Sorbonne Université Université Paris-Saclay

Master 2 Sciences de l'Océan, de l'Atmosphère et du Climat (SOAC) Parcours Météorologie, Océanographie, Climat et Ingénierie pour les Observations Spatiales (MOCIS)

Master 2 Water, Air, Pollution and Energy at local and regional scales (WAPE)

Année 2019-2020

Course Introduction to data assimilation

From numerical modelling to data assimilation

Olivier Talagrand

7 January 2020

- What is assimilation ?
 - Numerical weather prediction. Principles and performances
 - Definition of initial conditions
- Bayesian Estimation
- One first step towards assimilation : 'Optimal Interpolation'
- The temporal dimension : Kalman Filter and Variational Assimilation



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Fig. 1: Members of day 7 forecast of 500 hPa geopotential height for the ensemble originated from 25 January 1993.

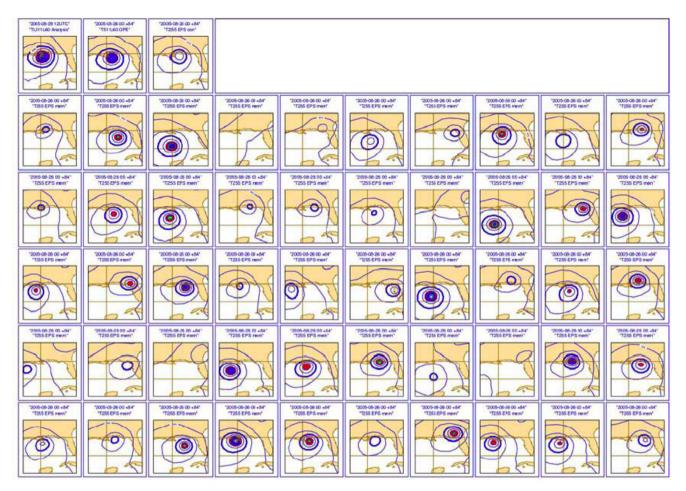


Figure 6 Hurricane Katrina mean-sea-level-pressure (MSLP) analysis for 12 UTC of 29 August 2005 and t+84h high-resolution and EPS forecasts started at 00 UTC of 26 August:

1st row: 1st panel: MSLP analysis for 12 UTC of 29 Aug 2nd panel: MSLP t+84h T_L511L60 forecast started at 00 UTC of 26 Aug 3rd panel: MSLP t+84h EPS-control T_L255L40 forecast started at 00 UTC of 26 Aug Other rows: 50 EPS-perturbed T_L255L40 forecast started at 00 UTC of 26 Aug.

The contour interval is 5 hPa, with shading patters for MSLP values lower than 990 hPa.

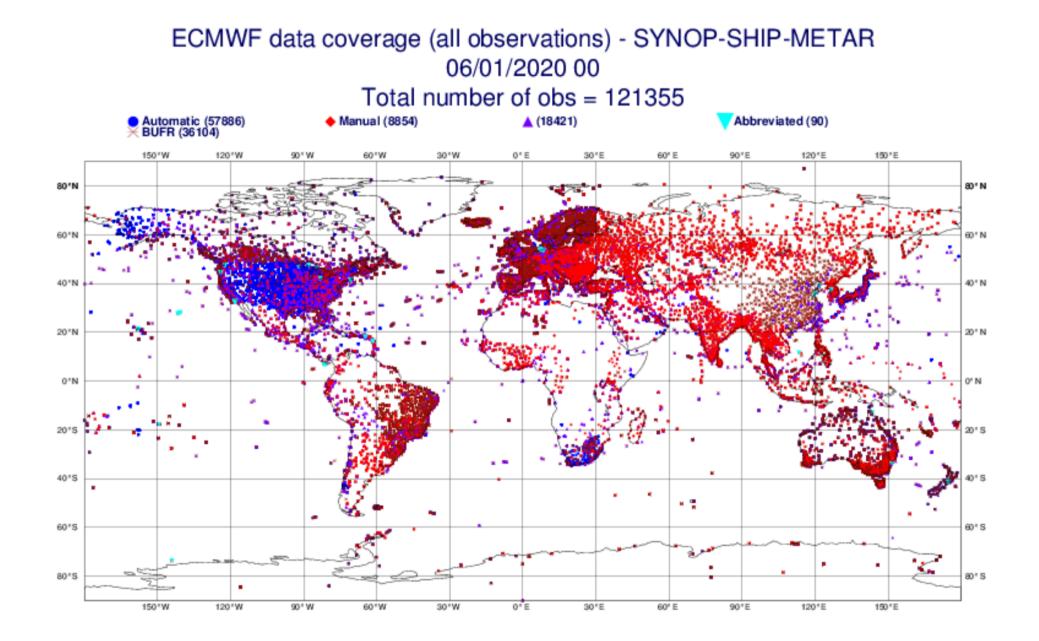
ECMWF, Technical Report 499, 2006

Pourquoi les météorologistes ont-ils tant de peine à prédire le temps avec quelque certitude ? Pourquoi les chutes de pluie, les tempêtes elles-mêmes nous semblent-elles arriver au hasard, de sorte que bien des gens trouvent tout naturel de prier pour avoir la pluie ou le beau temps, alors qu'ils jugeraient ridicule de demander une éclipse par une prière ? Nous voyons que les grandes perturbations se produisent généralement dans les régions où l'atmosphère est en équilibre instable. Les météorologistes voient bien que cet équilibre est instable, qu'un cyclone va naître quelque part ; mais où, ils sont hors d'état de le dire ; un dixième de degré en plus ou en moins en un point quelconque, le cyclone éclate ici et non pas là, et il étend ses ravages sur des contrées qu'il aurait épargnées. Si on avait connu ce dixième de degré, on aurait pu le savoir d'avance, mais les observations n'étaient ni assez serrées, ni assez précises, et c'est pour cela que tout semble dû à l'intervention du hasard.

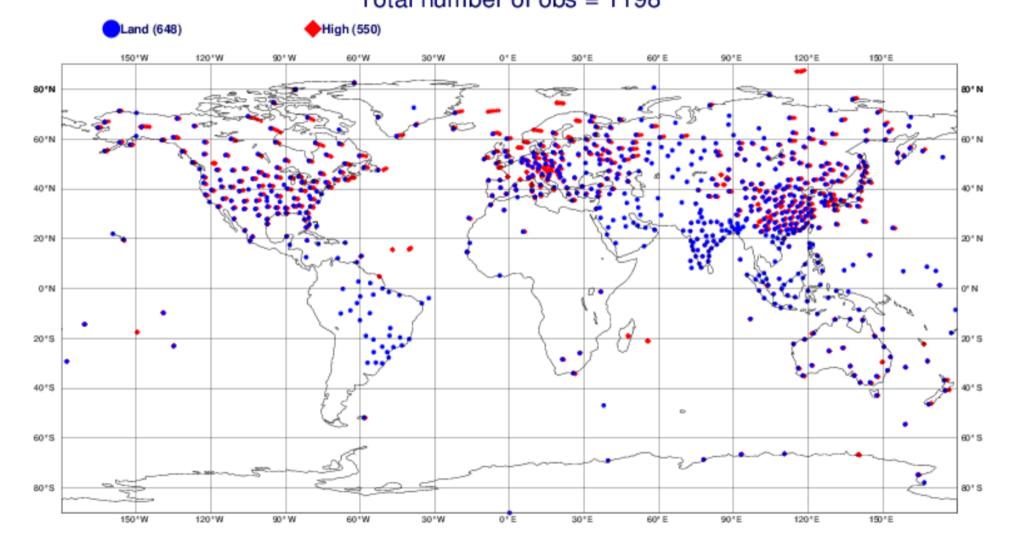
H. Poincaré, Science et Méthode, Paris, 1908

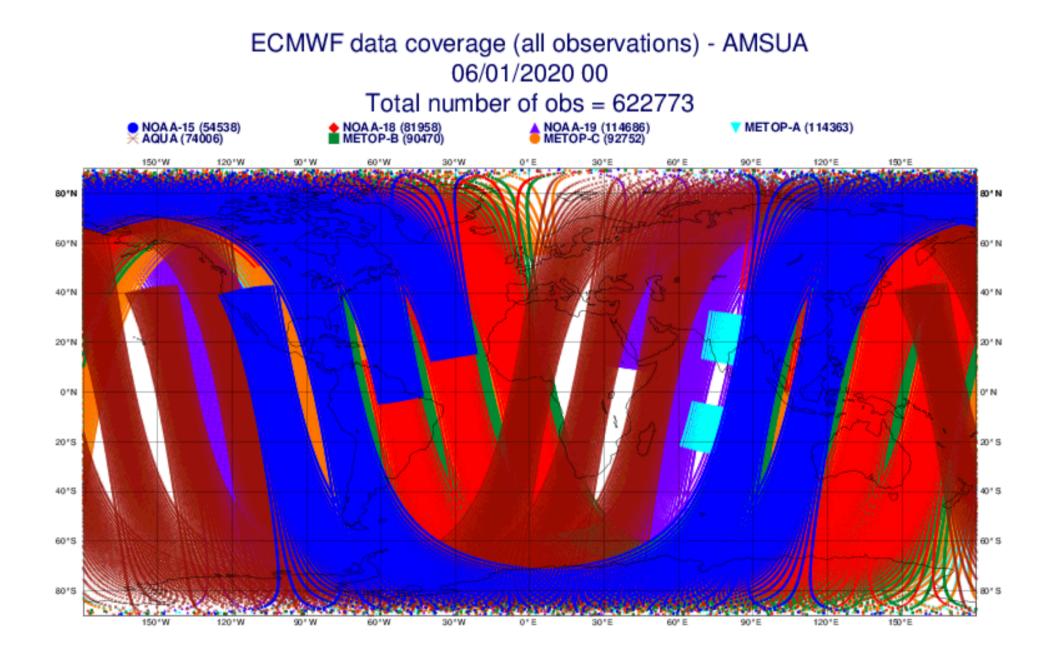
Why have meteorologists such difficulty in predicting the weather with any certainty? Why is it that showers and even storms seem to come by chance, so that many people think it quite natural to pray for rain or fine weather, though they would consider it ridiculous to ask for an eclipse by prayer? We see that great disturbances are generally produced in regions where the atmosphere is in unstable equilibrium. The meteorologists see very well that the equilibrium is unstable, that a cyclone will be formed somewhere, but exactly where they are not in a position to say; a tenth of a degree more or less at any given point, and the cyclone will burst here and not there, and extend its ravages over districts it would otherwise have spared. If they had been aware of this tenth of a degree they could have known it beforehand, but the observations were neither sufficiently comprehensive nor sufficiently precise, and that is the reason why it all seems due to the intervention of chance.

> H. Poincaré, *Science et Méthode*, Paris, 1908
> (English transl. by F. Maitland, *Science and Method*, T. Nelson and Sons, London, 1914)

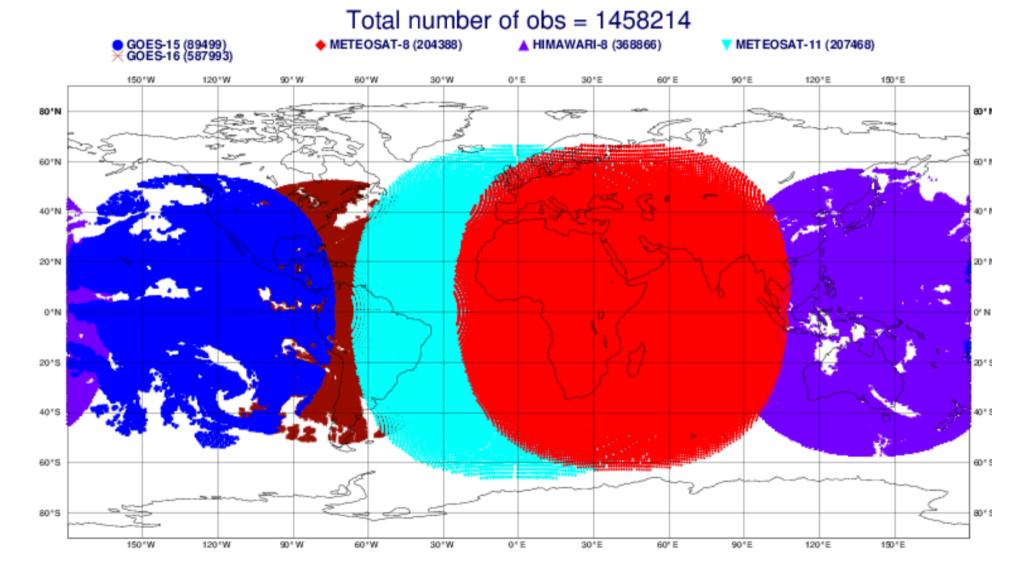


ECMWF data coverage (all observations) - RADIOSONDE 06/01/2020 00 Total number of obs = 1198

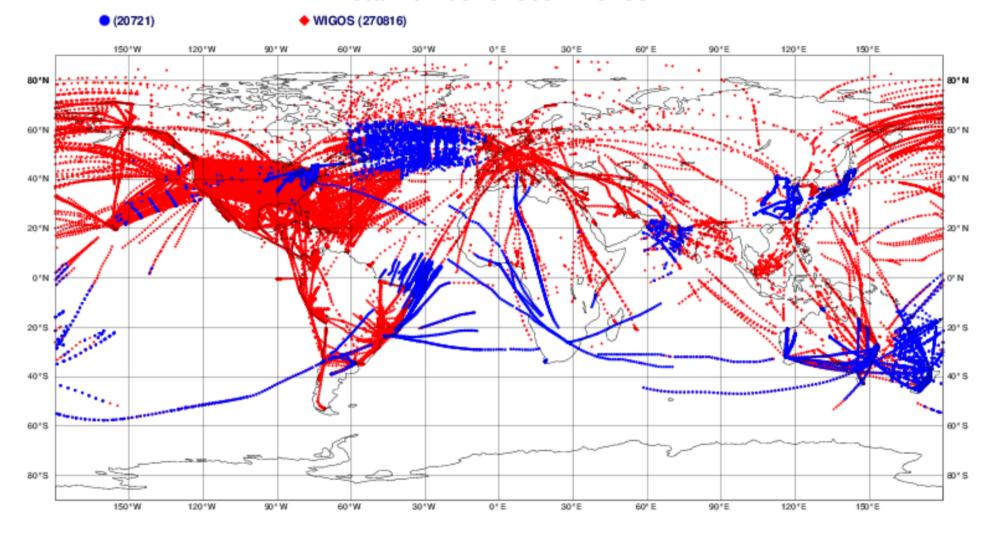


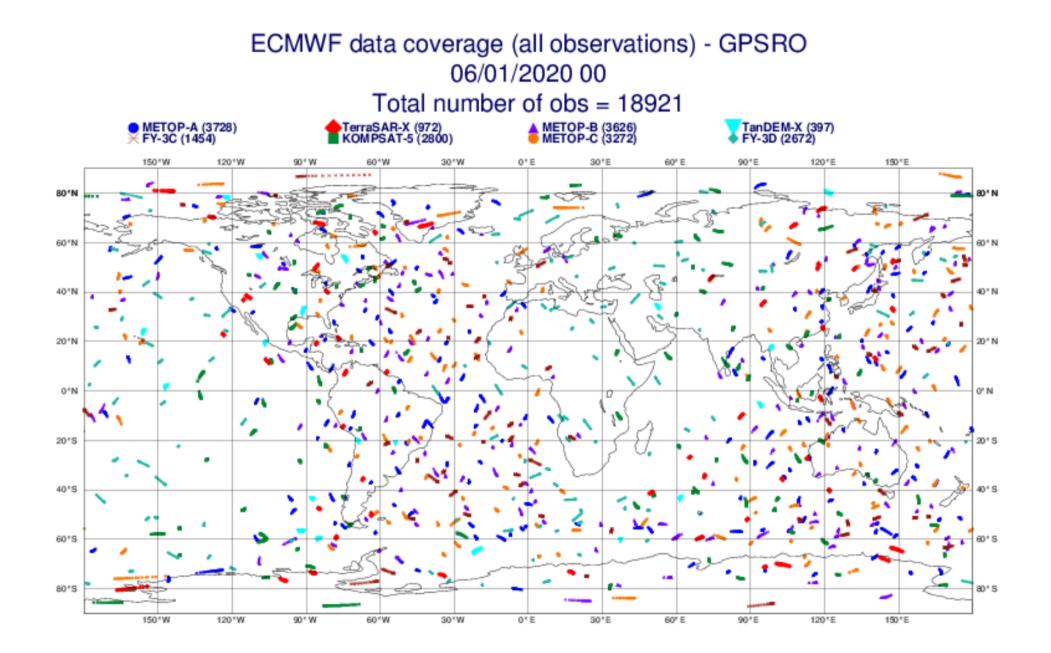


ECMWF data coverage (all observations) - GEOSTATIONARY RADIANCES 06/01/2020 00

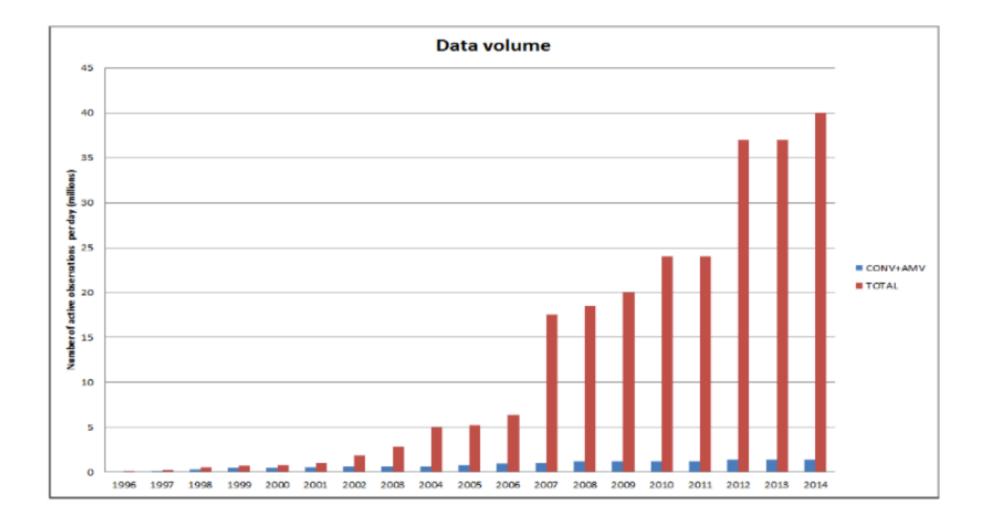


ECMWF data coverage (all observations) - AIRCRAFT 06/01/2020 00 Total number of obs = 291537





ECMWF



Satellite **ADM-Aeolus** was launched on August 22 2018. It carries a Lidar-Doppler instrument, called Aladin (Atmospheric LAser Doppler Instrument), that measures the wind in the volume of the atmosphere. Preliminary tests have shown that these new observations have a positive impact on the quality of the previsions, especially in the tropics and in the Southern Hemisphere.

- *Synoptic* observations (ground observations, radiosonde observations), performed simultaneously, by international agreement, in all meteorological stations around the world (00:00, 06:00, 12:00, 18:00 UTC), and are in practice concentrated over continents.
- Asynoptic observations (satellites, aircraft), performed more or less continuously in time.
- *Direct* observations (temperature, pressure, horizontal components of the wind, moisture), which are local and bear on the variables used for describing the flow in numerical models.
- *Indirect* observations (radiometric observations, ...), which bear on some more or less complex combination (most often, a one-dimensional spatial integral) of variables used for for describing the flow

$y = H(\boldsymbol{x})$

H : *observation operator* (for instance, radiative transfer equation)

Échantillonnage de la circulation océanique par les missions altimétriques sur 10 jours : combinaison Topex-Poséidon/ERS-1



S. Louvel, Doctoral Dissertation, 1999

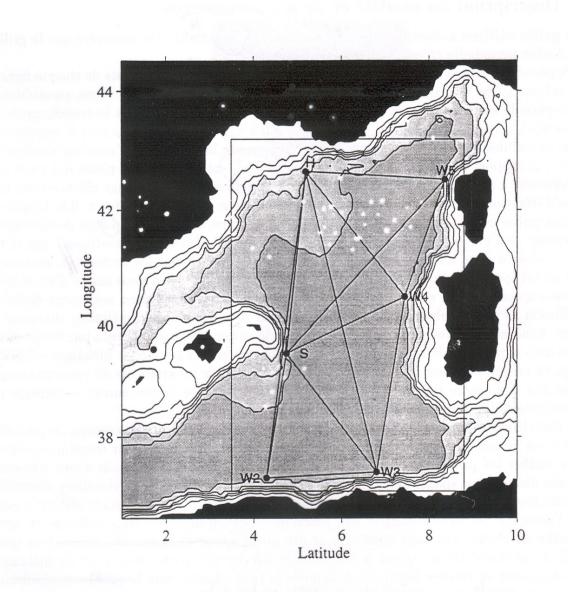


FIG. 1 – Bassin méditerranéen occidental: réseau d'observation tomographique de l'expérience Thétis 2 et limites du domaine spatial utilisé pour les expériences numériques d'assimilation.

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E. Rémy, Doctoral Dissertation, 1999

Physical laws governing the flow

Conservation of mass

 $D\rho/Dt + \rho \operatorname{div} U = 0$

- Conservation of energy $De/Dt - (p/\rho^2) D\rho/Dt = Q$
- Conservation of momentum $D\underline{U}/Dt + (1/\rho) \operatorname{grad} p - \underline{g} + 2 \underline{\Omega} \wedge \underline{U} = \underline{F}$
- Equation of state $f(p, \rho, e) = 0$ (for a perfect gas $p/\rho = rT$, $e = C_v T$)
- Conservation of mass of secondary components (water in the atmosphere, salt in the ocean, chemical species, ...) $Dq/Dt + q \operatorname{div} U = S$

These physical laws must be expressed in practice in discretized (and necessarily imperfect) form, both in space and time \Rightarrow *numerical model* 18

Parlance of the trade :

- Adiabatic and inviscid, and therefore thermodynamically reversible, processes (everything except Q, <u>F</u> and <u>S</u>) make up 'dynamics'
- Processes described by terms Q, <u>F</u> and <u>S</u> make up 'physics'

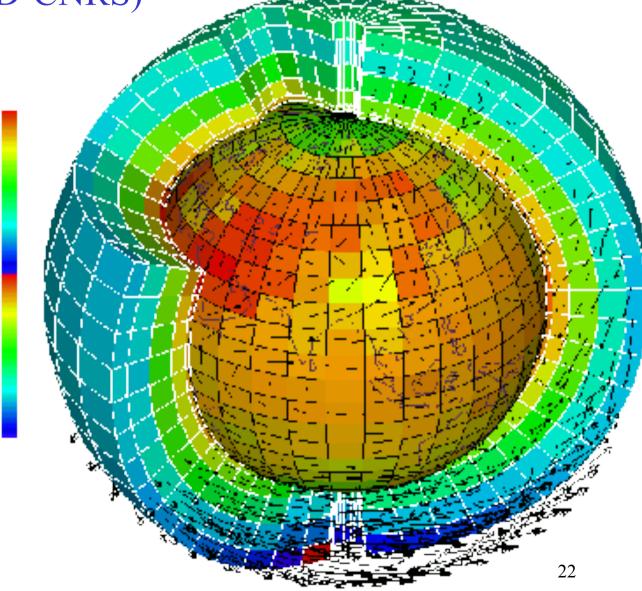
- All presently existing numerical models are built on simplified forms of the general physical laws. Global numerical models, used either for large-scale meteorological prediction or for climate simulation, are at present built on the so-called *primitive equations*. Those equations rely on several approximations, the most important of which being the *hydrostatic approximation*, which expresses balance, in the vertical direction, of the gravity and pressure gradient forces. This forbids explicit description of thermal convection, which must be parameterized in some appropriate way.
- More and more *limited-area models* have been developed over time. They require appropriate definition of lateral boundary conditions (not a simple problem). Most of them are non-hydrostatic, and therefore allow description of convection.

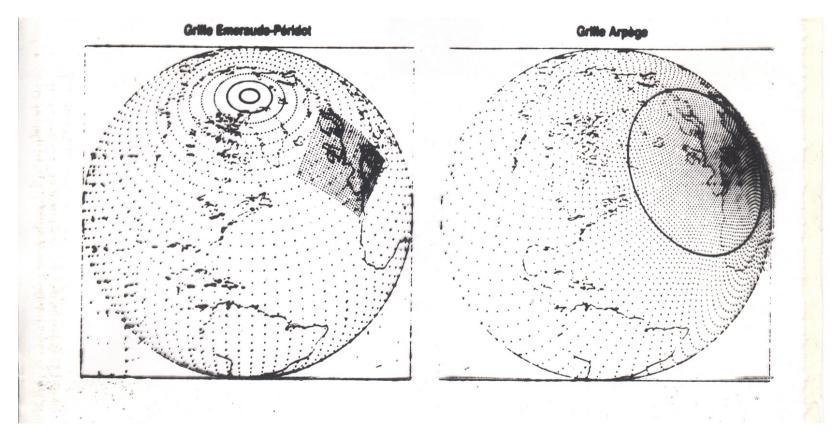
There exist at present two forms of discretization

- Gridpoint discretization
- (Semi-)spectral discretization (mostly for global models, and most often only in the horizontal direction)

Finite element discretization, which is very common in many forms of numerical modelling, is rarely used for modelling of the atmosphere. It is more frequently used for oceanic modelling, where it allows to take account of the complicated geometry of coast-lines.

Schematic of a gridpoint atmospheric model (L. Fairhead /LMD-CNRS)





The grids of two of the models of Météo-France (La Météorologie)

- In gridpoint models, meteorological fields are defined by values at the nodes of the grid. Spatial and temporal derivatives are expressed by finite differences.
- In spectral models, fields are defined by the coefficients of their expansion along a prescribed set of basic functions. In the case of global meteorological models, those basic functions are the *spherical harmonics* (eigenfunctions of the laplacian at the surface of the sphere).

Modèles (semi-)spectraux

 $T(\mu = \sin(\text{latitude}), \lambda = \text{longitude}) = \sum_{\substack{0 \le n < \infty \\ -n \le m \le n}} T_n^m Y_n^m(\mu, \lambda)$

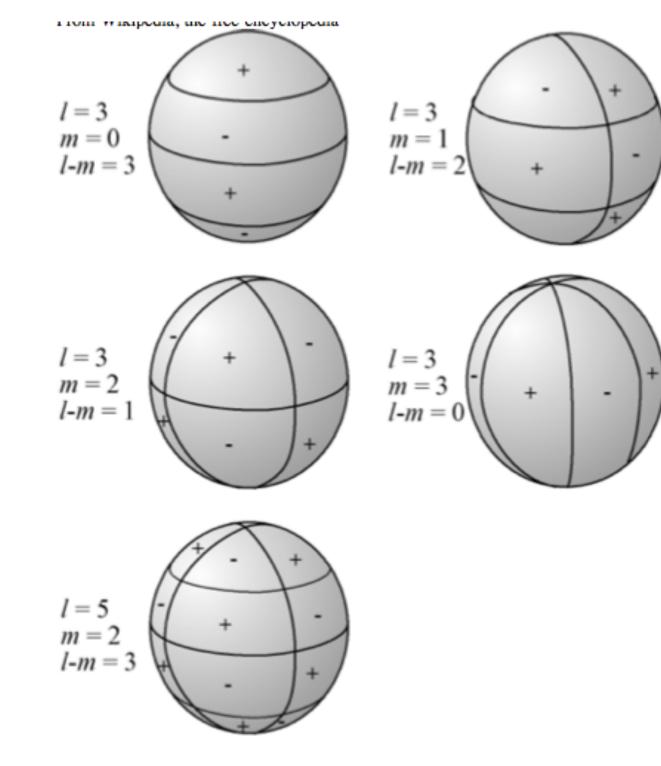
où les $Y_n^m(\mu,\lambda)$ sont les harmoniques sphériques

 $Y_n^m(\mu,\lambda) \propto P_n^m(\mu) \exp(im\lambda)$

 $P_n^m(\mu)$ est la *fonction de Legendre* de deuxième espèce.

$$P_n^m(\mu) \propto (1-\mu^2)^{\frac{m}{2}} \frac{d^{n+m}}{d\mu^{n+m}} (\mu^2 - 1)^n$$

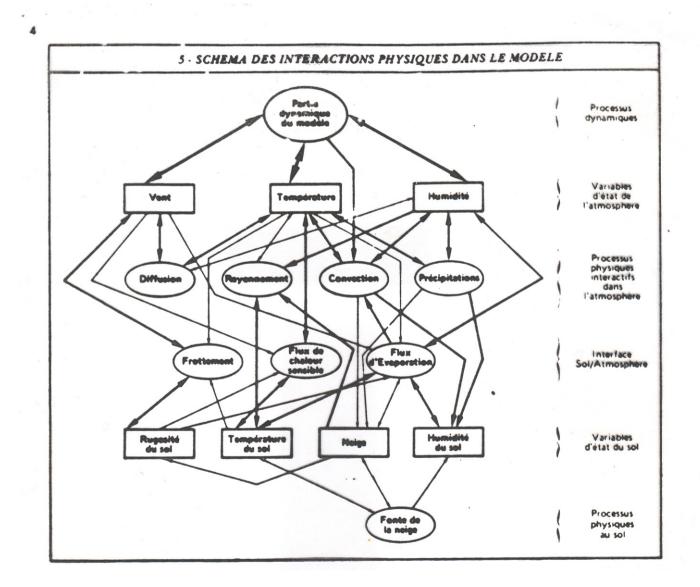
n et *m* sont respectivement le *degré* et l'*ordre* de l'harmonique $Y_n^m(\mu, \lambda)$



Linear operations, and in particular differentiation with respect to spatial variables, are performed in spectral space, while nonlinear operations and 'physical' computations (advection by the movement, diabatic heating and cooling, ...) are performed in gridpoint physical space. This requires constant transformations from one space to the other, which are made possible at an acceptable cost through the systematic use of Fast Fourier Transforms.

For that reason, those models are called *semi-spectral*.

- Numerical schemes have been progressively developed and validated for the 'dynamics' component of models, which are by and large considered now to work satisfactorily (although regular improvements are still being made).
- The situation is different as concerns 'physics', where many problems remain (as concerns for instance subgrid scales parameterization, the water cycle and the associated exchanges of energy, or the exchanges between the atmosphere and the underlying medium). 'Physics' as a whole remains the weaker point of models, and is still the object of active research.



Centre Européen pour les Prévisions Météorologiques à Moyen Terme (CEPMMT, Reading, GB)

(European Centre for Medium-range Weather Forecasts, ECMWF)

Modèle hydrostatique semi-spectral

Depuis mars 2016 :

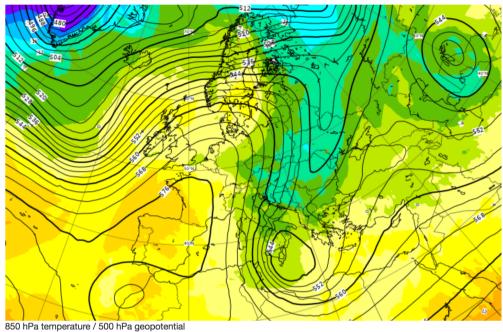
Troncature triangulaire TCO1279 / O1280 (résolution horizontale \approx 9 kilomètres)

137 niveaux dans la direction verticale (0 - 80 km)

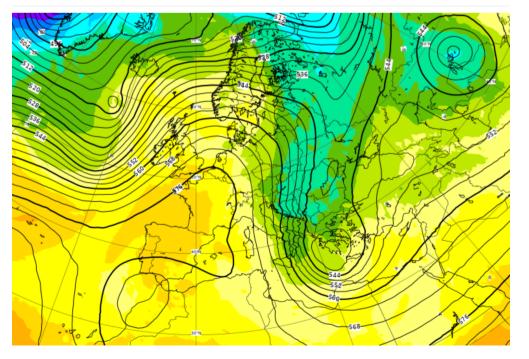
Discrétisation en éléments finis dans la direction verticale

Dimension du vecteur d'état correspondant $\approx 4.10^9$

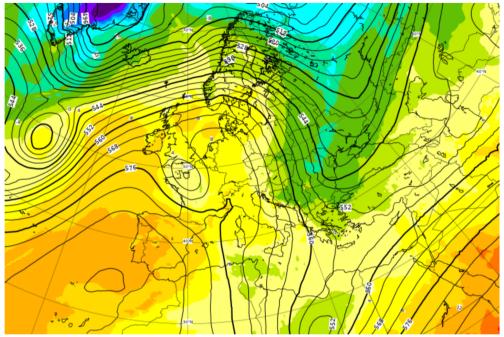
Pas de discrétisation temporelle (schéma semi-Lagrangien semiimplicite): 450 secondes 850 hPa temperature / 500 hPa geopotential Wednesday 1 Jan, 00 UTC T+120 Valid: Monday 6 Jan, 00 UTC 2020



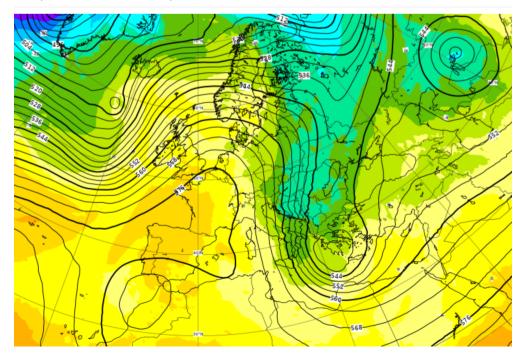
Monday 6 Jan, 00 UTC T+0 Valid: Monday 6 Jan, 00 UTC

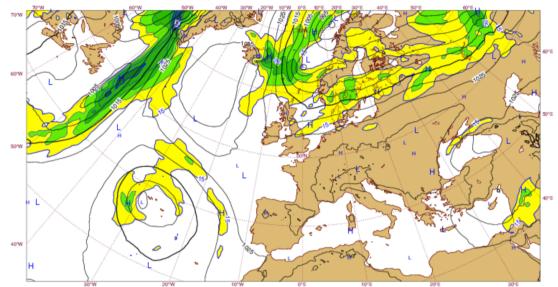


850 hPa temperature / 500 hPa geopotential Wednesday 1 Jan, 12 UTC T+0 Valid: Wednesday 1 Jan, 12 UTC



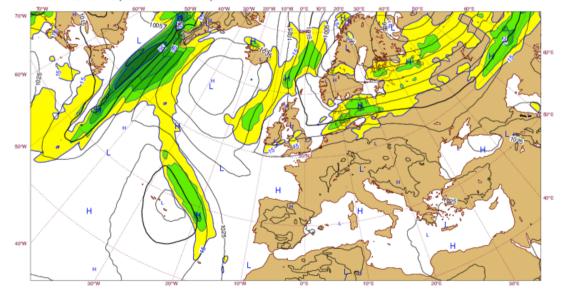
850 hPa temperature / 500 hPa geopotential Monday 6 Jan, 00 UTC T+0 Valid: Monday 6 Jan, 00 UTC

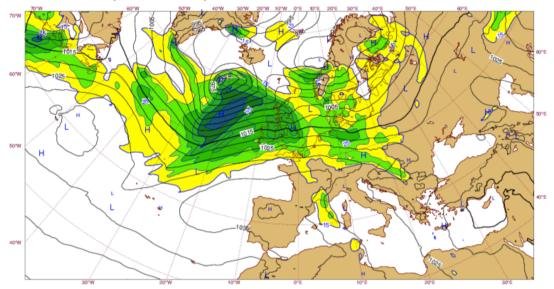




Sunday 25 December 2016 0000 UTC ECMWF t+168 VT: Sunday 01 January 2017 0000 UTC Surface: Mean sea level pressure / 850hPa wind speed

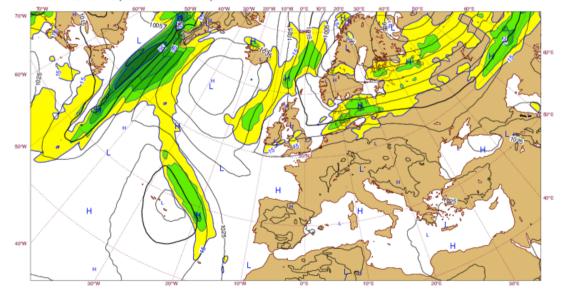
Sunday 01 January 2017 0000 UTC ECMWF t+0 VT: Sunday 01 January 2017 0000 UTC Surface: Mean sea level pressure / 850hPa wind speed

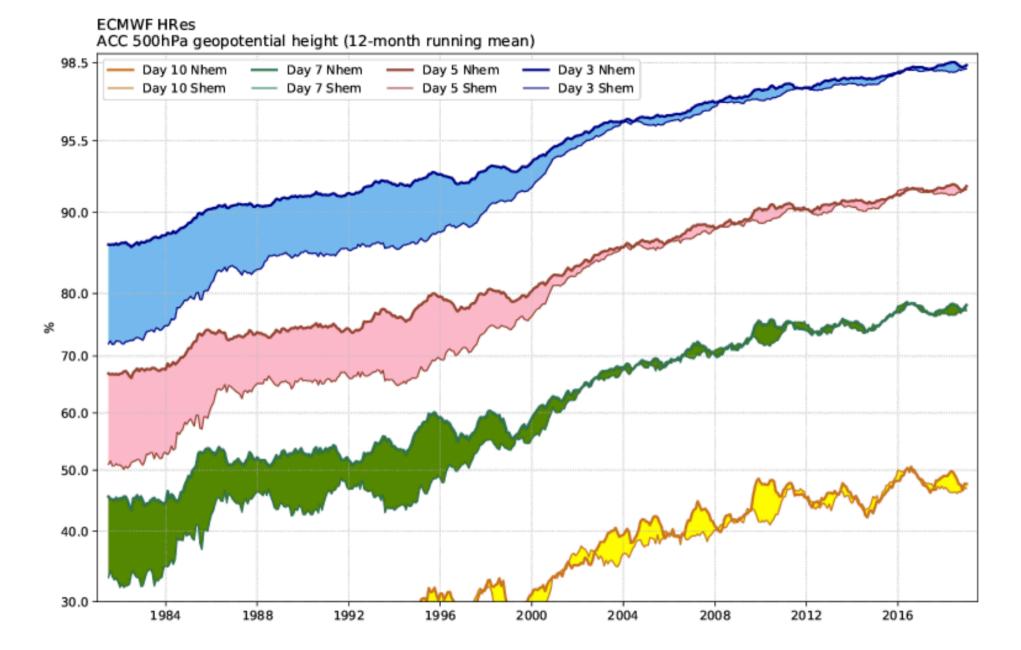




Sunday 25 December 2016 0000 UTC ECMWF t+0 VT: Sunday 25 December 2016 0000 UTC Surface: Mean sea level pressure / 850hPa wind speed

Sunday 01 January 2017 0000 UTC ECMWF t+0 VT: Sunday 01 January 2017 0000 UTC Surface: Mean sea level pressure / 850hPa wind speed

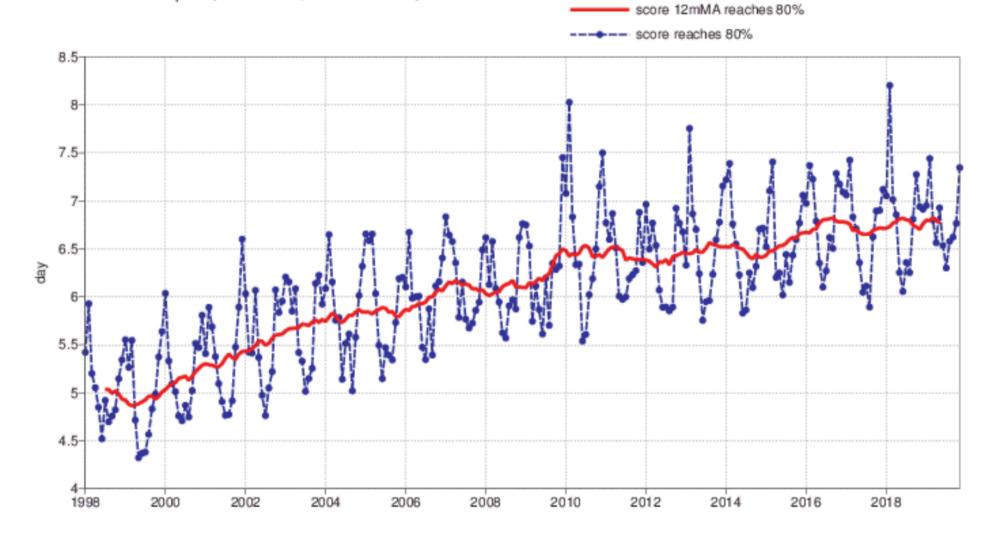




Anomaly correlation of ECMWF 500hPa height forecasts

ECMWF

500hPa geopotential Lead time of Anomaly correlation reaching 80% NHem Extratropics (lat 20.0 to 90.0, lon -180.0 to 180.0)





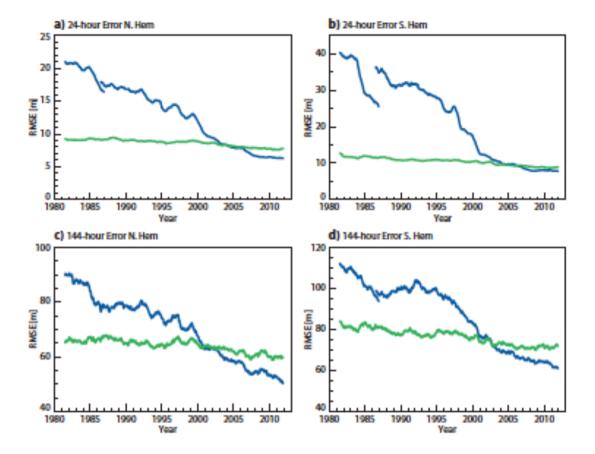


FIG. 3. Evolution of forecast errors from 1981 to 2012 for N.Hem (a and c) and S.Hem (b and d). Operational forecasts (blue) and ERA Interim (green). Note that before 1986 the operational analysis is used to verify the operational forecasts, after 1986 ERA Interim is used for the verification (with an overlap of 6 months present).

Remaining Problems

Mostly in the 'physics' of models (Q and \underline{F} terms in basic equations)

- Water cycle (evaporation, condensation, influence on radiation absorbed or emitted by the atmosphere)

- Exchanges with ocean or continental surface (heat, water, momentum, ...)

- ...

- What is assimilation ?

- Definition of initial conditions

Purpose of assimilation : reconstruct as accurately as possible the state of the atmospheric or oceanic flow, using all available appropriate information. The latter essentially consists of

- The observations proper, which vary in nature, resolution and accuracy, and are distributed more or less regularly in space and time.
- The physical laws governing the evolution of the flow, available in practice in the form of a discretized, and necessarily approximate, numerical model.
- 'Asymptotic' properties of the flow, such as, *e. g.*, geostrophic balance of middle latitudes. Although they basically are necessary consequences of the physical laws which govern the flow, these properties can usefully be explicitly introduced in the assimilation process.

Both observations and 'model' are affected with some uncertainty \Rightarrow uncertainty on the estimate.

For some reason, uncertainty is conveniently described by probability distributions (don't know too well why, but it works; see, *e.g.* Jaynes, 2007, *Probability Theory: The Logic of Science*, Cambridge University Press).

Assimilation is a problem in bayesian estimation.

Determine the conditional probability distribution for the state of the system, knowing everything we know (see Tarantola, A., 2005, *Inverse Problem Theory and Methods for Model Parameter Estimation*, SIAM).

Assimilation is one of many '*inverse problems*' encountered in many fields of science and technology

- solid Earth geophysics
- plasma physics
- 'nondestructive' probing
- navigation (spacecraft, aircraft,)
- ...

Solution most often (if not always) based on Bayesian, or probabilistic, estimation. 'Equations' are fundamentally the same.

Difficulties specific to assimilation of meteorological observations :

- Very large numerical dimensions ($n \approx 10^{6}$ -10⁹ parameters to be estimated, $p \approx 4.10^{7}$ observations per 24-hour period). Difficulty aggravated in Numerical Weather Prediction by the need for the forecast to be ready in time.

- Non-trivial, actually chaotic, underlying dynamics

Relative cost of the various components of the operational prediction suite at ECMWF (september 2015, J.-N. Thépaut) :

- 4DVAR: 9.5%

- Ensemble Data Assimilation (EDA) : 30%

EDA produces both the background error covariances for 4D-Var and the initial perturbations (in addition to Singular Vectors) for EPS.

- High resolution deterministic model : 4.5%

- Ensemble Prediction System (EPS) : 22%
- Ensemble hindcasts : 14%

- Others : 20% (among which 17% for computation of boundary conditions of a number of limited-area models ; those 17% include both assimilation and forecast)

Assimilation over 24 hours of observations takes more than 40% of the computing power devoted to 10-day operational prediction

$$z_1 = x + \zeta_1$$
 density function $p_1(\zeta) \propto \exp[-(\zeta^2)/2s_1]$

$$z_2 = x + \zeta_2$$
 density function $p_2(\zeta) \propto \exp[-(\zeta^2)/2s_2]$

 ζ_1 and ζ_2 mutually independent

 $P(x = \xi \mid z_1, z_2)$?

 $z_1 = x + \zeta_1$ density function $p_1(\zeta) \propto \exp[-(\zeta^2)/2s_1]$ $z_2 = x + \zeta_2$ density function $p_2(\zeta) \propto \exp[-(\zeta^2)/2s_2]$ ζ_1 and ζ_2 mutually independent

 $P(x = \xi \mid z_1, z_2)$?

 $x = \xi \iff \zeta_1 = z_1 - \xi \text{ and } \zeta_2 = z_2 - \xi$

• $P(x = \xi | z_1, z_2) \propto p_1(z_1 - \xi) p_2(z_2 - \xi)$ $\propto \exp[-(\xi - x^a)^2/2p^a]$

where $1/p^a = 1/s_1 + 1/s_2$, $x^a = p^a (z_1/s_1 + z_2/s_2)$

Conditional probability distribution of *x*, given z_1 and $z_2 : \mathcal{N}[x^a, p^a]$ $p^a < (s_1, s_2)$ independent of z_1 and z_2

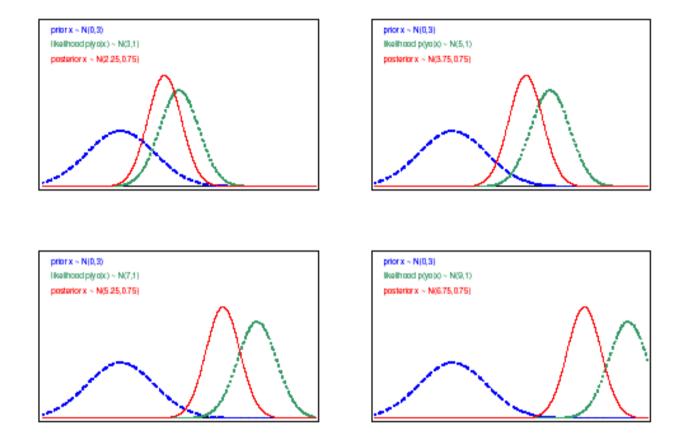


Fig. 1.1: Prior pdf p(x) (dashed line), posterior pdf $p(x|y^o)$ (solid line), and Gaussian likelihood of observation $p(y^o|x)$ (dotted line), plotted against x for various values of y^o . (Adapted from Lorenc and Hammon 1988.)

Conditional expectation x^a minimizes following scalar *objective function*, defined on ξ -space

$$\xi \rightarrow \mathcal{J}(\xi) \equiv (1/2) \left[(z_1 - \xi)^2 / s_1 + (z_2 - \xi)^2 / s_2 \right]$$

In addition

 $p^a = 1/\mathcal{J}^{\prime\prime}(x^a)$

Conditional probability distribution in Gaussian case

$$P(x = \xi \mid z_1, z_2) \propto \exp[-(\xi - x^a)^2/2p^a]$$
$$\mathcal{J}(\xi) + Cst$$

Estimate

 $x^{a} = p^{a} \left(z_{1}/s_{1} + z_{2}/s_{2} \right)$

with error p^a such that

$$1/p^a = 1/s_1 + 1/s_2$$

can also be obtained, independently of any Gaussian hypothesis, as simply corresponding to the linear combination of z_1 and z_2 that minimizes the error $E[(x^{a}-x)^{2}]$

Best Linear Unbiased Estimator (BLUE)

$$z_1 = x + \zeta_1$$
$$z_2 = x + \zeta_2$$

Same as before, but ζ_1 and ζ_2 are now distributed according to exponential law with parameter *a*, *i*. *e*.

```
p(\zeta) \propto \exp[-|\zeta|/a]; \operatorname{Var}(\zeta) = 2a^2
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Conditional probability density function is now uniform over interval $[z_1, z_2]$, exponential with parameter a/2 outside that interval

 $E(x \mid z_1, z_2) = (z_1 + z_2)/2$

Var $(x \mid z_1, z_2) = a^2 (2\delta^3/3 + \delta^2 + \delta + 1/2) / (1 + 2\delta)$, with $\delta = |z_1 - z_2| / (2a)$ Increases from $a^2/2$ to ∞ as δ increases from 0 to ∞ . Can be larger than variance $2a^2$ of original errors (probability 0.08)

Bayesian estimation

State vector x, belonging to state space $S(\dim S = n)$, to be estimated.

Data vector z, belonging to data space $\mathcal{D}(\dim \mathcal{D} = m)$, available.

 $z = F(x, \zeta) \tag{1}$

where ζ is a random element representing the uncertainty on the data (or, more precisely, on the link between the data and the unknown state vector).

For example

 $z = \Gamma x + \zeta$

Bayesian estimation (continued)

Probability that $x = \xi$ for given ξ ?

 $x = \xi \implies z = F(\xi, \zeta)$

$$P(x = \xi \mid z) = P[z = F(\xi, \zeta)] / \int_{\xi'} P[z = F(\xi', \zeta)]$$

Unambiguously defined iff, for any ζ , there is at most one ξ such that $z = F(\xi, \zeta)$.

 \Leftrightarrow data contain information, either directly or indirectly, on any component of *x*. *Determinacy* condition.

Bayesian estimation is however impossible in its general theoretical form in meteorological or oceanographical practice because

- It is impossible to explicitly describe a probability distribution in a space with dimension even as low as $n \approx 10^3$, not to speak of the dimension $n \approx 10^{6-9}$ of present Numerical Weather Prediction models (*'curse of dimensionality'*).
- Probability distribution of errors on data very poorly known (model errors in particular).

One has to restrict oneself to a much more modest goal. Two approaches exist at present

- Obtain some 'central' estimate of the conditional probability distribution (expectation, mode, ...), plus some estimate of the corresponding spread (standard deviations and a number of correlations).
- Produce an ensemble of estimates which are meant to sample the conditional probability distribution (dimension $N \approx O(10-100)$).

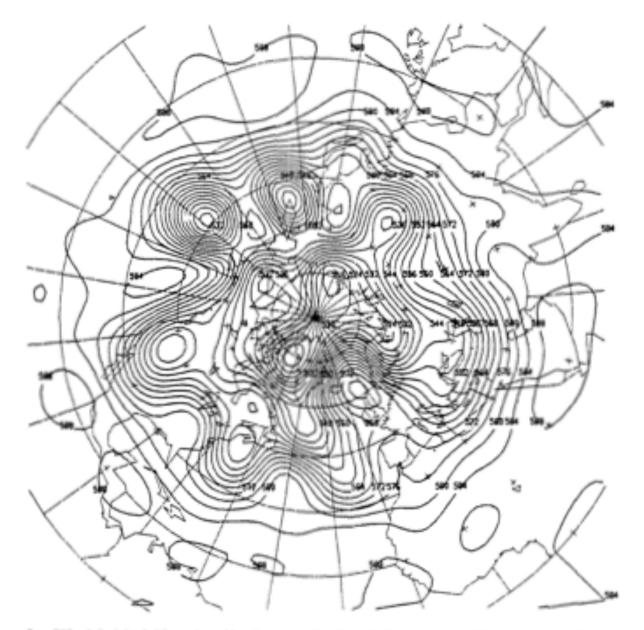


Figure 2. 500 mb height field produced by the operational analysis procedure of Direction de la Météorologie for 00 GMT, 26 April 1984. Units: dam, contour interval: 4 dam. The field has been truncated to the truncation of the model used for the experiments described in the article.

Courtier and Talagrand, QJRMS, 1987

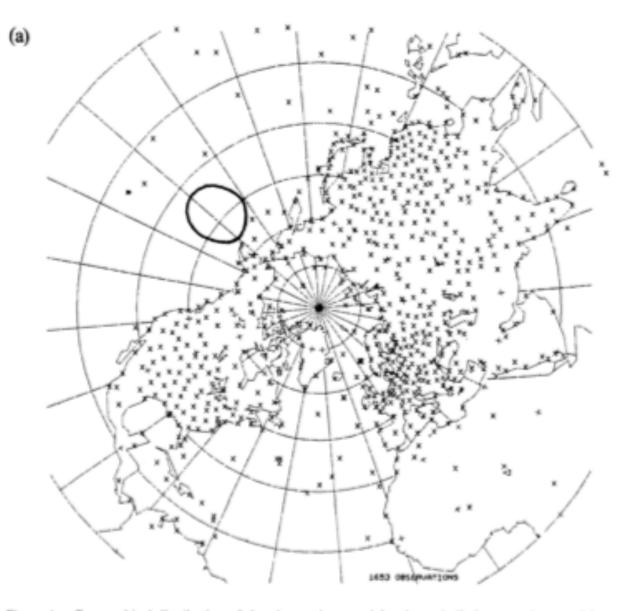


Figure 1. Geographical distribution of the observations used for the assimilation experiments. (a): geopotential observations; (b): wind observations. At most of the points plotted, several observations were made at successive synoptic hours. On each of the two charts, the heavy line delineates the Aleutian depression (see Figure 2).

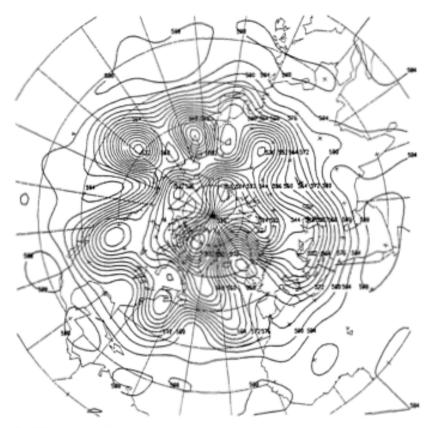


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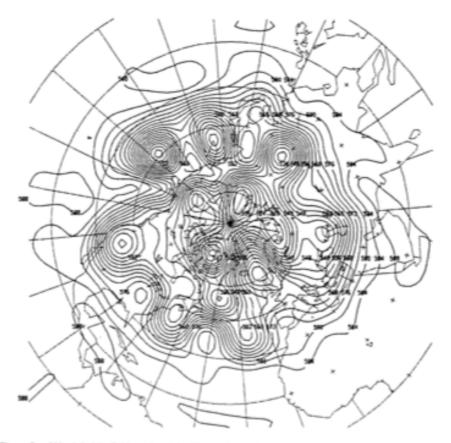


Figure 3. 500 mb height field produced for 00 GMT, 26 April 1984, by the variational analysis minimizing the distance function defined by Eqs. (1)-(2) over a 24-hour period. Units: dam; contour interval: 4 dam.

500-hPa geopotential field as determined by : (left) operational assimilation system of French Weather Service (3D, primitive equation) and (right) experimental variational system (2D, vorticity equation)

Courtier and Talagrand, QJRMS, 1987

Random vector $\mathbf{x} = (x_1, x_2, ..., x_n)^T = (x_i)$ (e. g. pressure, temperature, abundance of given chemical compound at *n* grid-points of a numerical model)

- Expectation $E(x) = [E(x_i)]$; centred vector x' = x E(x)
- Covariance matrix

$$E(\boldsymbol{x}^{\prime}\boldsymbol{x}^{\prime \mathrm{T}}) = [E(x_{i}^{\prime}x_{j}^{\prime})]$$

dimension nxn, symmetric non-negative (strictly definite positive except if linear relationship holds between the x_i 's with probability 1).

- Two random vectors
 - $\boldsymbol{x} = (x_1, x_2, ..., x_n)^{\mathrm{T}}$ $\boldsymbol{y} = (y_1, y_2, ..., y_p)^{\mathrm{T}}$

 $E(\mathbf{x}'\mathbf{y}'^{\mathrm{T}}) = E(x_i'y_i')$

dimension *nxp*

Covariance matrices will be denoted

$$C_{xx} \equiv E(x'x'^{\mathrm{T}})$$

$$C_{xy} \equiv E(x'y'^{\mathrm{T}})$$

Random function $\Phi(\xi)$ (field of pressure, temperature, abundance of given chemical compound, ...; ξ is now spatial and/or temporal coordinate)

- Expectation $E[\Phi(\xi)]$; $\Phi'(\xi) = \Phi(\xi) E[\Phi(\xi)]$
- Variance $Var[\Phi(\xi)] = E\{[\Phi'(\xi)]^2\}$
- Covariance function

$$(\xi_{1}, \xi_{2}) \rightarrow C_{\Phi}(\xi_{1}, \xi_{2}) \equiv E[\Phi'(\xi_{1}) \Phi'(\xi_{2})]$$

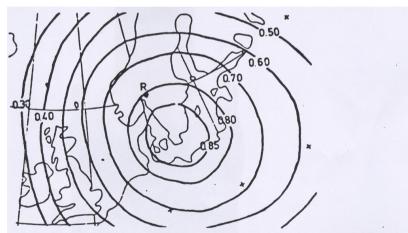
Correlation function

•

 $Cor_{\varphi}(\xi_{1}, \xi_{2}) = E[\Phi'(\xi_{1}) \Phi'(\xi_{2})] / \{Var[\Phi(\xi_{1})] Var[\Phi(\xi_{2})]\}^{1/2}$

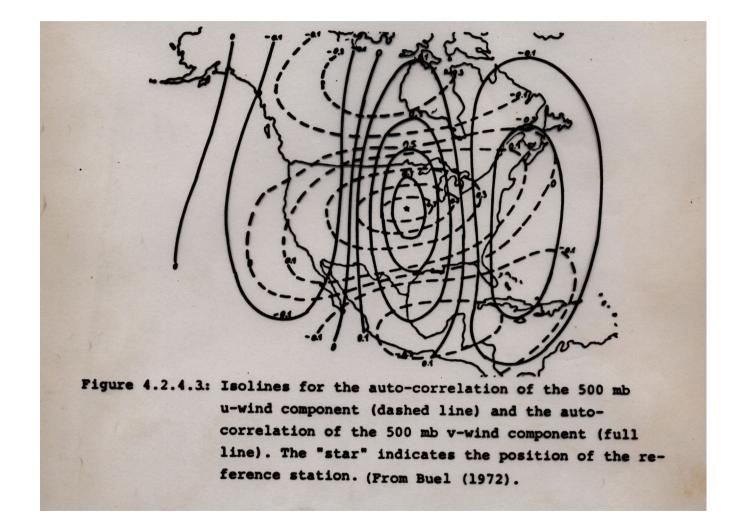


.: Isolines for the auto-correlations of the 500 mb geopotential between the station in Hannover and surrounding stations. From Bertoni and Lund (1963)

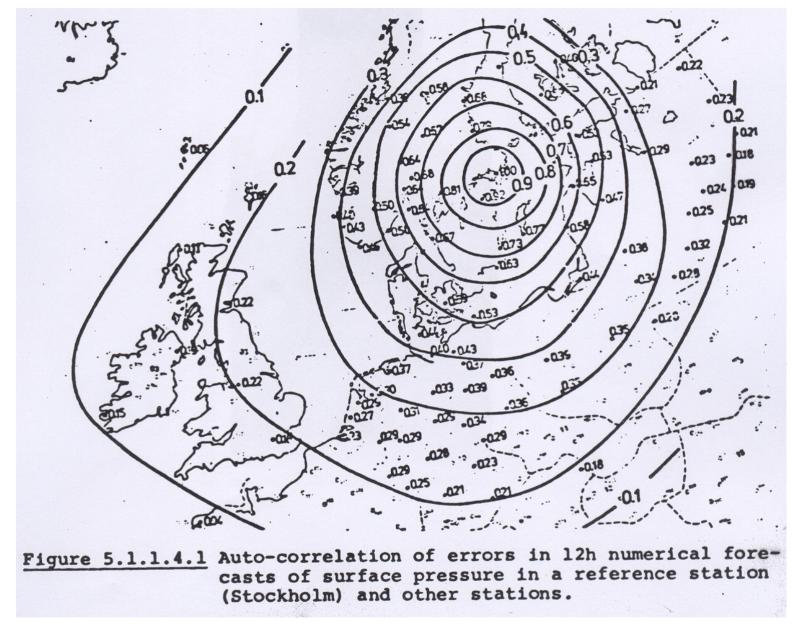


Isolines of the cross-correlation between the 500 mb geopotential in station 01 384 (R) and the surface pressure in surrounding stations.

After N. Gustafsson



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