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)

Institut polytechnique de Paris Master 2 Water, Air, Pollution and Energy at local and regional scales (WAPE)

Année 2023-2024

Course Introduction to data assimilation (ADOMO)

# From numerical modelling to data assimilation

Olivier Talagrand

9 January 2024

- 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

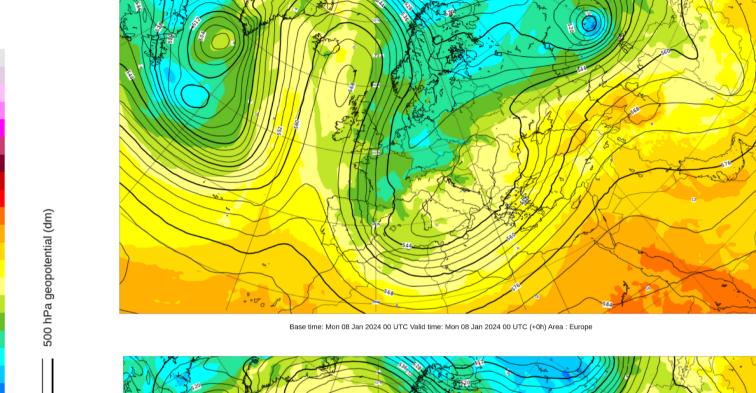
#### ECMWF

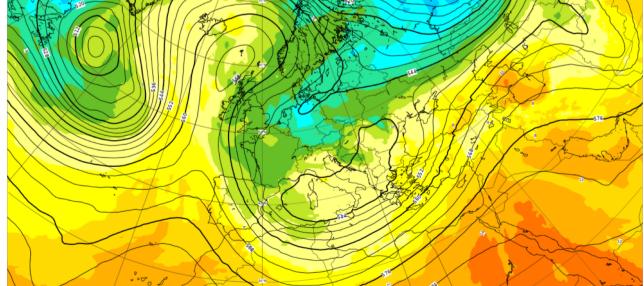
12 16

850 hPa temperature (C) 1.16 -12 -8 -4 0 4 8

-80 -70 -60 -52 -48 -44 -40 -36 -32 -28 -24 -20

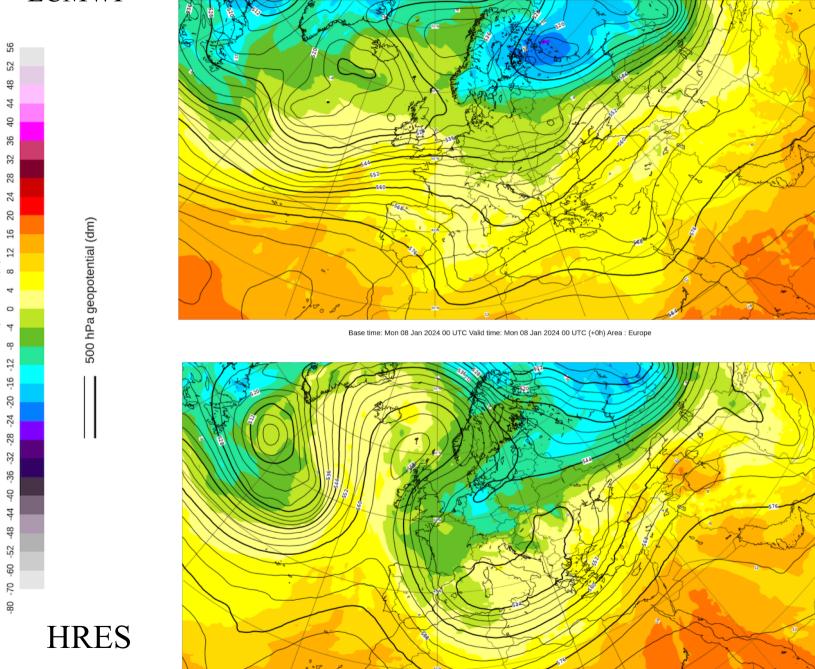
HRES

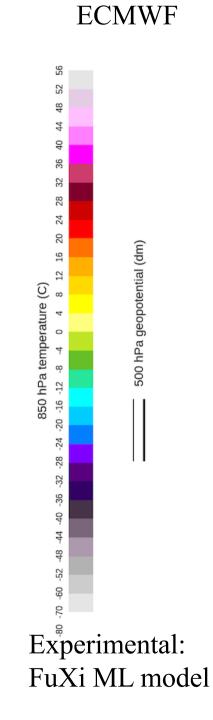


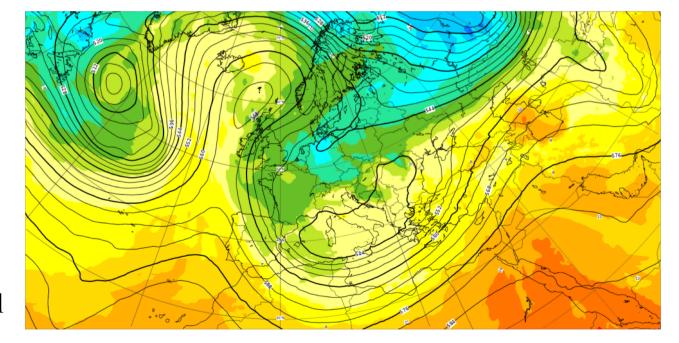


ECMWF

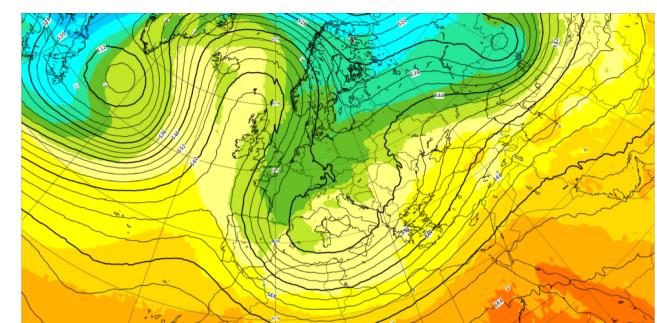
850 hPa temperature (C)





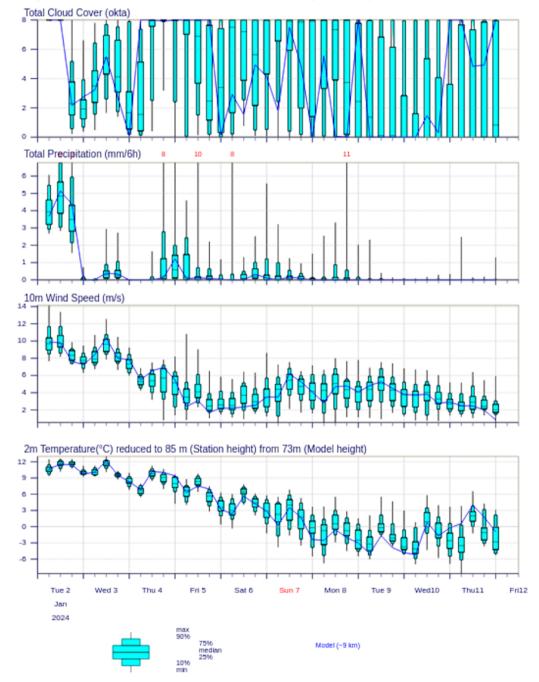


Base time: Mon 08 Jan 2024 00 UTC Valid time: Mon 08 Jan 2024 00 UTC (+0h) Area : Europe



**ECMWF** 

ENS Meteogram 48.82°N 2.29°E (ENS land point) 85 m High Resolution Forecast and ENS Distribution Tuesday 2 January 2024 00 UTC

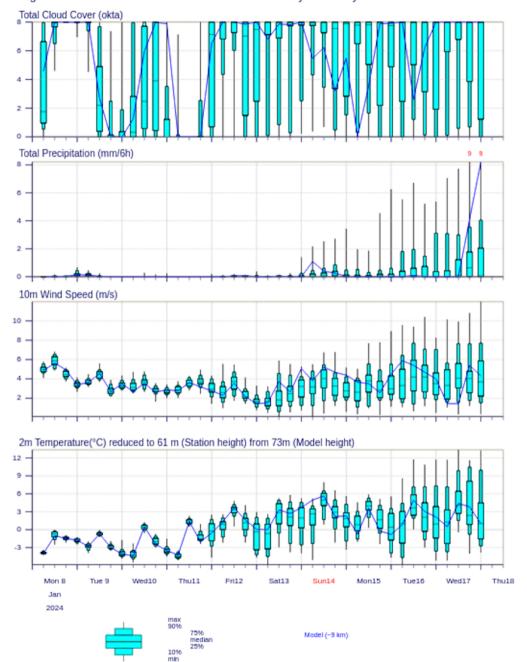




#### ENS Meteogram



48.82°N 2.29°E (ENS land point) 61 m High Resolution Forecast and ENS Distribution Monday 8 January 2024 00 UTC

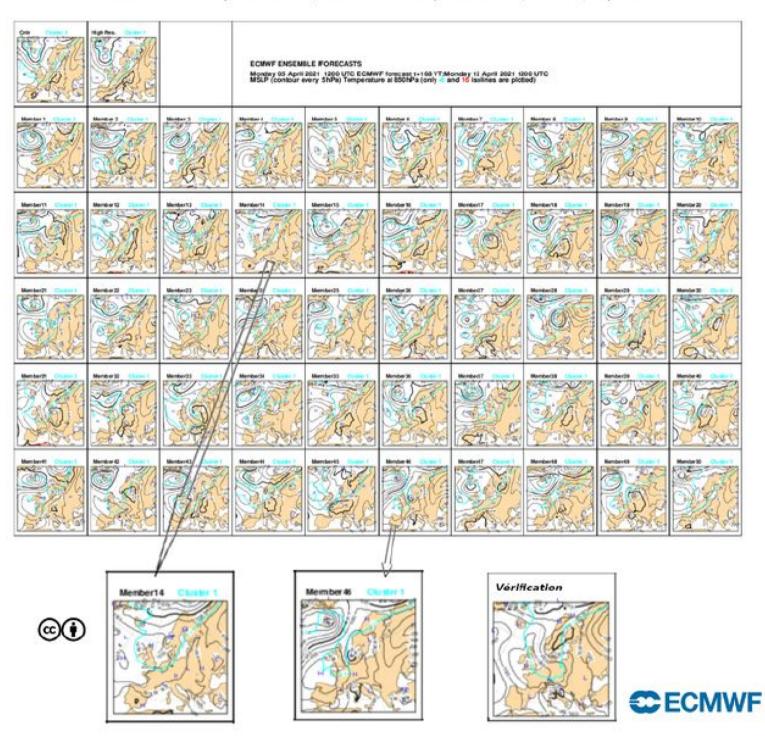


ENS



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



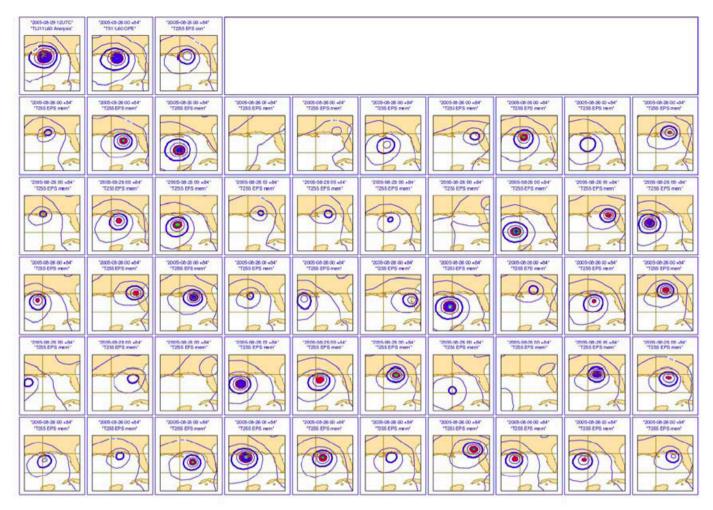


Figure 6 Hurricane Katrina mean-sea-level-pressure (MSLP) analysis for 12 UTC of 29 August 2005 and t+84h high-resolution and EPS forecasts started at 00 UTC of 26 August:

1st row: 1<sup>st</sup> panel: MSLP analysis for 12 UTC of 29 Aug 2<sup>nd</sup> panel: MSLP t+84h T<sub>L</sub>511L60 forecast started at 00 UTC of 26 Aug 3<sup>rd</sup> panel: MSLP t+84h EPS-control T<sub>L</sub>255L40 forecast started at 00 UTC of 26 Aug Other rows: 50 EPS-perturbed T<sub>L</sub>255L40 forecast started at 00 UTC of 26 Aug.

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

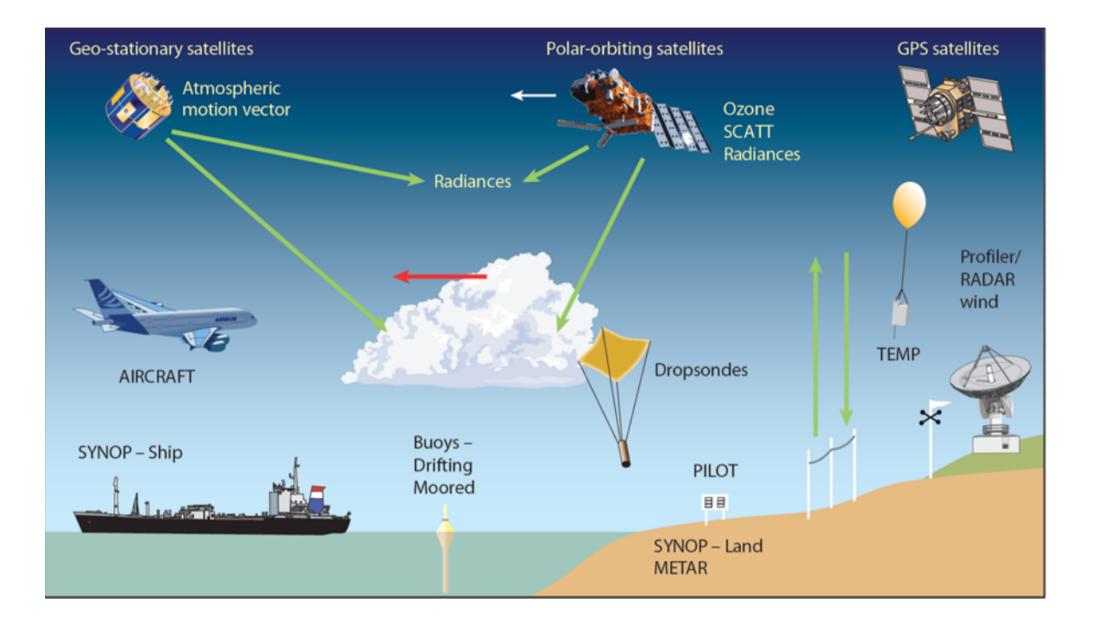
ECMWF, Technical Report 499, 2006

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.

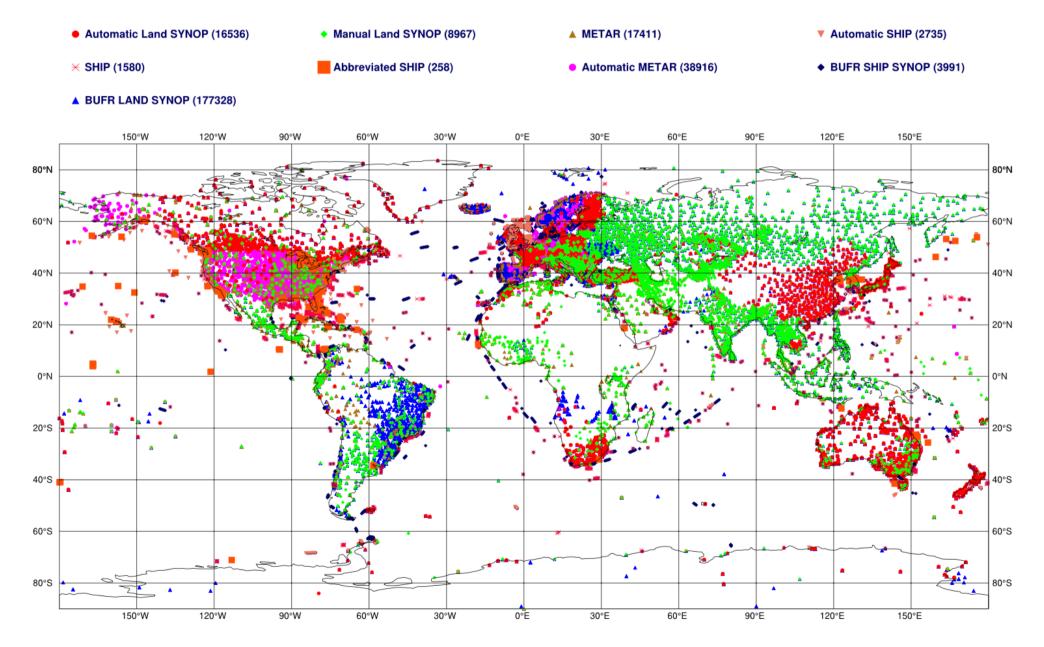
H. Poincaré, Science et Méthode, Paris, 1908

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.

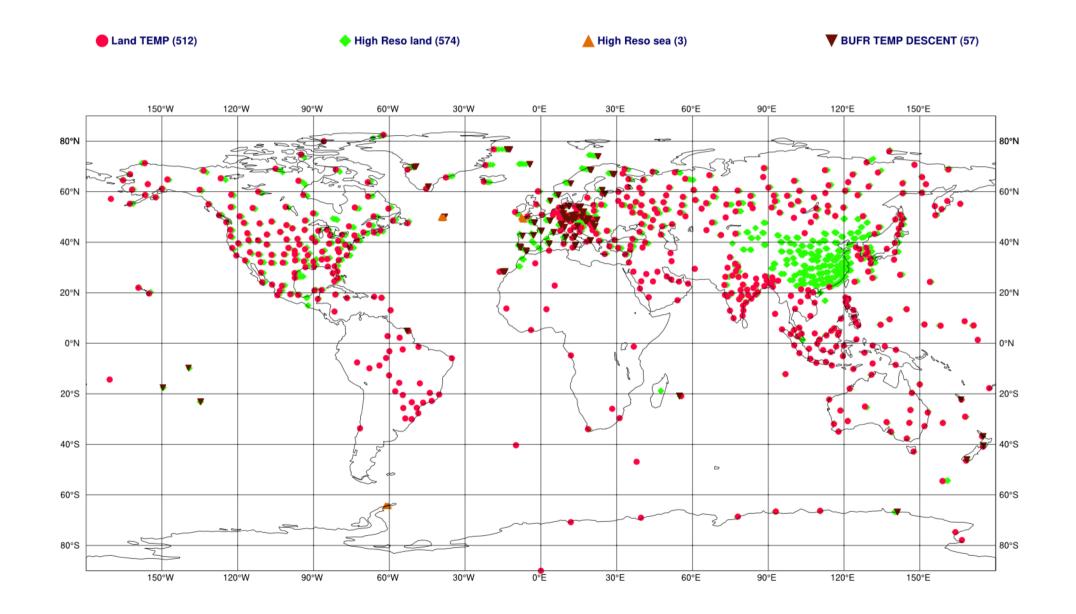
> H. Poincaré, *Science et Méthode*, Paris, 1908 (English transl. by F. Maitland, *Science and Method*, T. Nelson and Sons, London, 1914)



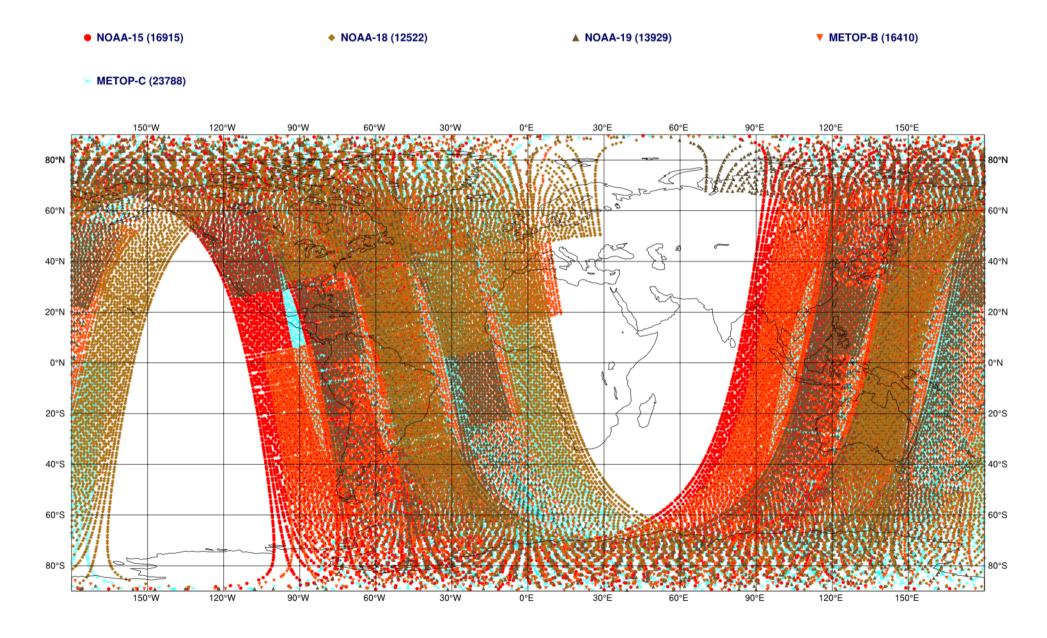
#### ECMWF data coverage (all observations) - SYNOP-SHIP-METAR 2024010521 to 2024010603 Total number of obs = 267722



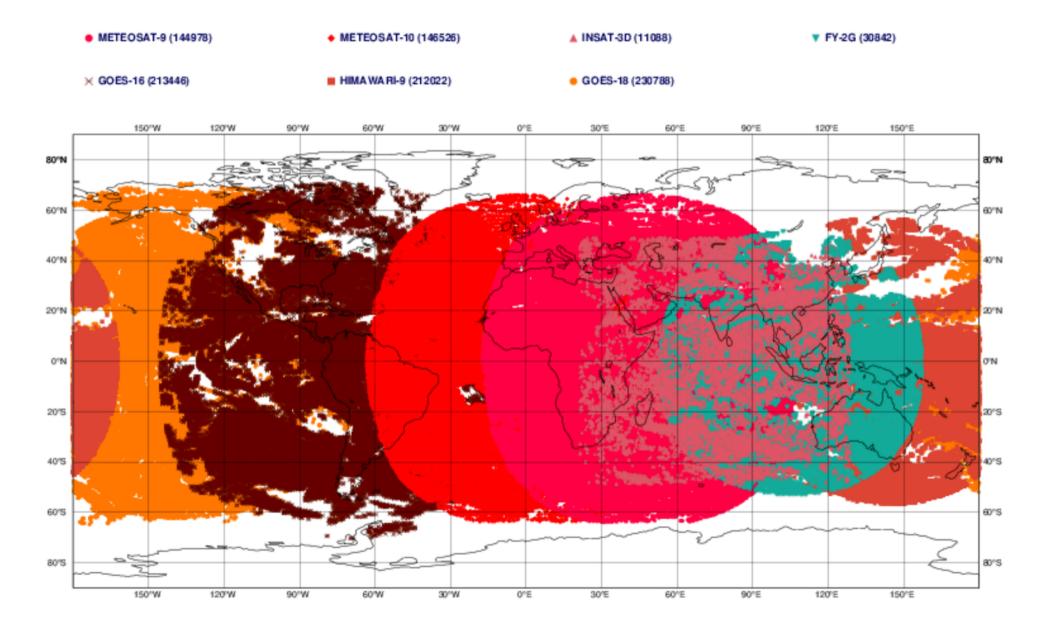
#### ECMWF data coverage (all observations) - RADIOSONDE 2024010521 to 2024010603 Total number of obs = 1146



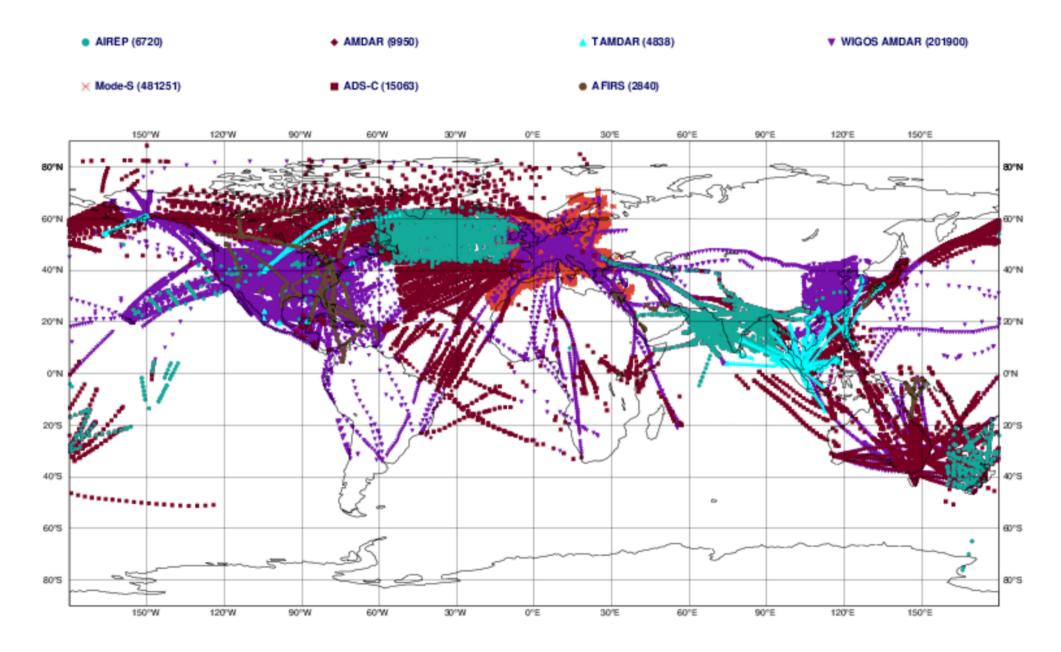
#### ECMWF data coverage (all observations) - AMSUA 2024010521 to 2024010603 Total number of obs = 83564



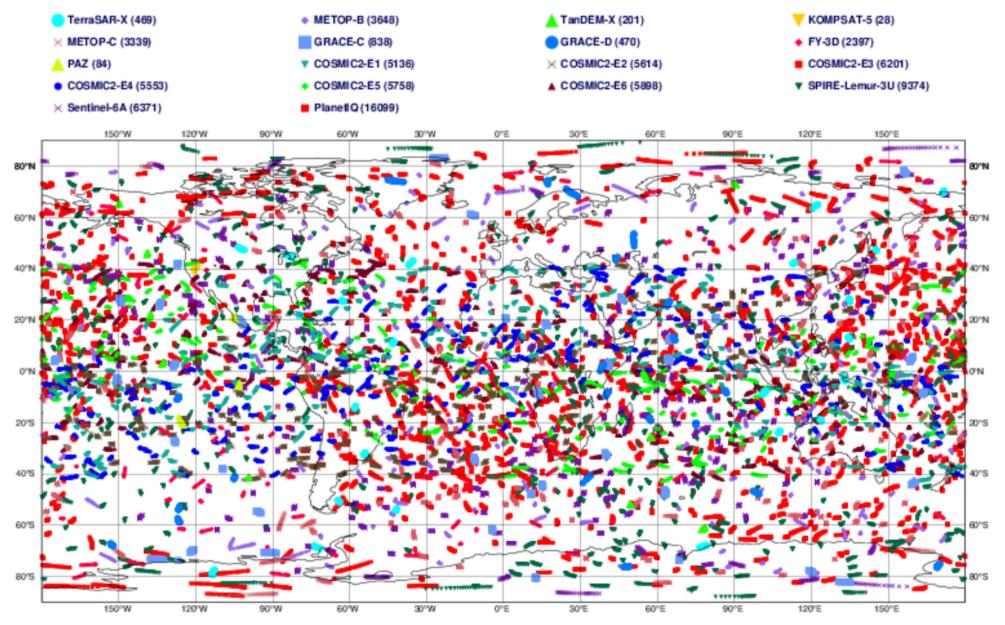
#### ECMWF data coverage (all observations) - AMV WV 2024010521 to 2024010603 Total number of obs = 989690



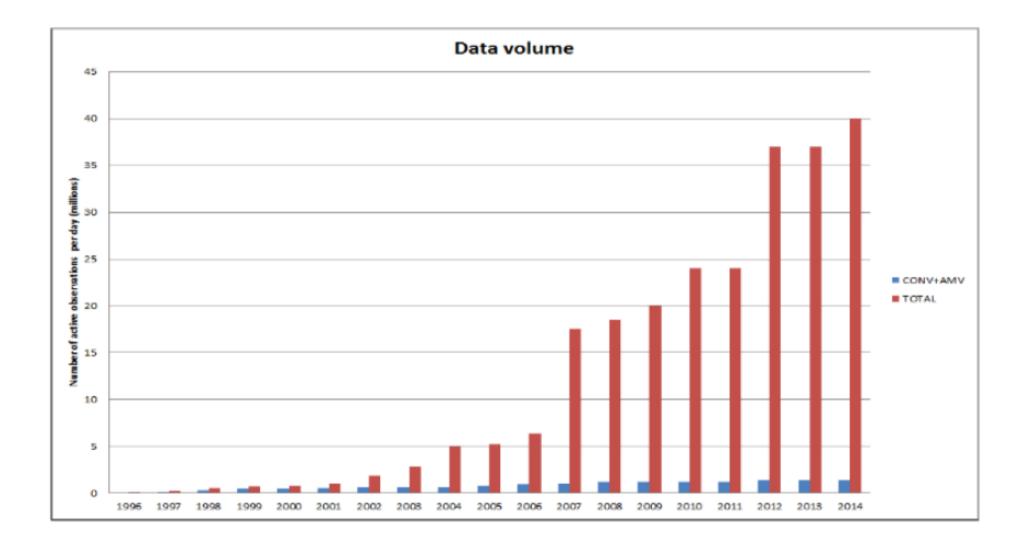
#### ECMWF data coverage (all observations) - AIRCRAFT 2024010521 to 2024010603 Total number of obs = 722562



#### ECMWF data coverage (all observations) - GPSRO 2024010521 to 2024010603 Total number of obs = 77478



## ECMWF



## As of 2023

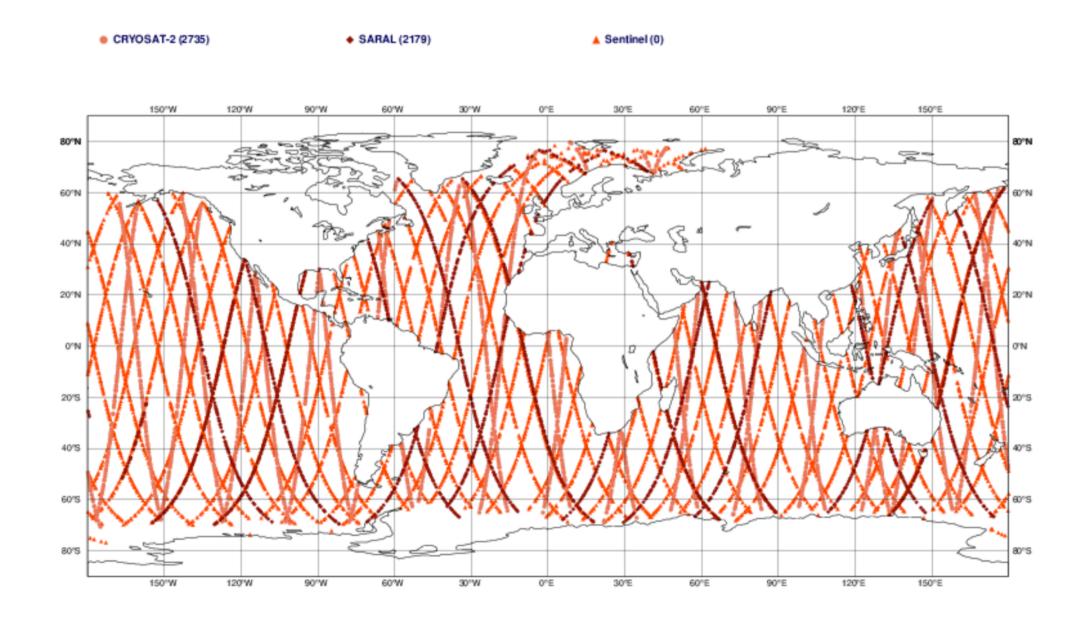
We receive 800 million observations daily, and 60 million quality-controlled observations are available daily for use in the Integrated Forecasting System (IFS); the vast majority of these are satellite measurements, but ECMWF also benefits from all available observations from non-satellite sources, including surfacebased and aircraft reports.

- 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

#### $y = H(\mathbf{x})$

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

#### ECMWF data coverage (all observations) - SEA LEVEL ANOMALY 20240105 00 Total number of obs = 4914



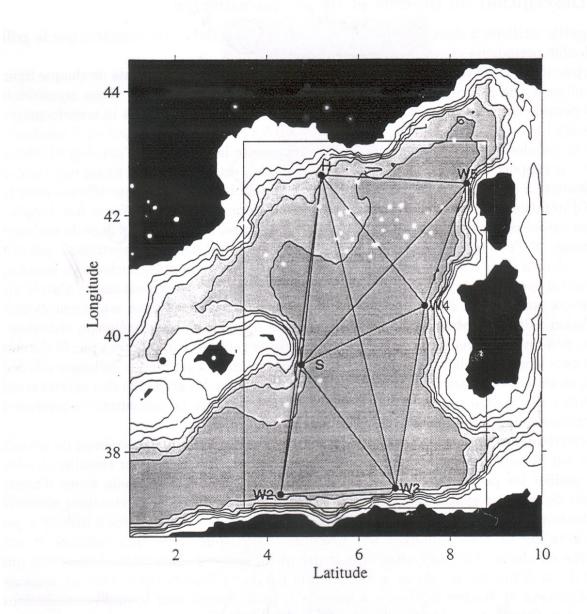


FIG. 1 – Bassin méditerranéen occidental: réseau d'observation tomographique de l'expérience Thétis 2 et limites du domaine spatial utilisé pour les expériences numériques d'assimilation.

24

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  $D\underline{U}/Dt + (1/\rho) \operatorname{grad} p - g + 2 \underline{\Omega} \wedge \underline{U} = \underline{F}$
- 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* 

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'

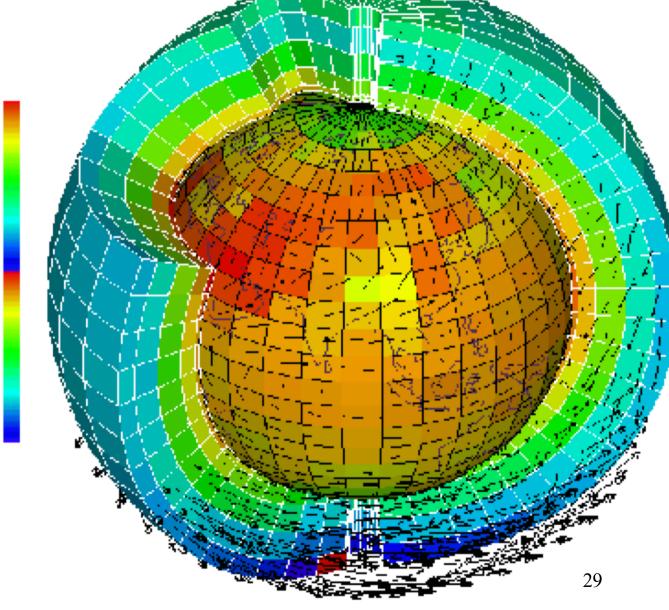
- All presently existing numerical models are built on simplified forms of the general physical laws. Global numerical models, used either for large-scale meteorological prediction or for climate simulation, are at present built on the so-called *primitive equations*. Those equations rely on several 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 horizontal spatial 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)



- 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

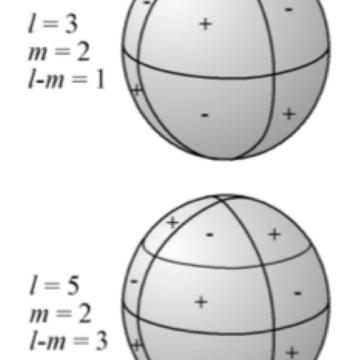
 $Y_n^m(\mu,\lambda) \propto P_n^m(\mu) \exp(im\lambda)$ 

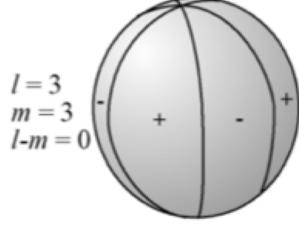
 $P_n^m(\mu)$  est la *fonction de Legendre* de deuxième espèce

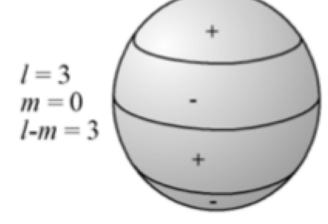
$$P_n^m(\mu) \propto (1-\mu^2)^{\frac{m}{2}} \frac{d^{n+m}}{d\mu^{n+m}} (\mu^2-1)^n$$

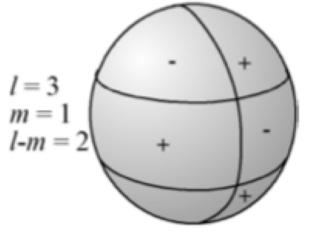
*n* et *m* sont respectivement le *degré* et l'*ordre* de l'harmonique  $Y_n^m(\mu, \lambda)$ 

$$n = 0, 1, \dots - n \le m \le n$$









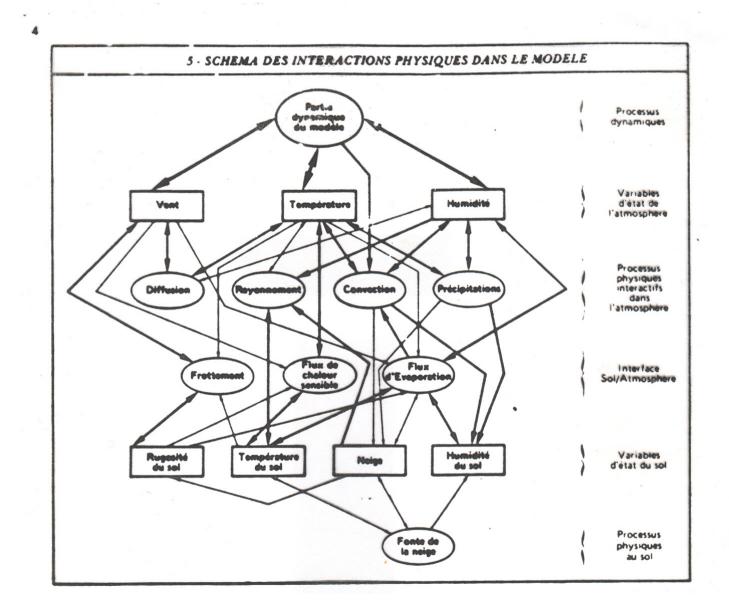
ritoni minipoula, une nec encyclopeula

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 motion, 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 gradually 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.



**European Centre for Medium-range Weather Forecasts** (ECMWF, Reading, GB, Bologna, Italy, Bonn, Germany)

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

June 2023 High-resolution (HRES) model

Triangular semi-spectral truncation TCO1279 / O1280 (horizontal resolution  $\approx$  9 kilometres)

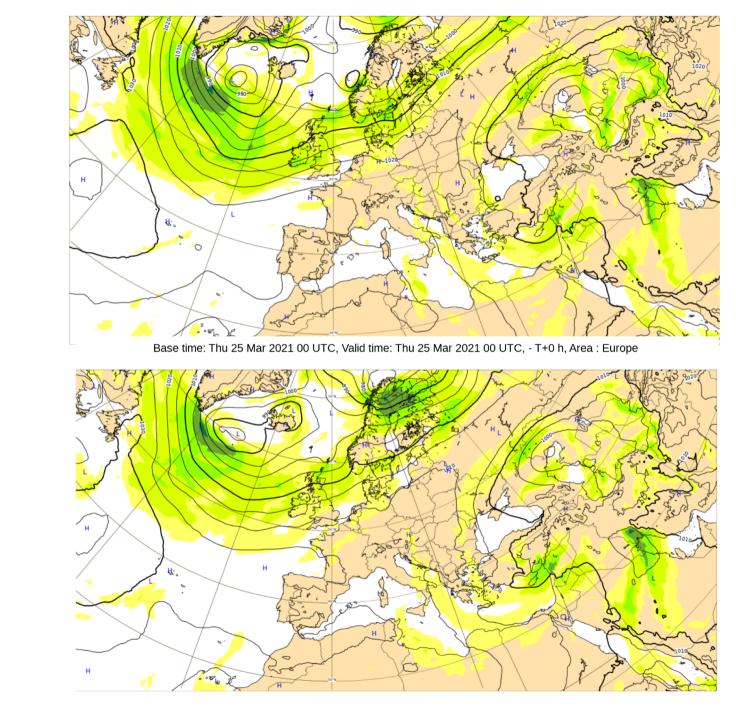
Hydrostatic primitive equations. 137 vertical levels (0 - 80 km)

Finite-element vertical discretisation (hybrid coordinate)

Dimension of corresponding state vector  $> 10^9$ 

Integration timestep (semi-Lagrangian semi-implicit scheme): 450 seconds

Integrated four times a day (from 00, 06, 12 and 18 UTC) to 10-36 day range

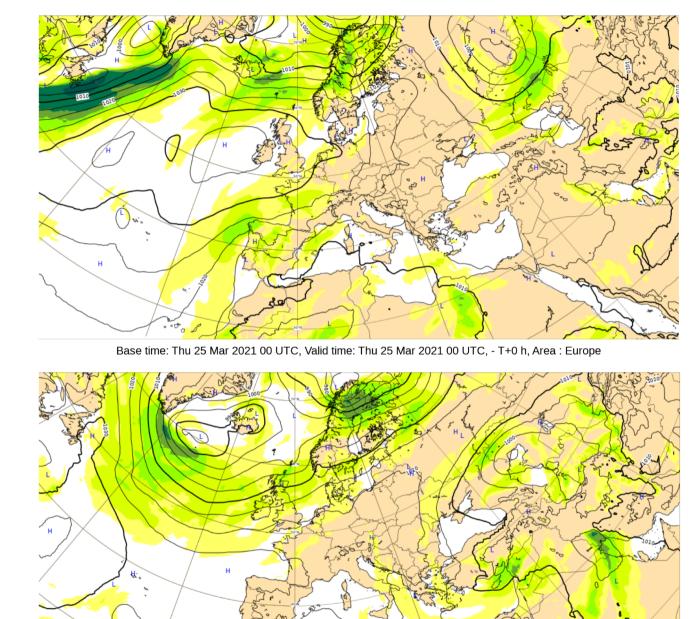


10

Mean sea level pressure (hPa)

[00]

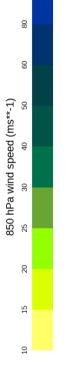
2021



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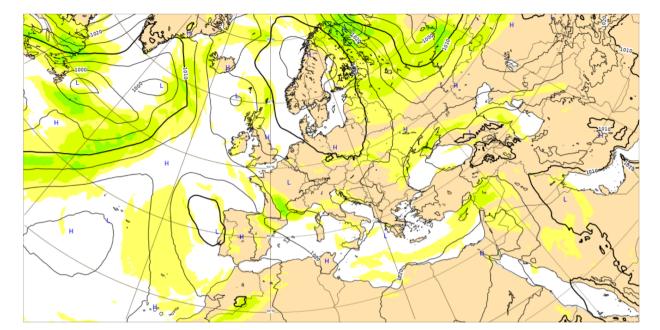
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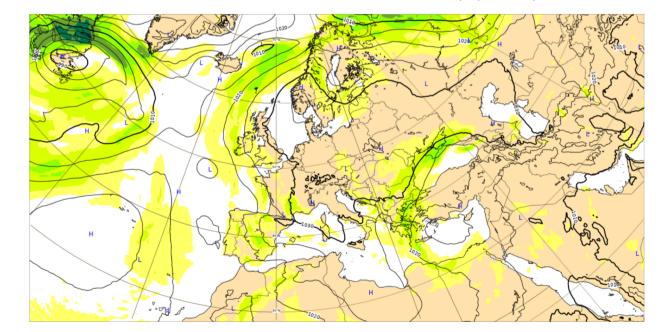
Mean sea level pressure (hPa)

[00]

2021

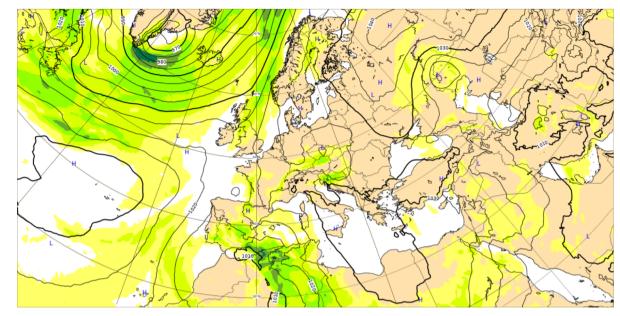


Base time: Wed 23 Mar 2022 00 UTC Valid time: Wed 23 Mar 2022 00 UTC (+0h) Area : Europe

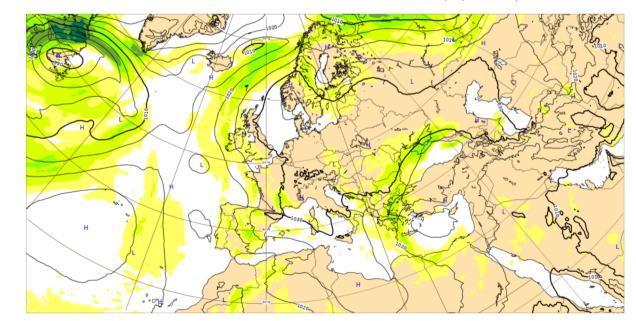




Mean sea level pressure (hPa)



Base time: Wed 23 Mar 2022 00 UTC Valid time: Wed 23 Mar 2022 00 UTC (+0h) Area : Europe



850 hPa wind speed (ms\*\*-1) 15 20 25 30 40 50 60

10

Mean sea level pressure (hPa)

100 m/s)

80

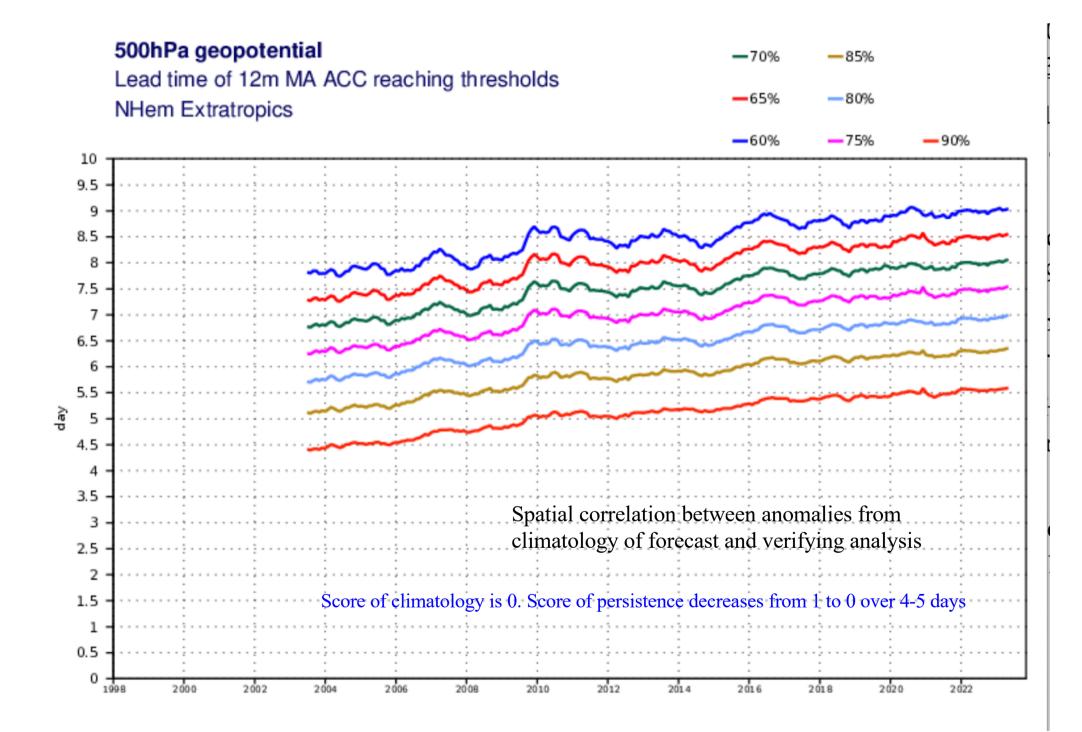
Results on site of ECMWF www.ecmwf.int

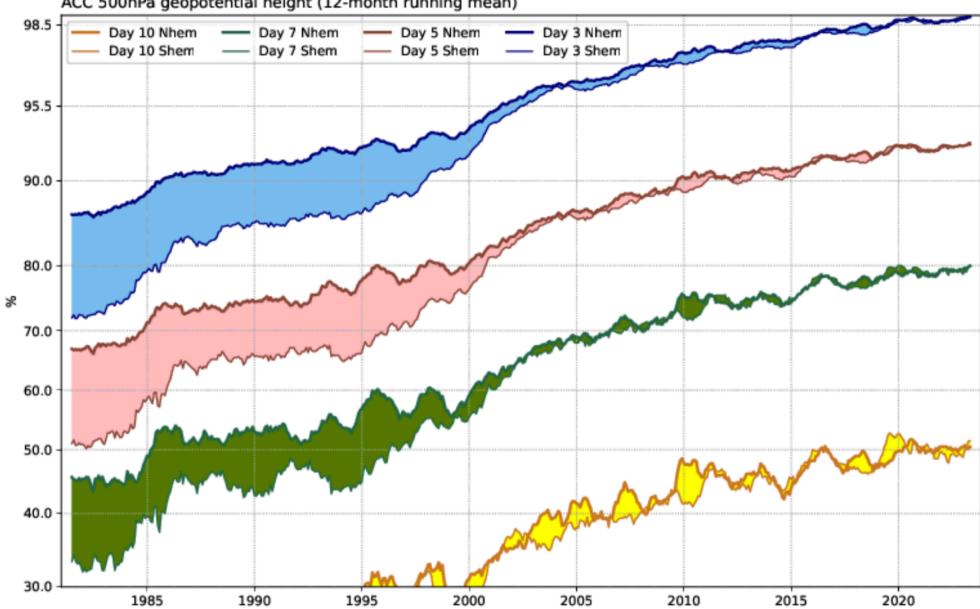
In particular

T. Haiden *et al., Evaluation of ECMWF forecasts, including the 2023 upgrade*, Technical Memorandum 911, September 2023, ECMWF, Reading, UK.

Available at the address :

https://www.ecmwf.int/en/elibrary/81389-evaluationecmwf-forecasts-including-2023-upgrade





ECMWF HRes ACC 500hPa geopotential height (12-month running mean)



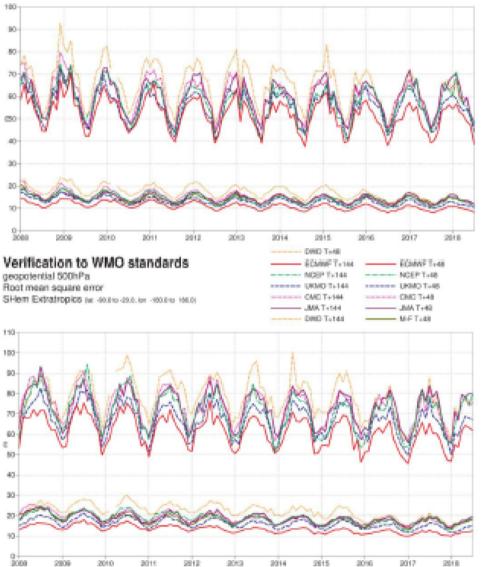


Figure 14: WMO-exchanged scores from global forecast centres. RMS error of 500 hPa geopotential height over northern (top) and southern (bottom) extratropics. In each panel, the upper curves show the six-day forecast error and the lower curves show the two-day forecast error of model runs initiated at 12 UTC. Each model is verified against its own analysis. JMA = Japan Meteorological Agency, CMC = Canadian Meteorological Centre, UKMO = the UK Met Office, NCEP = U.S. National Centers for Environmental Prediction, M-F = Météo France, DWD = Deutscher Wetterdienst.

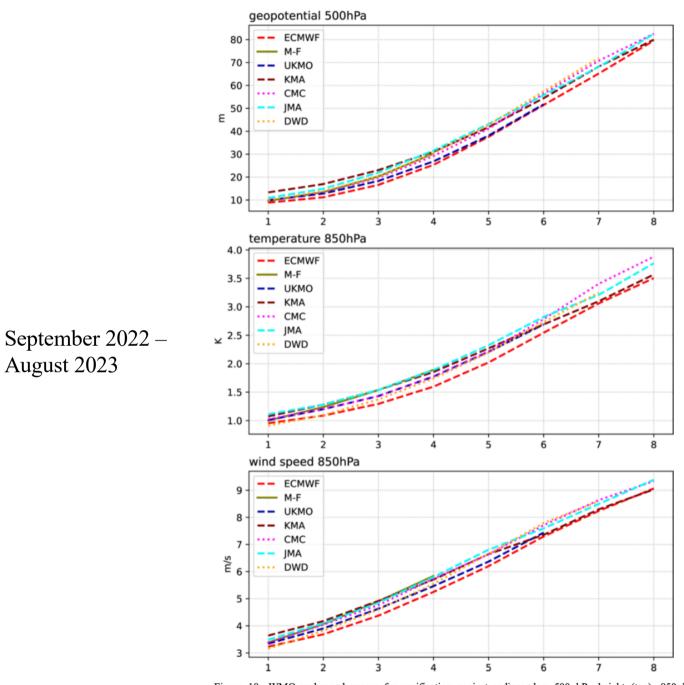


Figure 18: WMO-exchanged scores for verification against radiosondes: 500 hPa height (top), 850 hPa temperature (middle), and 850 hPa wind (bottom) RMS error over Europe and North Africa (annual mean August 2022–July 2023) of forecast runs initialized at 12 UTC. M-F = Météo-France, JMA = Japan Meteorological Agency, CMC = Canadian Meteorological Centre, UKMO = the UK Met Office, KMA = Korea Meteorological Administration, DWD = Deutscher Wetterdienst.

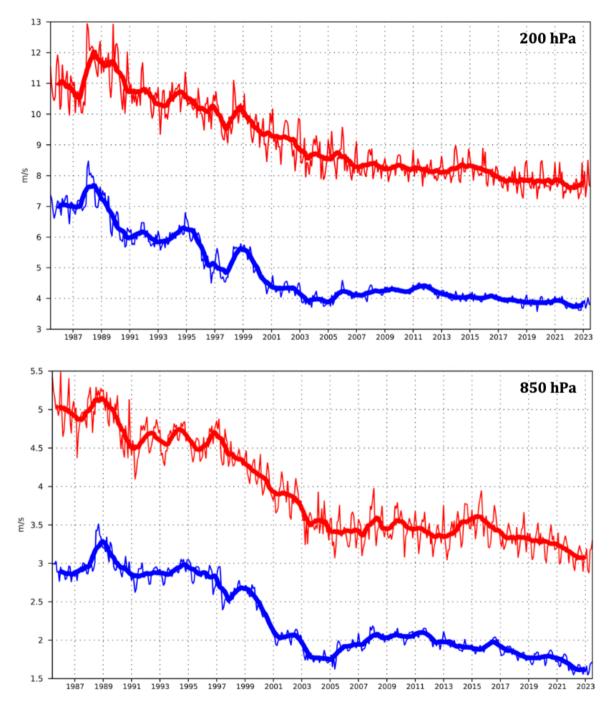


Figure 16: Forecast performance in the tropics. Curves show the monthly average RMS vector wind errors at 200 hPa (top) and 850 hPa (bottom) for one-day (blue) and five-day (red) forecasts, verified against analysis. 12-month moving average scores are also shown (in bold).

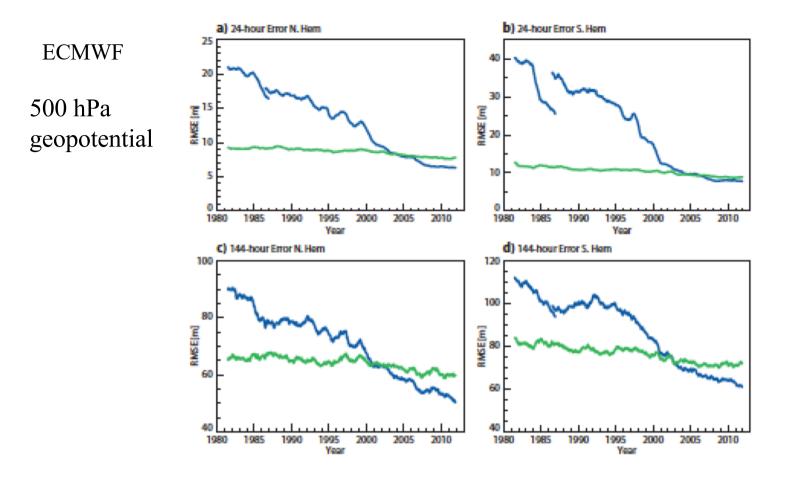


FIG. 3. Evolution of forecast errors from 1981 to 2012 for N.Hem (a and c) and S.Hem (b and d). Operational forecasts (blue) and ERA Interim (green). Note that before 1986 the operational analysis is used to verify the operational forecasts, after 1986 ERA Interim is used for the verification (with an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

- ...

## **Remaining Problems**

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

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

- ...

#### **Alternative Approach to Numerical Weather Prediction**

Machine Learning (aka Artificial Intelligence)

Set of empirical data

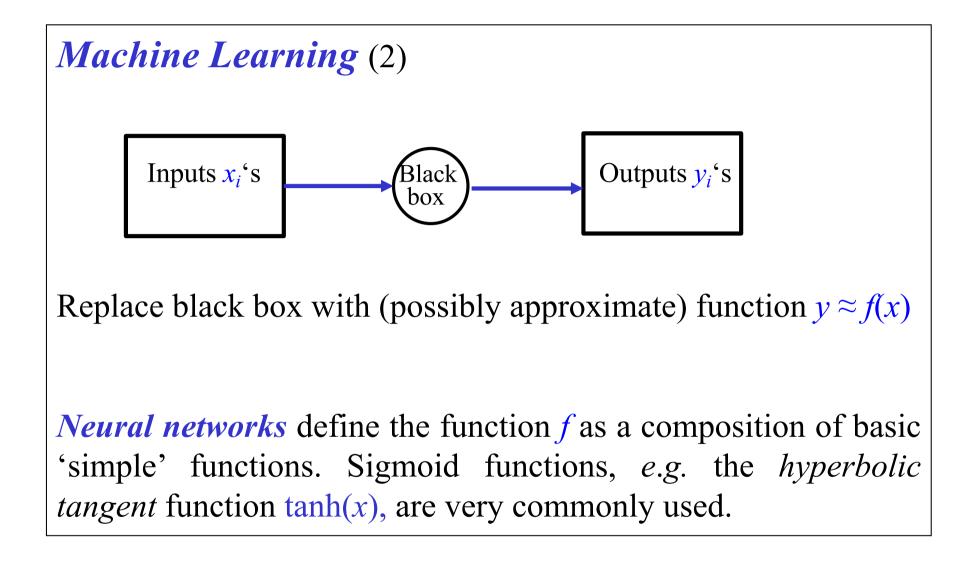
 $(x_i, y_i), i = 1, N$ 

with no *a prori* explicitly known relationship between the inputs  $x_i$ 's and the outputs  $y_i$ 's.

Look for an explicit relationship of the form

 $y \approx f(x)$ 

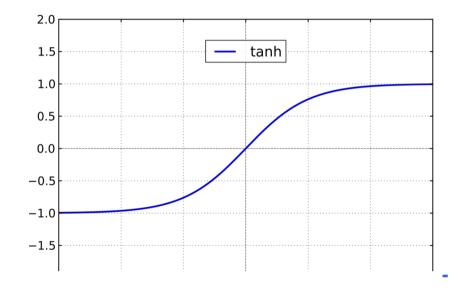
at least over a practically useful domain of variation of x.



**Machine Learning** (3)

#### Neural networks

 $tanh(x) = (e^{2x} - 1) / (e^{2x} + 1)$ 



Affine change of coordinates. Four degrees of freedom : two for the coordinates of the central point, and one for the range of variation in either direction.

# **Machine Learning** (4)

## Neural networks

The initial empirical dataset  $(x_i, y_i)$  is typically divided into two sets

- A *training set* over which the composition of basic functions is defined. This usually involves several layers of '*neurons*', the neurons in each layer being compositions of neurons in previous layers. The optimal combination is obtained by minimizing the misfit between the original and computed outputs, often on the basis of a least-squares criterion.
- A *validating set* used to estimate the quality of the adjustment obtained from the training set.

# **Machine Learning** (5)

## Neural networks

This approach, with many variants, has proved to be extremely efficient, and is now used for innumerable applications in many different domains.

It has been applied to numerical weather prediction. A number of recently developed softwares are

GraphCast

Pangu-Weather

FourCastNet

FuXi

## Machine Learning (5). Neural networks

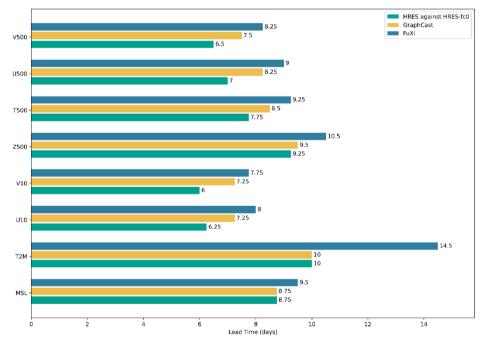
These software pieces have been trained on the ECMWF Reanalysis v5 (ERA5).

ERA5, which covers the period from January 1940 to present, provides hourly estimates of a large number of atmospheric, land and oceanic climate variables. The data cover the Earth on a 30km grid and resolve the atmosphere using 137 levels from the surface up to a height of 80km. ERA5 includes information about uncertainties for all variables. It is produced using 4D-Var data assimilation over 12-hour assimilation windows.

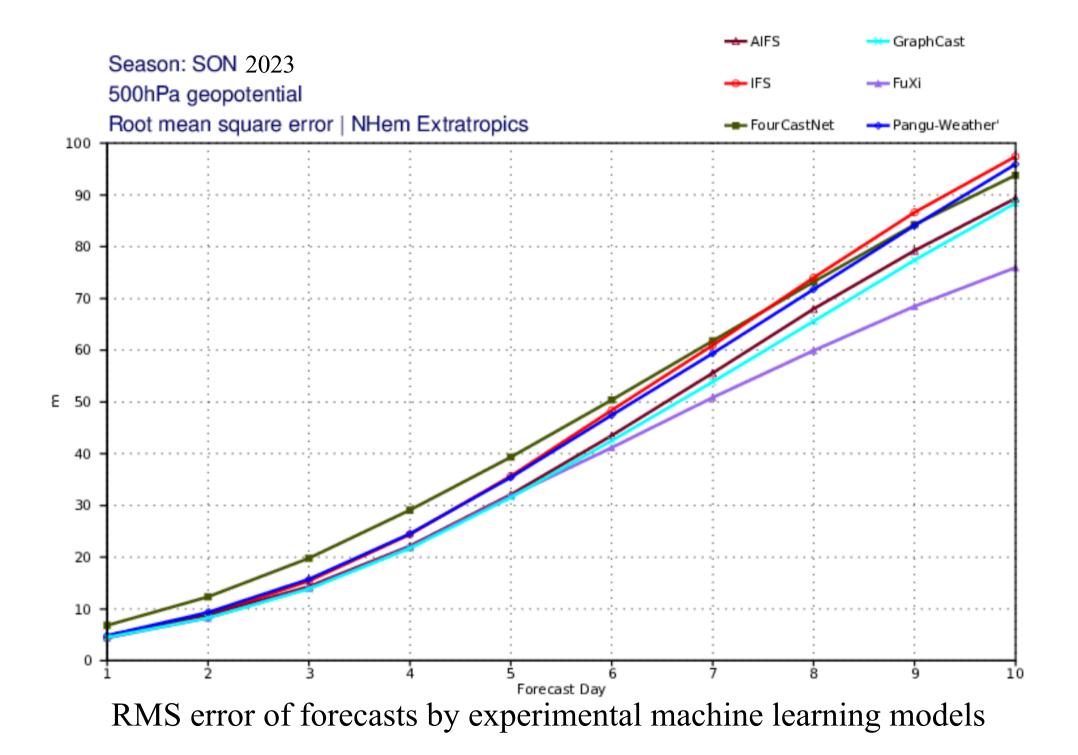
These neural networks trained on ERA5 produce forecasts of quality similar to, or better than, the ECMWF operational forecasts at a much lower numerical cost. Their results are accessible online on the Website of ECMWF.

# Machine Learning (6). Neural networks

FuXi (伏羲) has been trained on 39 years of ERA5. It has a spatial resolution of 0.25° (28 km, against 9 km for ECMWF HRES) and produces forecasts for a number of meteorological variables



**Fig. B.2**: Skillful forecast lead times (ACC >0.6) of ECMWF HRES, Graphcast, and FuXi for 4 surface variables (MSL, T2M, U10, and V10) and 4 upper-air variables (Z500, T500, U500, and V500) at 500 hPa pressure level.



# Machine Learning (7).

- Machine Learning forecasts are more accurate in terms of RMS error and correlation coefficients, but are also spatially much smoother.

- Machine learning can be implemented for estimating errors in deterministic forecasts

- But, at this stage, machine learning still depends totally on the availability of a training set produced by well-established and thoroughly validated means. How will these be updated ?

# Machine Learning (8).

- Machine Learning can be expected to have a significant impact on the way weather prediction is going to be performed, as well as on the quality of the corresponding forecasts.

- But what will precisely be that impact ? It is simply too soon to tell.

- 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 ( $n \approx 10^{6}$ -10<sup>9</sup> parameters to be estimated,  $p \approx 10^{7}$ -10<sup>8</sup> 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

Proportion of computing resources devoted to assimilation of observations in the whole process of Numerical Weather Prediction has gradually increased over time.

Definition of initial conditions originally required a simple interpolation from observation stations to model gridpoints, with negligible cost. As of now, assimilation over 24 hours of observations requires about the same amount of resources as a 10-day forecast, including probabilistic forecast.

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

 $\zeta_1$  and  $\zeta_2$  mutually independent

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

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

$$P(x = \xi | z_1, z_2) \propto p_1(z_1 - \xi) p_2(z_2 - \xi)$$
  

$$\propto \exp[-(z_1 - \xi)^2 / 2s_1] \exp[-(z_2 - \xi)^2 / 2s_2]$$
  

$$= \exp[-A/2]$$

with 
$$A = (z_1 - \xi)^2 / s_1 + (z_2 - \xi)^2 / s_2$$
  
=  $(\xi - x^a)^2 / p^a$  + terms independent of  $\xi$ 

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

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

Conditional probability distribution of *x*, given  $z_1$  and  $z_2 : \mathcal{N}[x^a, p^a]$ 

Conditional probability distribution of *x*, given  $z_1$  and  $z_2 : \mathcal{N}[x^a, p^a]$ 

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

 $p^a < (s_1, s_2)$  independent of  $z_1$  and  $z_2$ 

 $x^a = p^a (z_1/s_1 + z_2/s_2)$  is weighted average of  $z_1$  and  $z_2$ , with respective weights  $1/s_1$  and  $1/s_2$ . Larger weight is given to more accurate piece of data.

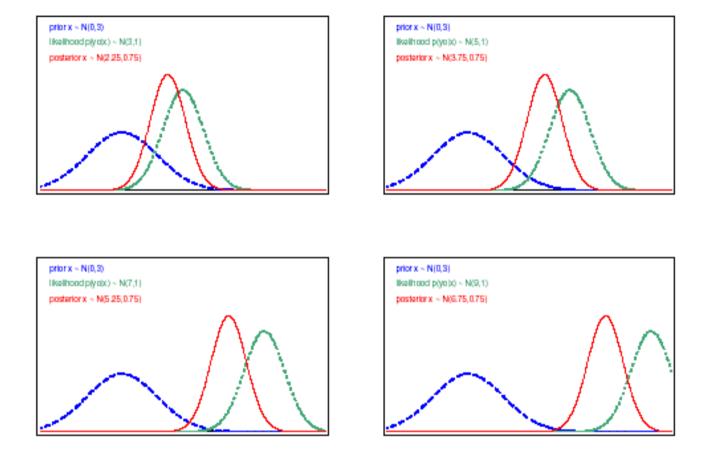


Fig. 1.1: Prior pdf p(x) (dashed line), posterior pdf  $p(x|y^o)$  (solid line), and Gaussian likelihood of observation  $p(y^o|x)$  (dotted line), plotted against x for various values of  $y^o$ . (Adapted from Lorenc and Hammon 1988.)

#### 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)

International Symposium on Data Assimilation - Online (ISDA-Online)

# "Machine Learning in Data Assimilation"

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