

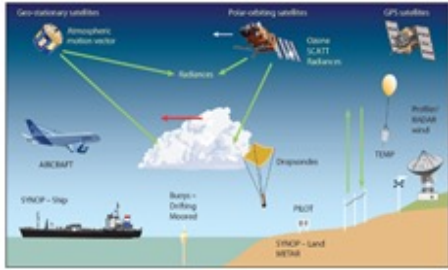
# Machine Learning for Model Error Estimation and Prediction

Massimo Bonavita

*Principal Scientist*

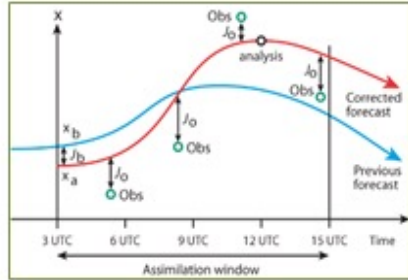
*Data Assimilation Team Leader*

*[massimo.bonavita@ecmwf.int](mailto:massimo.bonavita@ecmwf.int)*



## Observations

- quality control
- adaptive thinning
- bias correction
- Fast observation models



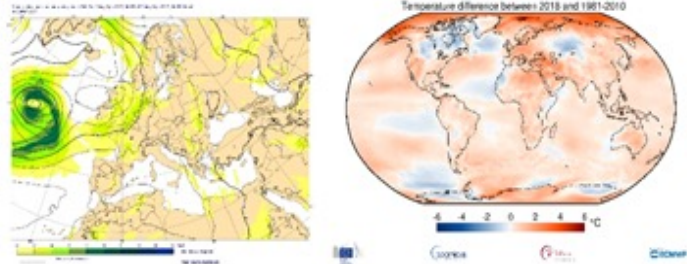
## Data assimilation

- Model error estimation
- Model parameter estimation
- Error covariance statistics



## Forecast Models

- Surrogate models
- Fast emulator models
- Linearised models for Var



## Product generation

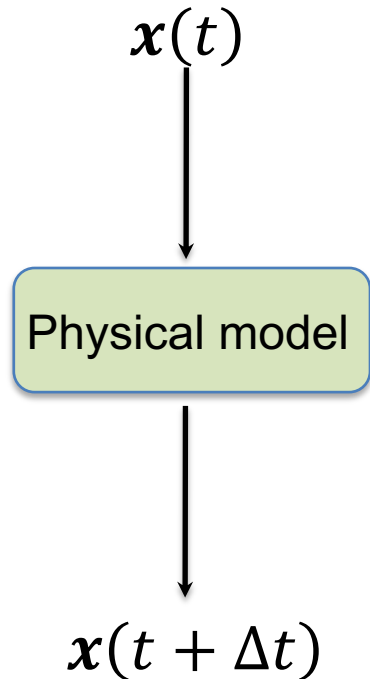
- information extraction (resolution, ensembles, weather features)
- data compression

# A taxonomy of forecast models

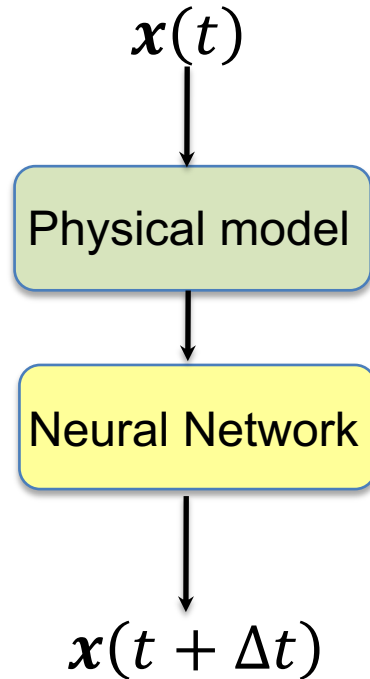
$$x(t + \Delta t) = M(x(t))$$

Physics-based

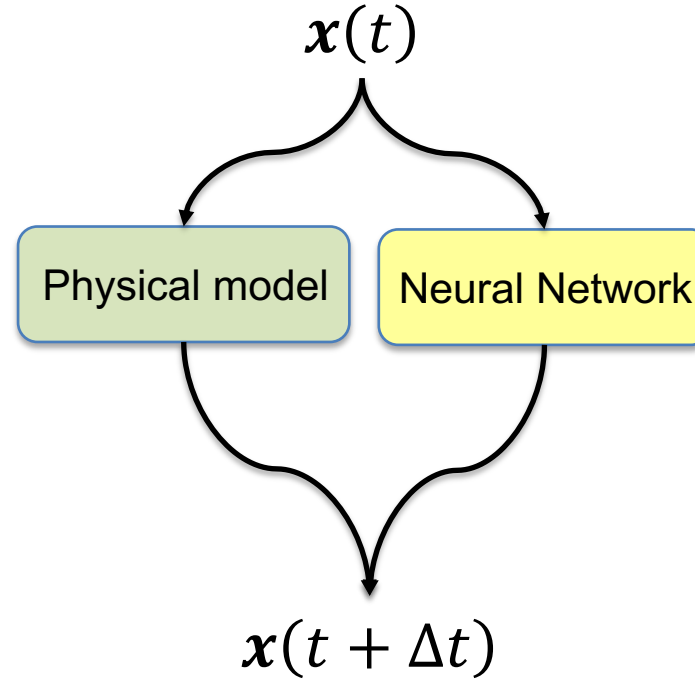
Data-driven



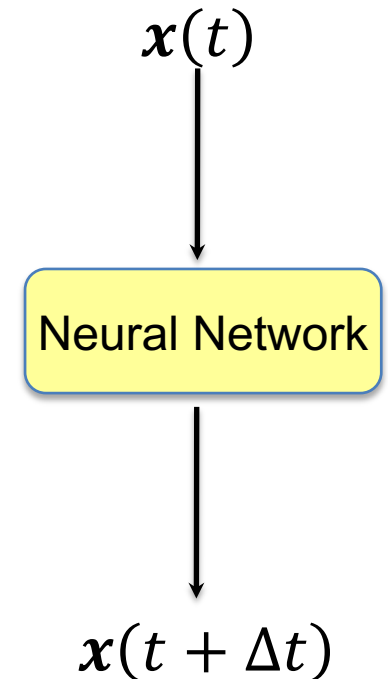
**Standard NWP models**  
(IFS, ICON, FVM,...)



**Model error correction**  
(e.g. Bonavita and Laloyaux, 2020; Farchi et al., 2022, 2023)

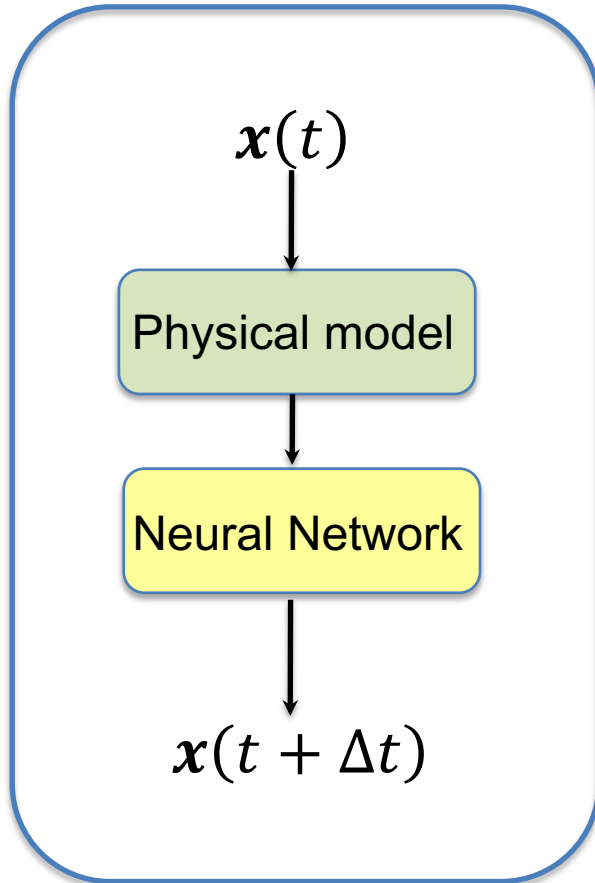


**Partial model emulation**  
(e.g. Chantry et al., 2021; Kochkov et al., 2023, NeuroGCM)



**Full model emulation**  
(e.g. Keisler, 2021, PanguWeather, 2022, GraphCast, 2023, ...)

# Data-driven model error correction



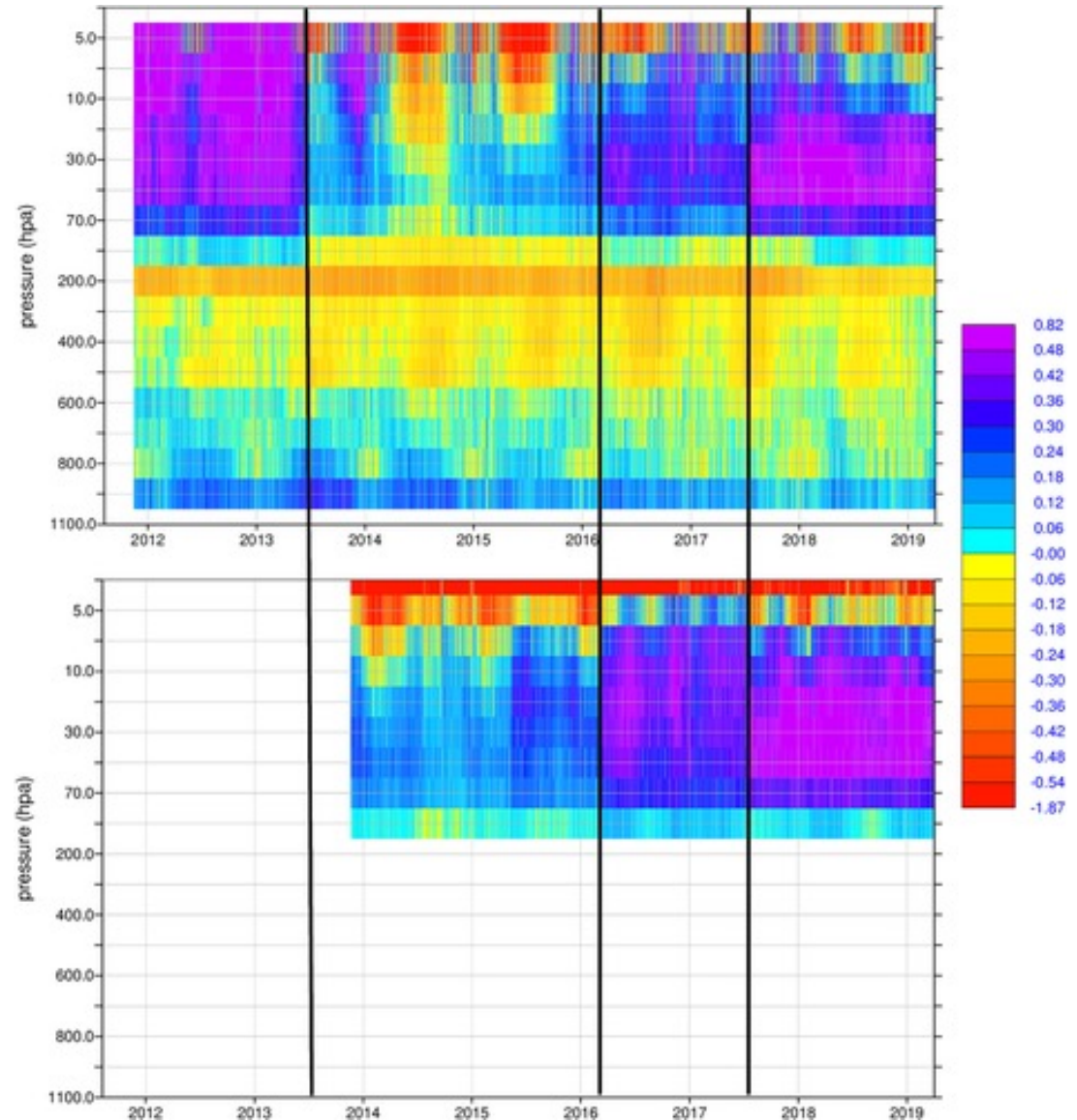
- The physical model will always be affected by systematic, predictable errors due to a variety of causes (unresolved, unrepresented physics, discretisation errors, wrong model forcings, etc.)
- The NN is used as a data-driven (statistical) online correction to the time tendencies forecasted by the physical model:

$$\frac{dx}{dt} = \Phi_{adv}(x(t)) + \Phi_{phys}(x(t)) + \Phi_{ML}(x(t))$$

- Is model error a big deal?

# Model Error: Atmosphere

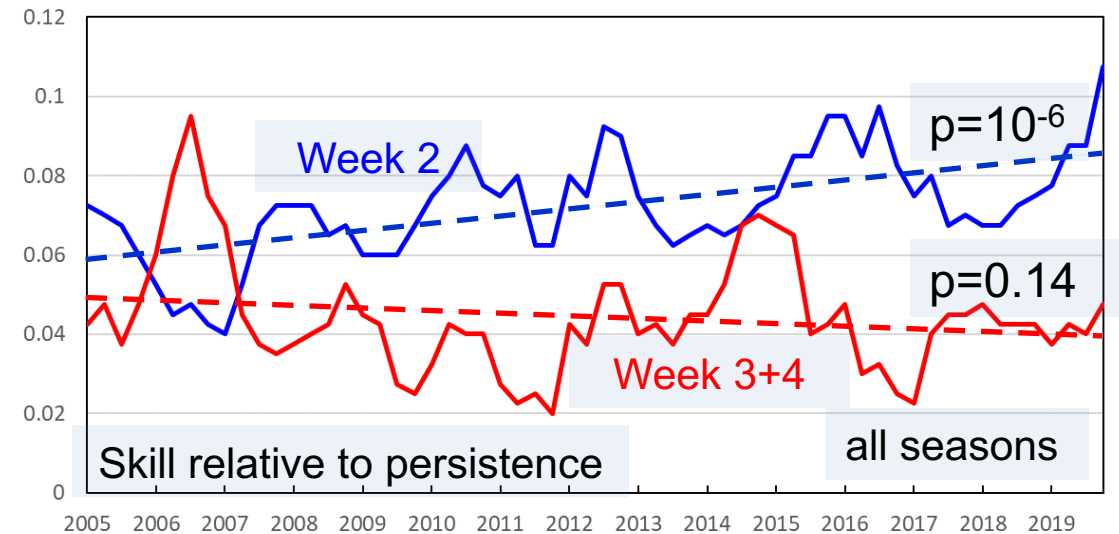
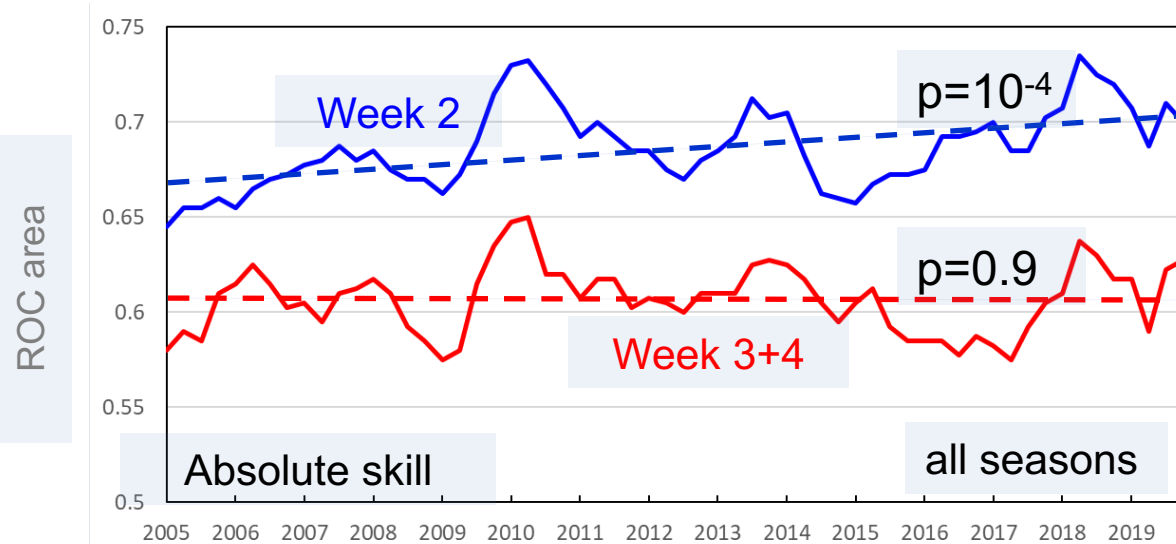
Time series of the difference between observations and temperature first-guess trajectory from the ECMWF operational analysis cycle for radiosonde (top) and Radio Occultations (bottom)



Laloyaux et al., 2020

# Model Error: Atmosphere

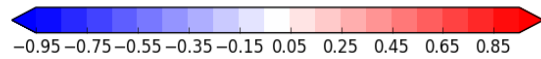
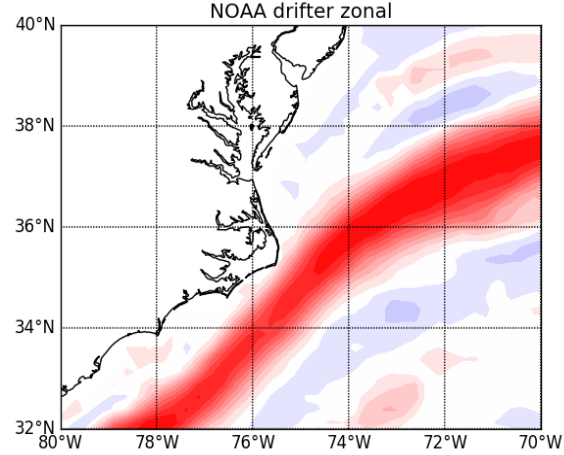
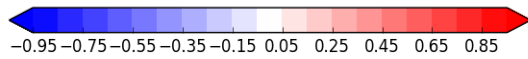
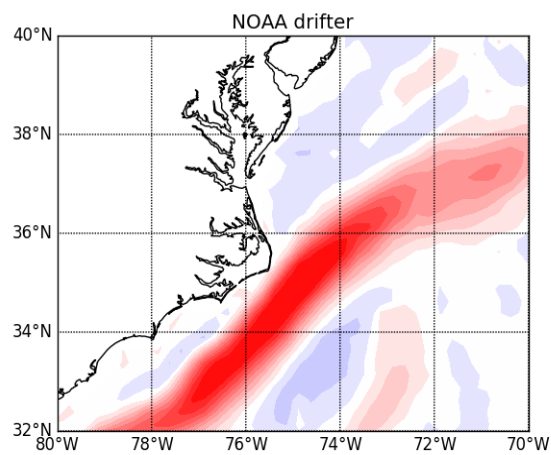
- Traditionally, DA algorithms have used a perfect model assumption and aimed at reducing random initial conditions errors: this approach brings steady progress up to ~2 weeks, but not beyond
- Can Machine Learning help break the 2-week Lorenz predictability barrier?



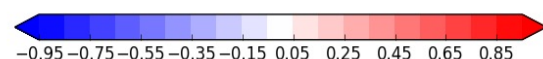
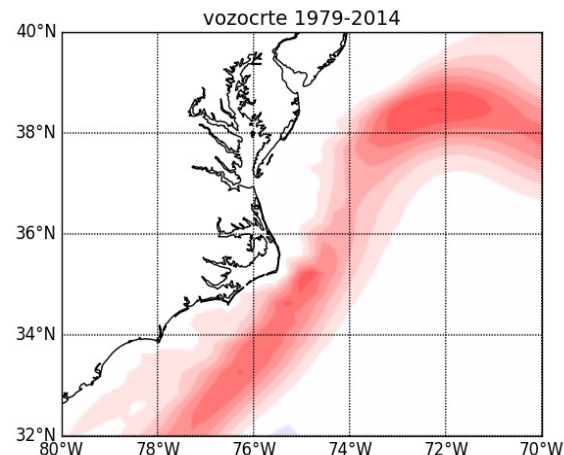
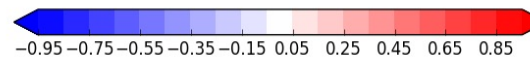
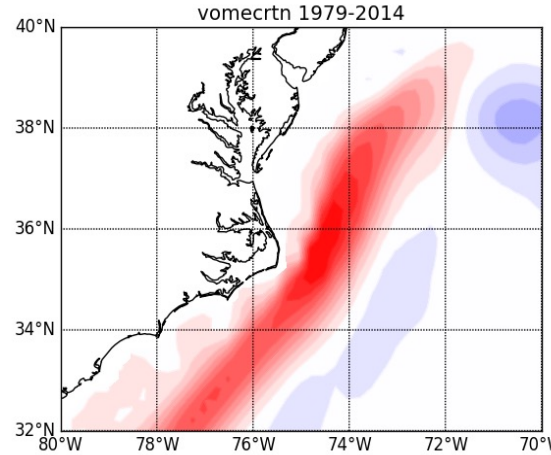
From Frederic Vitart and Thomas Haiden

# Model Error: Ocean

## NOAA drifter climatology

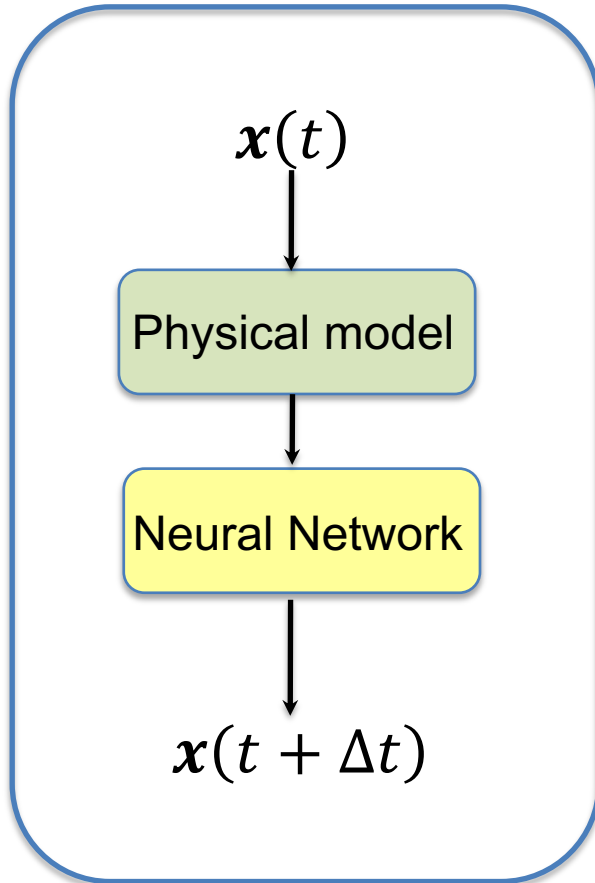


## ORAS5 1985-2012.



From Hao Zuo

# Model error estimation

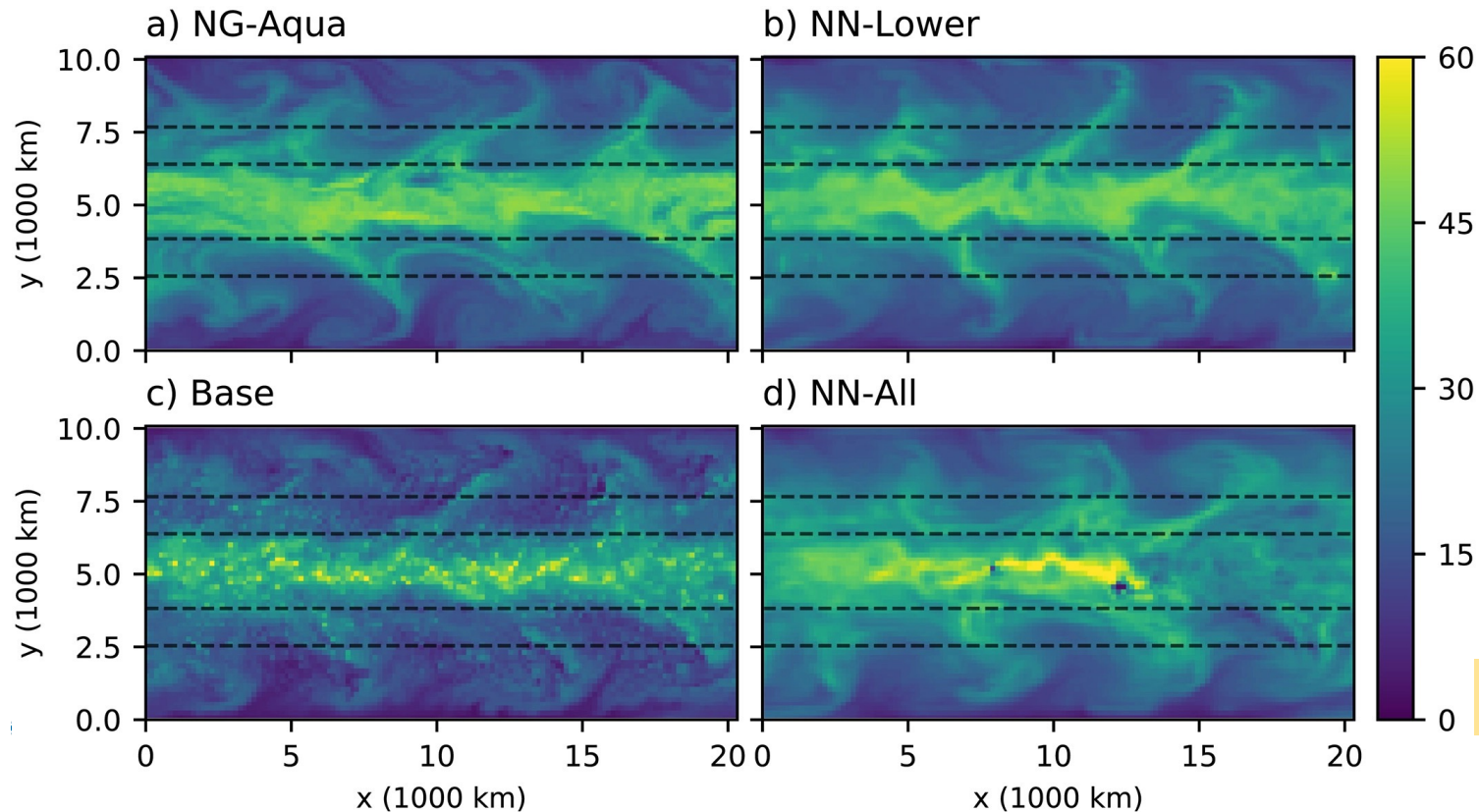


- The first challenge is the estimation of model error
- Using a statistical model like a NN requires choosing a ground truth to build the training dataset
- We have different options here...



# Model error estimation

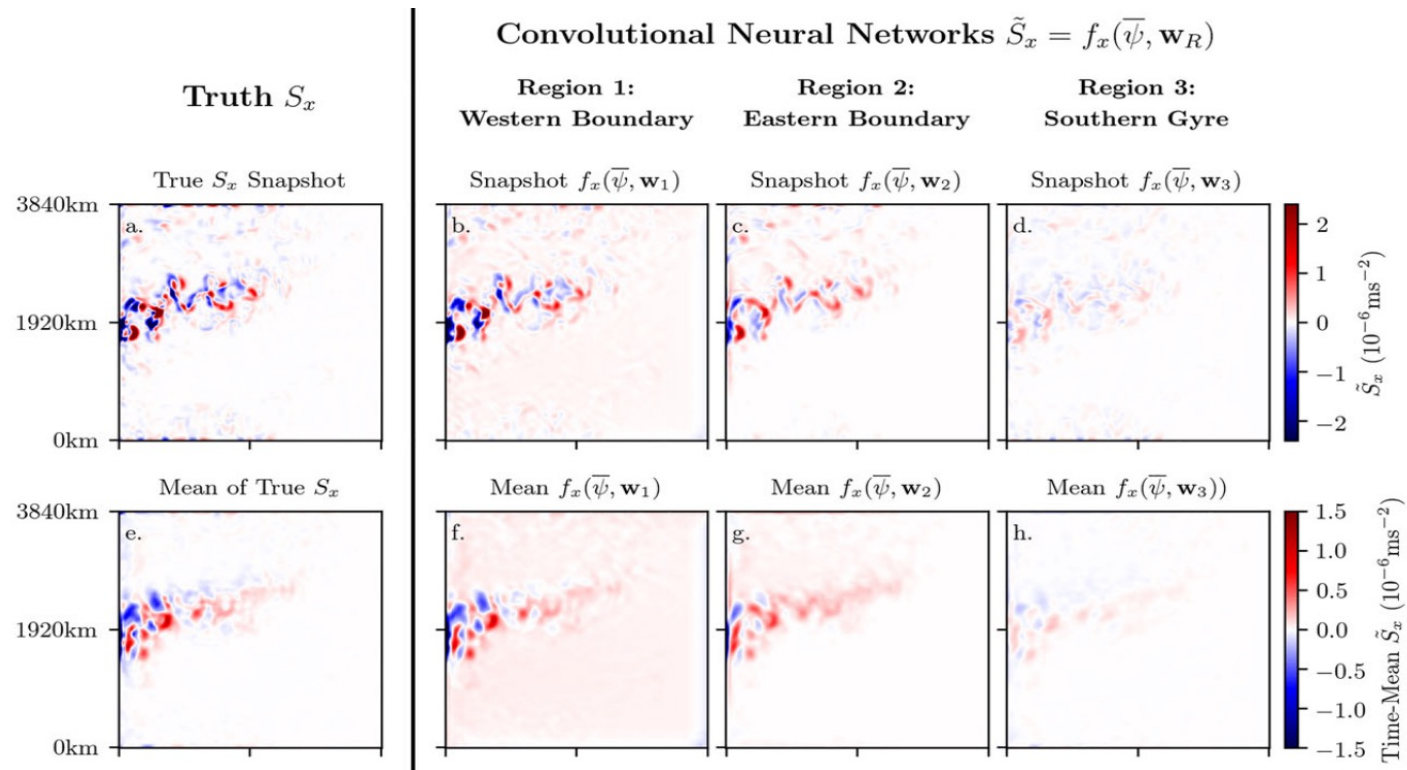
- One option is to train the NN using a more complex, more accurate, higher resolution version of the model as a proxy for the truth
- The goal is to train the NN to learn the effect of the parameterised and unresolved dynamical and physical processes onto the resolved dynamics (e.g., Brenowitz and Bretherton, 2018, 2019; Rasp et al., 2018)



Brenowitz and Bretherton, 2019

# Model error estimation

- In Ocean Modelling one of the main sources of errors come from insufficient resolution -> need to account for unresolved physical processes
- This problem has been tackled with ML tools (CNN, DNN, RVM) to build offline data-driven parameterizations of the unresolved dynamics for a fully observed system (Bolton and Zanna, 2019, Zanna and Bolton, 2020, Kutz, 2017, Ling et al., 2016)



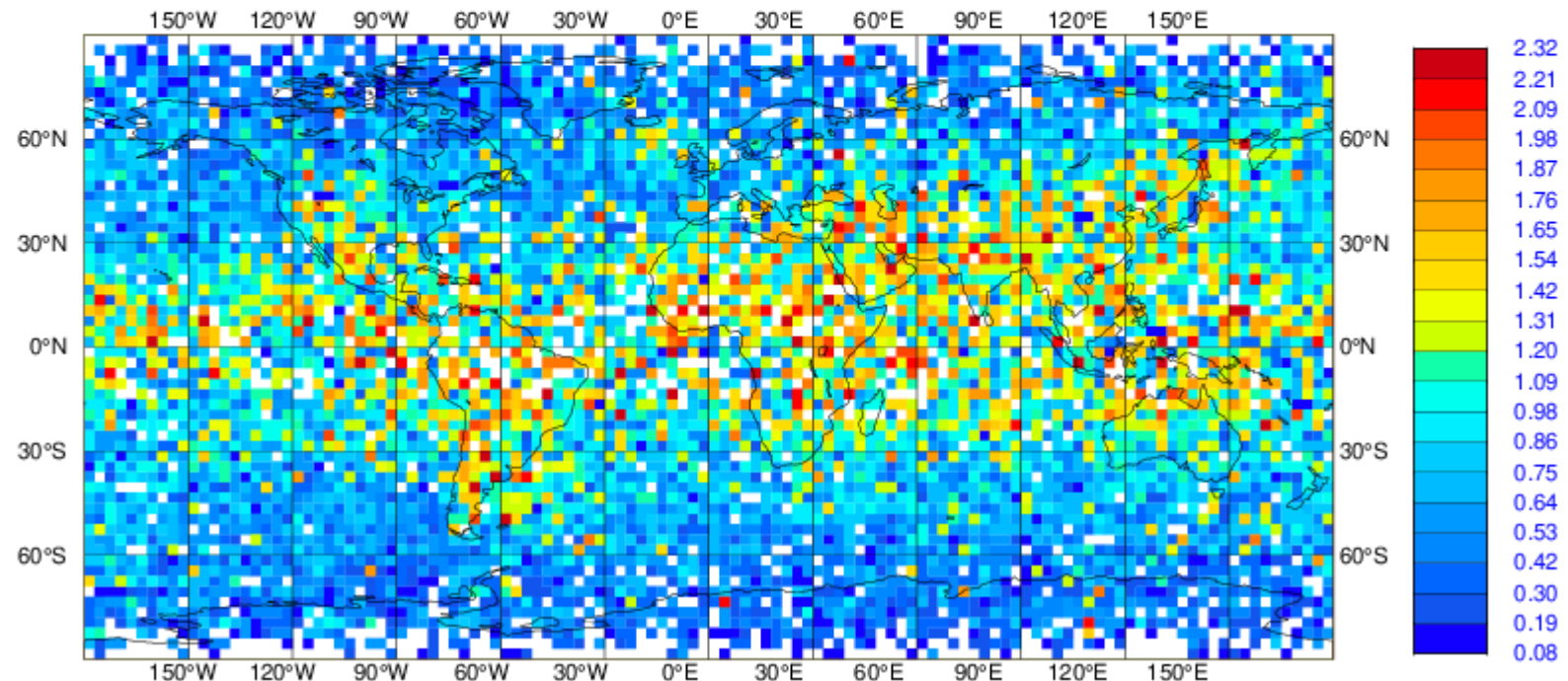
Bolton and Zanna, 2019



# Model error estimation

- Another option is to train the NN using observations of the system as a proxy for the truth
- The training dataset is built using observations minus (short range) forecasts (O-B departures)
- The NN is trained to learn the O-B departures from a set of available predictors (state, location, time of day, season, etc.)

STATISTICS FOR SETTING RO FROM METOP-B  
STDV OF NORMALISED FIRST GUESS DEPARTURE (PASSED\_FGCHECK)  
DATA PERIOD = 2022-02-28 21 - 2022-04-22 21  
EXP =, IMPACT HEIGHT = 20 KM  
Min: 0.000 Max: 3.464 Mean: 0.894  
GRID: 3.00x 3.00

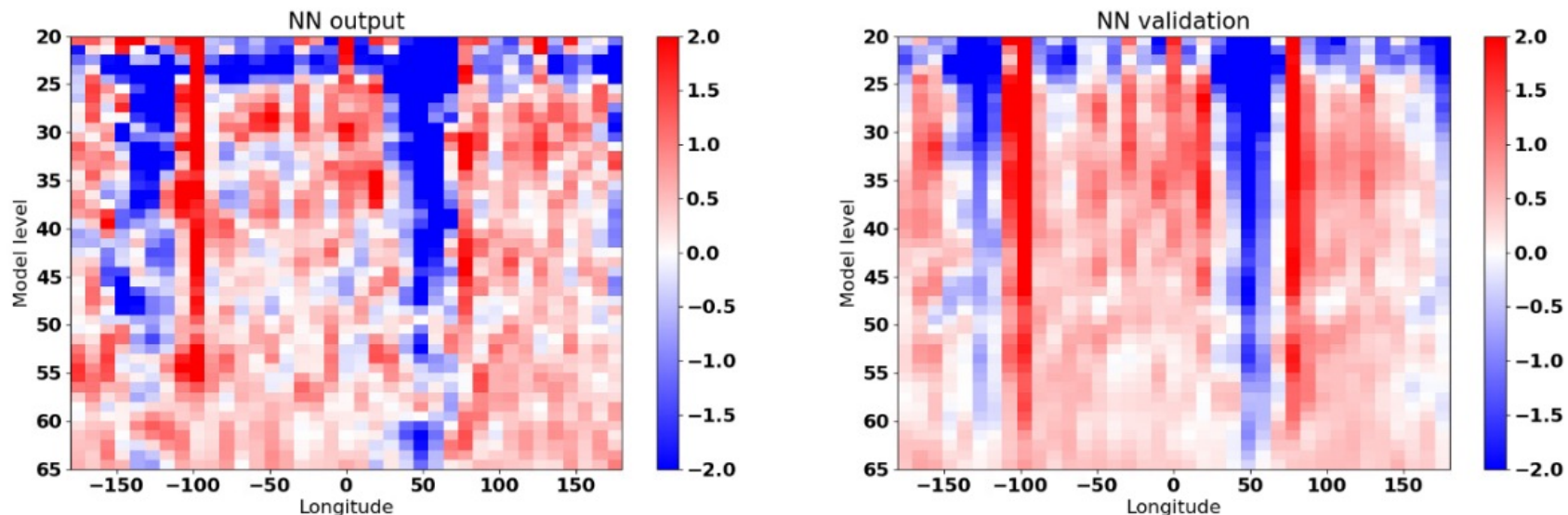


ECMWF Observation Monitoring

# Model error estimation

- The idea of using observations as the truth is attractive because it directly introduces independent information on the model errors we want to correct
- It also comes with its own caveats: observation errors, observation coverage, how to extrapolate the corrections in space, time and to other variables in a physically consistent manner?

O-B departures on 01-05-2019 averaged between 10S and 20N (left) and their prediction with a Convolutional Neural Network (right)



# Model error estimation

- Option #3 is to train the NN using analysed states of the system as a proxy for the truth
- The training dataset is built using analysis minus (short range) forecasts (A-B increments)
- The NN is trained to learn the A-B increments from a set of available predictors (state, location, time of day, season, local solar zenith angle, SST, etc)
- Advantages:
  1. The model error estimates are directly available in model space and globally;
  2. Analyses are more accurate than any individual observation type
- Disadvantages:
  1. The analyses will be affected to some extent by the model error we want to estimate
  2. The (A-B) increments will also be affected by "errors of the day" (i.e., initial condition errors)

# Model error estimation: weak constraint 4D-Var

- We already do model error estimation inside the 4D-Var analysis cycle: it is called weak constraint 4D-Var!

$$J_{wc4DVar}(\mathbf{x}_0, \boldsymbol{\eta}) = J_B + J_O + J_Q = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T B^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2} \sum_{i=0}^N (H_i(\mathbf{x}_i) - \mathbf{y}_i)^T R_i^{-1} (H_i(\mathbf{x}_i) - \mathbf{y}_i) + \frac{1}{2} \sum_{i=1}^N \left( \mathbf{x}_i - M_i(\mathbf{x}_{i-1}, \boldsymbol{\eta}) \right)^T Q_i^{-1} \left( \mathbf{x}_i - M_i(\mathbf{x}_{i-1}, \boldsymbol{\eta}) \right)$$

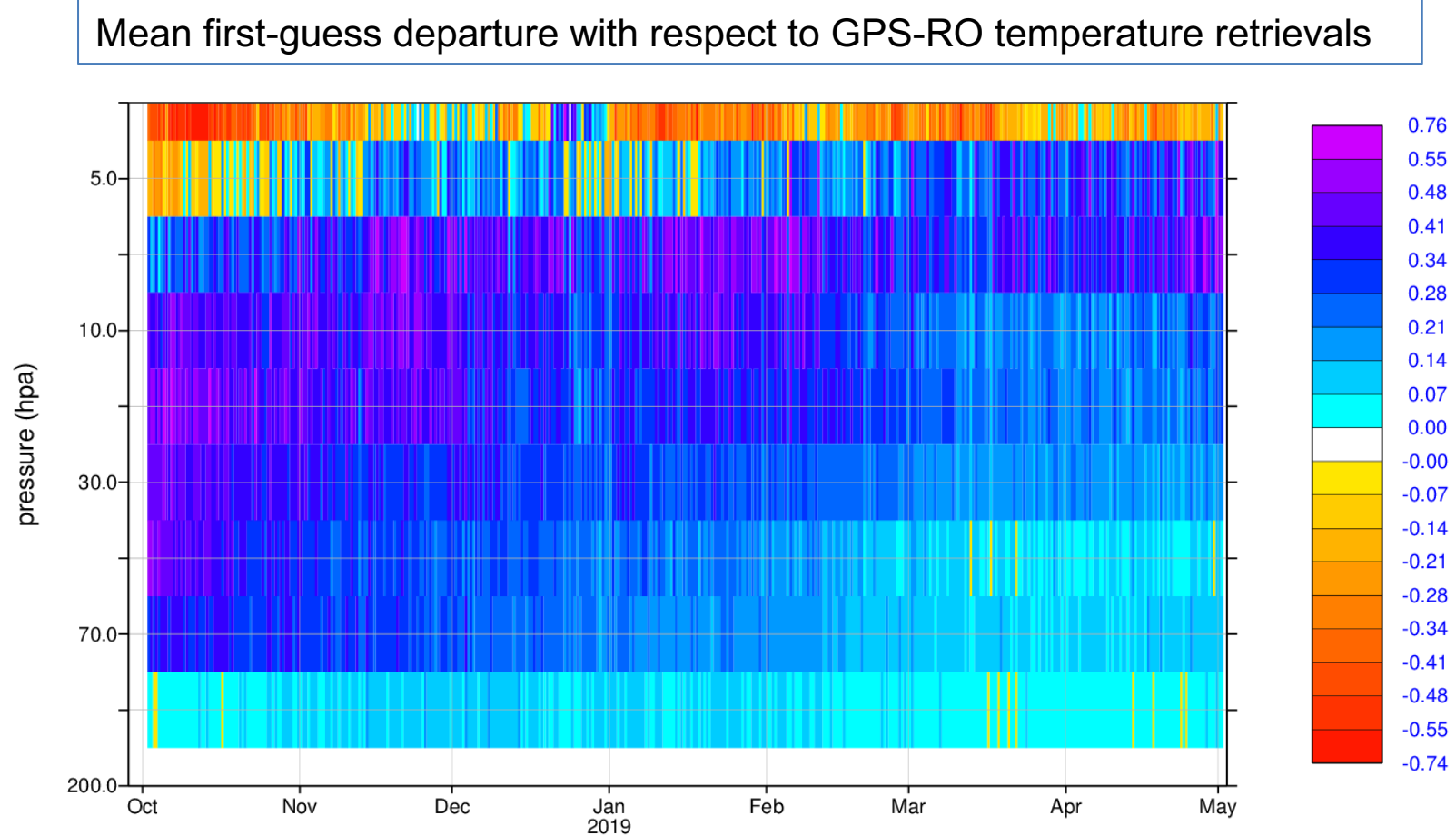
$\mathbf{x}_0 = \text{state estimate}$   
 $\boldsymbol{\eta} = \text{model error estimate}$

Loss functions common in ML/DL can be obtained as particularisations of wc-4DVar (Brajard et al., 2020; Bocquet et al., 2020; Farchi et al., 2020):

1. ML/DL models are not used for state estimation  $\rightarrow J_B = 0$
2. ML/DL loss functions typically assume full, noiseless observations ( $H_i = I, R_i \rightarrow 0$ )  $\rightarrow J_O = 0$
3. ML/DL models can optionally have a regularization term function of the NN model parameters  $\mathbf{L}(\boldsymbol{\eta}) = \mathbf{L}(\mathbf{W}, \mathbf{b})$ , e.g. Tikhonov regularisation, drop-out, etc.

# Model error estimation: weak constraint 4D-Var

- wc-4DVar progressively learns a model error tendency correction and applies it to subsequent background forecasts in the DA cycle
- wc-4DVar is an online machine learning algorithm for model error estimation and correction!



From Laloyaux et al, 2020

# Model error estimation: weak constraint 4D-Var

- What can Machine Learning bring to table?
- wc-4DVar produces an estimate of model error valid over the length of the assimilation window:  
 $J_{wc4DVar}(\mathbf{x}_0, \boldsymbol{\eta})$
- The NN will produce a model of model error, which can be applied and used at any point in time:

$$\mathbf{M}_W(\mathit{predictors}) = \mathbf{M}_W(\mathit{x}, \mathit{time}, \mathit{lat}, \mathit{lon}, \mathit{SST}, \dots)$$



# Hybrid ML-DA

- Option #3 is to train the NN using analysed states of the system as a proxy for the truth
- In this approach we have a number of possibilities on how to fuse the Data Assimilation system with the ML estimate of model error:
  1. Offline training of NN and use it in a data assimilation cycle (e.g, Bonavita and Laloyaux, 2020, Watson, 2019);
  2. Online training of NN in a data assimilation cycle with a coordinate descent approach (e.g. Brajard et al., 2020, Bocquet et al., 2020),
  3. Full online training of NN inside data assimilation system (e.g., Farchi et al., 2021b)

# Hybrid ML-DA in low-order systems

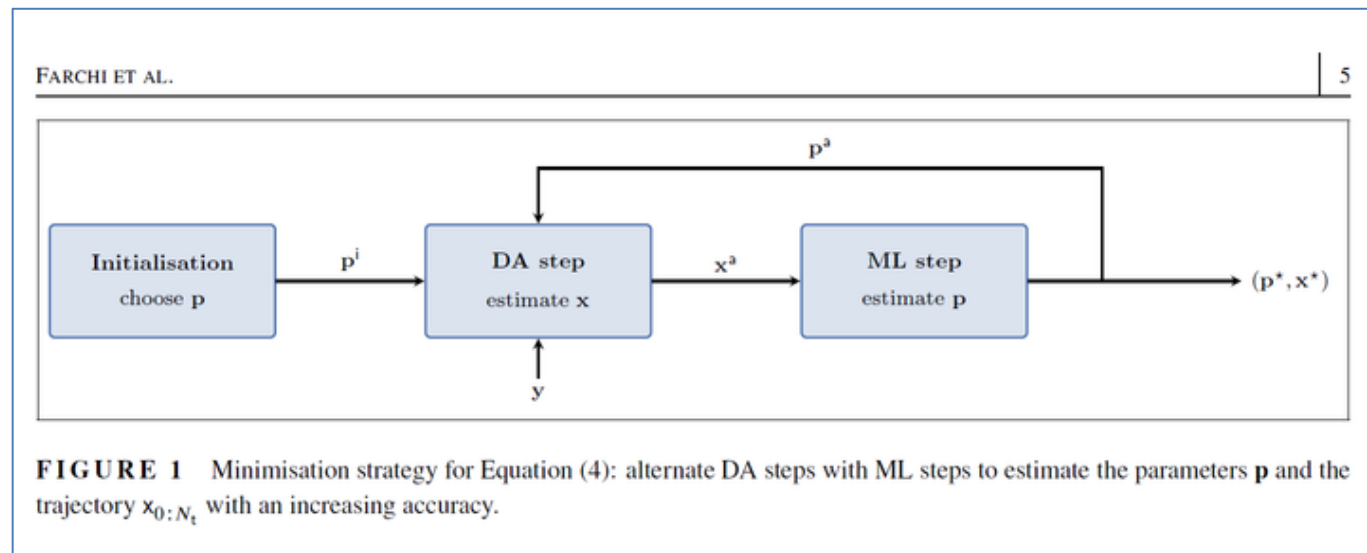
- In all generality we would like to minimise the following cost function of the state ( $\mathbf{x}_{0:N}$ ) and the NN parameters ( $\mathbf{p}$ ) (Farchi et al., 2021):

$$\begin{aligned} \mathcal{J}(\mathbf{p}, \mathbf{x}_{0:N_t}) &\triangleq \frac{1}{2} \|\mathbf{x}_0 - \mathbf{x}_0^b\|_{\mathbf{B}^{-1}}^2 + \frac{1}{2} \sum_{k=0}^{N_t} \|\mathbf{y}_k - \mathcal{H}_k(\mathbf{x}_k)\|_{\mathbf{R}_k^{-1}}^2 \\ &\quad + \frac{1}{2} \sum_{k=0}^{N_t-1} \|\mathbf{x}_{k+1} - \mathcal{M}_k(\mathbf{p}, \mathbf{x}_k)\|_{\mathbf{Q}_k^{-1}}^2 + \mathcal{L}(\mathbf{p}), \end{aligned} \tag{4}$$

- Here the background error ( $\mathbf{x}_0 - \mathbf{x}_0^b$ )  $\sim \mathcal{N}(\mathbf{0}, \mathbf{B})$ , the observations are sparse and are related to the system state by  $\mathbf{y}_k = \mathbf{H}_k(\mathbf{x}_k) + \mathbf{v}_k$ , ( $\mathbf{v}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$ )
- Model errors ( $\mathbf{x}_{k+1} - \mathcal{M}(\mathbf{p}, \mathbf{x}_k)$ ) follow a Gaussian distribution with covariance  $\mathbf{Q}_k$ , and are assumed uncorrelated with other error sources

# Hybrid ML-DA in low-order systems

- How to optimise this cost function of  $(\mathbf{p}, \mathbf{x}_{0:N})$ ?
- One way is to alternate DA steps (to estimate  $\mathbf{x}_{0:N}$ ) and ML steps (to estimate the model error parameters  $\mathbf{p}$ ) in a coordinate-descent framework:

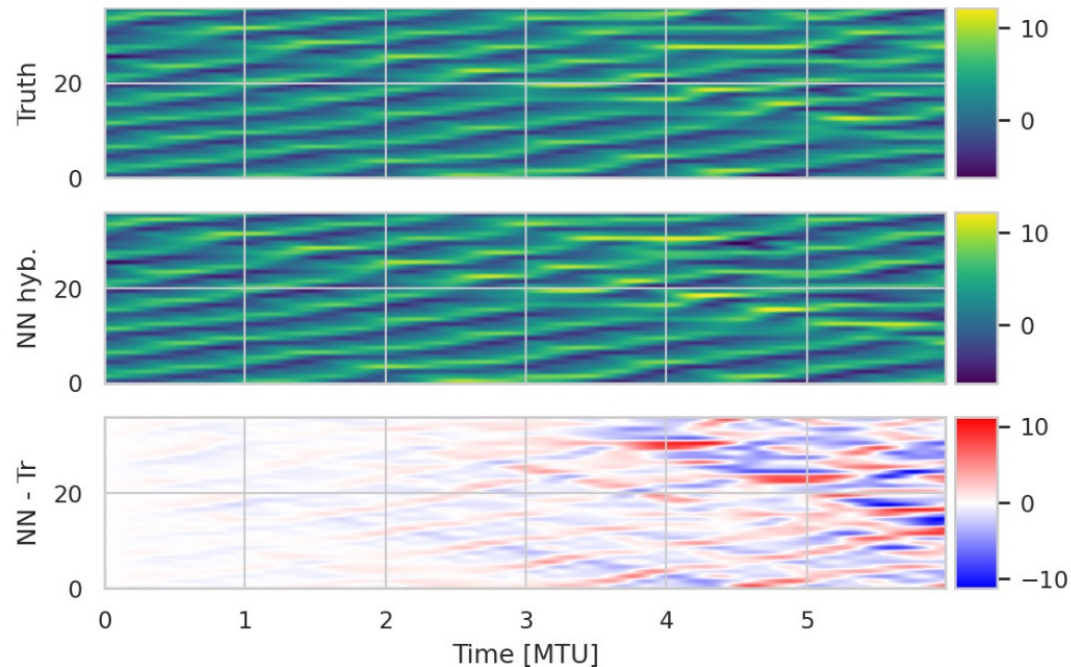


Coordinate descent approach for the online training of a NN

From Farchi et al., 2020

# Hybrid ML-DA in low-order systems

- This coordinate-descent idea was used with good results, e.g. in Brajard et al., 2021 to reconstruct the state and the dynamics of Lorenz-96 model using convolutional neural networks



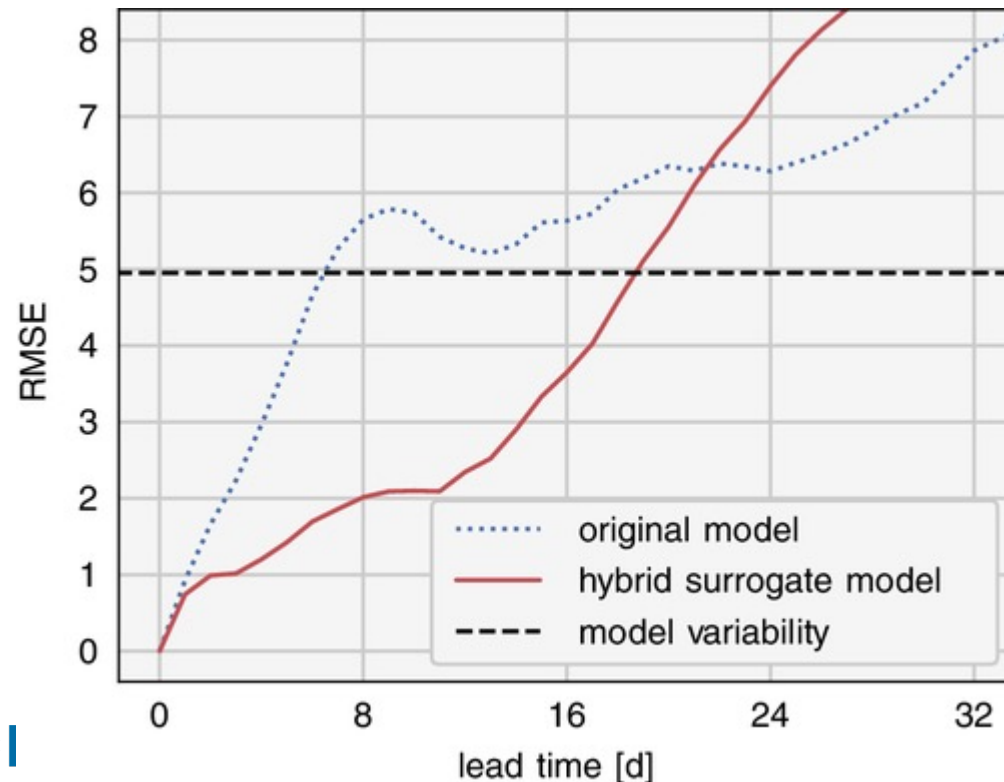
State estimation with the coordinate descent approach for the online training of a NN

from Brajard et al., 2021

- However: 1) the initialization of  $\mathbf{p}$  is critical and cold-starting can easily lead to divergence, and 2) the number of DA-ML cycles required to reach convergence can be high, problematic for a realistic application

# Hybrid ML-DA in low-order systems

- Farchi et al., 2021a, have used an offline training approach to construct a hybrid ML-physics model for a quasi-geostrophic system
- Their surrogate model based on Convolutional Neural Networks was shown to be able to significantly improve on the original perturbed model both in forecast mode and in the assimilation cycle

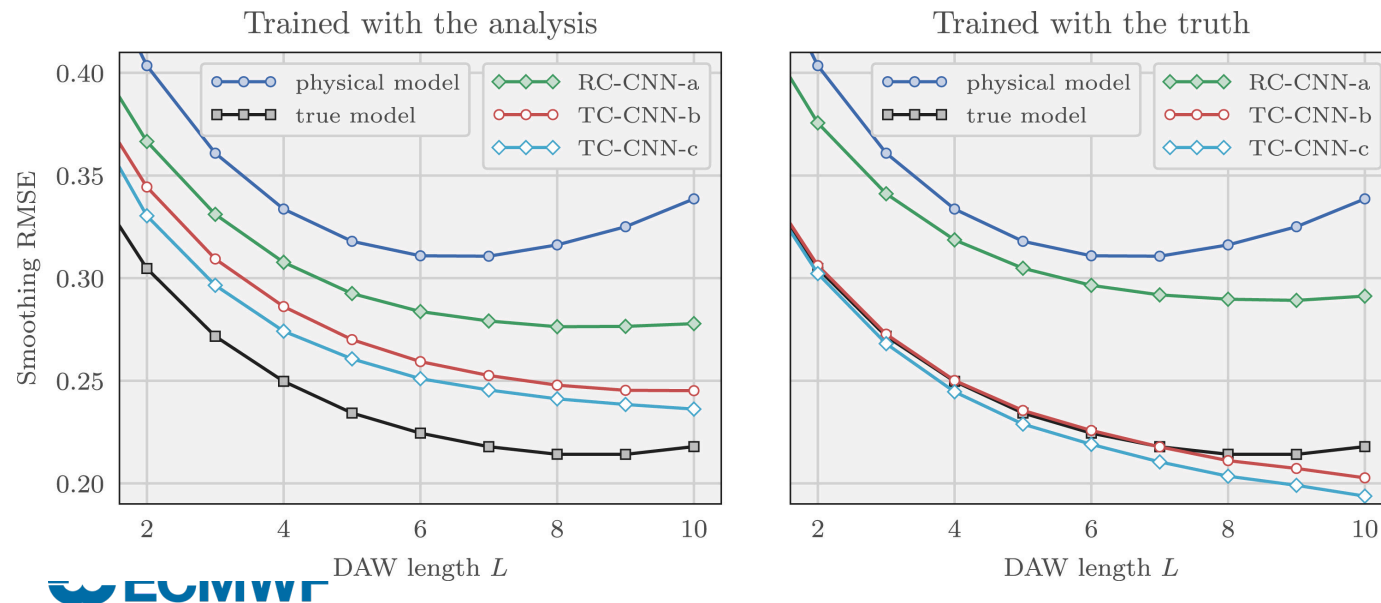


Forecast skill of the original model (dotted line) and the hybrid surrogate model (continuous line) as a function of the lead time in days

From Farchi et al., 2021a

# Hybrid ML-DA in low-order systems

- In Farchi et al., 2021b, two crucial aspects of the training process have been studied using the two-scale Lorenz model
- One aspect was whether it is more efficient to correct the integrated-in-time model error (i.e., the model resolvent), or the model error tendencies
- Results show that both techniques perform well in forecast mode, but tendency correction is preferable when the hybrid model is used in a DA cycle

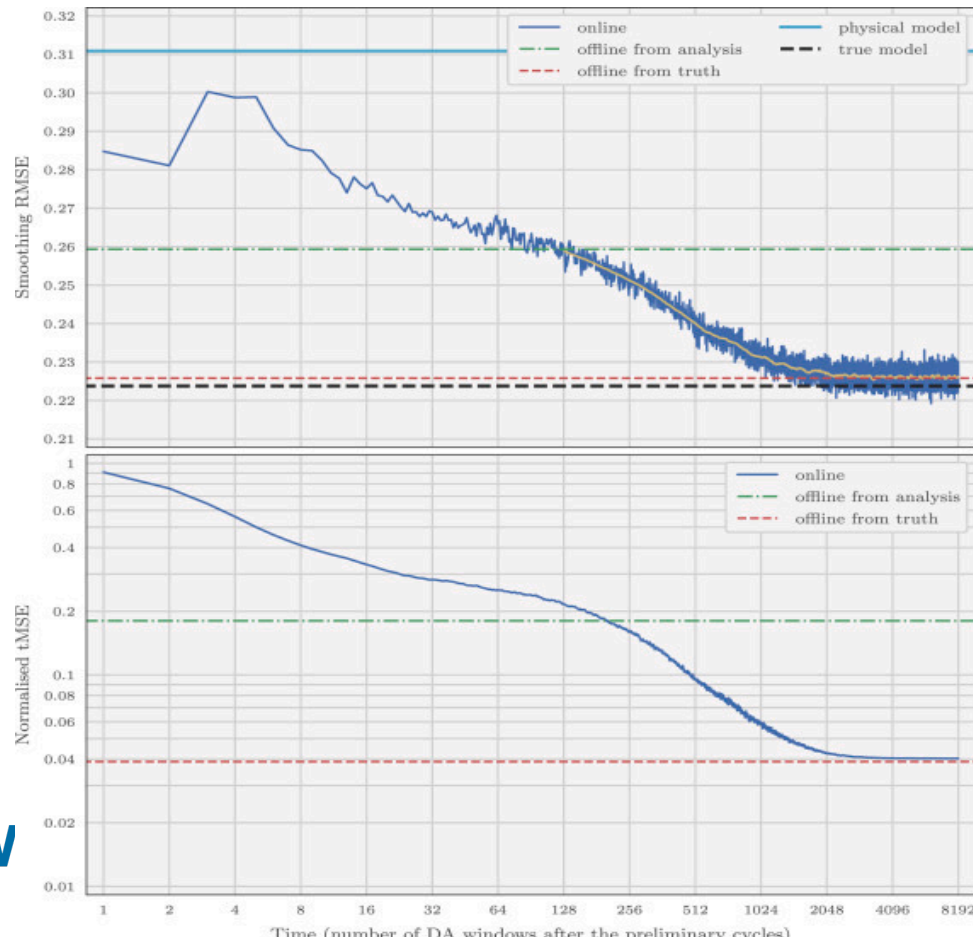


Analysis RMSE for the physical model (in blue), the true model (in black), and the trained surrogate models: RC-CNN-a (in green), TC-CNN-b (in red), and TC-CNN-c (in cyan). The surrogate models are trained either with the analysis (left panel) or with the truth (right panel).

From Farchi et al., 2021b

# Hybrid ML-DA in low-order systems

- The other aspect that was investigated was the effectiveness of offline vs online (i.e., inside 4D-Var) model error learning
- Online learning appears to give best results in this experimental setup



Time series of sRMSE (top panel) and tMSE (bottom panel) for the online experiment with TC-CNN-b (in blue). For comparison, the horizontal lines show the scores for the physical model (in cyan), the true model (in black), TC-CNN-b trained offline with the analysis (in green) and trained offline with the truth (in red).

From Farchi et al., 2021b

# Hybrid ML-DA in operational systems

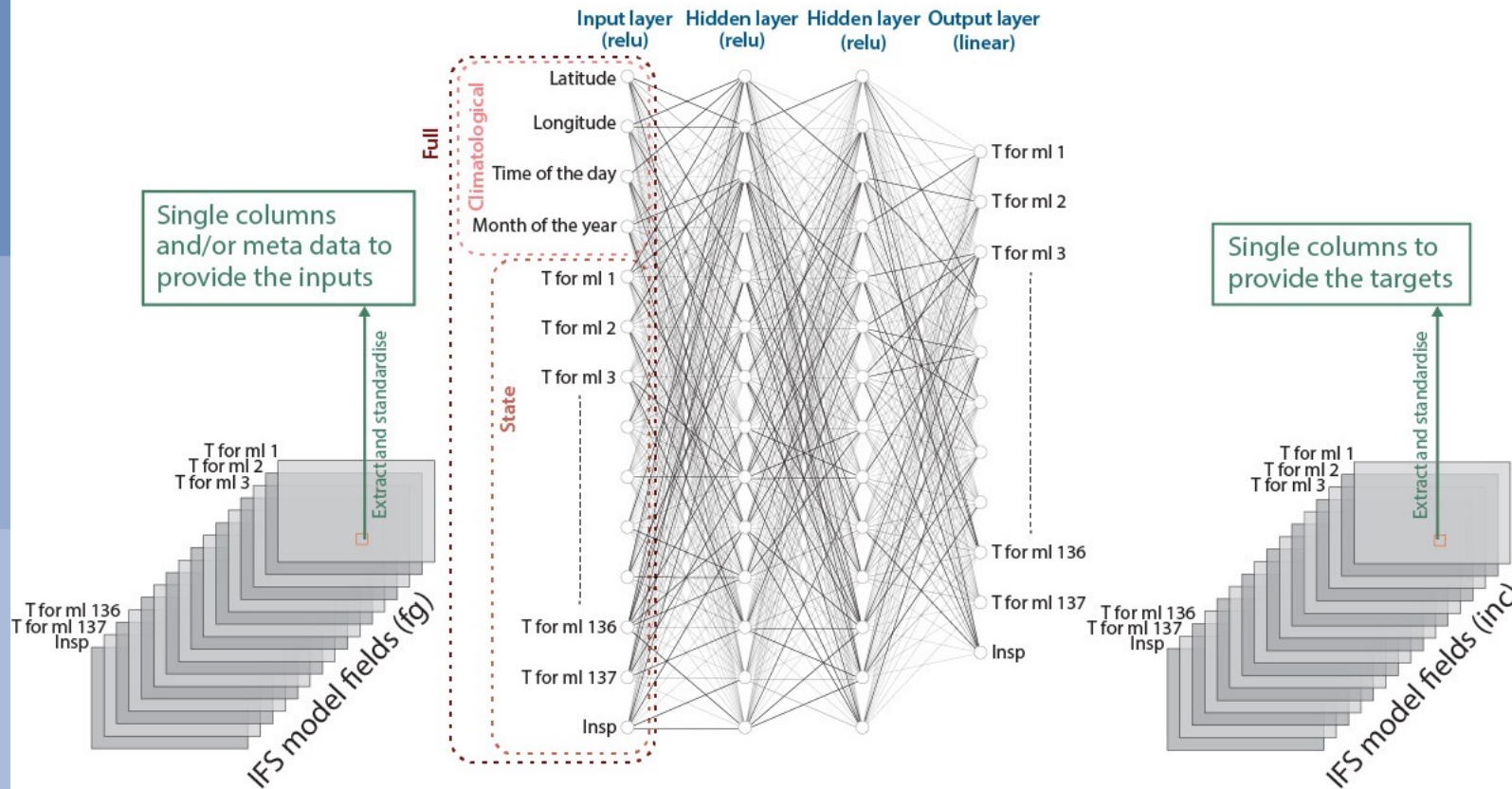
- How can we adapt these ideas to operational NWP and Climate prediction? There are some issues:
  1. Typically there is not enough time to iterate to convergence the DA and ML steps in operational NWP;
  2. We have a much more complex model, but a very good one!
  3. Most importantly, the size of the model error space is orders of magnitude bigger than in low-order models



# Hybrid ML-DA in operational systems

- What kind of prior knowledge do we have on the atmospheric model error generating distribution?
- Prior assumptions:
  1. *We can consider the atmospheric flow to be subject to homogeneous dynamics and heterogeneous forcings;*
  2. *Physical parameterisations of unresolved motions and radiation plus surface forcings are the dominant sources of model error*
  3. *Physical parameterisations are computed and applied over model columns.*
- This led us to define a set of predictors made up of the concatenation of climatological predictors (time of day, month, lat, lon) and the vertical columns (137 levels) of the model first guess prognostic variables of the model (t, Insp, vo, div, q).
- This choice amounts to splitting the full 3d regression problem into a 1d x 2d problem and is conceptually similar to having a separable representation of a 3D covariance matrix

# Hybrid ML-DA in operational systems

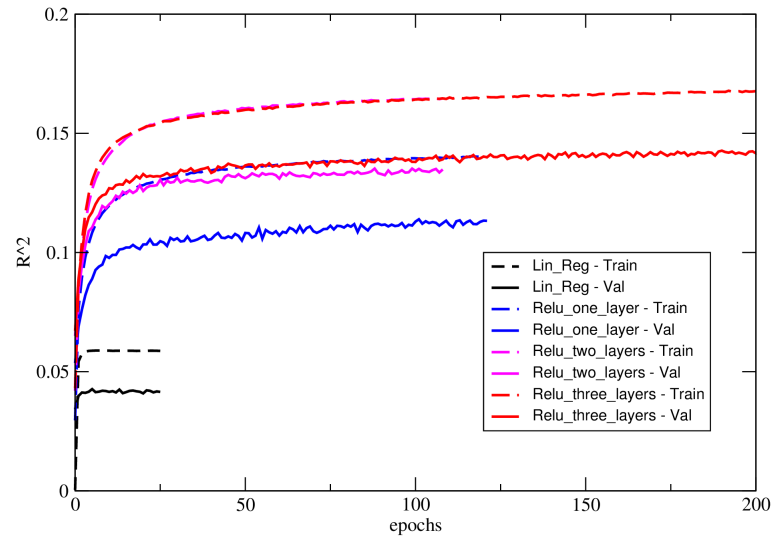


- Dense Neural Network with Relu activations
- Three layers with nonlinear activations give best results: problem with only moderate nonlinearities
- Dropout layers used to control overfitting, input/outputs pre-normalised for training, Adam minimiser
- **Number of trainable parameters  $\sim 6 \cdot 10^4$** , size of training dataset  $\sim 10^6$

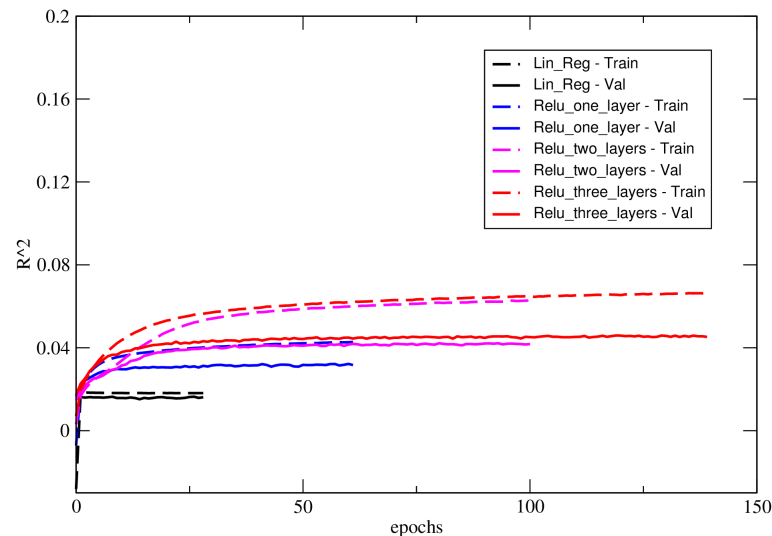
Bonavita & Laloyaux, 2020

# Hybrid ML-DA in operational systems

T\_LNSP - Full Regressors



Vo\_D - Full Regressors



- Training/Testing curves are shown in terms of explained variance ( $R^2$ )
- Saturation of explained variance is used as stopping criterion during training
- Mass (T, Insp) errors can be better predicted (~14-15% explained variance) than wind (~4-5% explained variance) and humidity (~0%) errors.
- State-dependent predictors (first guess values) have more predictive power than climatological predictors
- The NN model provides a state-dependent correction beyond climatological bias correction.

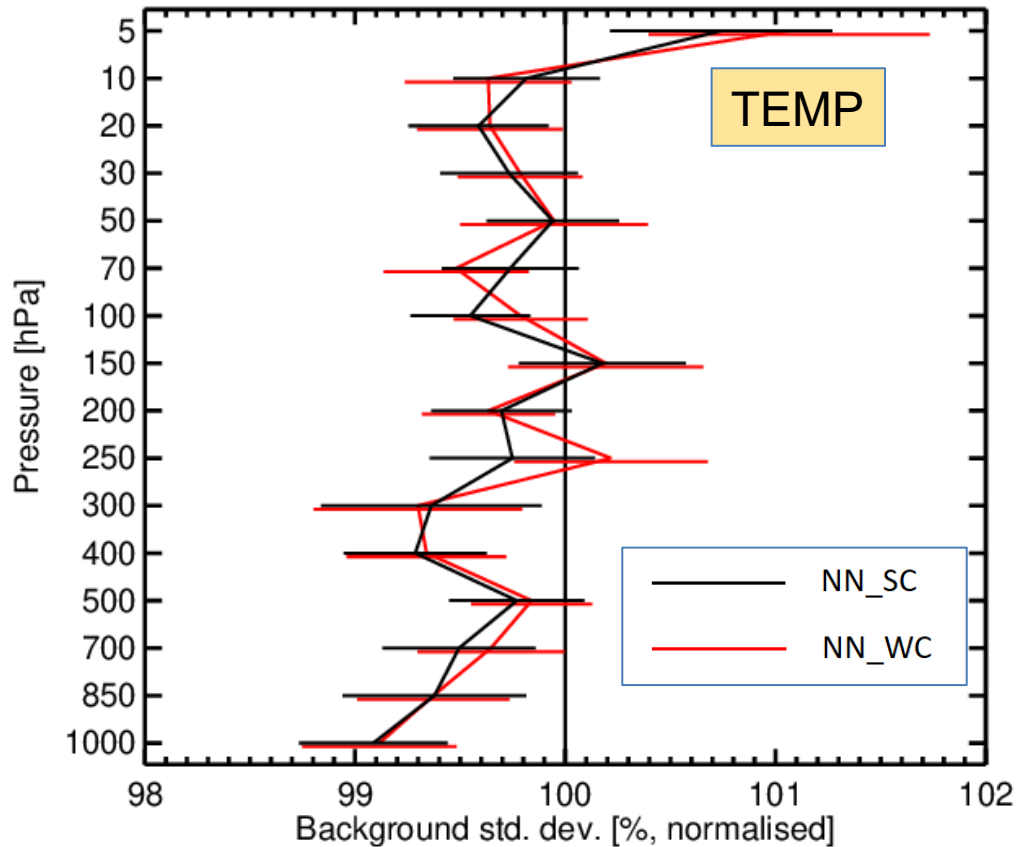
Bonavita & Laloyaux, 2020



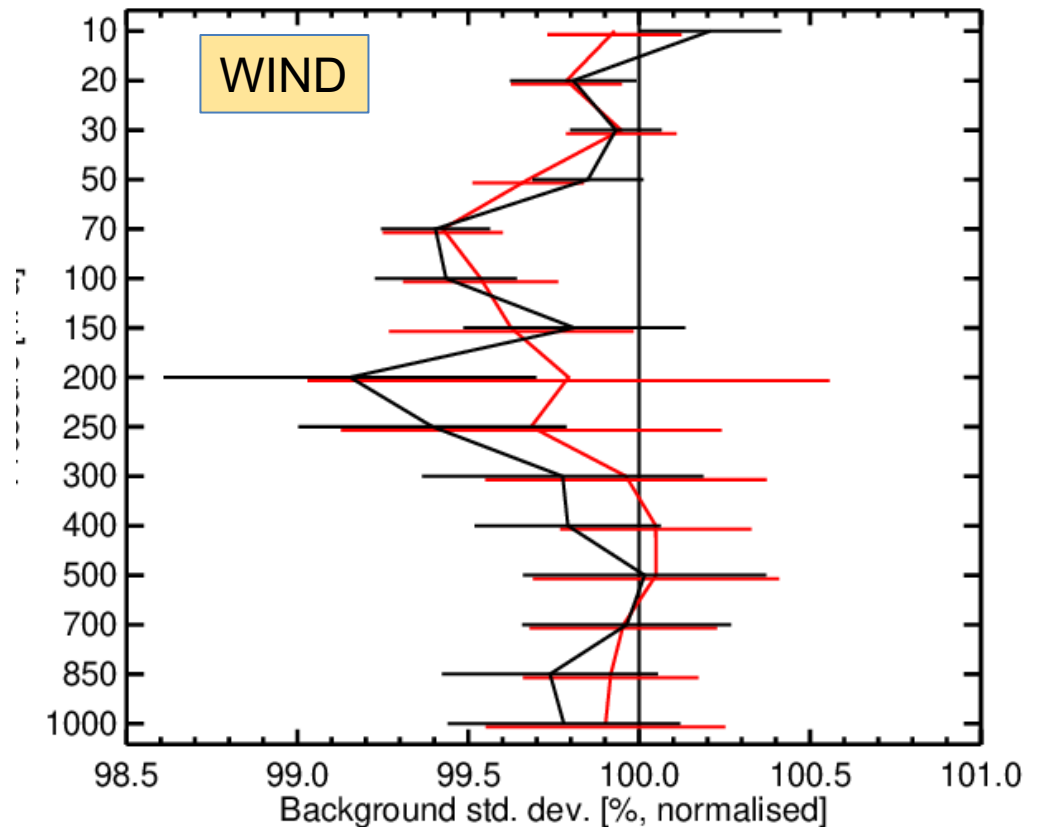
# Model Error Estimation and Correction in the IFS: Random errors

Globally-averaged Observation-First Guess StDev norm. diff.

Instrument(s): TEMP – T Area(s): N.Hemis S.Hemis Tropics  
From 00Z 16-Jul-2019 to 12Z 22-Aug-2019



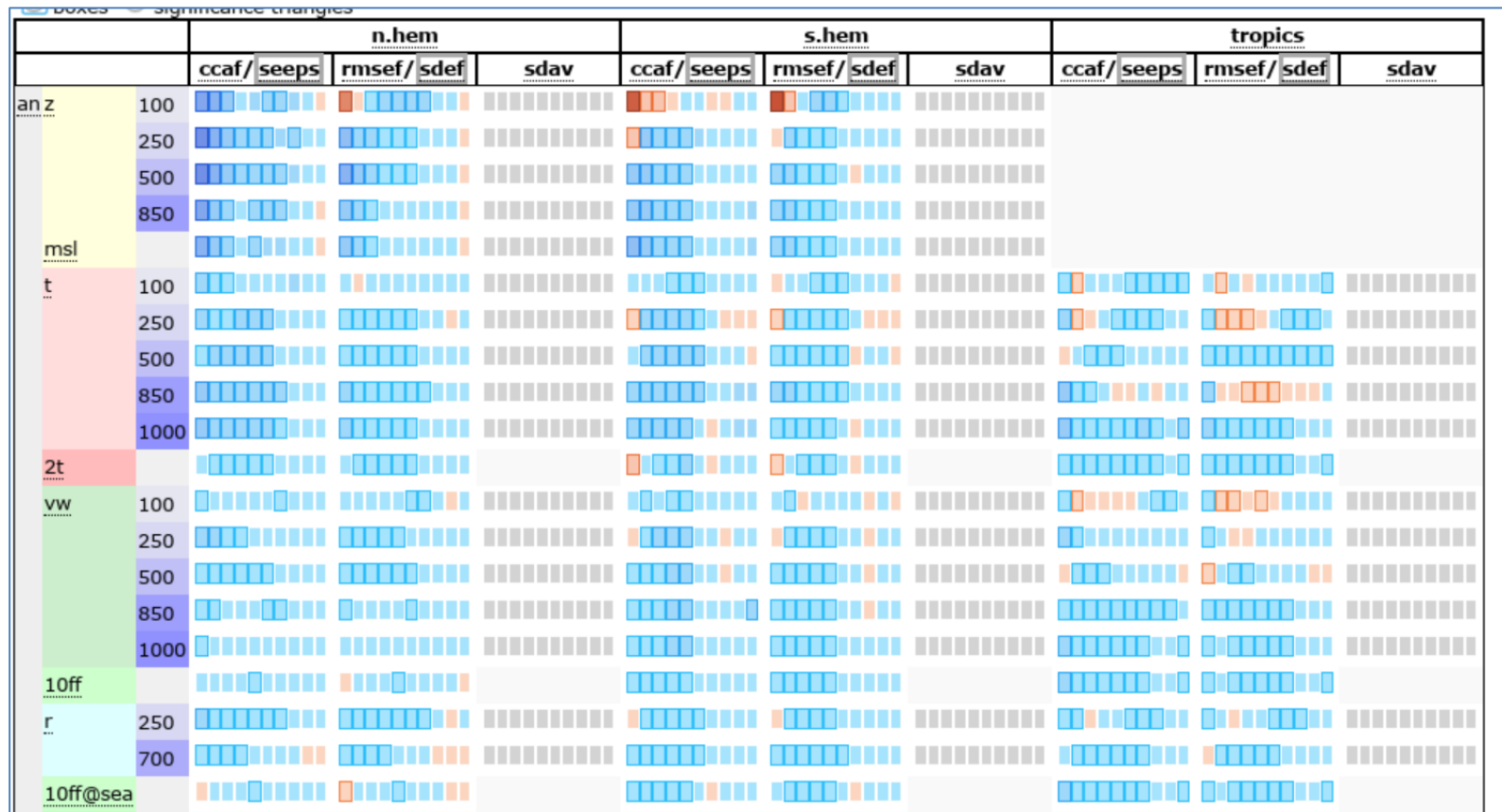
Instrument(s): AIRP PILOT PROF TEMP – U V  
Area(s): Europe Japan N.Hemis S.Hemis Tropics  
From 00Z 16-Jul-2019 to 12Z 22-Aug-2019



Note: 100% Baseline is current operational Weak Constraint 4D-Var

# Model Error Estimation and Correction in the IFS: Forecast Skill

- ANN in combination with Weak Constraint 4DVar improves the fit of observations to the model, both in the mean and in the random component.
- What can the ANN bring to **forecast skill**?



# Model Error Estimation and Correction in the IFS

- The original idea of Bonavita and Laloyaux, 2020 has been further developed
- Specifically, the NN training can now be done inside the IFS 4DVar (NN 4D-Var, Farchi et al., 2023)
- Where are we with this line of development?

# Model Error Estimation and Correction in the IFS

Training the NN parameters inside 4D-Var results in further forecast skill improvements for most variables.

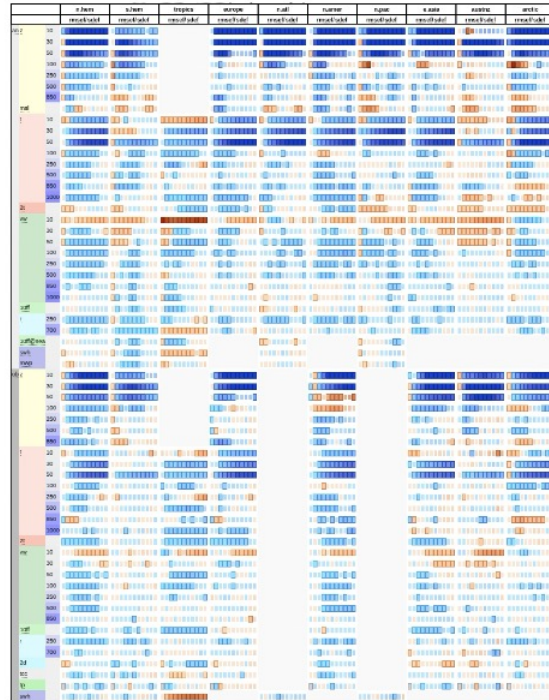


Figure: Score card 2022/06/03 to 2022/08/31. 12H assimilation window with NN model error correction trained **online**.

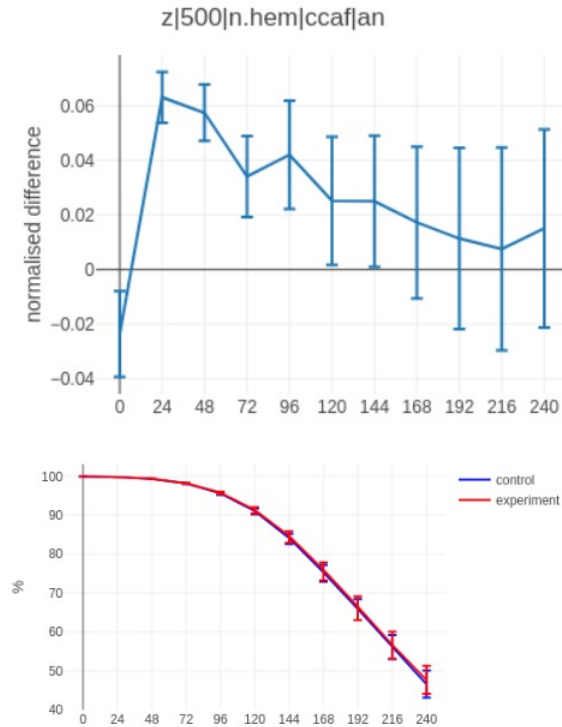


Figure: Z500 NH anomaly correlation. 2022/06/03 to 2022/08/31. 12H assimilation window with NN model error correction trained **online**.

# Model Error Estimation and Correction in the IFS

- Up to now we have been learning model errors optimising NN 4D-Var over the standard 12-hour assimilation window
- The problem with this approach is that some of the errors of the initial conditions (analysis) will get aliased into the model error estimates
- Initial conditions errors will be less of a factor if we do the NN 4D-Var optimisation over a longer assimilation window



# Model Error Estimation and Correction in the IFS

Impact of online model error training with a 24h DA window.

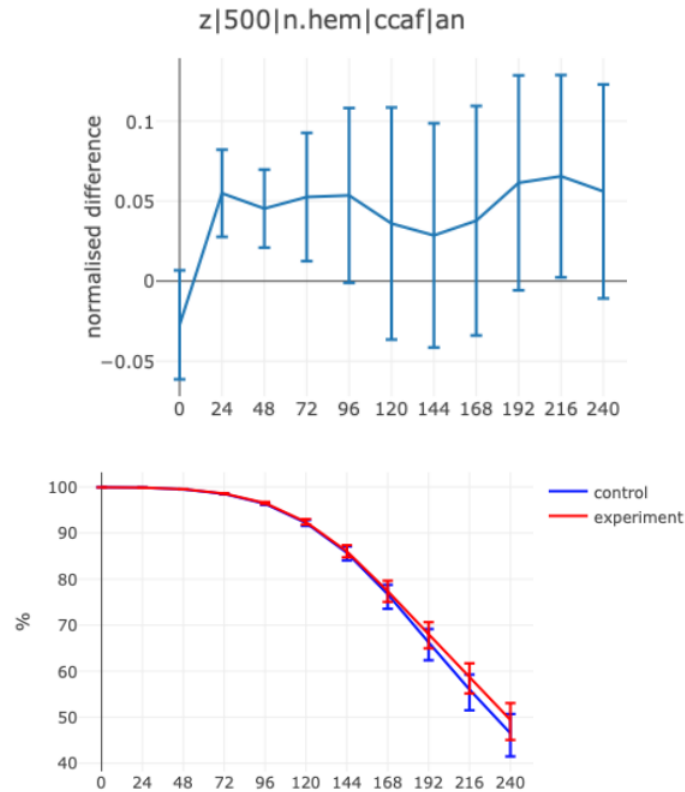


Figure: Z500 NH anomaly correlation. 2022/06/03 to 2022/07/28. 24H assimilation window with **offline** NN model error correction.

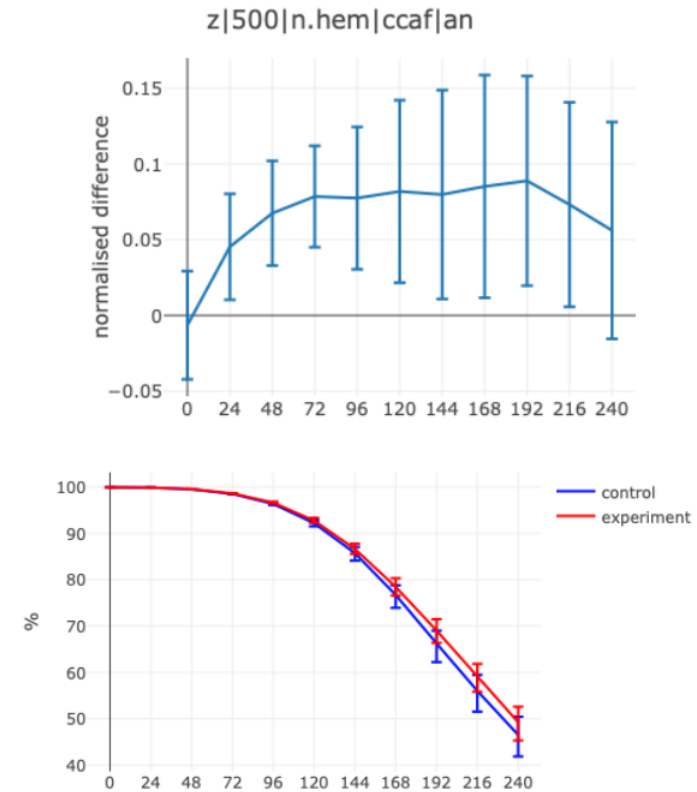


Figure: Z500 NH anomaly correlation. 2022/06/03 to 2022/07/28. 24H assimilation window with **online** NN model error correction.

# Model Error Estimation and Correction in the IFS

- Optimising over a 24-hour assimilation window shows clear improvement over 12-hour window (it recovers ~ half the gap in performance between the IFS and GraphCast/AIFS)
- Can we do better with an even longer assimilation window?
- Up to now we have used the original fully connected NN column model in NN 4D-Var. What if we use more expressive 3D NN architectures\* (CNN, Graph networks, Transformers, etc.)?
- To be continued...

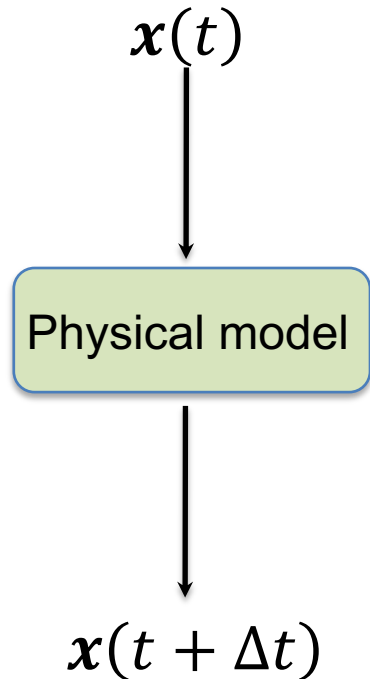
\* Note that this is more complex than putting together NN blocks in Tensorflow/Pytorch, as it requires coding the NN machinery inside 4D-Var

# A taxonomy of forecast models

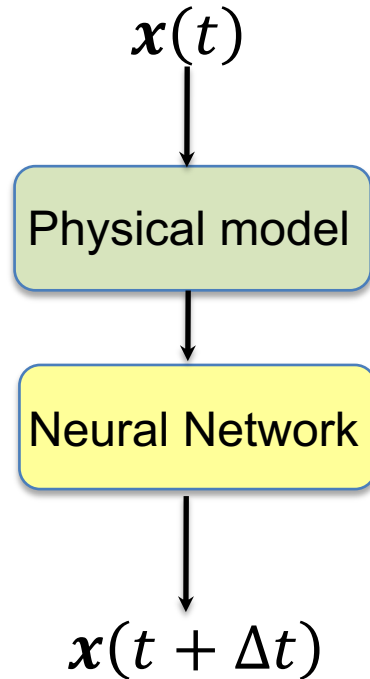
$$x(t + \Delta t) = M(x(t))$$

Physics-based

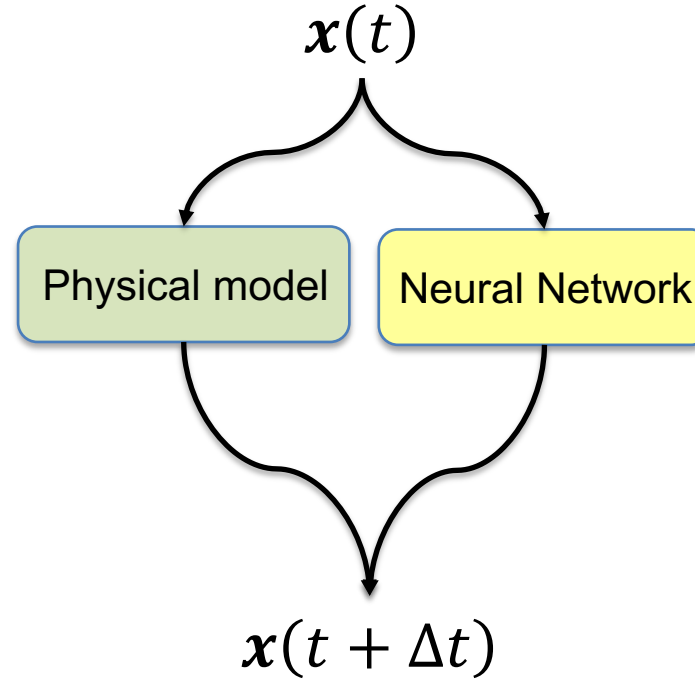
Data-driven



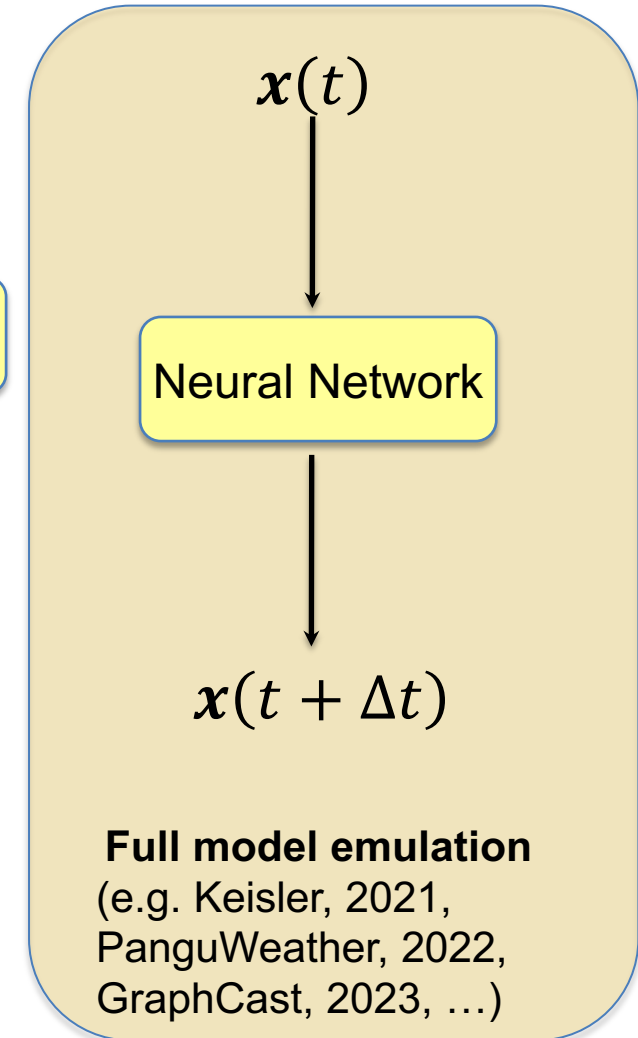
**Standard NWP models**  
(IFS, ICON, FVM,...)



**Model error correction**  
(e.g. Bonavita and Laloyaux, 2020; Farchi et al., 2022, 2023)

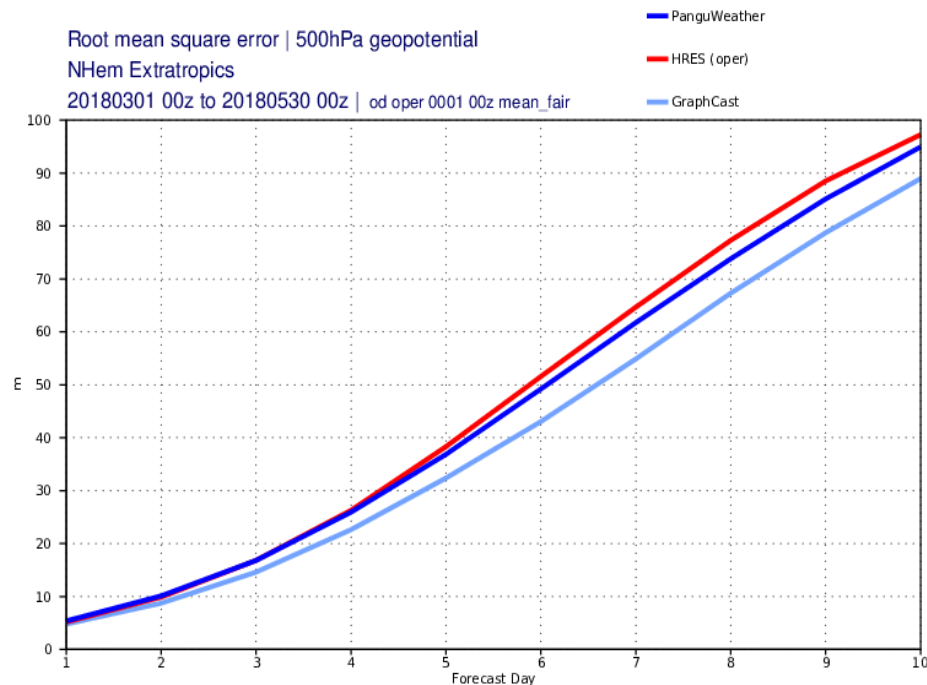


**Partial model emulation**  
(e.g. Chantry et al., 2021; Kochkov et al., 2023, aka NeuroGCM)



**Full model emulation**  
(e.g. Keisler, 2021, PanguWeather, 2022, GraphCast, 2023, ...)

# ML forecast models



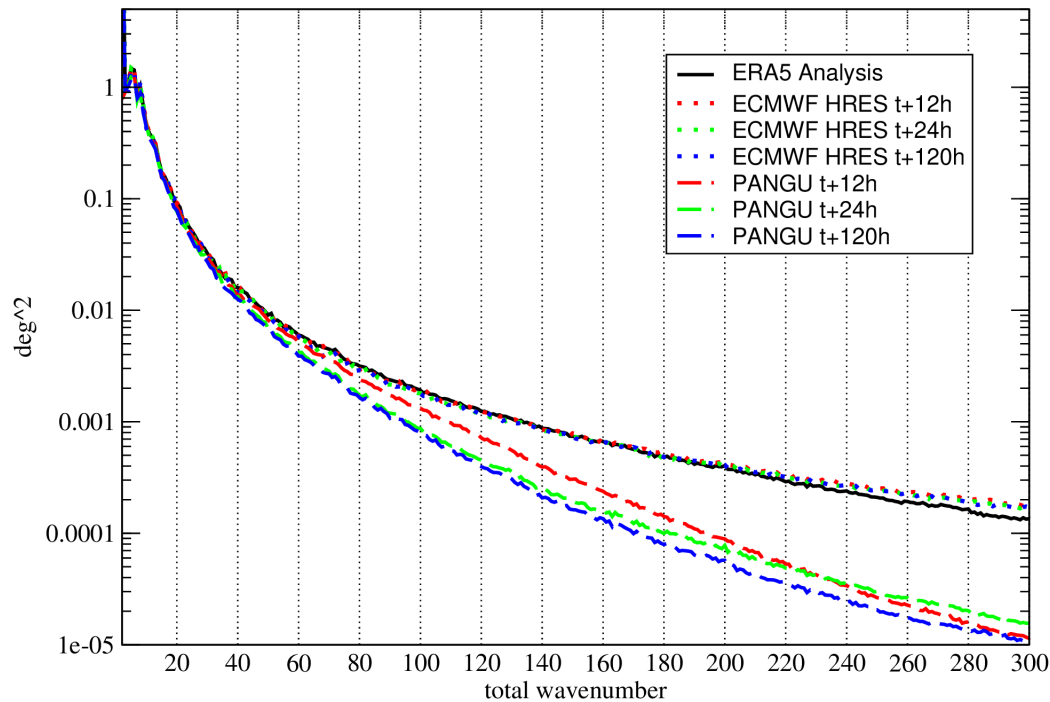
From Zied Ben Bouallegue (ECMWF)

- Field took off with Keisler, 2022, then in rapid succession FourCastNet (NVIDIA, Pathak et al., 2022), Pangu-weather (Huawei, Bi et al., 2022), GraphCast (Google-DeepMind, Lam et al., 2022), FengWu (Academic, Chen et al., 2023)...
- All trained on ERA5 re-analysis (deterministic + EDA)
- Superior forecast scores, 3-4 order of magnitude cheaper to run (not to train!)
- What's not to like?

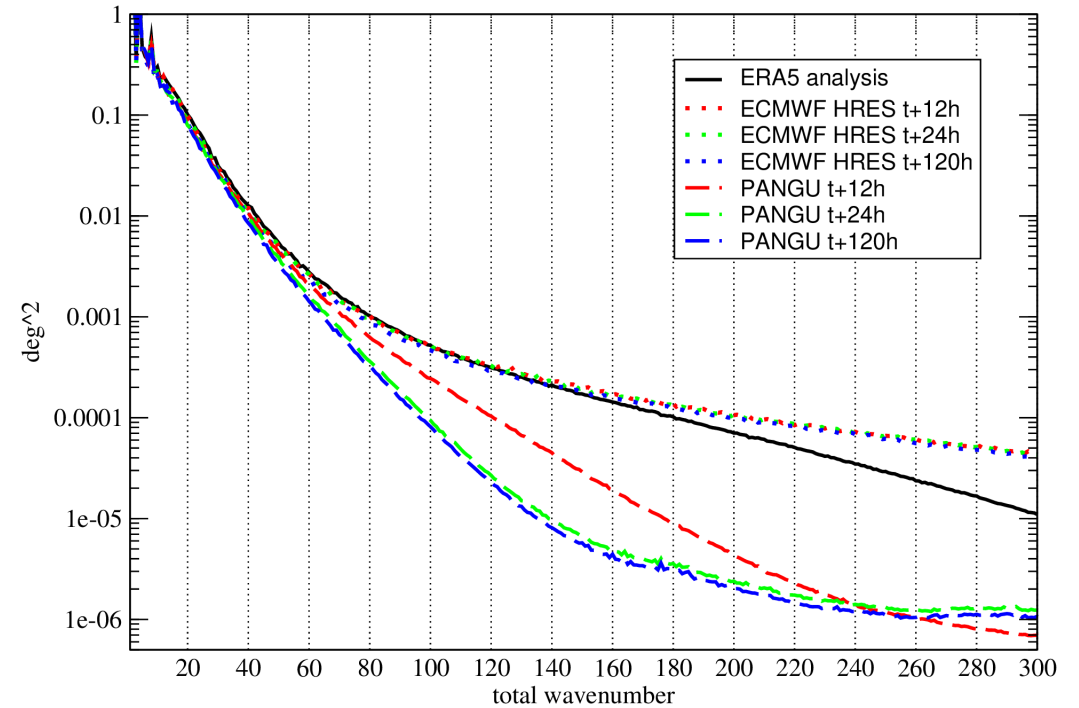
# A look under the hood of MLWP models: Pangu-weather

- Are Pangu-weather (and other DLWP models) **realistic atmosphere emulators**?

Temperature 850hPA



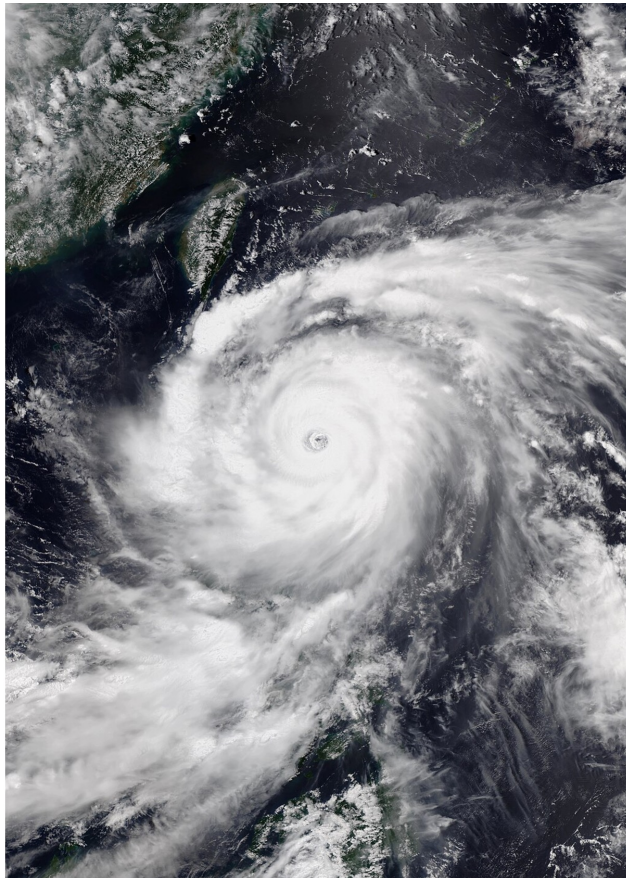
Temperature 250hPA



# A look under the hood of MLWP models: Pangu-weather

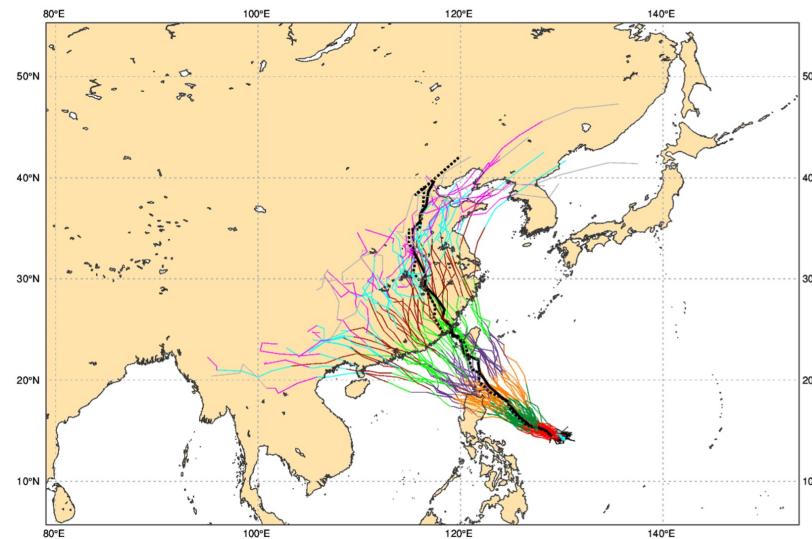
- Are Pangu-Weather (and other DLWP models) **realistic atmosphere emulators**?
- Pangu-Weather forecasts show sharply **decreased levels of variability** wrto ERA5 analyses beyond ~wavenumber 50 (**~400 km**) from the start of the forecast
- Differently from IFS forecasts, which show consistent variability at all forecast ranges, **PW forecast variability decreases with forecast range**, noticeable jump at t+24h and beyond -> increasing “**blurriness**” of predictions
- Does it matter?

# A look under the hood of MLWP models: Pangu-Weather



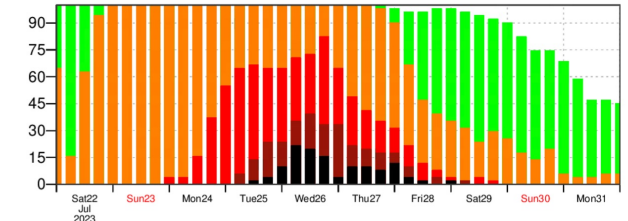
Typhoon Doksuri (Egay) of the 2023 Pacific typhoon season near its peak intensity while off the coast of Luzon during the afternoon of July 25, 2023. It had 10-min sustained winds of 175 km/h (110 mph) (JMA) and 1-min sustained winds of 230 km/h (145 mph) (JTWC) and an official minimum central pressure of 935 mbar (27.6 inHg) at the time this image was captured.

Date 20230722 00 UTC @ECMWF  
 Individual trajectories for **DOKSURI** during the next **240** hours  
 tracks: **thick solid**=HRES; **thick dot**=CTRL; **thin solid**=EPS members [coloured]  
**0-24h 24-48h 48-72h 72-96h 96-120h 120-144h 144-168h 168-192h 192-216h 216-240h**

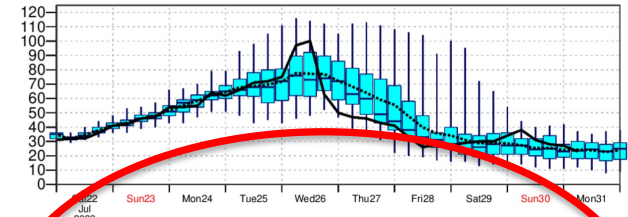


List of ensemble members numbers forecast Tropical Cyclone  
 Intensity category in colours: **TD**[up to 33] **TS**[34-63] **HR1**[64-82] **HR2**[83-95] **HR3**[> 95 kt]  
 +024 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +048 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +072 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +096 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +120 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +144 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +168 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50  
 +192 h : hr:ct01 02 03 04 05 06 07 08 09 10 11 12 14 15 16 17 18 19 21 22 23 24 25 26 27 29 30 31 32 33 35 36 37 39 40 41 42 43 44 45 46 47 48 49 50  
 +216 h : hr:ct01 02 03 05 06 07 10 11 12 14 15 17 18 19 21 22 24 25 26 27 29 30 32 33 34 35 36 37 40 43 44 45 47 49 50  
 +240 h : ct 01 02 07 10 11 12 15 18 19 21 24 25 26 27 32 33 34 36 37 40 42 44 45 49 50

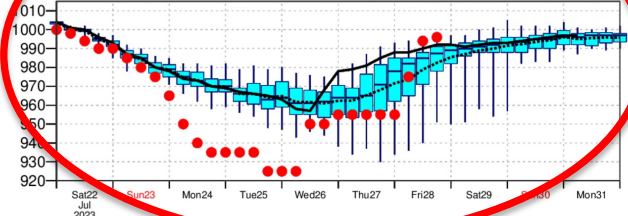
Probability (%) of Tropical Cyclone Intensity falling in each category  
**TD**[up to 33] **TS** [34-63] **HR1**[64-82] **HR2** [83-95] **HR3** [> 95 kt]



10m Wind Speed (kt) **solid**=HRES; **dot**=Ens Mean



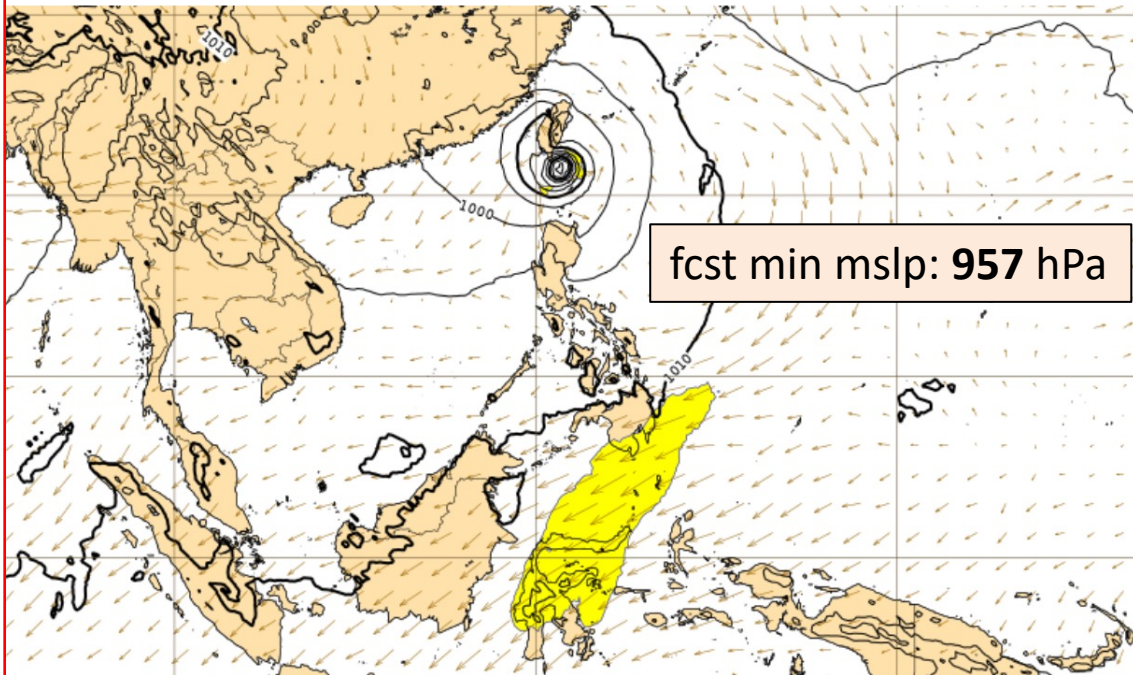
Mean Sea Level Pressure in Tropical Cyclone Centre (hPa) **solid**=HRES; **dot**=Ens Mean



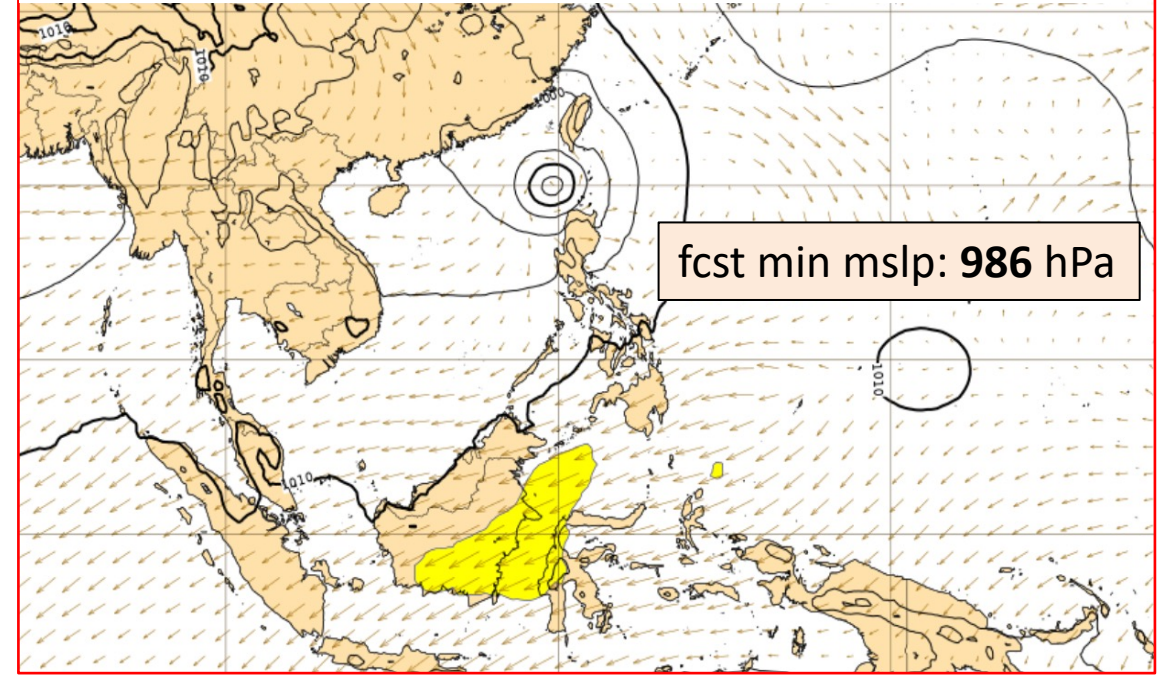
# A look under the hood of MLWP models: Pangu-Weather

TC Doksuri 26 Jul 2023 12Z  
Estimated Best Track min mslp: **944 hPa**

ECMWF HRES t+132h valid 26/07/23 12Z



Pangu-weather t+132h valid 26/07/23 12Z



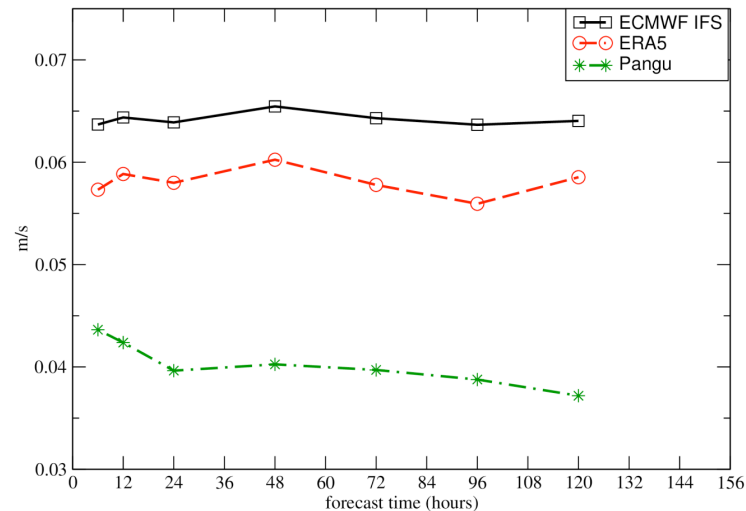


# Pangu-Weather dynamical fields

**Vertical velocity** is not predicted by Pangu-Weather (and others) but can be diagnosed by integrating the continuity equation on forecasted pressure-level fields (Holton and Hakim, 2012):

$$\omega(p) = \omega(p_s) - \int_{p_s}^p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dp$$

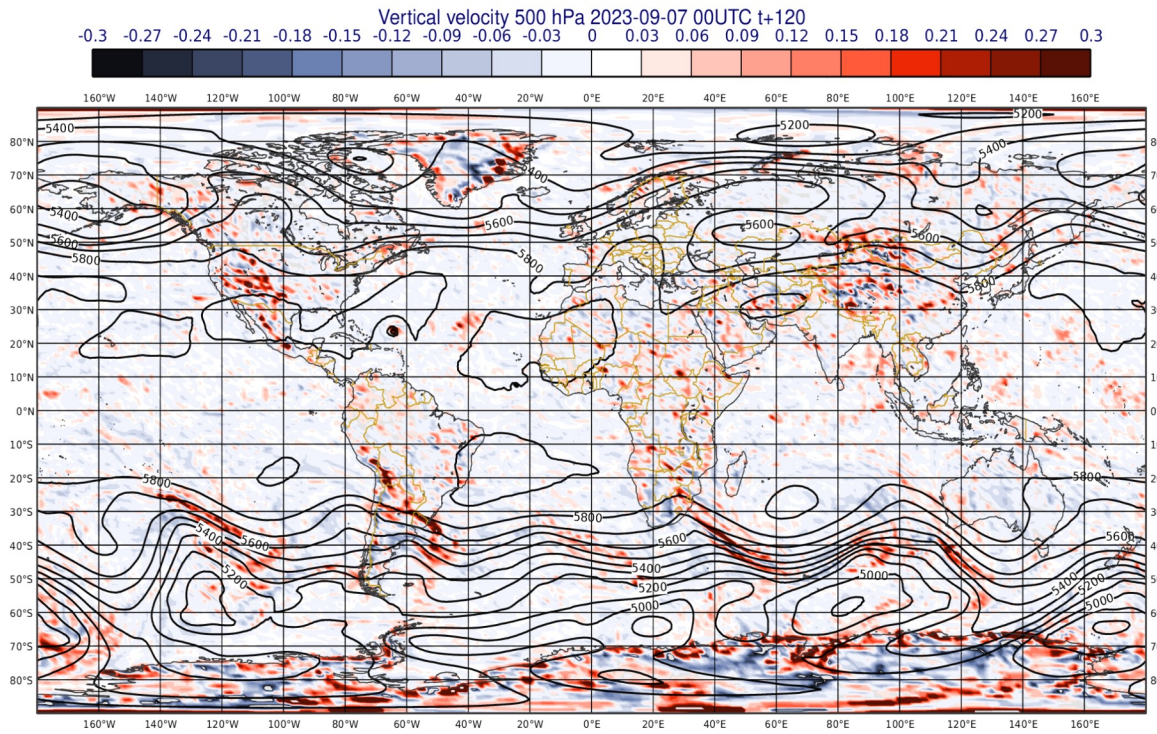
Unsurprisingly, the progressive reduction in the magnitude of the predicted divergence field leads to increasingly weak vertical velocity predictions:



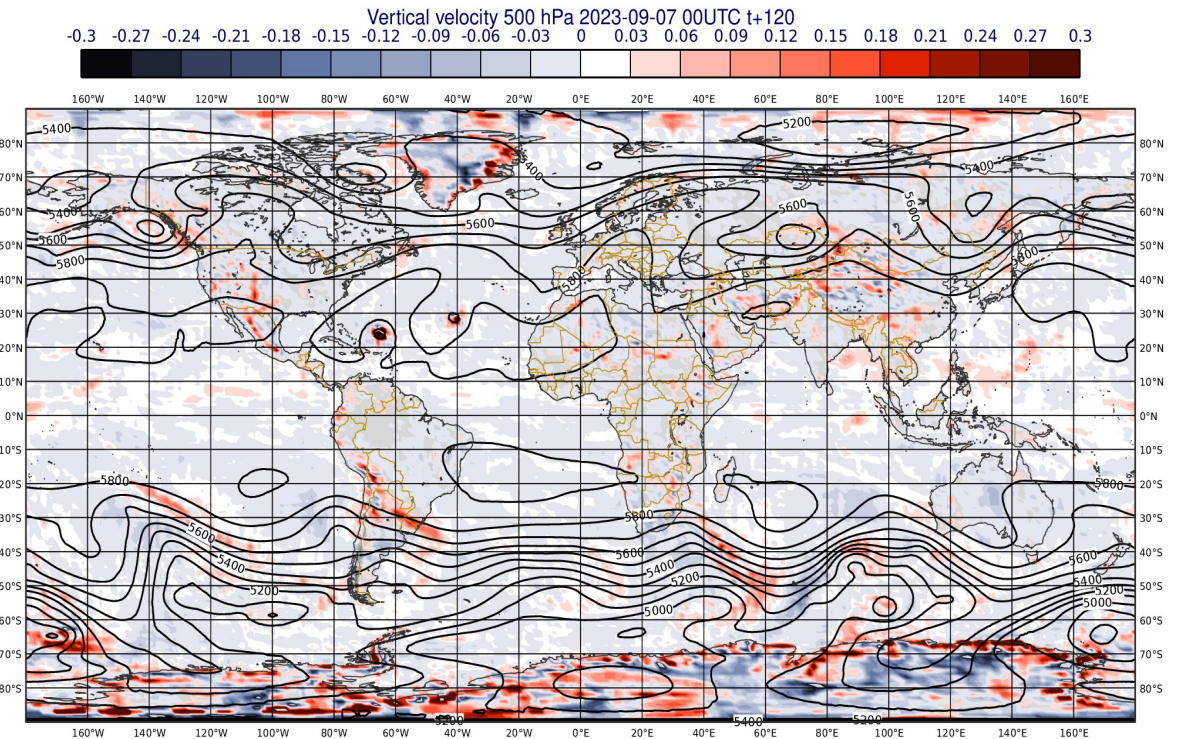
Evolution of stdev of fcst vertical velocity field  
IFS, ERA5, Pangu

# Pangu-Weather dynamical fields (3)

ERA5 fcst vert. vel.  
2023-09-07 00UTC t+120h



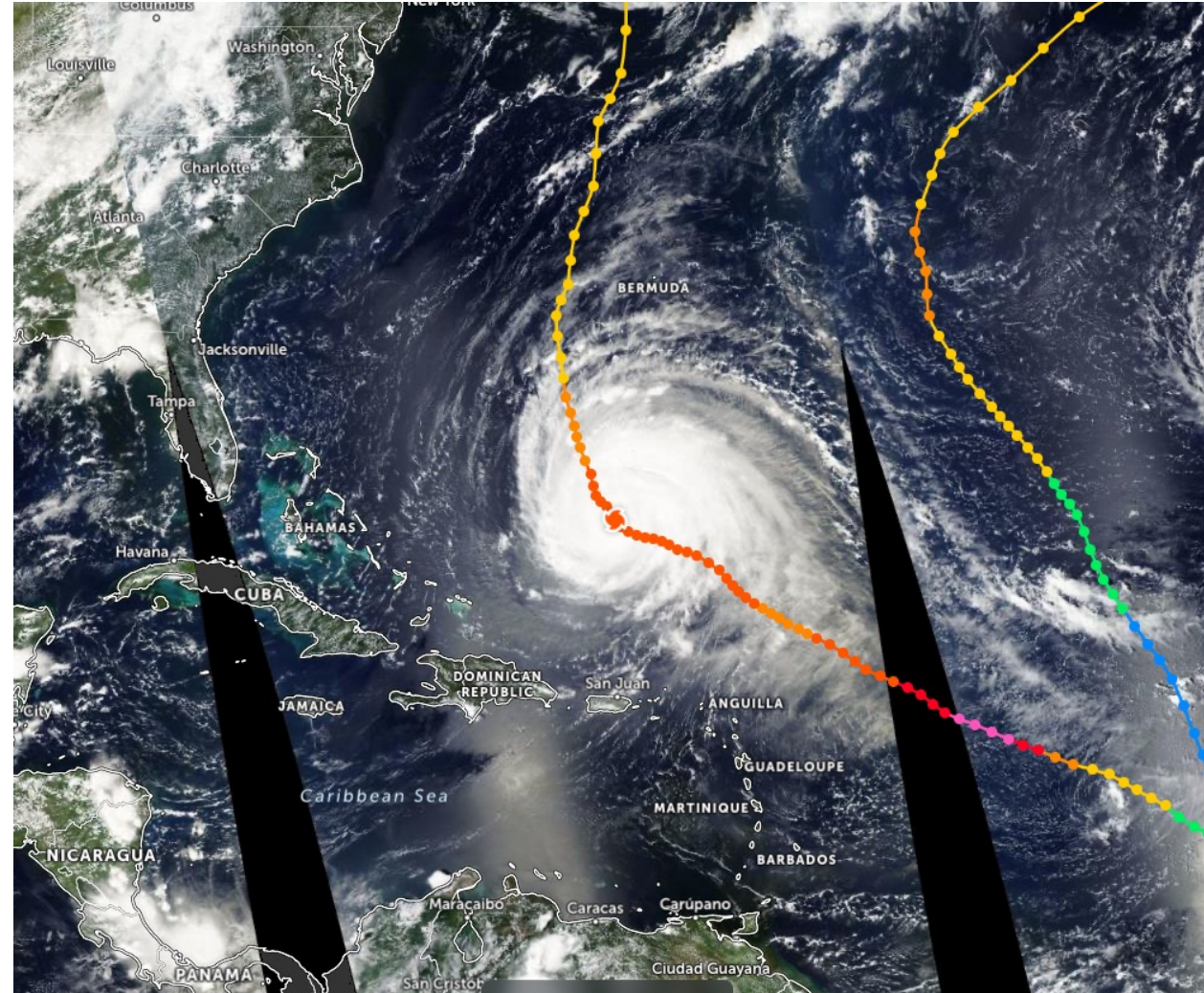
Pangu-Weather fcst vert. vel.  
2023-09-07 00UTC t+120h



# Pangu-Weather dynamical fields (3)

Hurricane Lee, 12 September 2023  
01UTC

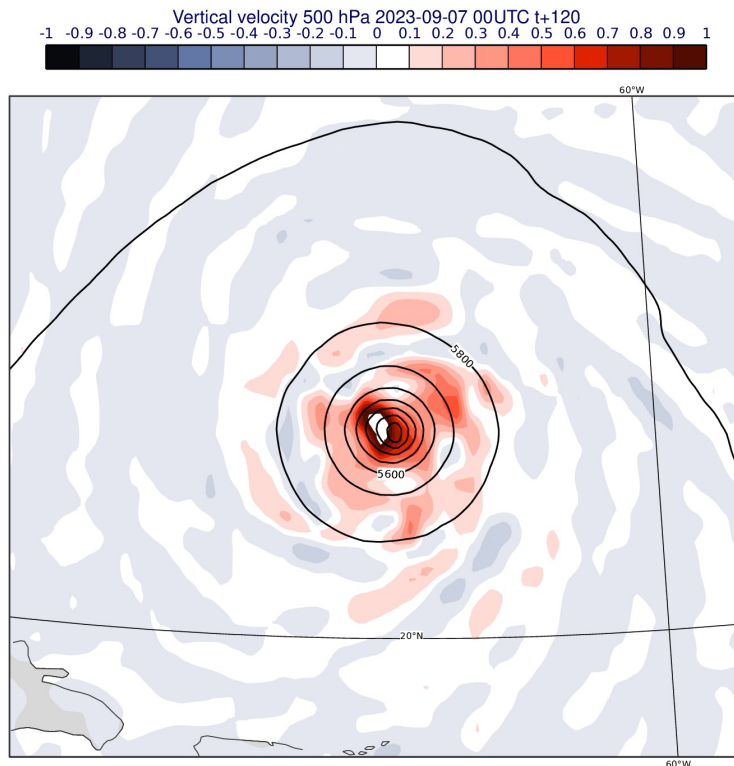
Strongest TC of the 2023 Atlantic  
Season so far, Category 3 at the time



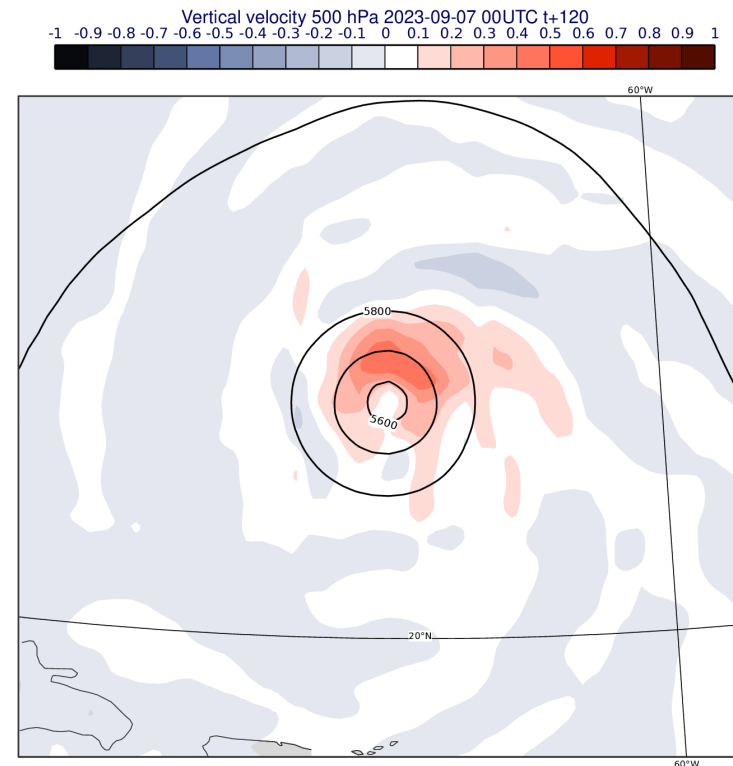
<https://zoom.earth/storms/lee-2023/#map=satellite-hd>

# Pangu-Weather dynamical fields (3)

**IFS** vert. vel. (m/s) + Z500  
2023-09-07 00UTC t+120h



**ERA5** vert. vel. (m/s) + Z500  
2023-09-07 00UTC t+120h

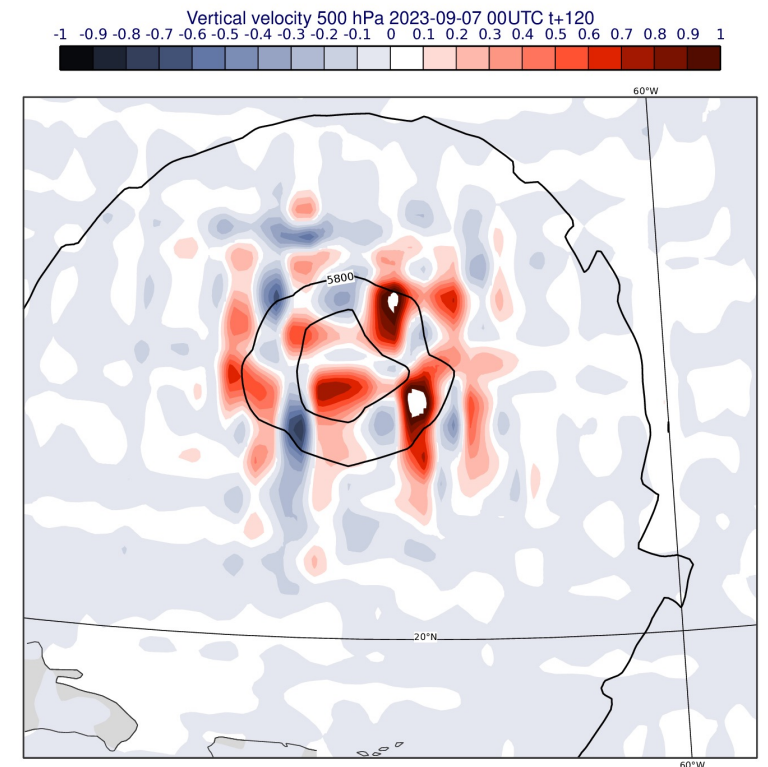
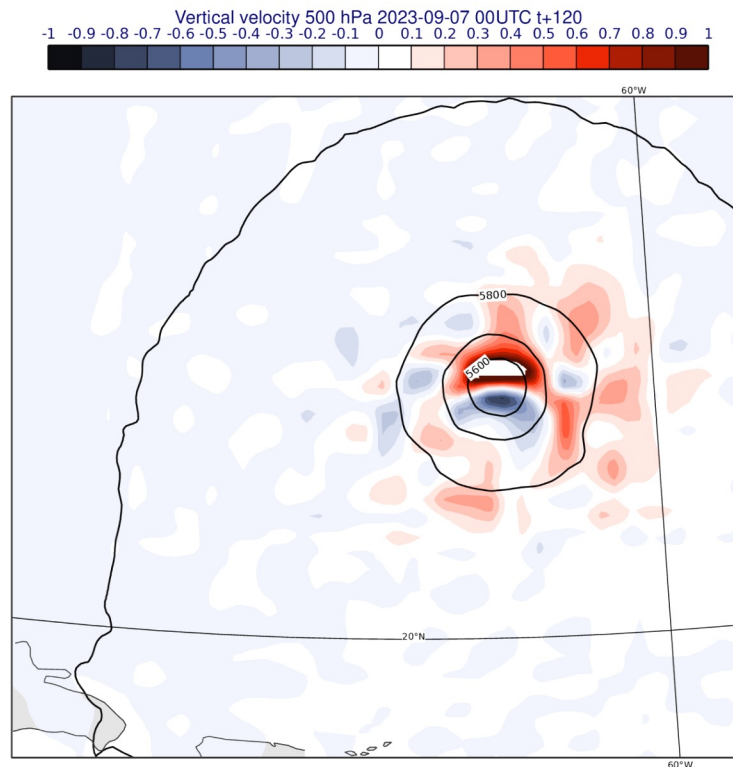
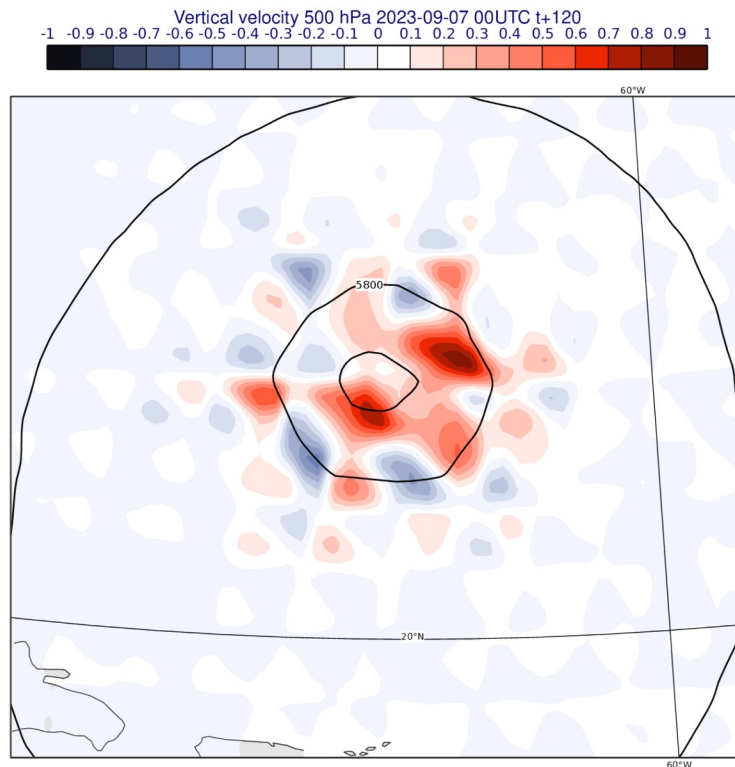


# Pangu-Weather dynamical fields

**AIFS v0.1** vert. vel. (m/s) + Z500  
2023-09-07 00UTC t+120h

**GraphCast** vert. vel. (m/s) + Z500  
2023-09-07 00UTC t+120h

**Pangu-Weather** vert. vel. (m/s) + Z500  
2023-09-07 00UTC t+120h



# Take-home Messages

- We are in the **Big Data** era! There is an unprecedented and rapidly growing amount of geophysical data ready to be used, both online (at ECMWF we use ~80 million obs a day in 4DVar: this is still less than 5% of the total amount of obs that reach the building every day!) and through reanalysis datasets
- This means that we have enough data not only to improve the initial state estimates, but also the models (both forecast model and forward models for observations)
- Machine Learning techniques can play a crucial role in tackling model deficiencies and improving predictive capabilities in both NWP and Climate.
- This field is evolving rapidly, next year's presentation will likely be quite different from this year's! Stay tuned...

# Outlook

- For the next generation of MLWP models the challenge will be to produce physically consistent forecasts with realistic activity levels and maintain forecast skill
- Can MLWP extend to DA, i.e. from observations to forecasts? (no examples of this yet, contrary to what is sometimes claimed)
- For the traditional DA-NWP community the challenge is to speed up adoption of ML techniques to make traditional DA and NWP processes significantly more effective and efficient: Can we match ML models forecast accuracy and provide physically credible forecasts?
- Too early to say which approach will prevail, but certainly things are moving at speed!  
4<sup>th</sup> ECMWF-ESA Workshop on ML for Earth Observation and Prediction, Frascati, Rome, 7-10 May 2024 (<https://www.ml4esop.esa.int>)

# Thanks for your attention!

Bocquet, M., Brajard, J., Carrassi, A. and Bertino, L. , 2019: Data assimilation as a learning tool to infer ordinary differential equation representations of dynamical models. *Nonlinear Processes in Geophysics*, 26 (3), 143–162. [doi:10.5194/npg-26-143-2019](https://doi.org/10.5194/npg-26-143-2019).

Bocquet, M., Brajard, J., Carrassi, A. and Bertino, L. (2020). Bayesian inference of chaotic dynamics by merging data assimilation, machine learning and expectation-maximization. *Foundations of Data Science*, 2 (1), 55–80. [doi:10.3934/fods.2020004](https://doi.org/10.3934/fods.2020004)

Bolton, T., & Zanna, L. (2019). Applications of deep learning to ocean data inference and subgrid parameterization. *Journal of Advances in Modeling Earth Systems*, 11, 376– 399. <https://doi.org/10.1029/2018MS001472>

Bonavita, M. and P. Laloyaux, 2020: Machine Learning for Model Error Inference and Correction, *JAMES*  
<https://doi.org/10.1002/essoar.10503695.1>

Bonavita, M., Arcucci, R., Carrassi, A., Dueben, P., Geer, A. J., Le Saux, B., Longép  , N., Mathieu, P., & Raynaud, L. (2021). Machine Learning for Earth System Observation and Prediction, *Bulletin of the American Meteorological Society*, 102(4), E710-E716, DOI: [10.1175/BAMS-D-20-0307.1](https://doi.org/10.1175/BAMS-D-20-0307.1)

Bonavita, M.. (2021) Exploring the structure of time-correlated model errors in the ECMWF data assimilation system. *Q J R Meteorol Soc*, 147( 739), 3454– 3471. Available from: <https://doi.org/10.1002/qj.4137>

Continued...



Bonavita, M. (2023). On some limitations of data-driven weather forecasting models. GRL, under review.  
<https://doi.org/10.48550/arXiv.2309.08473>

Brajard, J., Carrassi, A., Bocquet, M. and Bertino, L. (2020). Combining data assimilation and machine learning to emulate a dynamical model from sparse and noisy observations: A case study with the Lorenz 96 model. *Journal of Computational Science*, 44, 101171. [doi:10.1016/j.jocs.2020.101171](https://doi.org/10.1016/j.jocs.2020.101171).

Brenowitz, N. D., & Bretherton, C. S. (2018). Prognostic validation of a neural network unified physics parameterization. *Geophysical Research Letters*, 17, 6289–6298. <https://doi.org/10.1029/2018GL078510>

Brenowitz, N. D., and Bretherton, C. S. (2019), Spatially Extended Tests of a Neural Network Parametrization Trained by Coarse-Graining, *J. Adv. Model. Earth Syst.*, 11, 2728– 2744. <https://doi.org/10.1029/2019MS001711>.

Chantry, M., S. Hatfield, P. Dueben, I. Polichtchouk, and T. Palmer. Machine learning emulation of gravity wave drag in numerical weather forecasting. *Journal of Advances in Modeling Earth Systems*, 13(7):e2021MS002477, 2021. doi:  
<https://doi.org/10.1029/2021MS002477>

Farchi, A., Laloyaux, P., Bonavita, M. & Bocquet, M.(2021a) Using machine learning to correct model error in data assimilation and forecast applications. *Q J R Meteorol Soc*, 147( 739), 3067– 3084. Available from: <https://doi.org/10.1002/qj.4116>

Farchi, A., M. Bocquet, P. Laloyaux, M. Bonavita and Q. Malartic, (2021b) A comparison of combined data assimilation and machine learning methods for offline and online model error correction, *Journal of Computational Science*, Volume 55, 2021,101468, ISSN 1877-7503, <https://doi.org/10.1016/j.jocs.2021.101468>.

Keisler, R., (2021) Forecasting Global Weather with Graph Neural Networks, <https://arxiv.org/pdf/2202.07575.pdf>

Kutz, J. N. (2017). Deep learning in fluid dynamics. *Journal of Fluid Mechanics*, 814, 1–4.

Laloyaux, P, Bonavita, M, Dahoui, M, et al. 2020: Towards an unbiased stratospheric analysis. *Q J R Meteorol Soc.* 146: 2392–2409. <https://doi.org/10.1002/qj.3798>

Ling, J., Kurzawski, A., & Templeton, J. (2016). Reynolds averaged turbulence modelling using deep neural networks with embedded invariance. *Journal of Fluid Mechanics*, 807, 155–166.

Navon, I.M., 1998: Practical and theoretical aspects of adjoint parameter estimation and identifiability in meteorology and oceanography, *Dynamics of Atmospheres and Oceans*, Volume 27, Issues 1–4, 55-79

Rasp, S., Pritchard, M. S., & Gentine, P. (2018). Deep learning to represent subgrid processes in climate models. *Proceedings of the National Academy of Sciences of the United States of America*, 115(39), 9684–9689. <https://doi.org/10.1073/pnas.1810286115>

Ruiz, J.J., Pulido, M. and T. Miyoshi, 2013: Estimating Model Parameters with Ensemble-Based Data Assimilation: A Review, *Journal of the Meteorological Society of Japan. Ser. II*, 91, 2, 79-99. <https://doi.org/10.2151/jmsj.2013-201>

# Additional Material

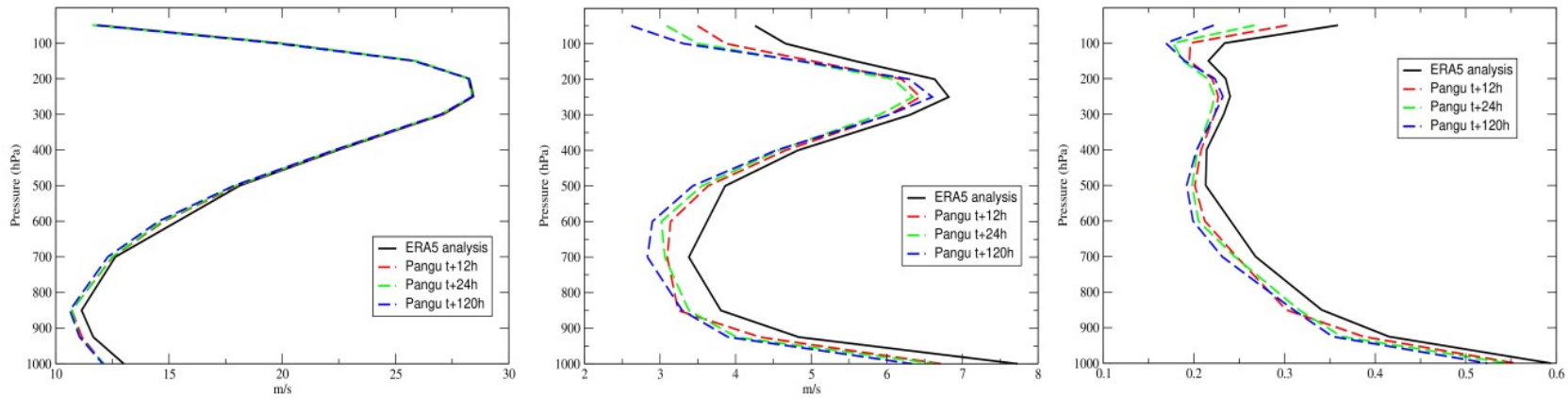
# A look under the hood of MLWP models: Pangu-Weather

Unrealistic forecast energy spectra imply **dynamically inconsistent forecast** fields

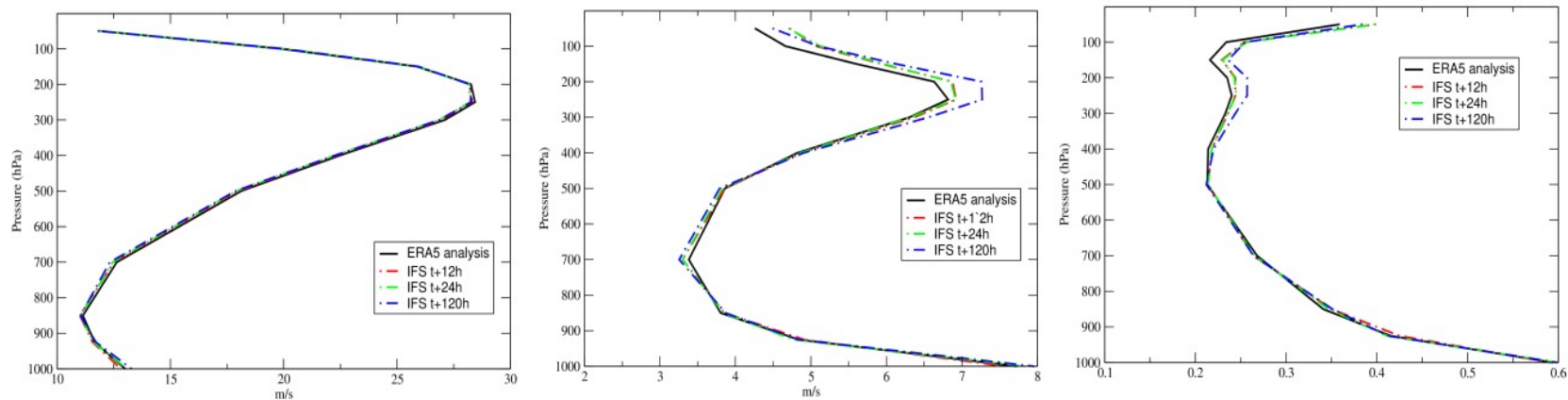
# Pangu-Weather dynamical fields (1)

Geostrophic wind ( $\mathbf{V}_g = \frac{1}{f} \hat{\mathbf{k}} \times \nabla_p \Phi$ ) vs ageostrophic wind  $\mathbf{V}_{ag} \equiv \mathbf{V} - \mathbf{V}_g$

Pangu



IFS



$|\mathbf{V}_g|$

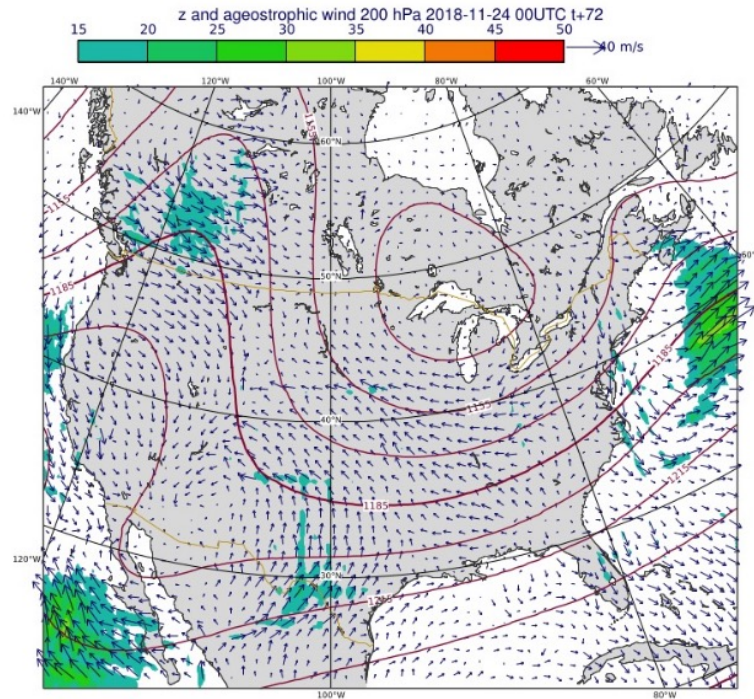
$|\mathbf{V}_{ag}|$

$|\mathbf{V}_{ag}| / |\mathbf{V}_g|$

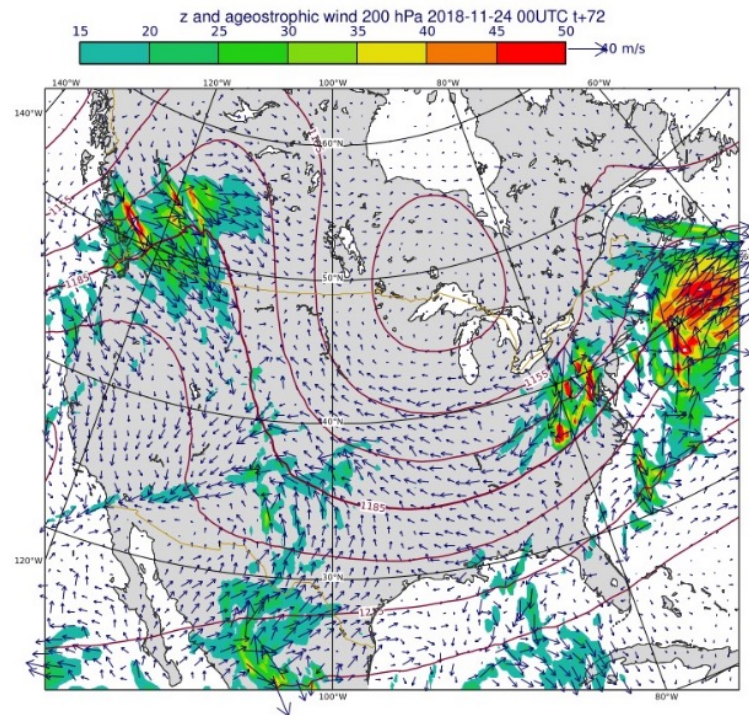
# Pangu-Weather dynamical fields (1)

Geostrophic wind ( $\mathbf{V}_g = \frac{1}{f} \hat{\mathbf{k}} \times \nabla_p \Phi$ ) vs ageostrophic wind  $\mathbf{V}_{ag} \equiv \mathbf{V} - \mathbf{V}_g$

Pangu



IFS



$|\mathbf{V}_{ag}|$

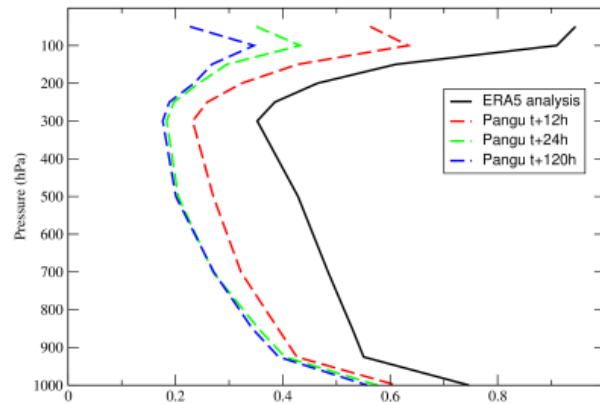
# Pangu-Weather dynamical fields (2)

Vorticity and divergence decomposition of the circulation

$$\mathbf{u} = \mathbf{u}_d + \mathbf{u}_v = -\nabla\chi + \mathbf{k} \times \nabla\psi$$

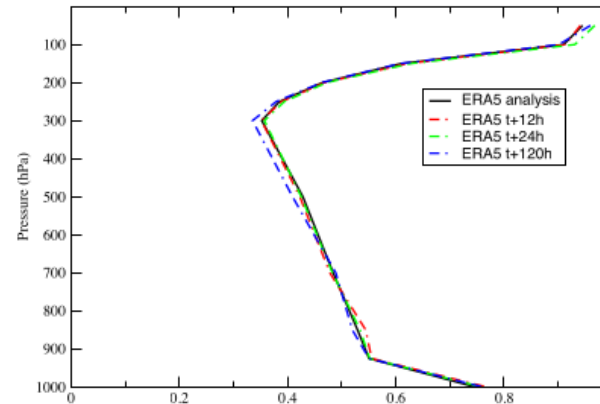
$$\nabla^2\chi = \delta, \quad \nabla^2\psi = \zeta$$

Pangu



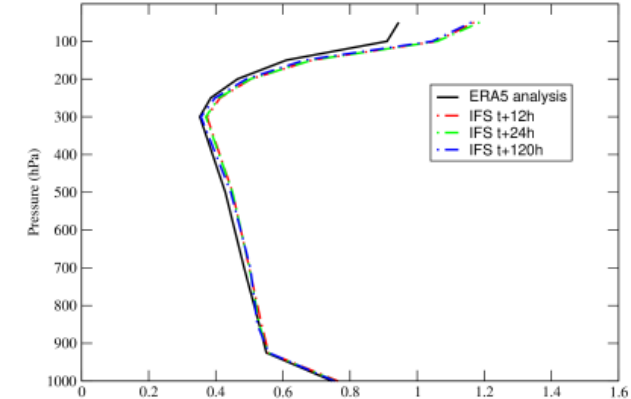
$\delta/\zeta$

ERA5-fcst



$\delta/\zeta$

IFS



$\delta/\zeta$