sum_{i=0}^{N} \left\langle \mathbf{H}_i(\mathbf{X}(t_i)) - \mathbf{y}_i, \mathbf{H}_i(\mathbf{X}(t_i)) - \mathbf{y}_i \right\rangle$$

  – Here $\langle \mathbf{f}, \mathbf{g} \rangle = \mathbf{f}^T \mathbf{R}^{-1} \mathbf{g}$ .

- The discretized form of inner product can be written as

$$\langle F, G \rangle = F^T \mathbf{Q} G$$

- Variation of the cost function (or *functional*) J($X_0$):

$$\delta J(\mathbf{X}_0) = J(\mathbf{X}_0 + \delta\mathbf{X}_0) - J(\mathbf{X}_0) \cong \langle \delta\mathbf{X}_0, \nabla J(\mathbf{X}_0) \rangle$$

## Definition and properties of an adjoint operator

- Definition of $H^*$ depends on the norm used:

$$\langle f, \mathbf{H} g \rangle = \langle \mathbf{H}^* f, g \rangle$$
$$f^T \mathbf{Q}\mathbf{H}\, g = (\mathbf{H}^* f)^T \mathbf{Q}\, g$$
$$\mathbf{H}^* = (\mathbf{Q}\mathbf{H}\mathbf{Q}^{-1})^T = \mathbf{Q}^{-1}\mathbf{H}^T\mathbf{Q}$$

- Case where $\mathbf{Q} = \mathbf{I}_d$: $\mathbf{H}^* = \mathbf{H}^T$
- **H** must be a linear operator

- **Properties**:
  - If **C** = **AB** then, $\mathbf{C}^* = \mathbf{B}^* \mathbf{A}^*$
  - An adjoint can be obtained by composing the adjoints of simpler operators

## Computation of the gradient using the adjoint model

- Variation of the functional

$$\delta J(\mathbf{X}_0) \cong 2\sum_{i=0}^{N}\left\langle \mathbf{H}_i^{'}\delta\mathbf{X}(t_i), \left(\mathbf{H}_i\left(\mathbf{X}(t_i)\right)-\mathbf{y}_i\right)\right\rangle = 2\sum_{i=0}^{N}\left\langle \mathbf{H}_i^{'}R(t_0,t_i)\delta\mathbf{X}_0, \left(\mathbf{H}_i\left(\mathbf{X}(t_i)\right)-\mathbf{y}_i\right)\right\rangle$$

$$= 2\sum_{i=0}^{N}\left\langle \delta\mathbf{X}_0, R^*(t_0,t_i)\mathbf{H}_i^{'*}\left(\mathbf{H}_i\left(\mathbf{X}(t_i)\right)-\mathbf{y}_i\right)\right\rangle = \left\langle \delta\mathbf{X}_0, 2\sum_{i=0}^{N}R^*(t_0,t_i)\mathbf{H}_i^{'*}\left(\mathbf{H}_i\left(\mathbf{X}(t_i)\right)-\mathbf{y}_i\right)\right\rangle$$

with $\mathbf{H}_i' = (\partial\mathbf{H}_i/\partial\mathbf{X})(\mathbf{X}(t_i))$, the Jacobian of **H** evaluated at $\mathbf{X}(t_i)$

- **Expression for the gradient**

$$\nabla_{\mathbf{X}_0} J(\mathbf{X}_0) = 2\sum_{i=0}^{N} R^*(t_0,t_i)\left[\mathbf{H}'^*(\mathbf{H}\mathbf{X}(t_i)-\mathbf{y}_i)\right]$$

- **Need an expression for the adjoint of the propagator of the TLM**

## Tangent Linear model and Adjoint Model (LeDimet and Talagrand, 1986)

* **Direct Model** : $\dfrac{d\mathbf{X}}{dt} = \mathbf{F}(\mathbf{X})$

* **Tangent Linear Model :** $\dfrac{d\delta\mathbf{X}}{dt} = \left(\dfrac{\partial\mathbf{F}}{\partial\mathbf{X}}(\mathbf{X}_R(t))\right)\delta\mathbf{X}$

$$\equiv L\delta\mathbf{X}$$

* **Adjoint Model** : $\dfrac{d\delta^*\mathbf{X}}{dt} = -\left(\dfrac{\partial\mathbf{F}}{\partial\mathbf{X}}(\mathbf{X}_R(t))\right)^*\delta^*\mathbf{X}$

$$\equiv -L^*\delta^*\mathbf{X}$$

# Example: the Lorenz (1963) model

- Direct Model

$$\frac{dX}{dt} = \sigma(-X + Y),$$
$$\frac{dY}{dt} = -XZ + rX - Y,$$
$$\frac{dZ}{dt} = XY - bZ,$$

- Tangent Linear Model (TLM)

$$\frac{d}{dt}\begin{pmatrix}\delta X\\ \delta Y\\ \delta Z\end{pmatrix} = \begin{pmatrix}-\sigma & +\sigma & 0\\ -Z_R(t)+r & -1 & -X_R(t)\\ Y_R(t) & X_R(t) & -b\end{pmatrix}\begin{pmatrix}\delta X\\ \delta Y\\ \delta Z\end{pmatrix}$$

- Adjoint Model

$$\frac{d}{dt}\begin{pmatrix}\delta^* X\\ \delta^* Y\\ \delta^* Z\end{pmatrix} = -\begin{pmatrix}-\sigma & -Z_R(t)+r & Y_R(t)\\ +\sigma & -1 & X_R(t)\\ 0 & -X_R(t) & -b\end{pmatrix}\begin{pmatrix}\delta X\\ \delta Y\\ \delta Z\end{pmatrix}$$

# Adjoint of the propagator $R(t_0,t_i)$ of the TLM

- **Computation of the gradient lead to**

$$\langle \delta\mathbf{X}(t_i), \mathbf{Z}(t_i)\rangle = \langle R(t_0,t_i)\delta\mathbf{X}_0, \mathbf{Z}(t_i)\rangle = \langle \delta\mathbf{X}_0, R^*(t_0,t_i)\mathbf{Z}(t_i)\rangle$$

- **Property**

$$\frac{d}{dt}\langle \delta\mathbf{X}(t), \delta^*\mathbf{X}(t)\rangle = \left\langle \frac{d\delta\mathbf{X}(t)}{dt}, \delta^*\mathbf{X}(t)\right\rangle + \left\langle \delta\mathbf{X}(t), \frac{d}{dt}\delta^*\mathbf{X}(t)\right\rangle$$
$$= \langle \mathbf{L}\delta\mathbf{X}, \delta^*\mathbf{X}\rangle - \langle \delta\mathbf{X}(t), \mathbf{L}^*\delta^*\mathbf{X}\rangle$$
$$= 0$$
$$\langle \delta\mathbf{X}(t), \delta^*\mathbf{X}(t)\rangle = \langle \delta\mathbf{X}(t_0), \delta^*\mathbf{X}(t_0)\rangle$$

- **Propagator associated with the adjoint model: $S(t_0,t)$**

$$\langle \delta\mathbf{X}(t_0), S(t,t_0)\delta^*\mathbf{X}(t)\rangle = \langle \delta\mathbf{X}(t_0), \delta^*\mathbf{X}(t_0)\rangle = \langle \delta\mathbf{X}(t), \delta^*\mathbf{X}(t)\rangle$$
$$= \langle R(t_0,t)\delta\mathbf{X}(t_0), \delta^*\mathbf{X}(t)\rangle$$
$$= \langle \delta\mathbf{X}(t_0), R^*(t_0,t)\delta^*\mathbf{X}(t)\rangle$$

- **$R^*(t_0,t) = S(t,t_0)$ = backward integration of the adjoint model**

## Steps involved in one iteration of 4D-Var

- Integration of the direct model and evaluation of the functional

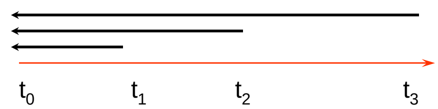
$$J(\mathbf{X}_0) = \sum_{i=0}^{N} \langle \mathbf{HX}(t_i) - \mathbf{y}_i, \mathbf{HX}(t_i) - \mathbf{y}_i \rangle$$

  - Retain the *trajectory* obtained from this integration which defines the coefficients of the adjoint model

- Evaluation of the gradient of the cost function from a backward integration of the adjoint model from $t_i \rightarrow t_0$.

$$\nabla_{\mathbf{X}_0} J(\mathbf{X}_0) = \sum_{i=0}^{N} R^*(t_0, t_i) \left[ \mathbf{H}^* (\mathbf{HX}(t_i) - \mathbf{y}_i) \right]$$

Backward integration of the adjoint model

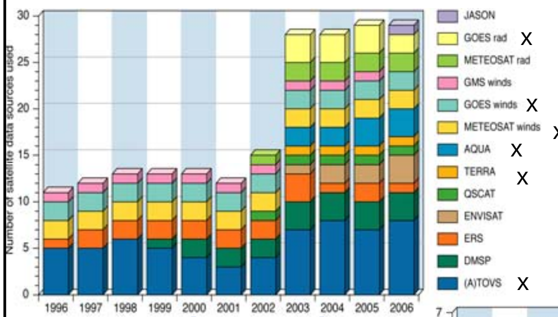



## **Computational cost**

- Minimization of 4D-Var with a preconditioned conjugate gradient or quasi-newton algorithm
  - Algorithm is based on orthogonalization within the Krylov subspace
  - Convergence can be reached with reasonable accuracy in less than a 100 iterations (200 model integrations of 6-h)
  - One hour of wall-clock time with 200 CPUs

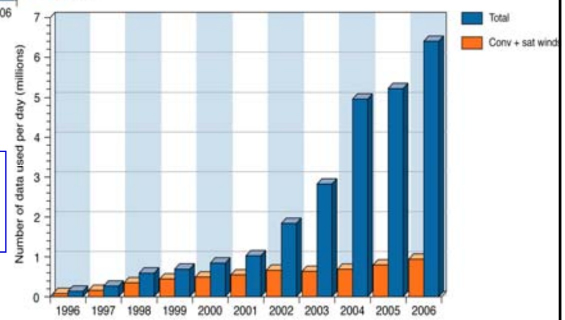
Data from twenty-eight sources used daily

Courtesy of J.-N. Thépaut
ECMWF




X = assimilated at MSC

**Large increase in number of data used daily**

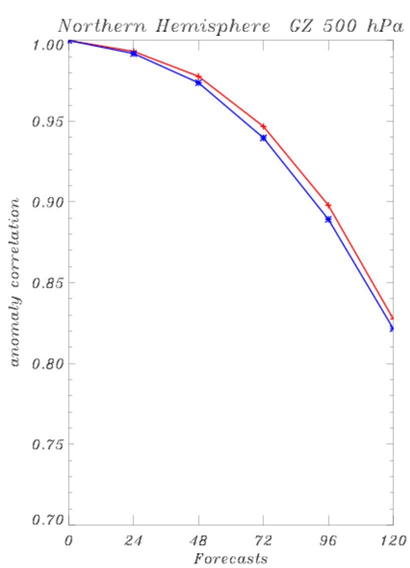


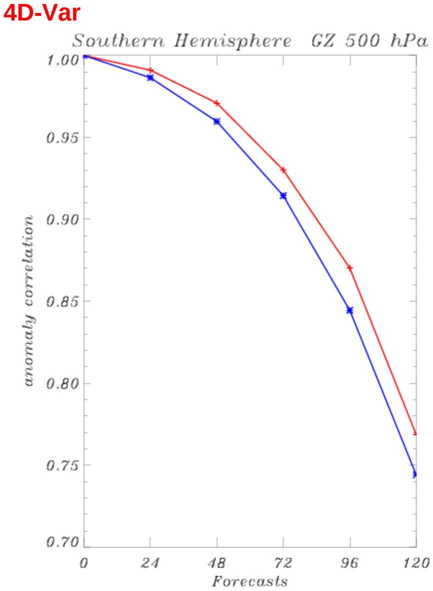

Use of satellite data today at ECMWF

# Anomaly correlation: NH winter

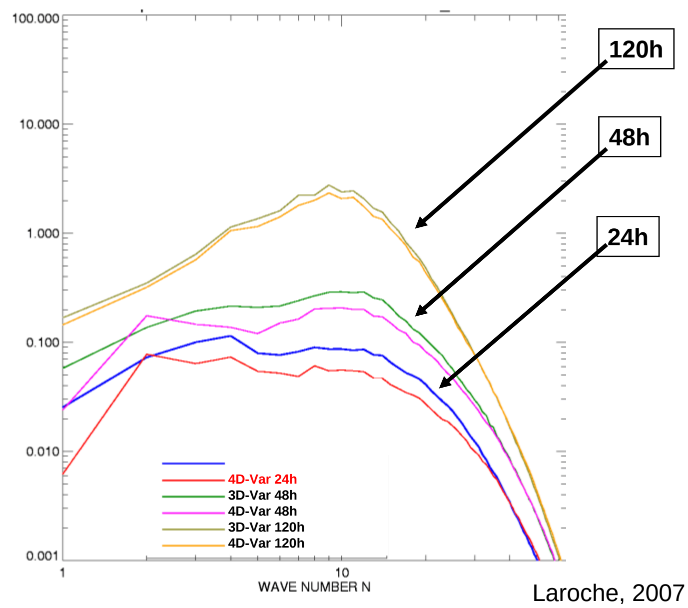
Laroche, 2007

**3D-Var**
**4D-Var**



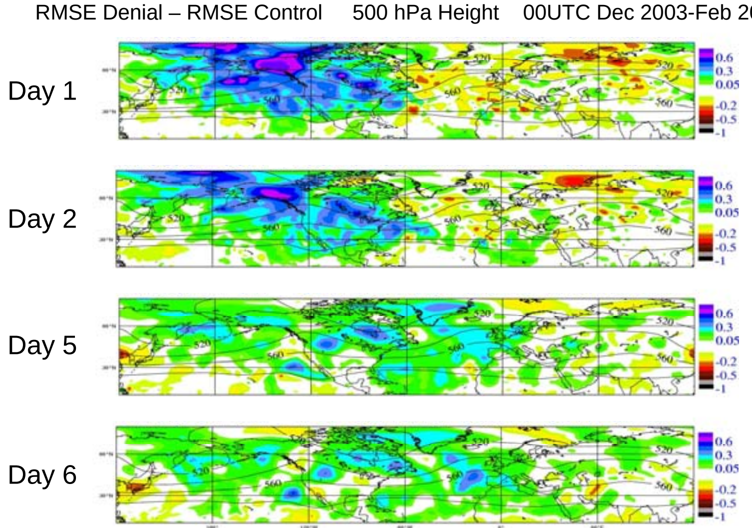
## Erreur spectrum GZ 500 hPa (summer 2003)




Laroche, 2007

## Impact of denying observations over the Pacific on forecasts of increasing length in 3D-VAR

RMSE Denial – RMSE Control 500 hPa Height 00UTC Dec 2003-Feb 2004




Kelly et al. 2007, *QJRMS*

***…signal becomes global and diffused in the medium range***

Impact of denying observations over the Pacific
on forecasts of increasing length in **4D-VAR**

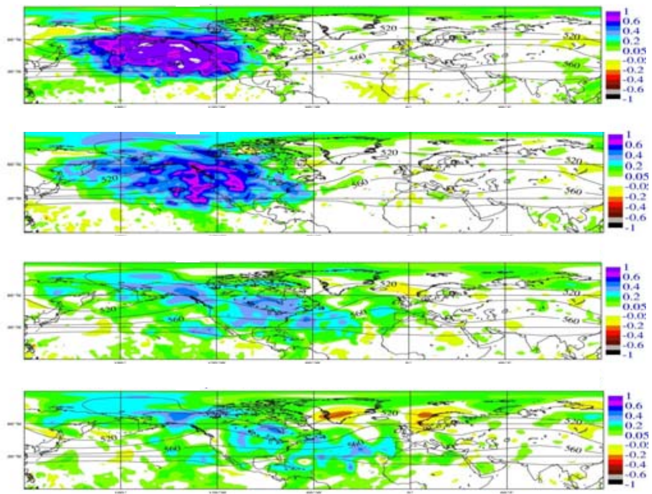
RMSE Denial – RMSE Control     500 hPa Height     00UTC Dec 2003-Feb 2004

Day 1

Day 2

Day 5

Day 6



Kelly et al. 2007, *QJRMS*

***…medium range signal is even weaker in 4D-VAR (but less diffused)***

## Application of the adjoint of a numerical model

- Singular vector decomposition (Lacarra and Talagrand, 1988)
  - Leading structure that identify perturbations in initial conditions that would lead to the most significant error growth at a given lead time

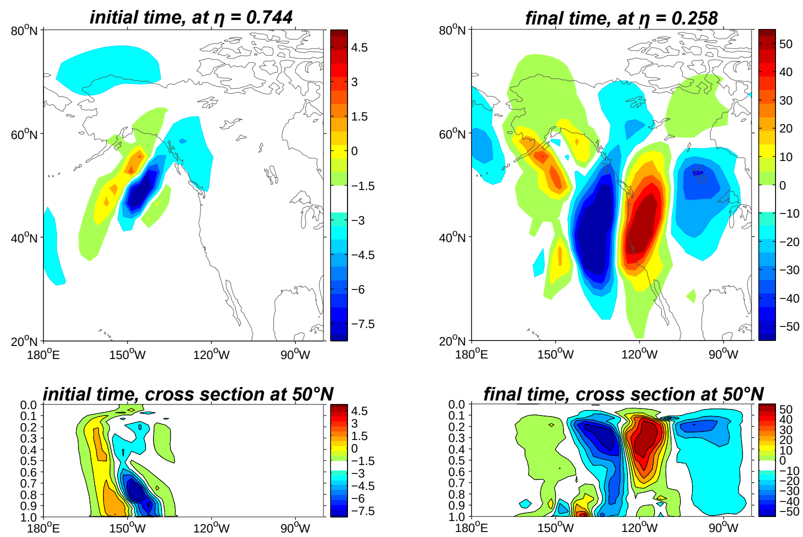
$$\langle \delta\mathbf{X}(t), \delta\mathbf{X}(t) \rangle = \langle L\,\delta\mathbf{X}_0, L\,\delta\mathbf{X}_0 \rangle = \langle L^* L\,\delta\mathbf{X}_0, \delta\mathbf{X}_0 \rangle$$

$$L^* L \mathbf{v}_k = \lambda_k \mathbf{v}_k$$

  - Eigenvalue problem can be solved with a Lanczos algorithm (does not require the explicit form of $L^*L$)

## Meridional wind structure of the leading SV

**(energy amplification factor = 60.4)**




Mahidjiba *et al.* (2006)

# Conclusion

- Information about the atmosphere and its evolution is gathered from both numerical models that include increasingly complex physical processes
- Observations of the Earth are needed to validate our models and to evaluate the current state of the Earth system (atmosphere, oceans, ice, land)
- Data assimilation methods have evolved enormously over the last two decades and have made it possible to make use of the large volume of satellite data
- Significant research is focused on improving the models, and the assimilation methods
- All these areas bring up significant mathematical challenges to lead to accurate and efficient algorithms to solve these problems