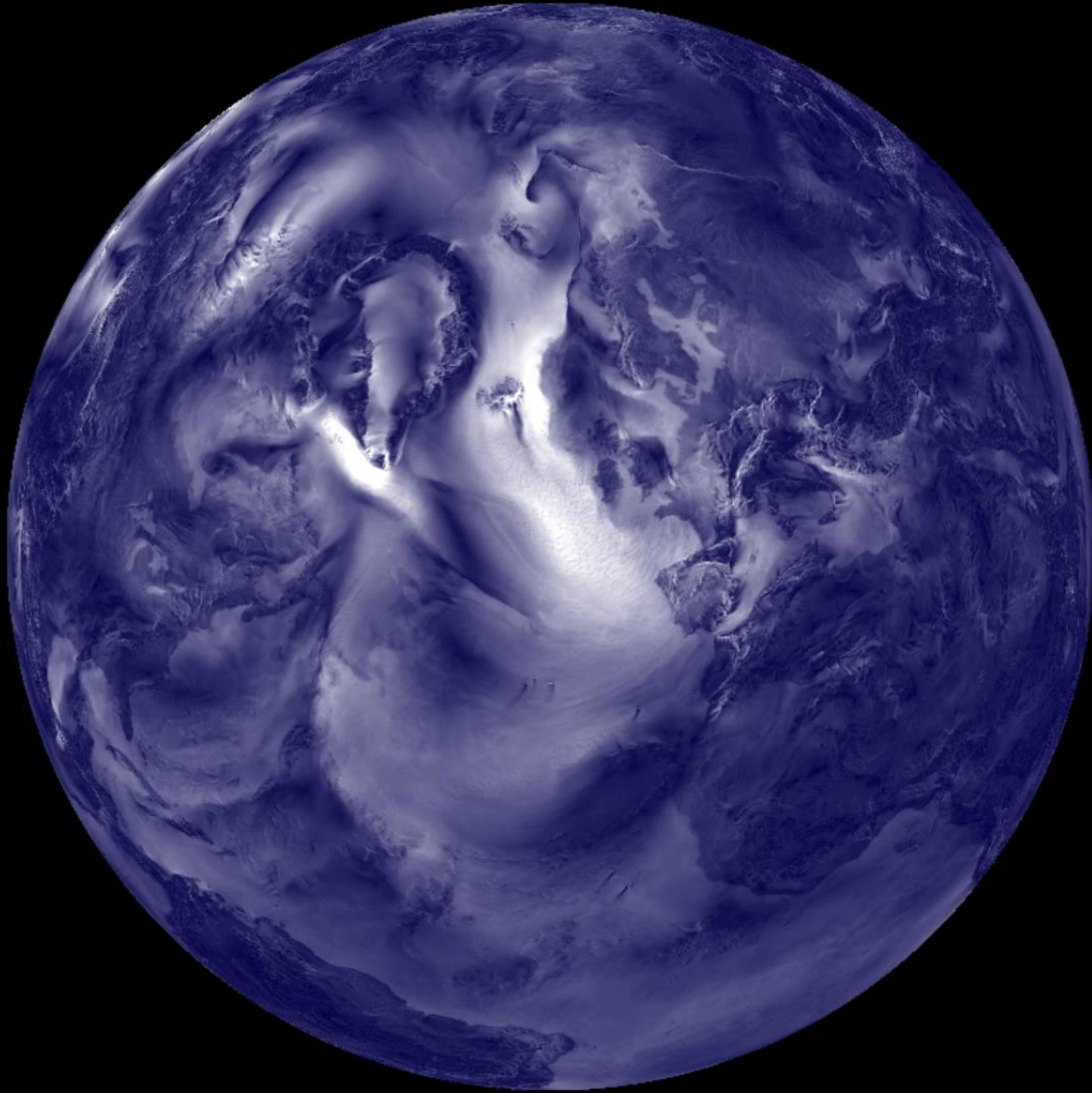


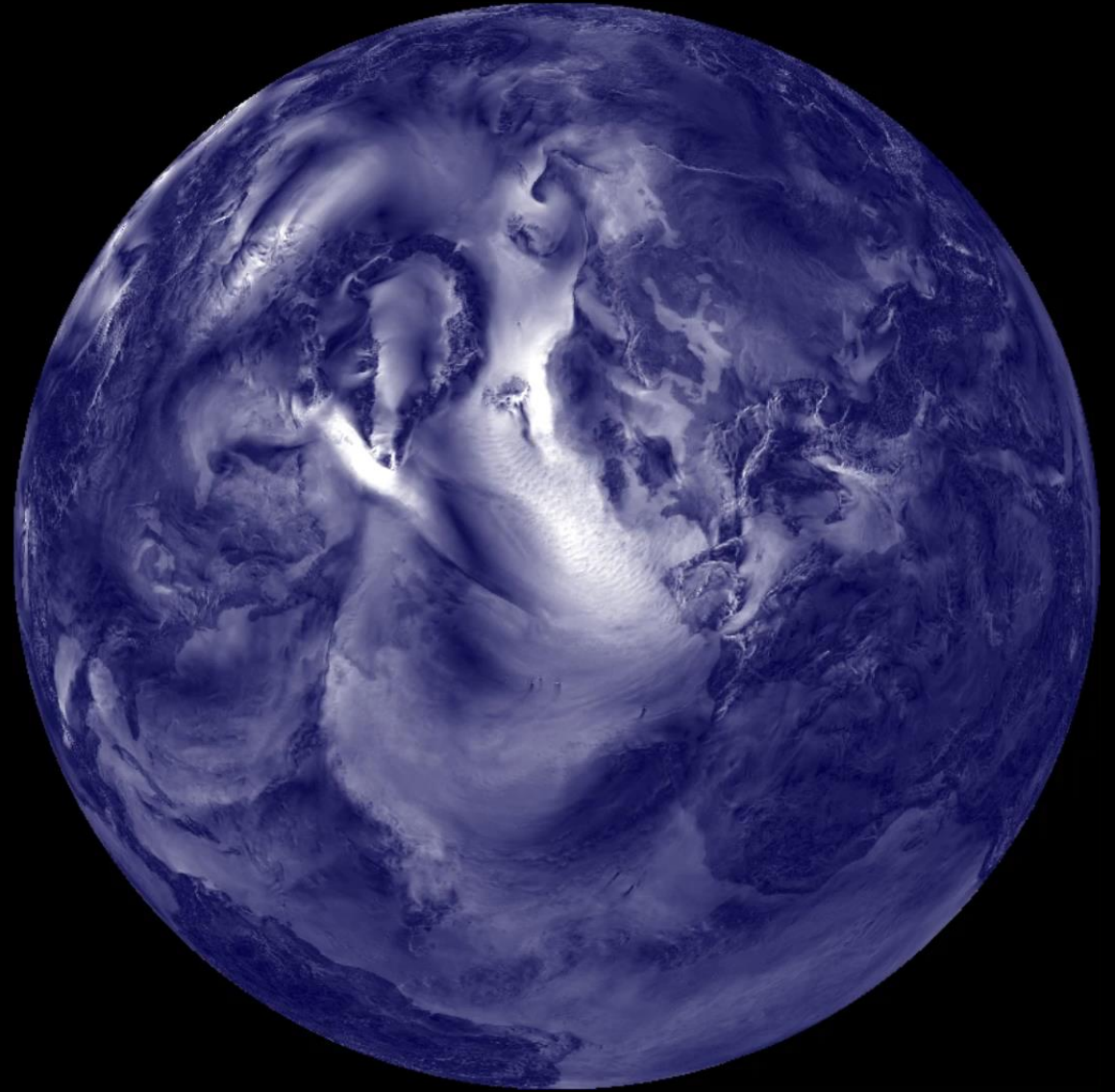
# Ensemble Forecasts Initial Perturbation

Simon Lang

IFS 10m wind gusts, 2020-12-04 00 UTC 720h forecasts, 9 km spatial resolution



Control Member



Perturbed member 1

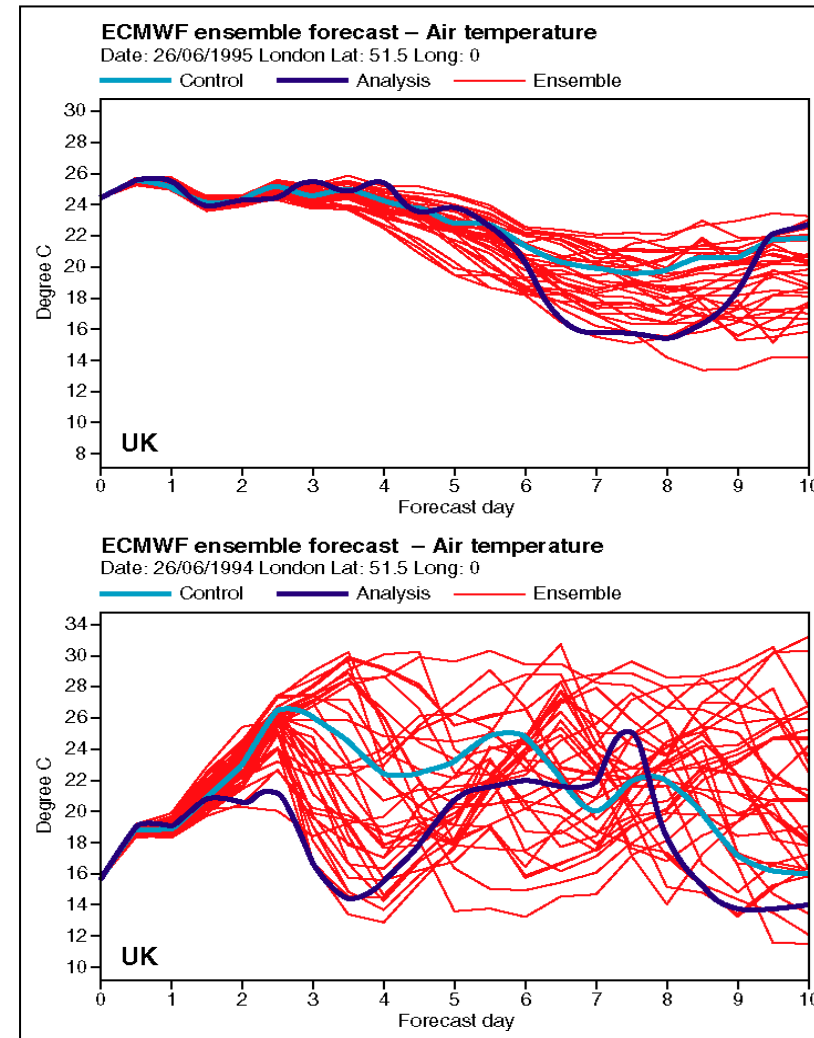
# Chaos and weather prediction

The atmosphere is a chaotic system

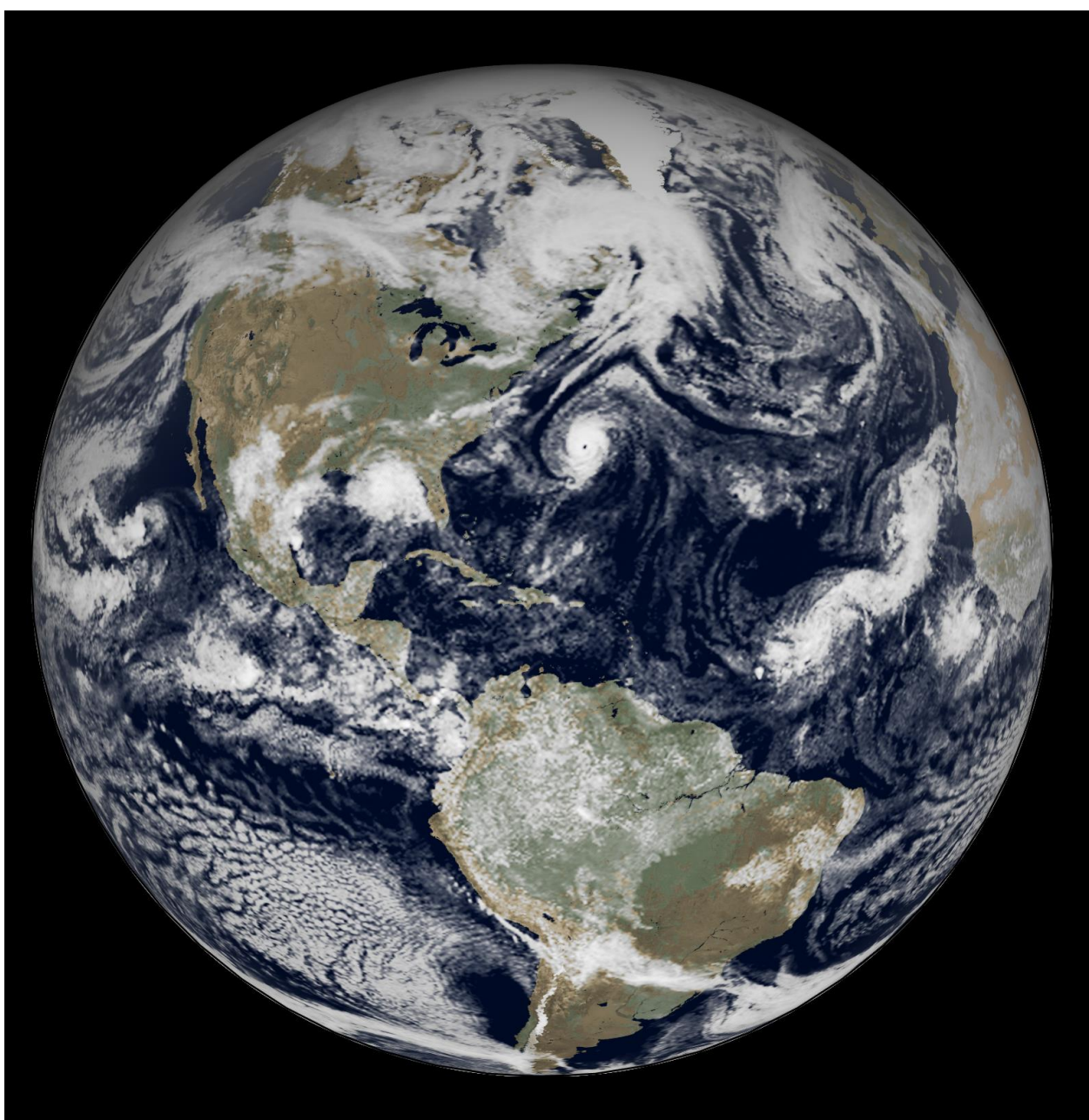
- Small errors can grow to have major impact
- We can never perfectly measure the current state of the whole atmosphere

Ensemble Forecasts

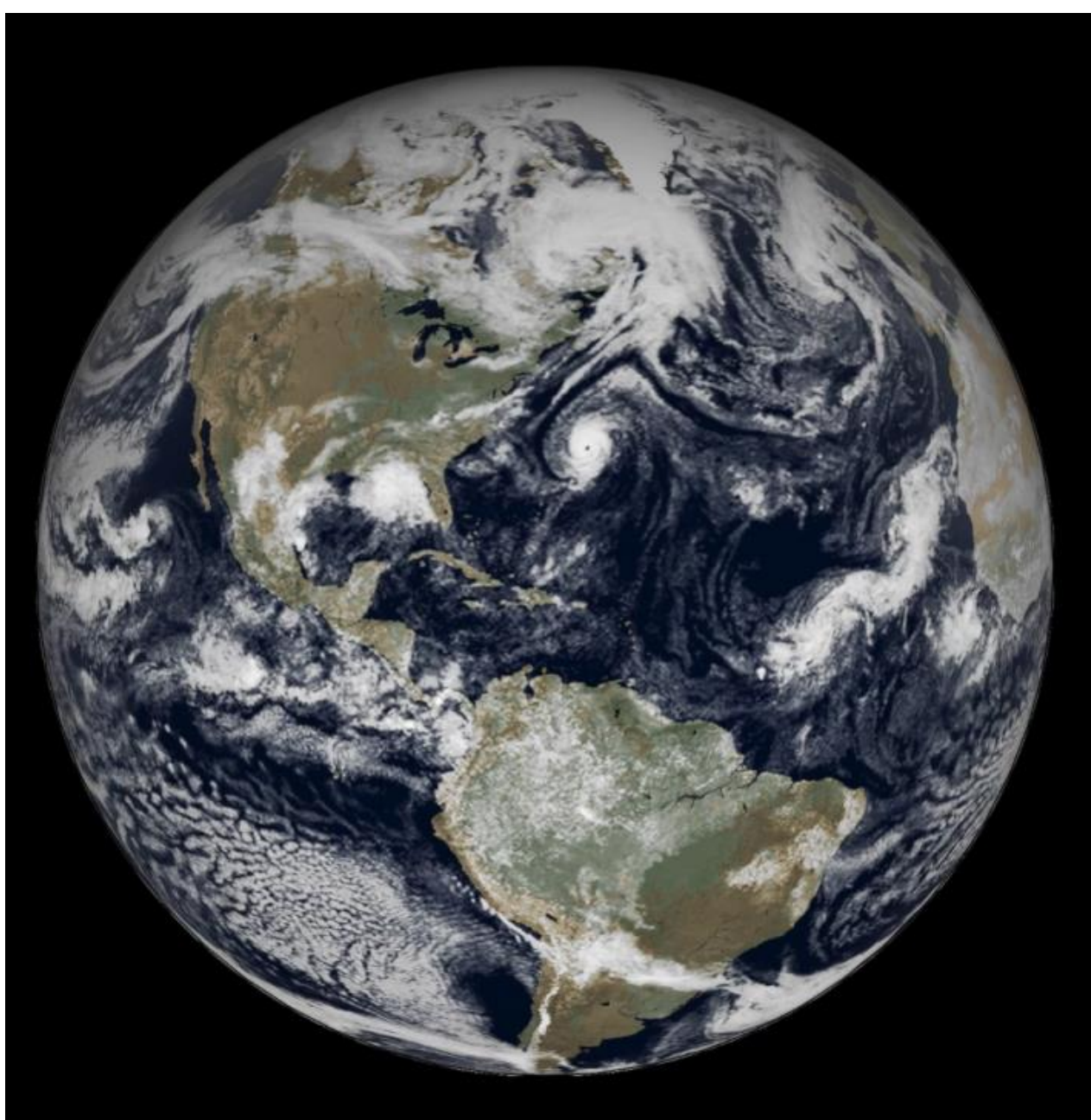
- Parallel set of forecasts from very slightly different initial conditions and model formulation
- Assess uncertainty of today's forecast







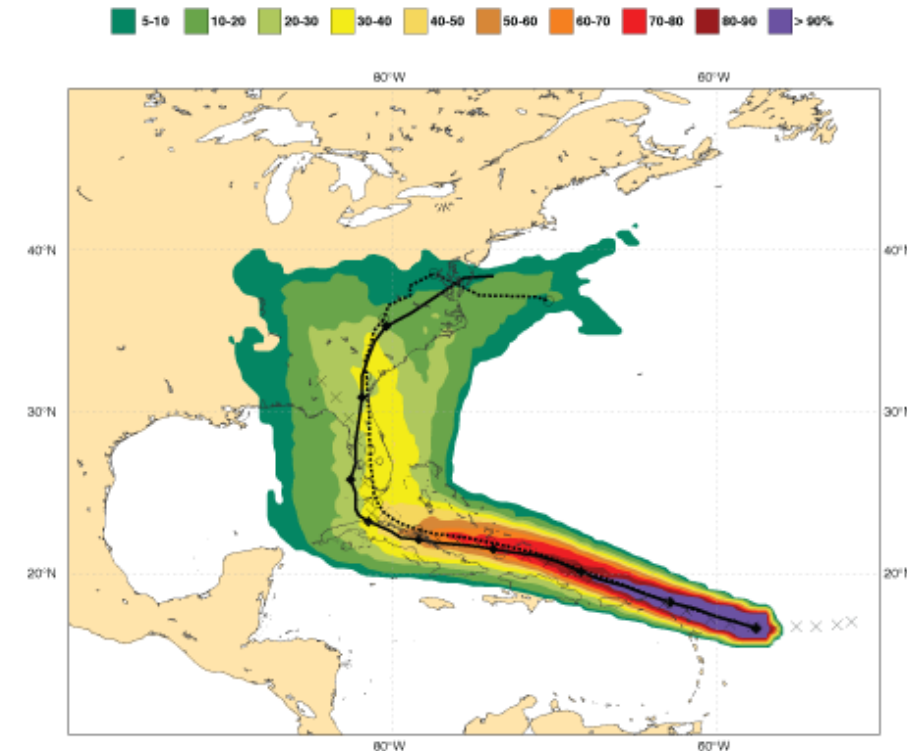




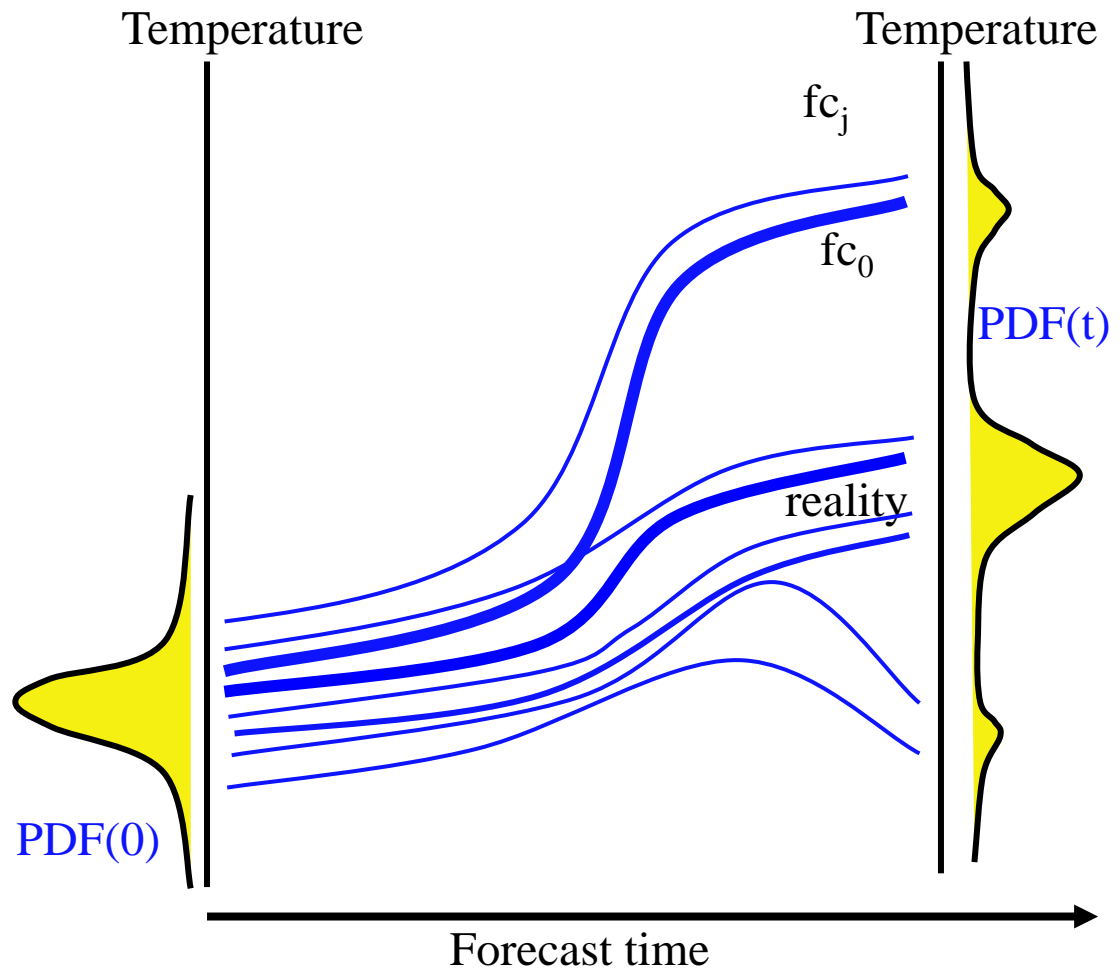
NOAA

TCo1279L137 ENS, 51 Members,  
20200913 00 UTC + 41 h

- 51 Members (50 perturbed + control member without perturbations), CY48R1 -> TCo1279 (~ 9 km) to day 15, extended-range, 100 member TCo319, ~ 36 km (see Lang. et al., 2023 for model cycle description).
- 137 vertical levels
- Coupled to NEMO ocean model (1/4 degree), ecWAM wave model and LIM2 ice model
- Initial perturbation via an ensemble of data assimilations and singular vectors, 5 member ocean data assimilation
- Model error representation – currently SPPT







Sources of Uncertainty:

- Initial Conditions
- Model Formulation

from R. Buizza

## Perturbations to the initial conditions:

Methods that rely on the dynamics only, e.g.:

- bred vectors
- singular vectors

Ensemble data assimilation methods, e.g.:

- Ensemble of 4D-Var data assimilations (EDA)
- Ensemble Kalman Filter

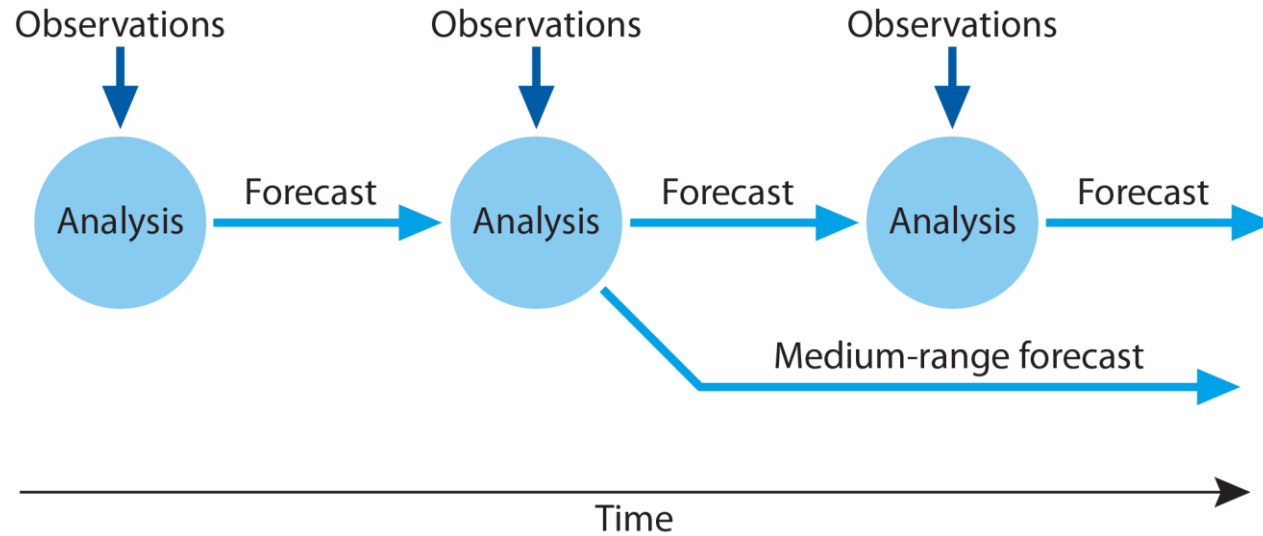
ECMWF: combination of EDA and singular vectors

-> data assimilation methods know about obs coverage etc



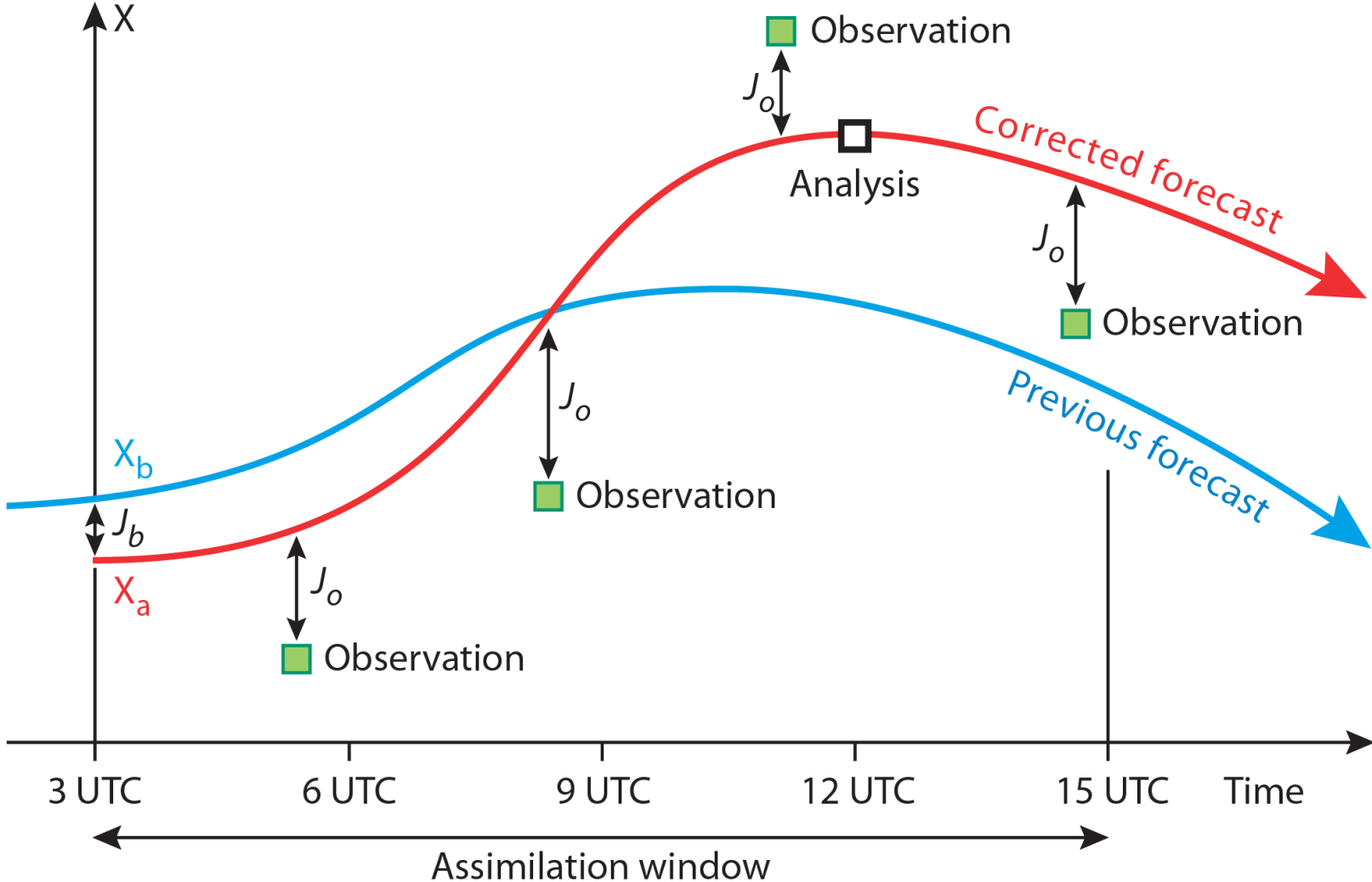
## Starting the Medium-Range Forecast – the ‘Analysis’

Analysis: 3 dimensional virtual image of the atmosphere at a given time.



- The short range forecast from the previous analysis is our ‘first estimate’ of the current state of the atmosphere.

# 4D-Var assimilation

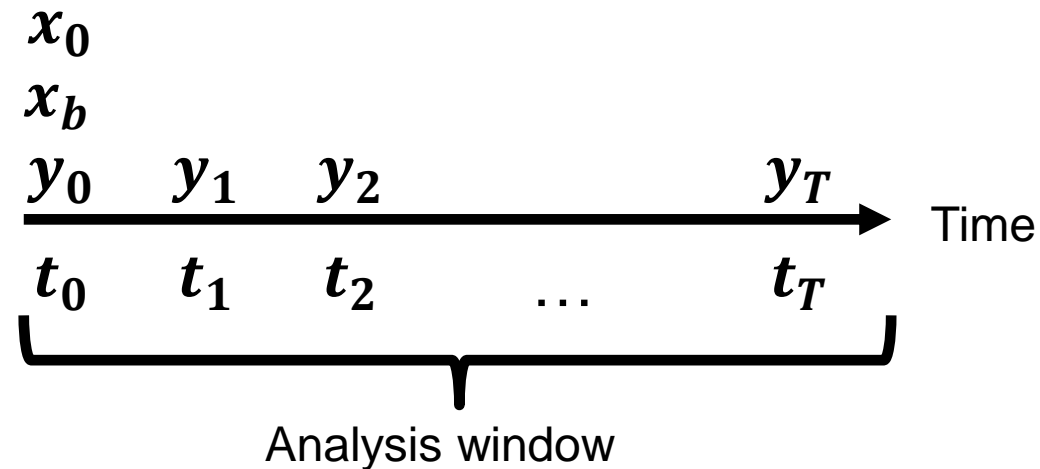




# 4D-Var assimilation

To find model trajectory that best fits the observations over an assimilation interval ( $t=0,1,\dots,T$ ) - > finding the minimum of the 4DVar cost function:

$$J(\mathbf{x}_0) = (\mathbf{x}_b - \mathbf{x}_o)^T (\mathbf{P}^b)^{-1} (\mathbf{x}_b - \mathbf{x}_o) + \sum_{t=0}^T (\mathbf{y}_t - H_t M_{0 \rightarrow t}(\mathbf{x}_0))^T \mathbf{R}_t^{-1} (\mathbf{y}_t - H_t M_{0 \rightarrow t}(\mathbf{x}_0))$$



See lectures in DA Training

## Ensemble of 4D-Var data assimilations (EDA)

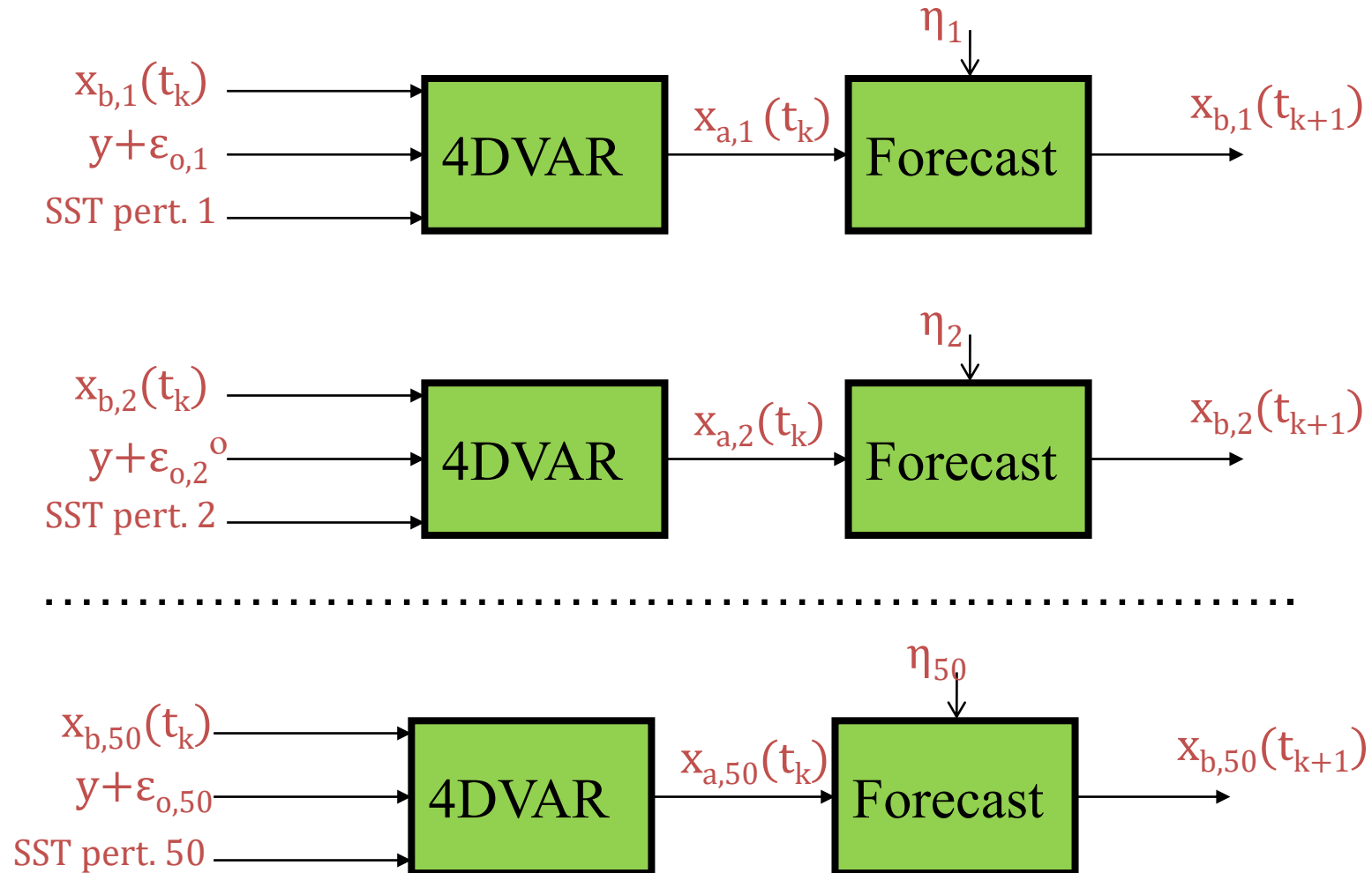
- 50 perturbed ensemble members + 1 control:  
TCo639 outer loops (~ 18 km), 137 levels, TL191/TL191 inner loops.  
(HRES DA: TCo1279 outer loops (~ 9 km), TL255/TL319/TL399/TL511 inner loops).
- Observations randomly perturbed according to their estimated error covariances (R)
- SST perturbed with climatological error structures
- Model error representation via Stochastically Perturbed Parametrization Tendencies (SPPT)

The EDA simulates the error evolution of the 4DVar analysis cycle:

→ uncertainty estimates to initialize ensemble forecasts

→ Flow dependent estimates of background error covariances for use in 4D-Var

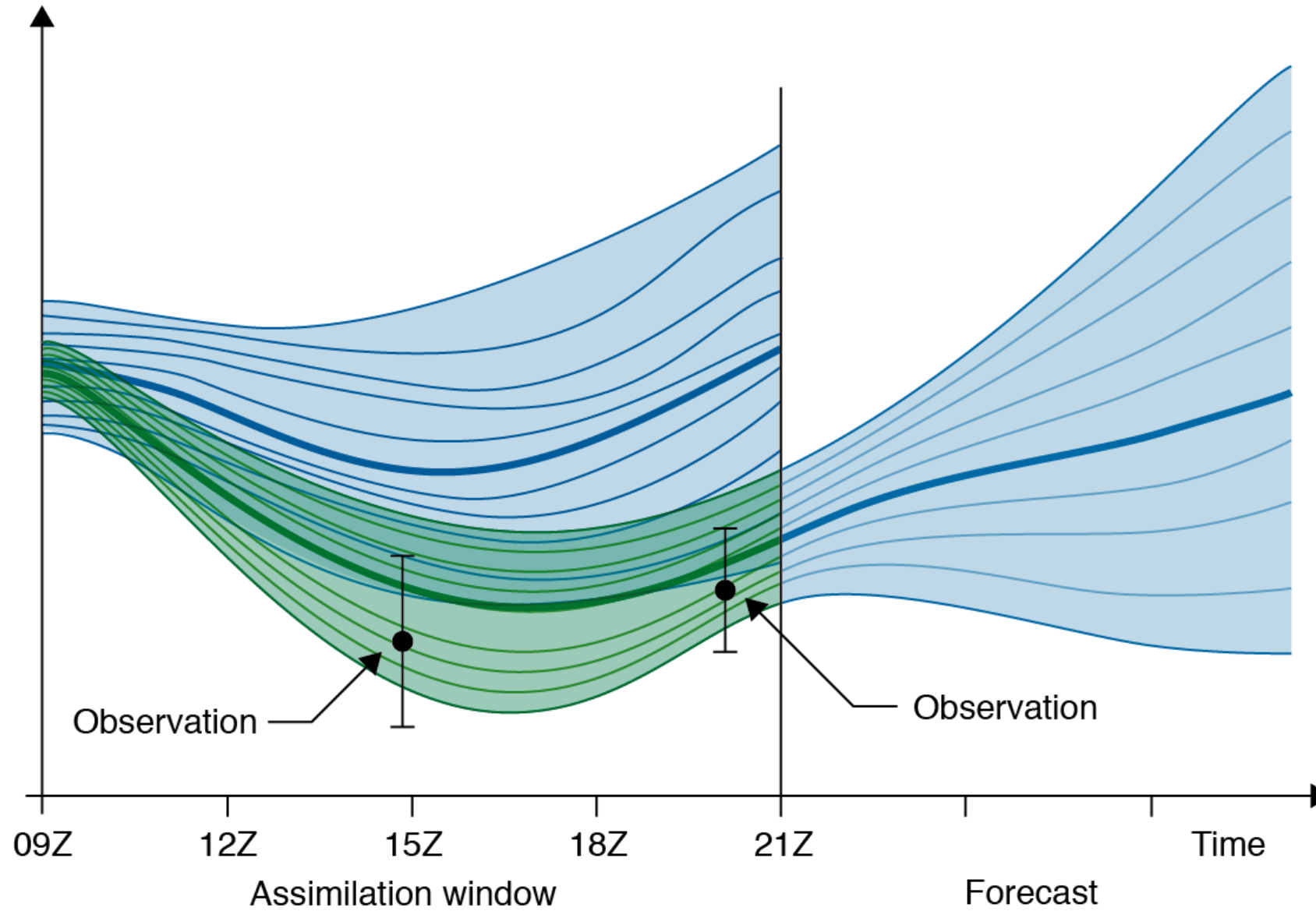




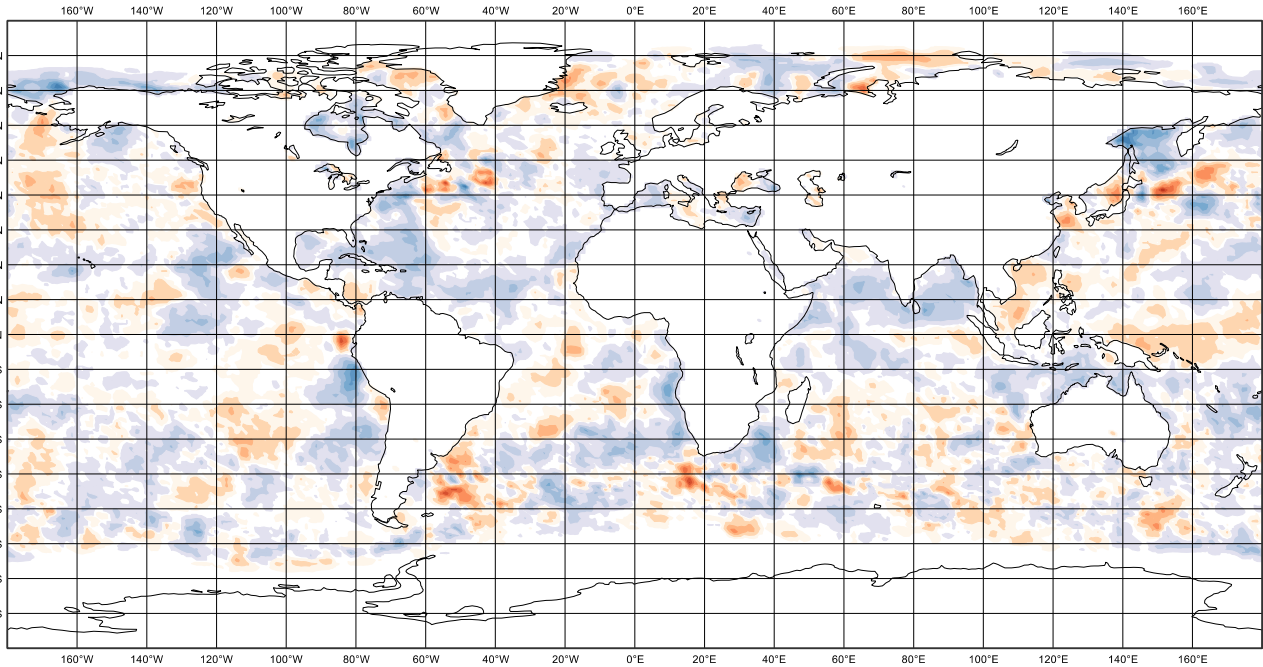
See also Massimo Bonavita's Talk in DA Training

# Ensemble Data Assimilation

# Ensemble Forecast

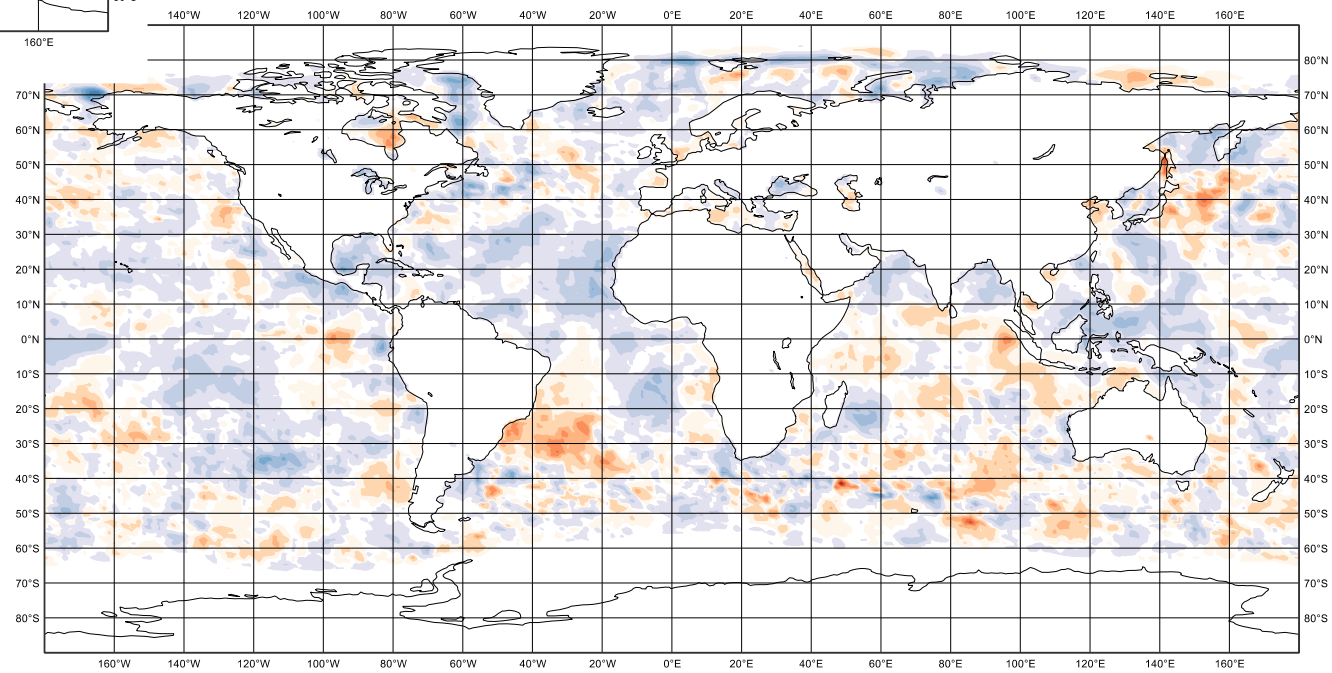


Thursday 30 September 2021 06 UTC ecmf t+3 VT:Thursday 30 September 2021 09 UTC surface Sea surface temperature



Example: SST perturbations

Thursday 30 September 2021 06 UTC ecmf t+3 VT:Thursday 30 September 2021 09 UTC surface Sea surface temperature





# Current Model Error Representation: SPPT

See Leutbecher et al., 2017 and  
Lock et. al, 2019 for details

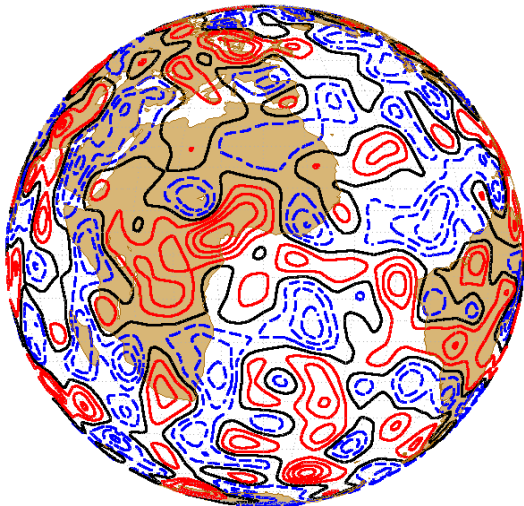
Perturb model tendencies during the forecast:

$$\mathbf{x}_p = \mathbf{x} + \alpha \mathbf{x}$$

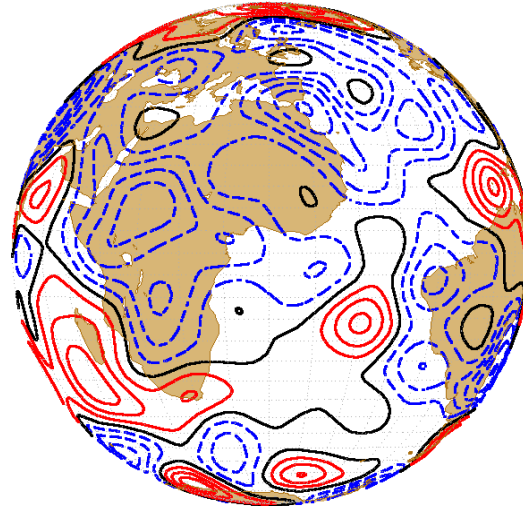
$\mathbf{x}$  sum of tendencies from parametrization schemes  
(convection, radiation, cloud etc.)

$\alpha$  includes random time and space correlations, provided by a pattern generator

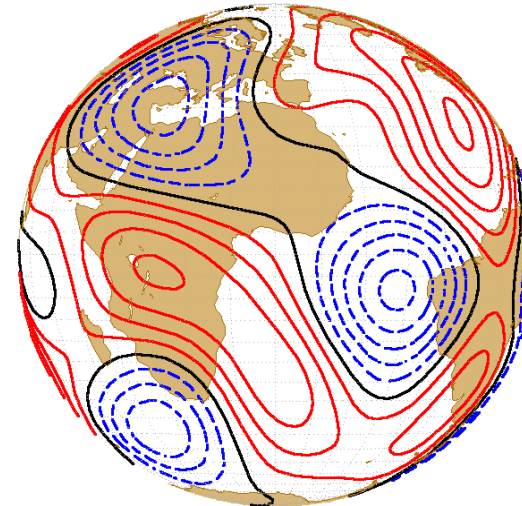
Scale 1



Scale 2



Scale 3



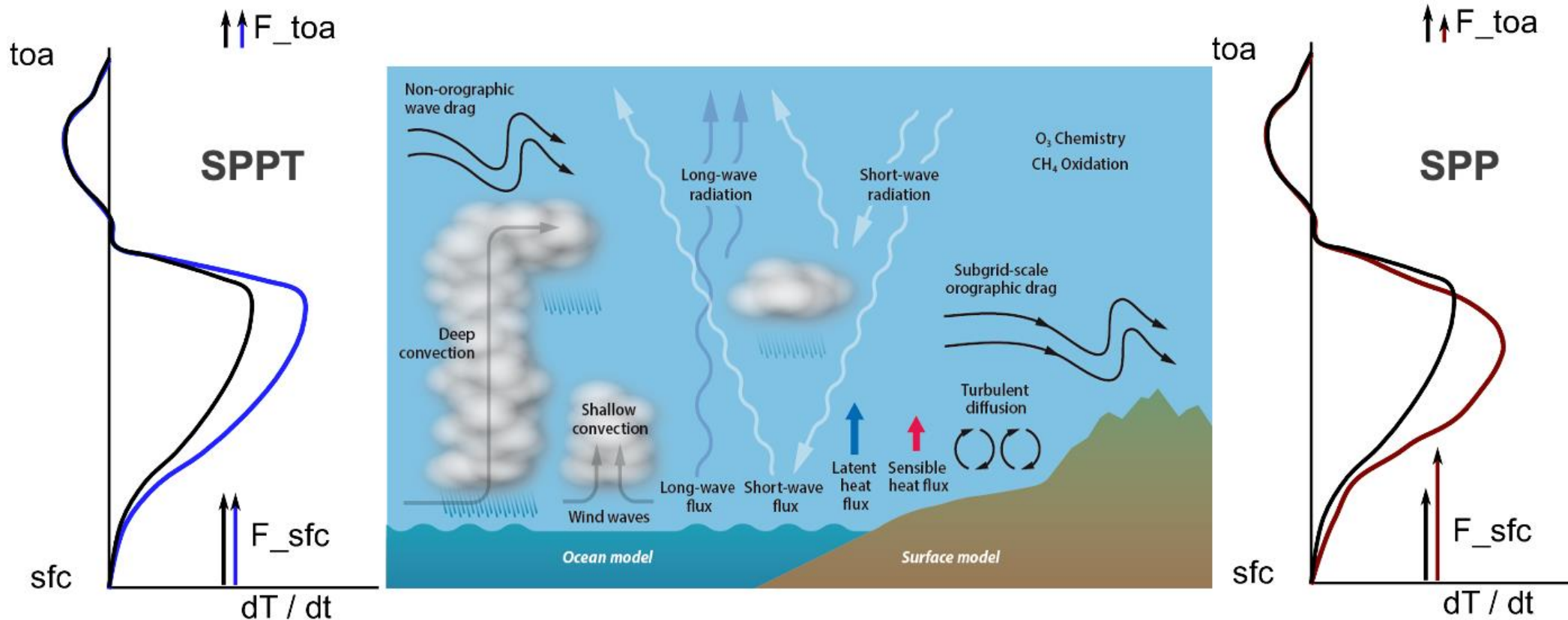
Same model uncertainty representation in ensemble forecasts and ensemble data assimilation

# Future Model Error representation: SPP

Ollinaho et al (2017), <https://doi.org/10.1002/qj.2931>  
Leutbecher et al (2017), <https://doi.org/10.1002/qj.3094>  
Lang et al (2021), <https://doi.org/10.1002/qj.3978>

## Key differences between SPPT and SPP:

- SPP represents model uncertainties closer to the assumed sources of the errors
- SPP better maintains physical consistency: e.g. local budgets and flux perturbations
- SPPT only represents amplitude errors while SPP can also represent errors in the shape of a heating profile

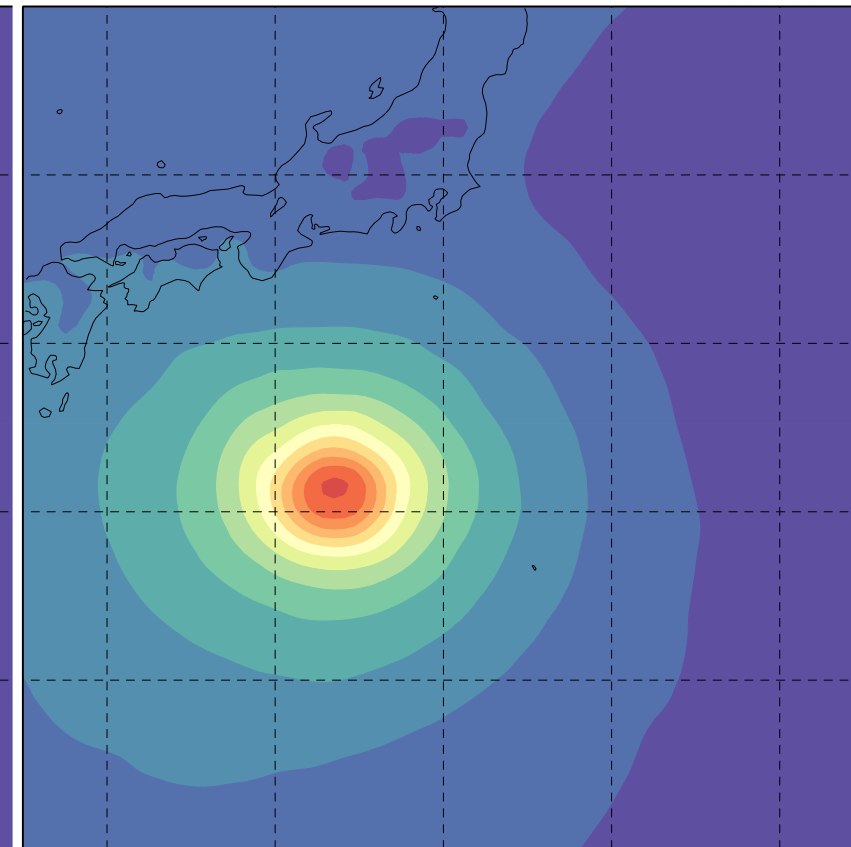
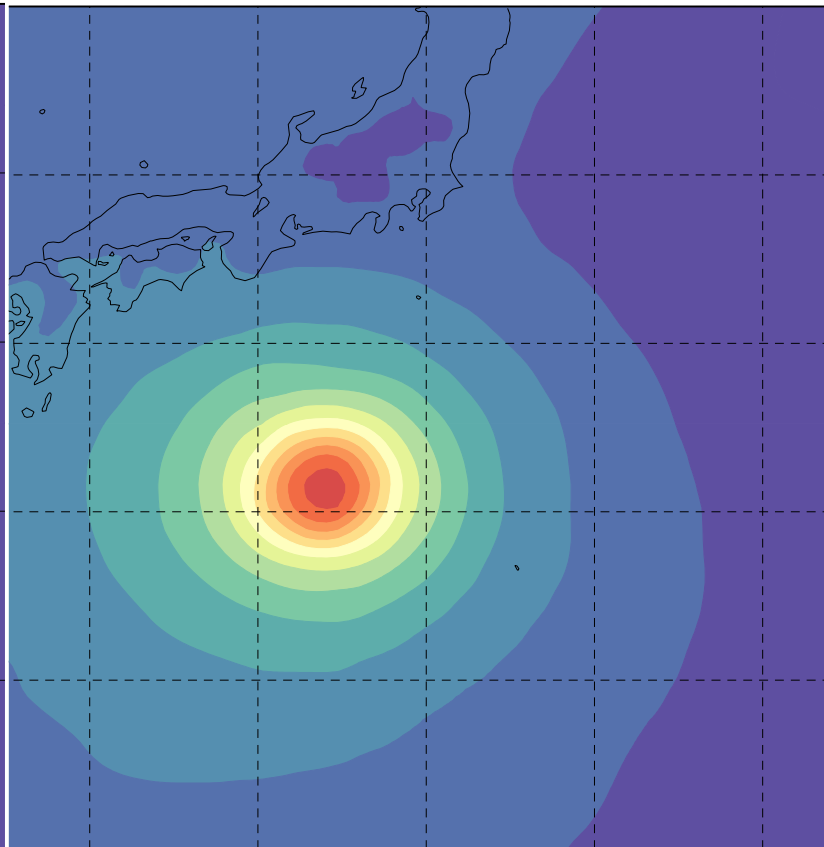
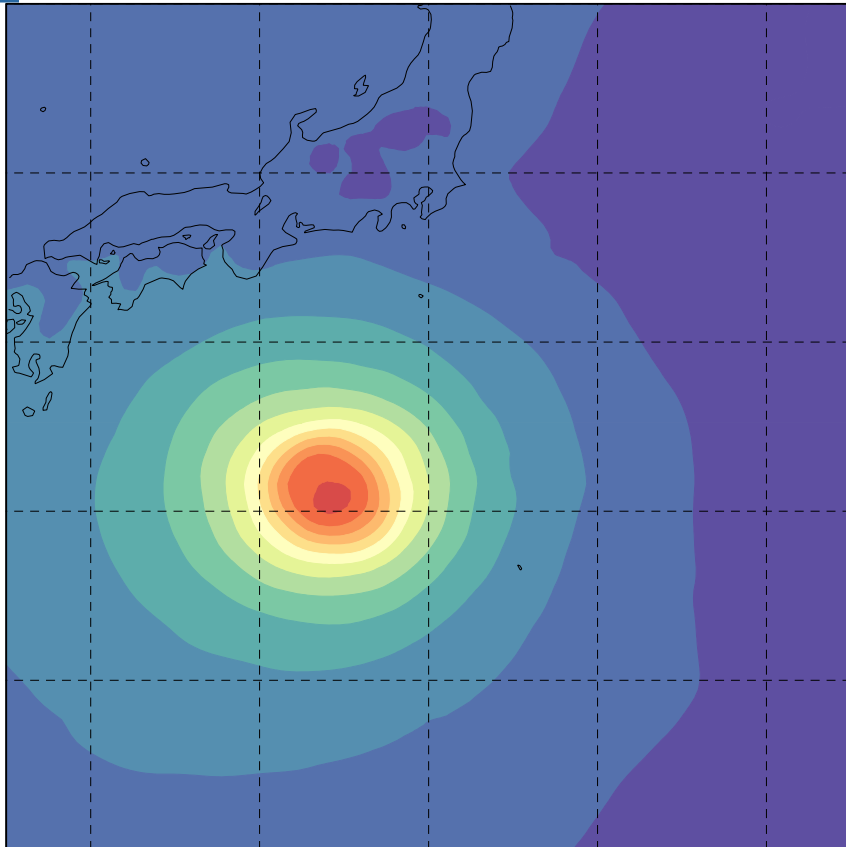


# MSLP

EDA member 2

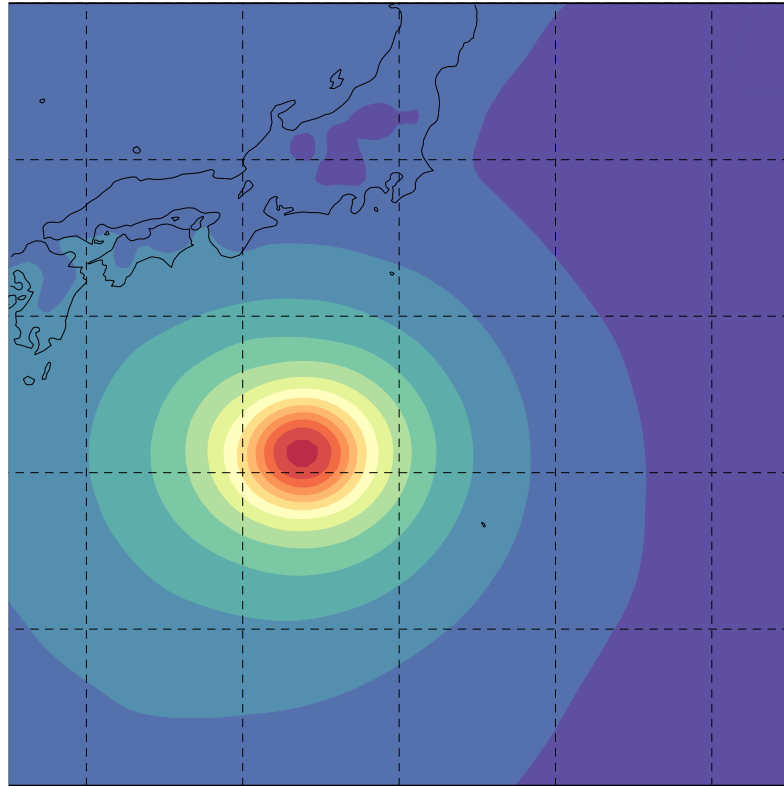
EDA member 4

EDA member 22

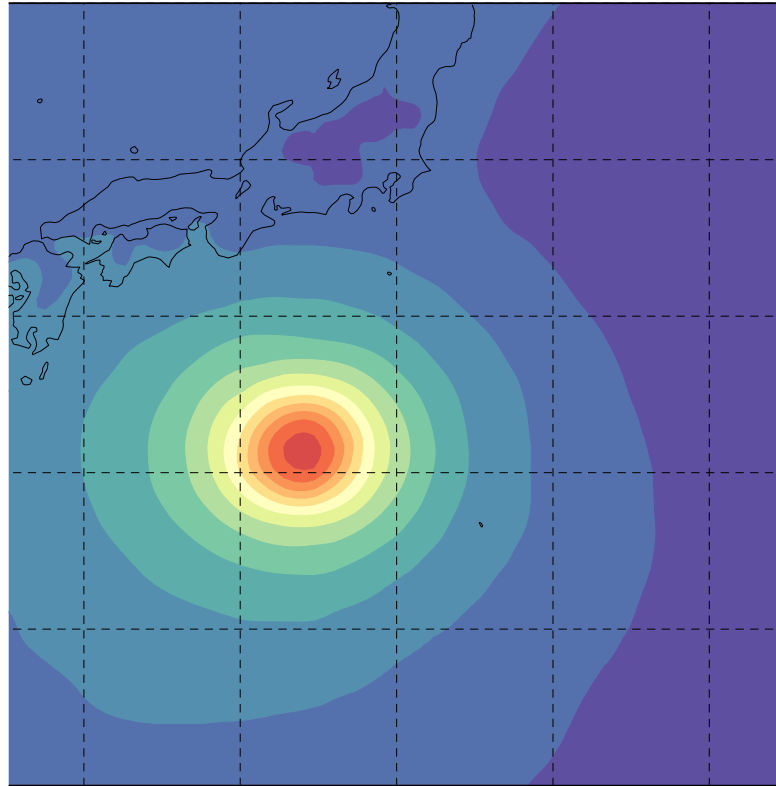


# MSLP

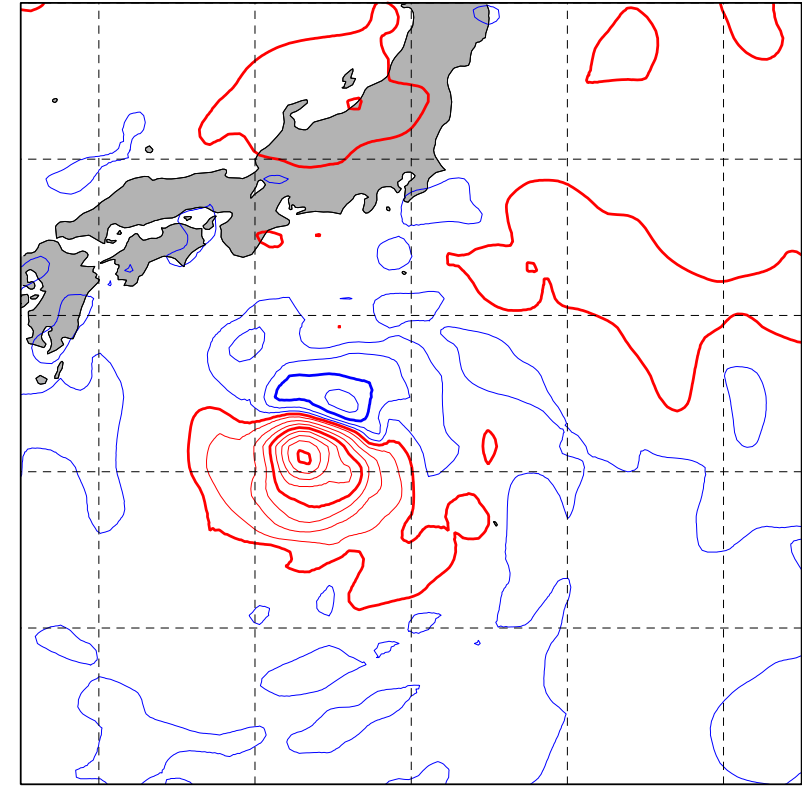
## EDA mean



## EDA member 2

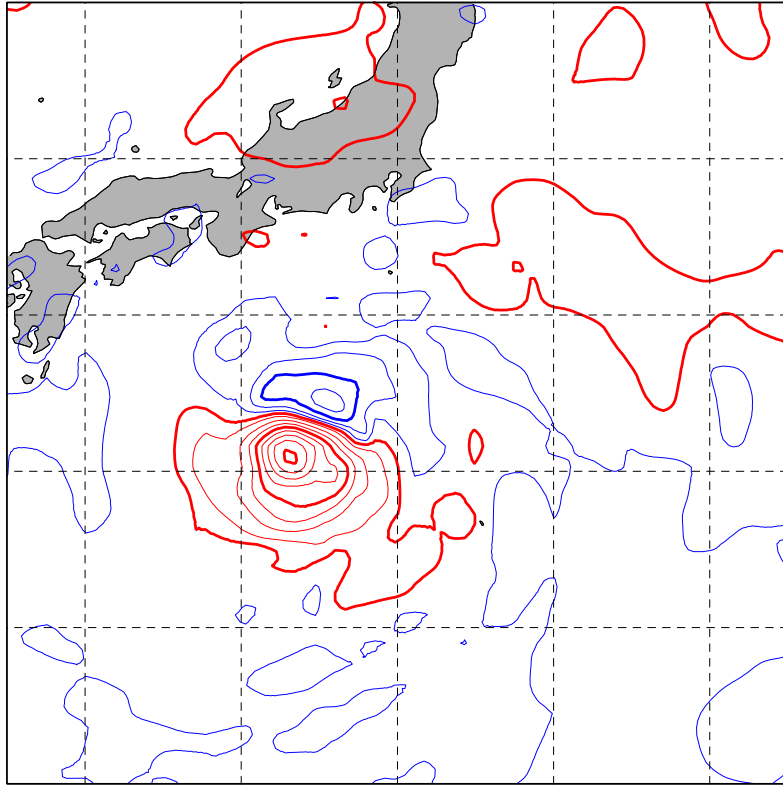


## EDA member 2 – EDA mean

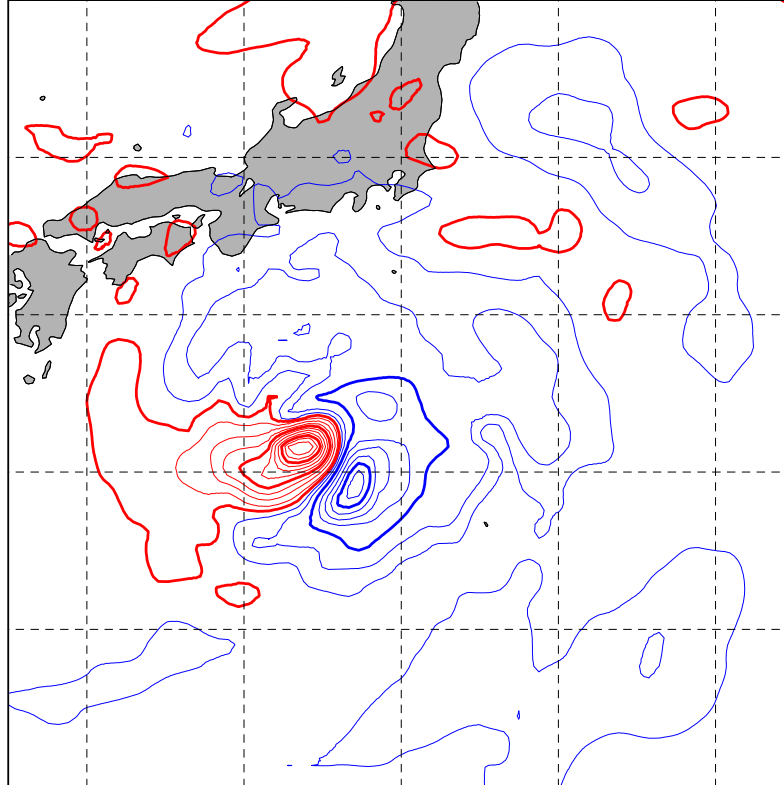




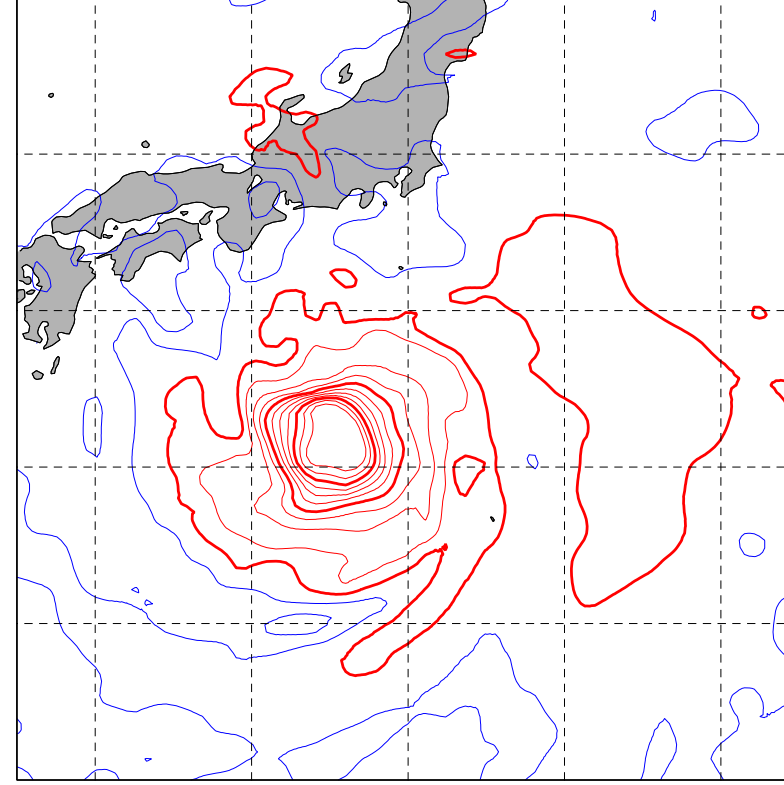
EDA member 2 – EDA mean



EDA member 4 – EDA mean

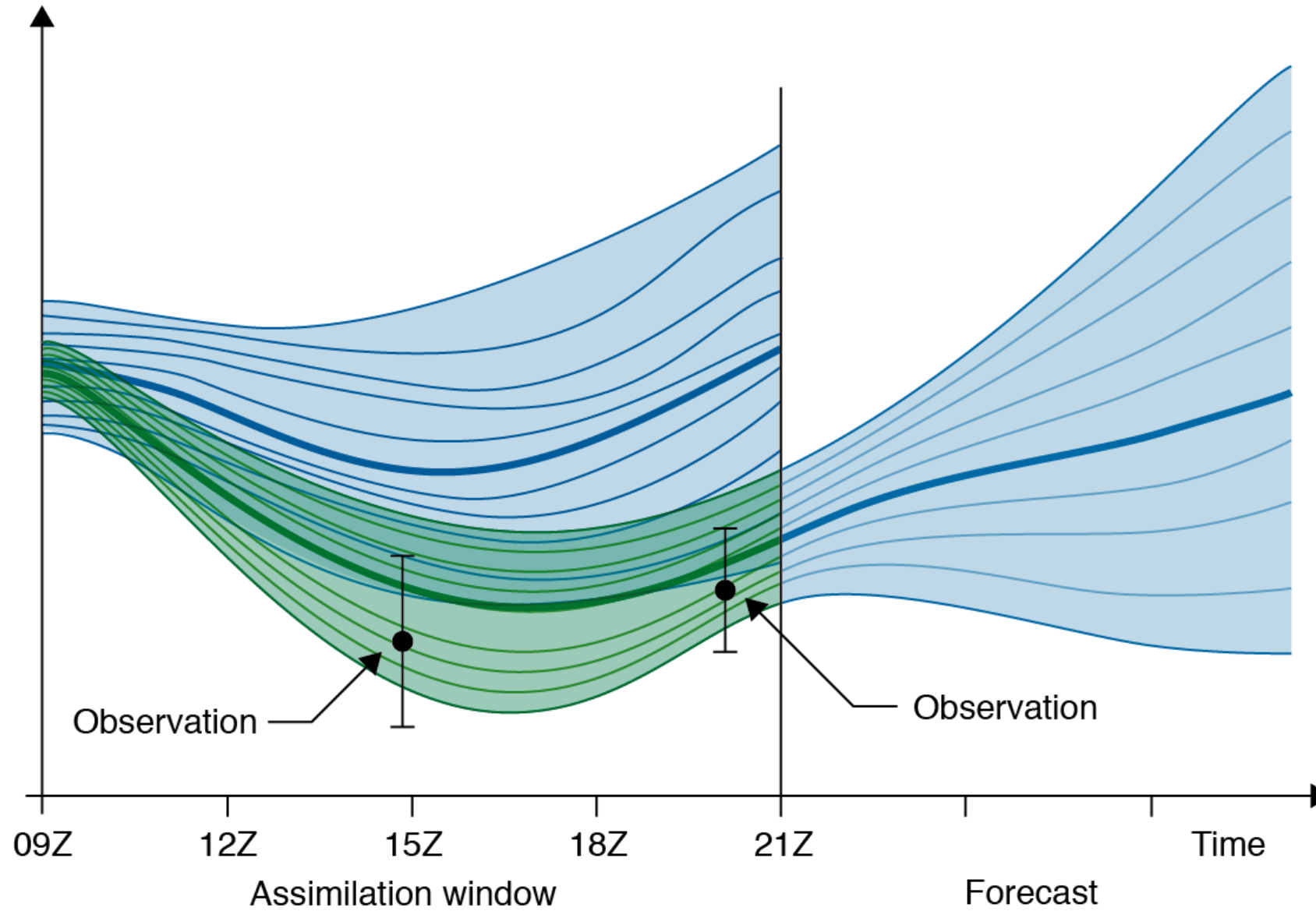


EDA member 22 – EDA mean



# Ensemble Data Assimilation

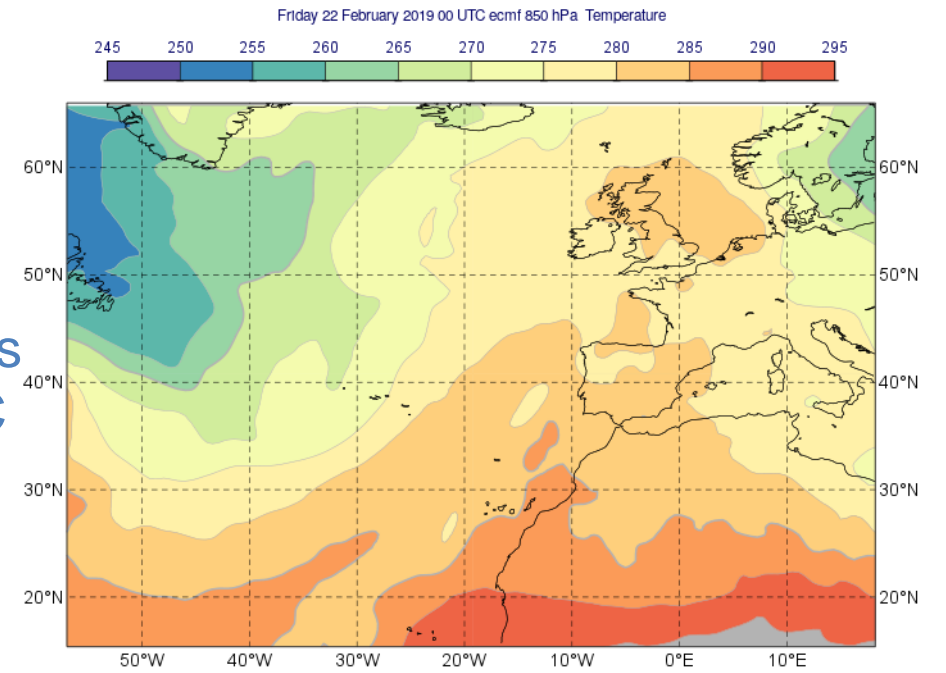
# Ensemble Forecast



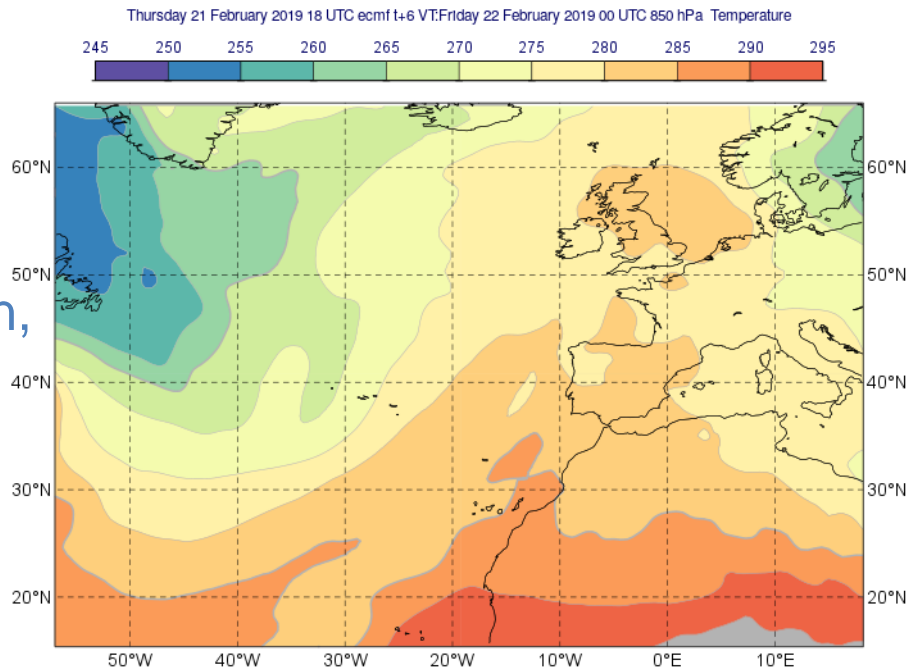
# T850hPa

What is available when we start the 00 UTC ensemble forecasts?

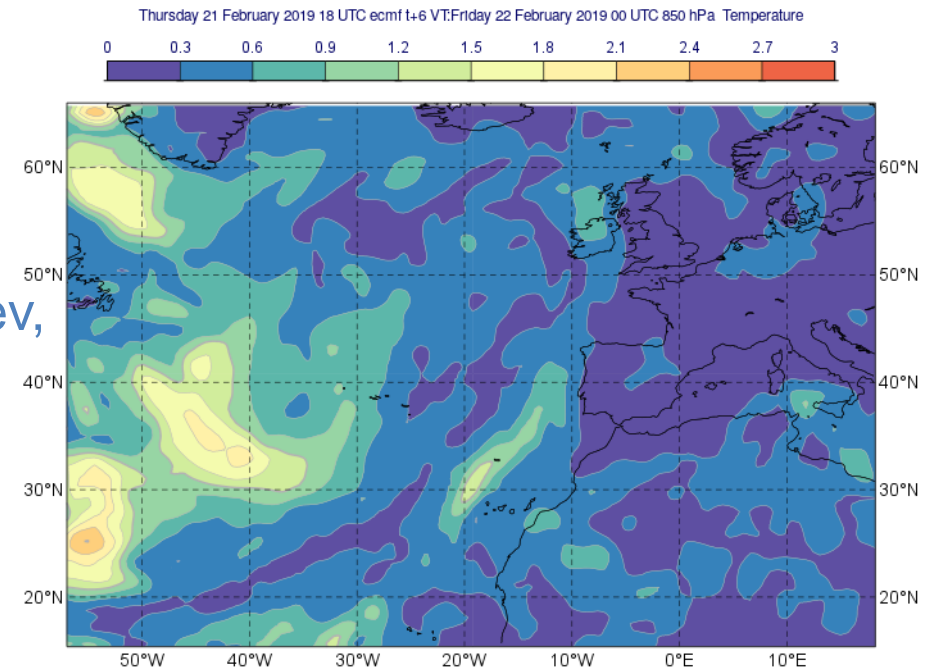
HRES  
Analysis  
00 UTC



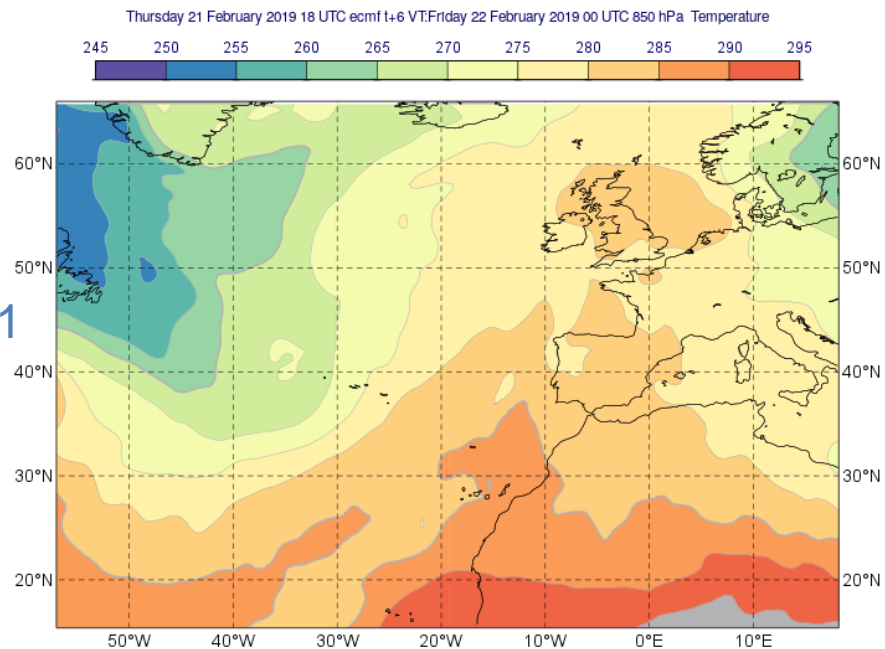
EDA Mean,  
18 UTC,  
6h Fcsts



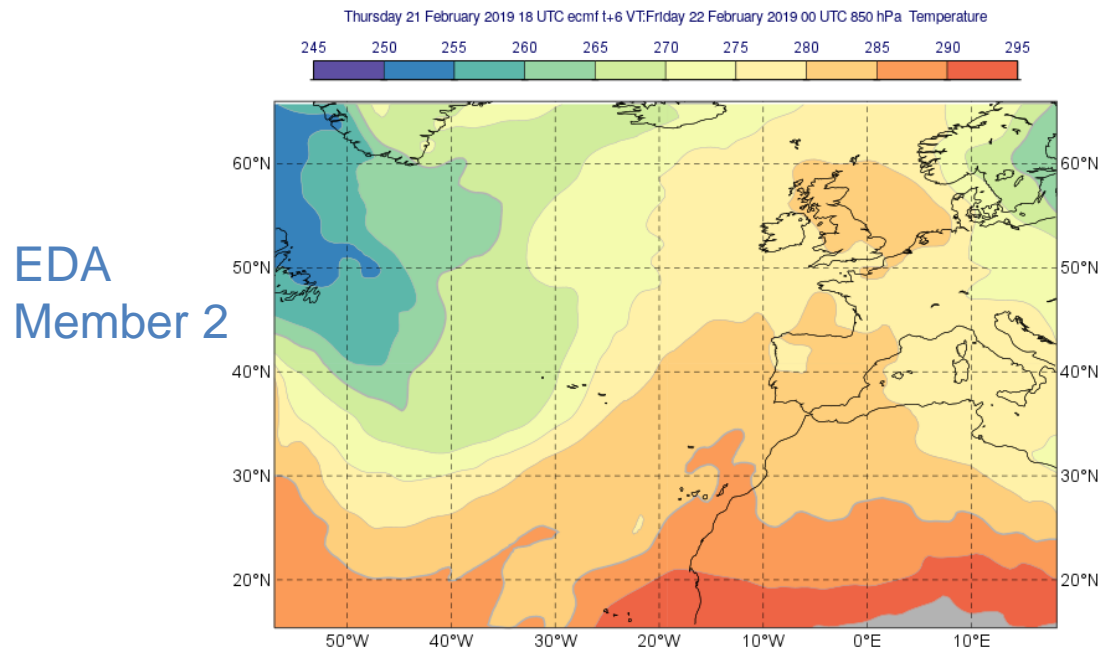
EDA StDev,  
18 UTC,  
6h Fcsts



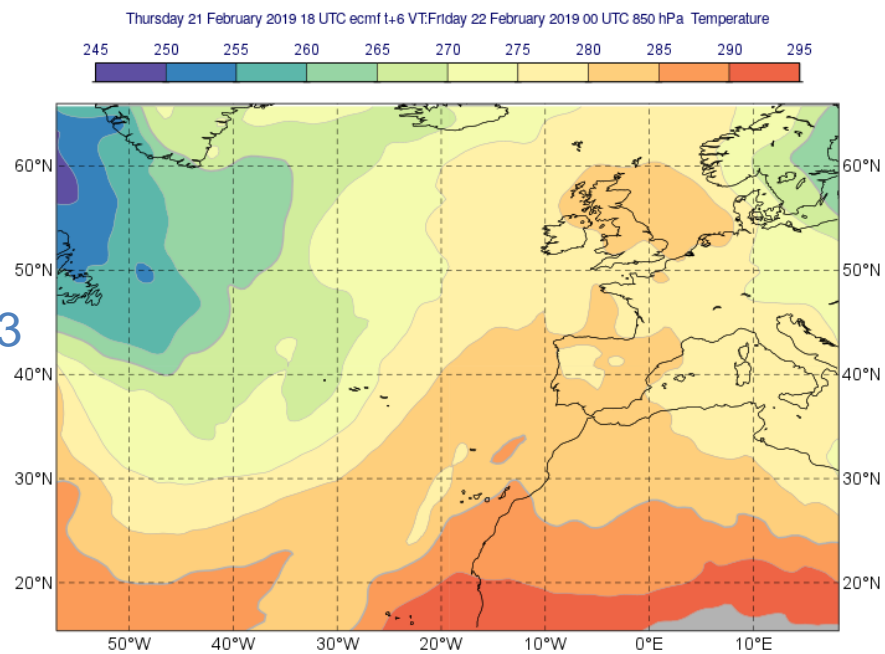
# EDA FC, 6h, T850hPa



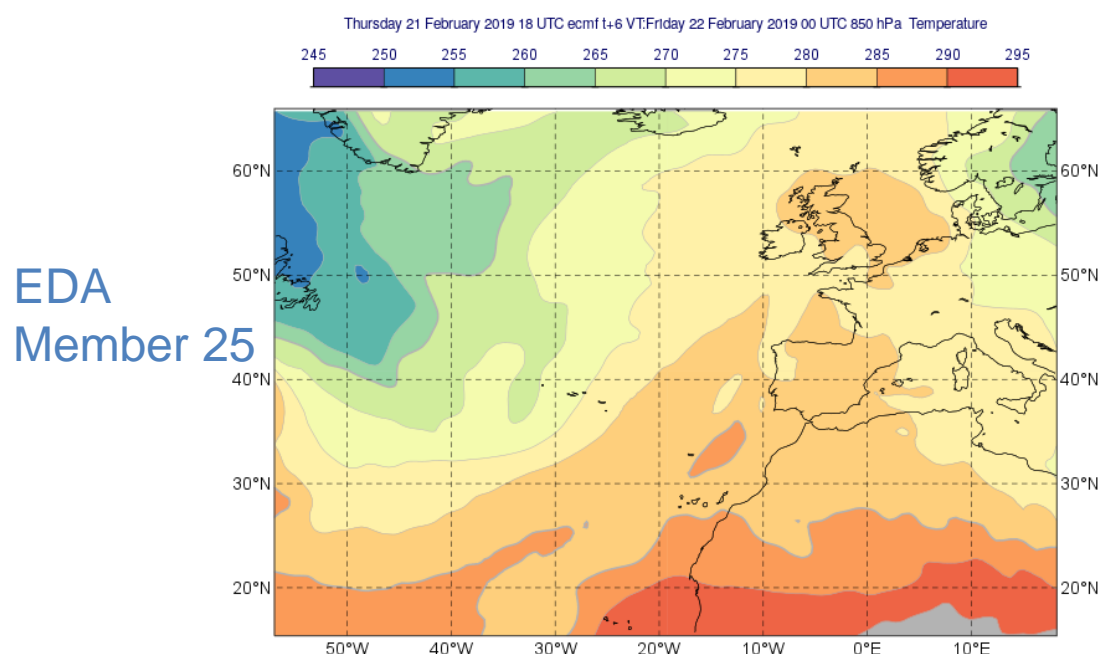
EDA  
Member 1



EDA  
Member 2



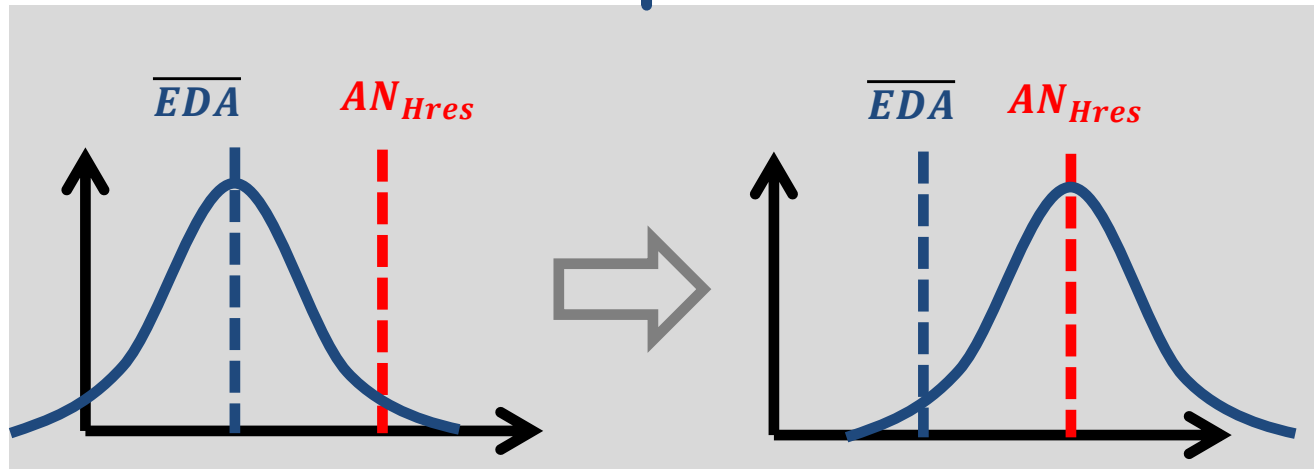
EDA  
Member 3



EDA  
Member 25

# Generation of initial conditions for the ensemble forecasts:

$$AN_{pf} = AN_{Hres} + (EDA_i - \overline{EDA}) + SVPERT_j \quad \begin{matrix} i = 1..50 \\ j = 1..50 \end{matrix}$$



EDA : 6h  
Forecasts

Re-centre EDA-Distribution on Hres-Analysis

$$SVPERT_j = \sum_l^{NSET} \sum_k^{NSV_l} \alpha_{lk} SV_{lk}$$

$\alpha$  random number drawn from Truncated gaussian

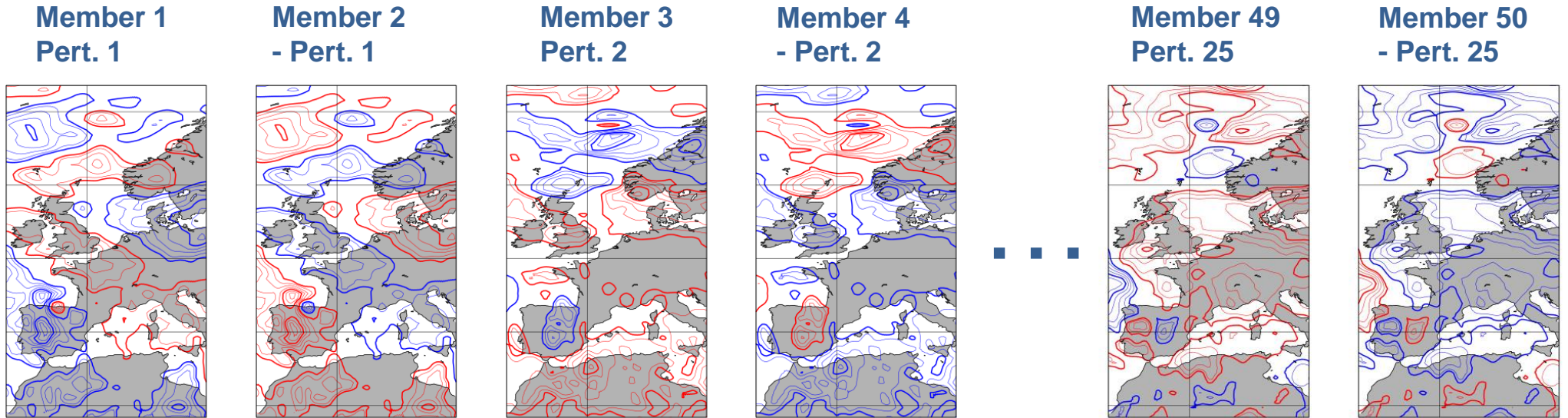
NSET : nhem, shem, TCs1-6

NSV : 50 for nhem and shem, 5 for TCs



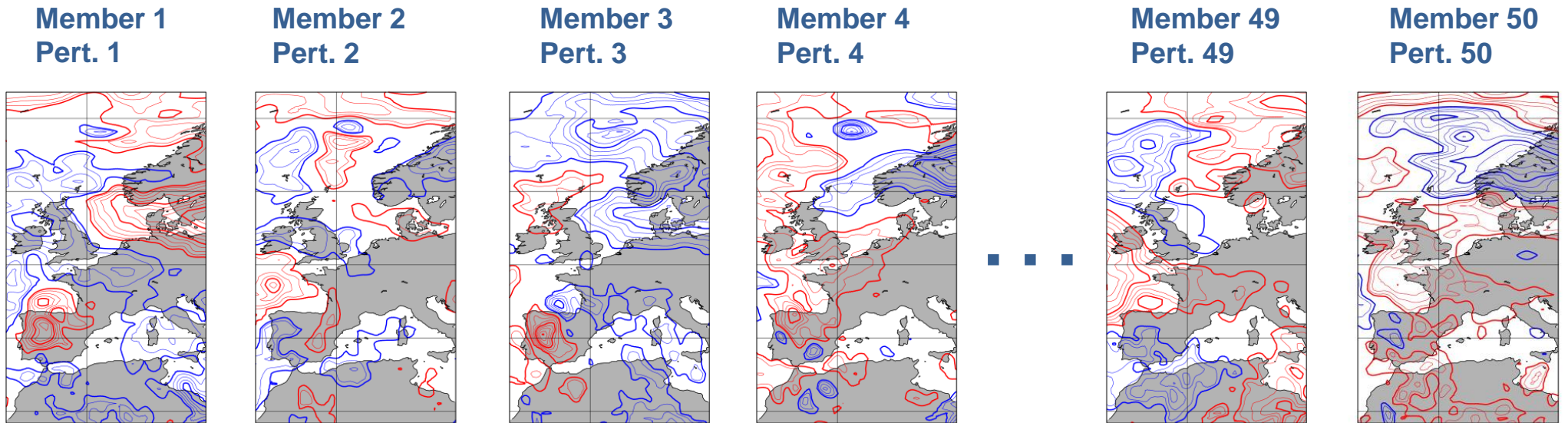
# New way to perturb the ensemble initial conditions for 50 Ensemble Members

Old:  
Plus-Minus  
Symmetry with  
Perturbations from  
25-Member EDA



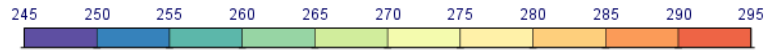
z500hPa

New:  
Perturbations  
from new  
50-Member EDA

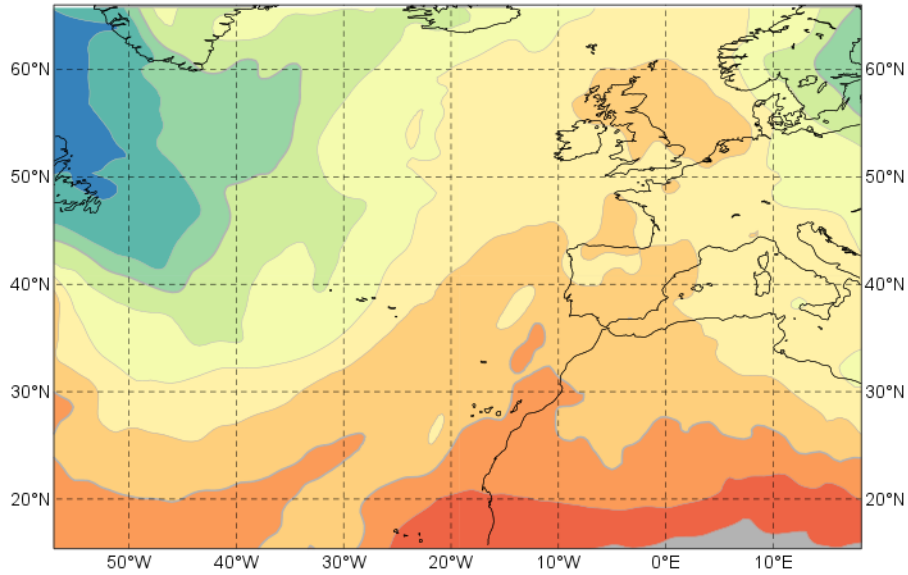


T850hPa

Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



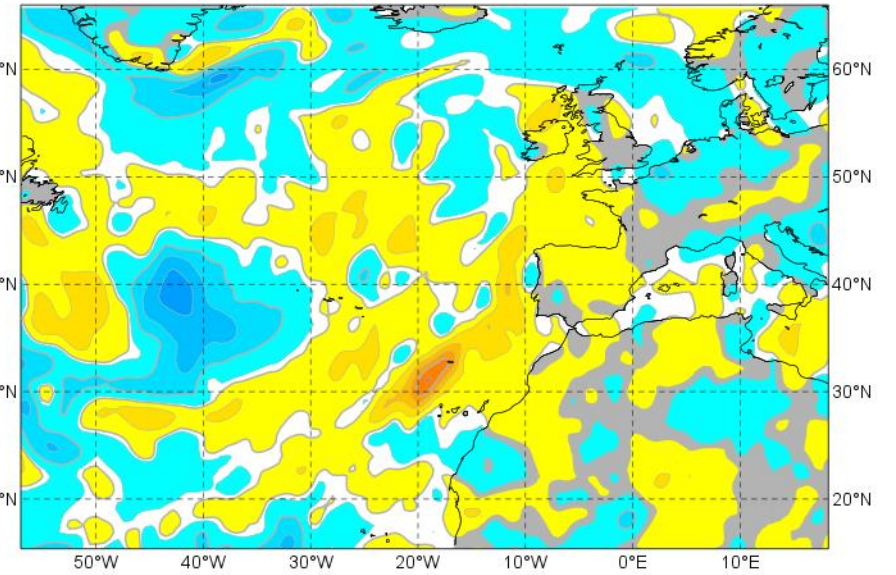
HRES  
Analysis  
00 UTC



Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



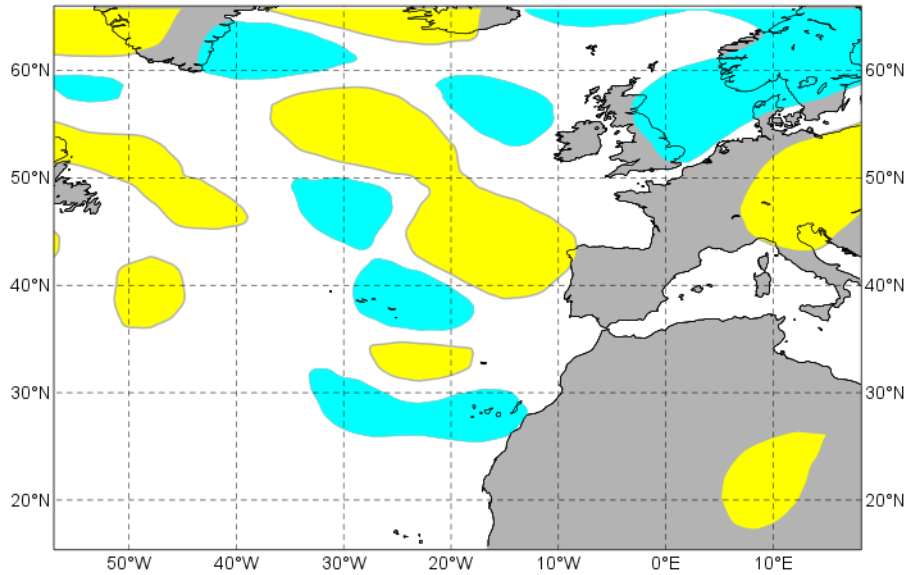
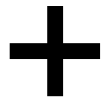
EDA-  
Pert 1



Friday 22 February 2019 00 UTC ecmf t+0 VT Friday 22 February 2019 00 UTC Model level 78 Temperature



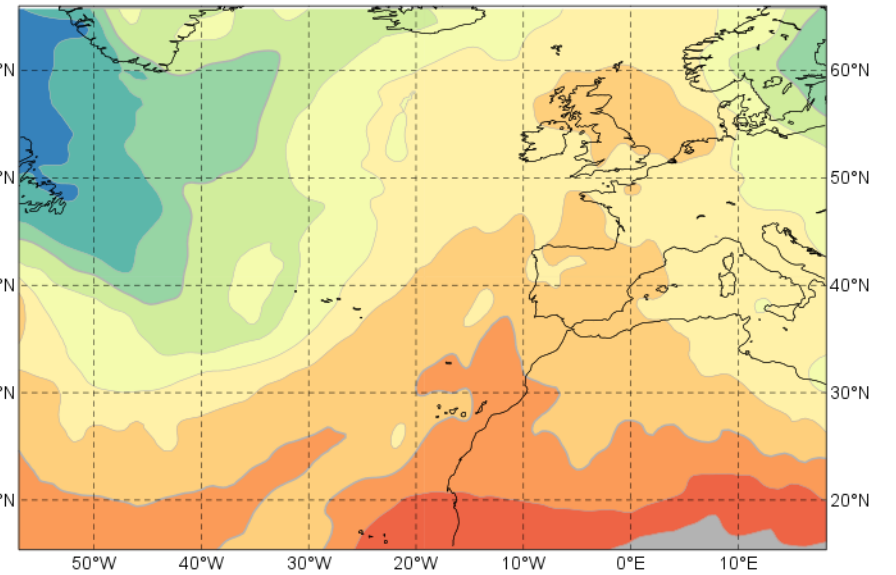
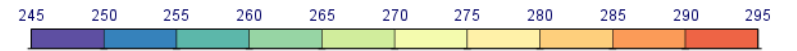
SV-  
Pert 1



Initial  
conditions  
for ENS  
member 1



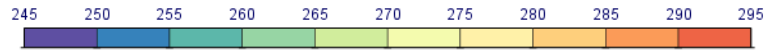
Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



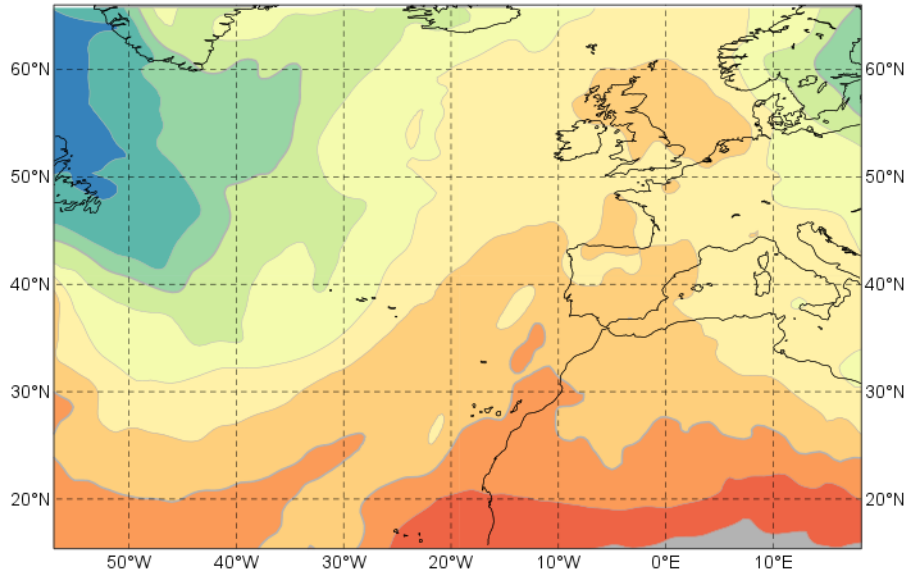


T850hPa

Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



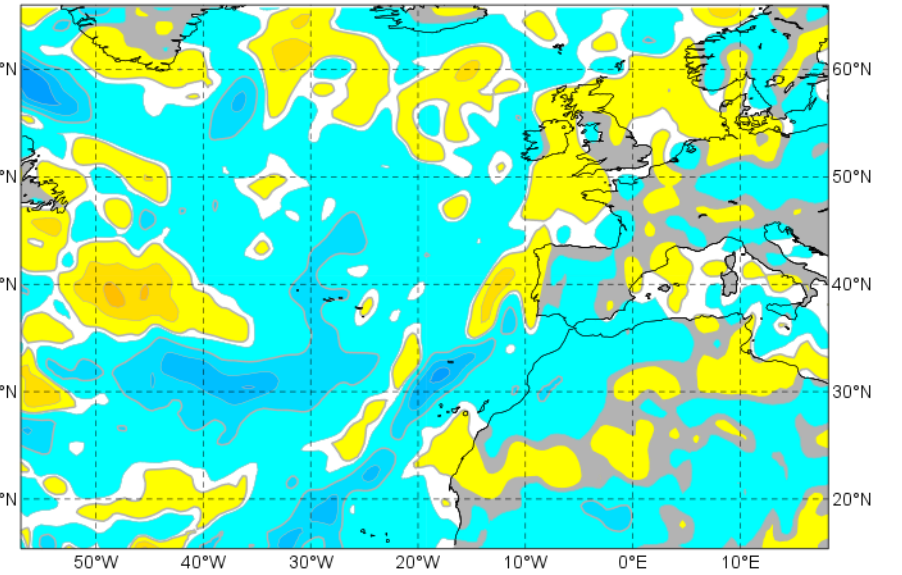
HRES  
Analysis  
00 UTC



EDA-  
Pert 3



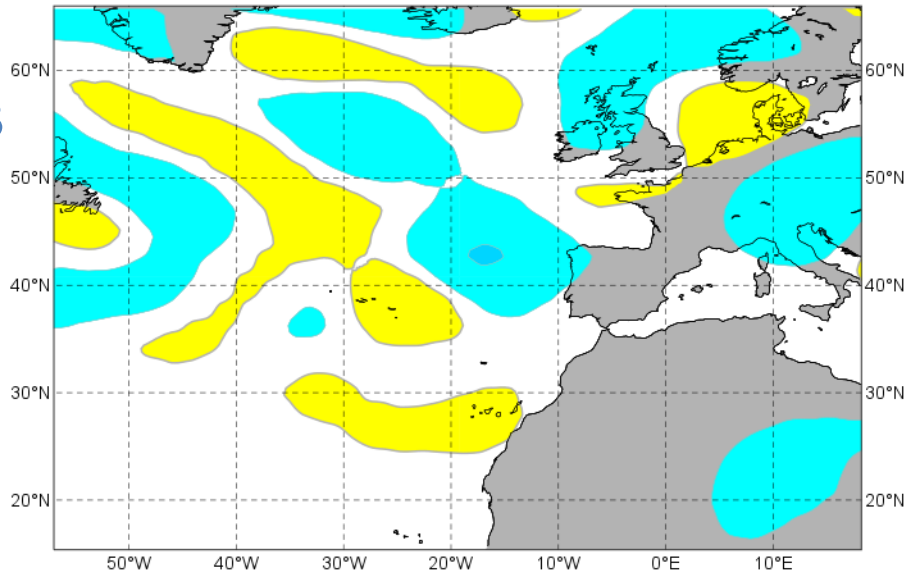
Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



Friday 22 February 2019 00 UTC ecmf t+0 VT Friday 22 February 2019 00 UTC Model level 78 Temperature

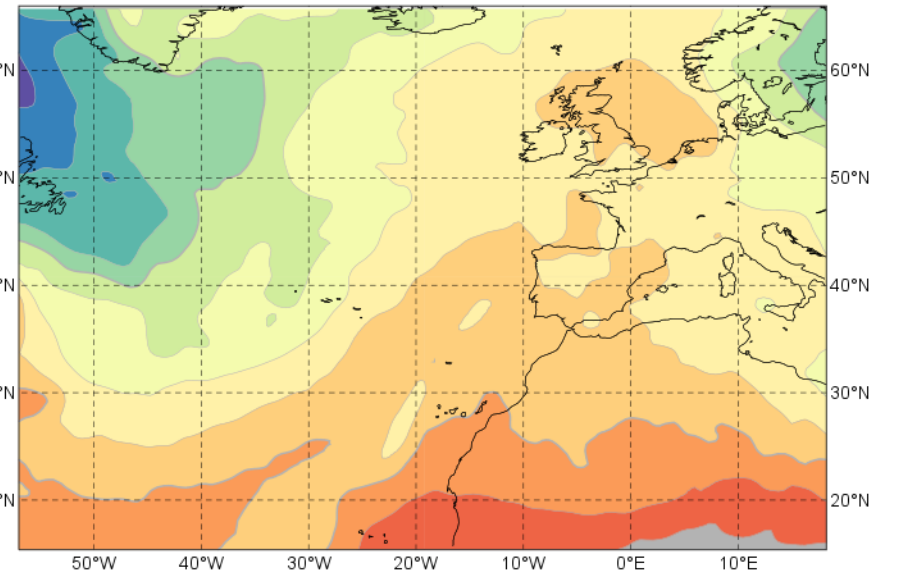
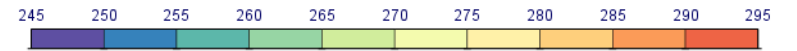


SV-  
Pert 3



Initial  
conditions  
for ENS  
member 3

Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature

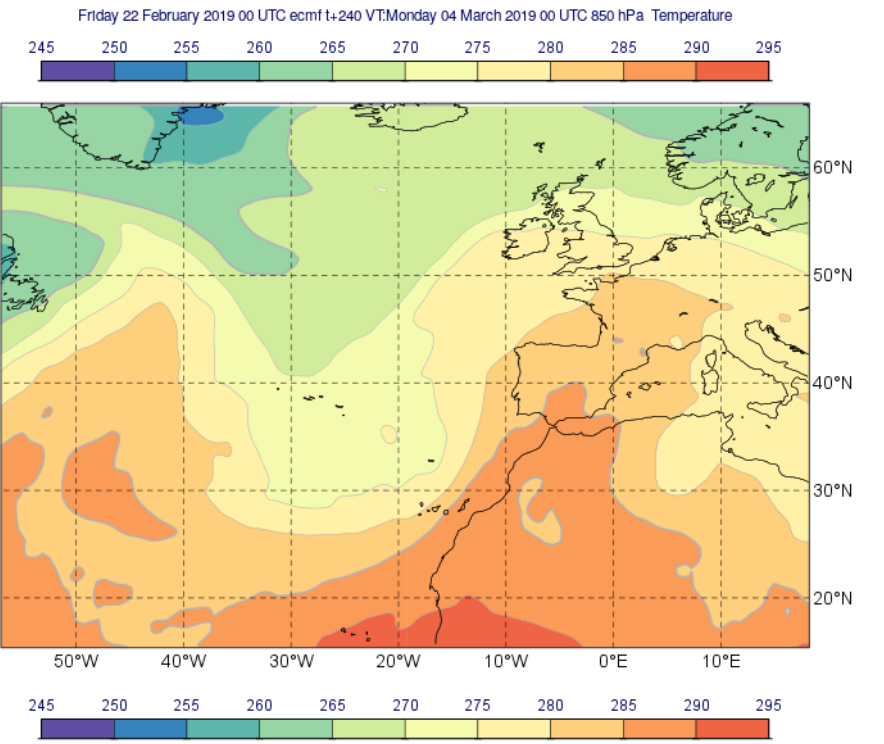
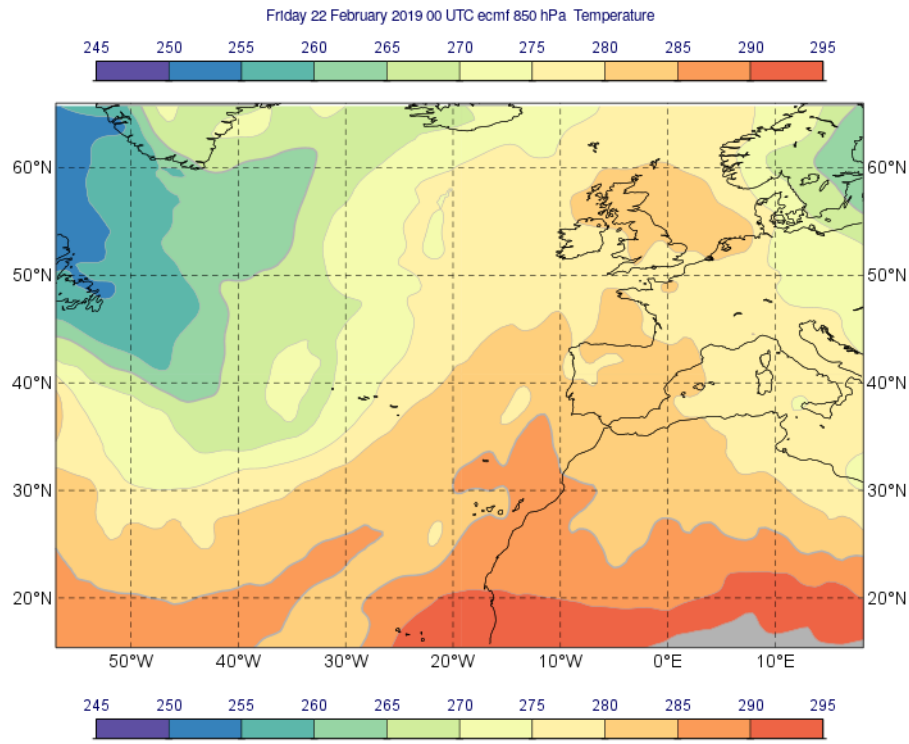


T850hPa

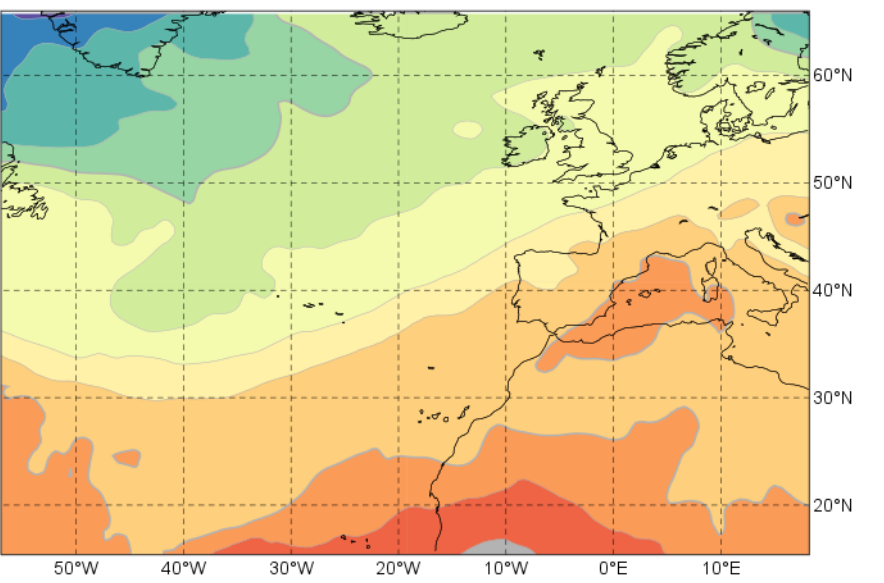
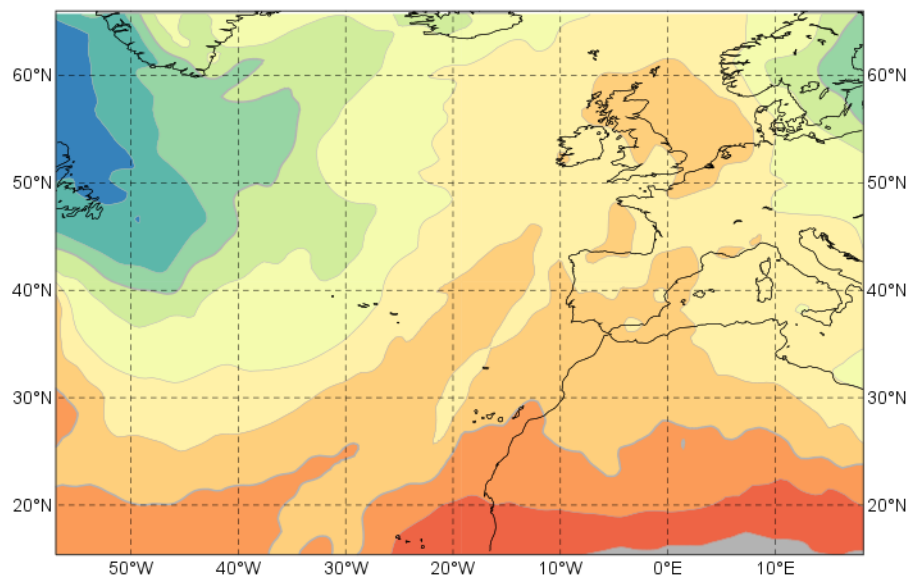
T+0h

T+240h

Member 1:



Member 2:





# Ocean initial state:

50 Members + 1 Control, 5 Ocean analyses

Member	Ocean analysis
Control	1
Member 1	2
Member 2	3
Member 3	4
Member 5	5
Member 6	1
Member 7	2
...	
Member 50	1

## Reliability of the ensemble spread

- Consider ensemble variance (“spread”) for an  $M$ -member ensemble

$$\frac{1}{M} \sum_{j=1}^M (x_j - \bar{x})^2$$

and the squared error of the ensemble mean

$$(\bar{x} - y)^2$$

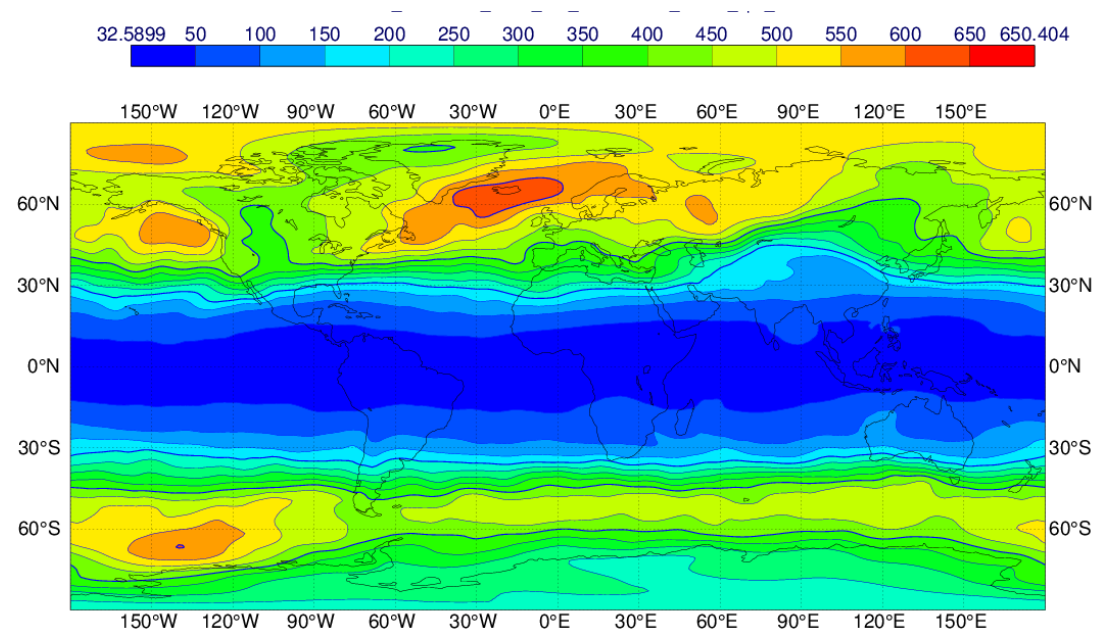
- Average the two quantities for many locations and/or start times.
- The averaged quantities have to match for a reliable ensemble (within sampling uncertainty).

From Martin Leutbecher’s lecture “Ensemble Verification 1”

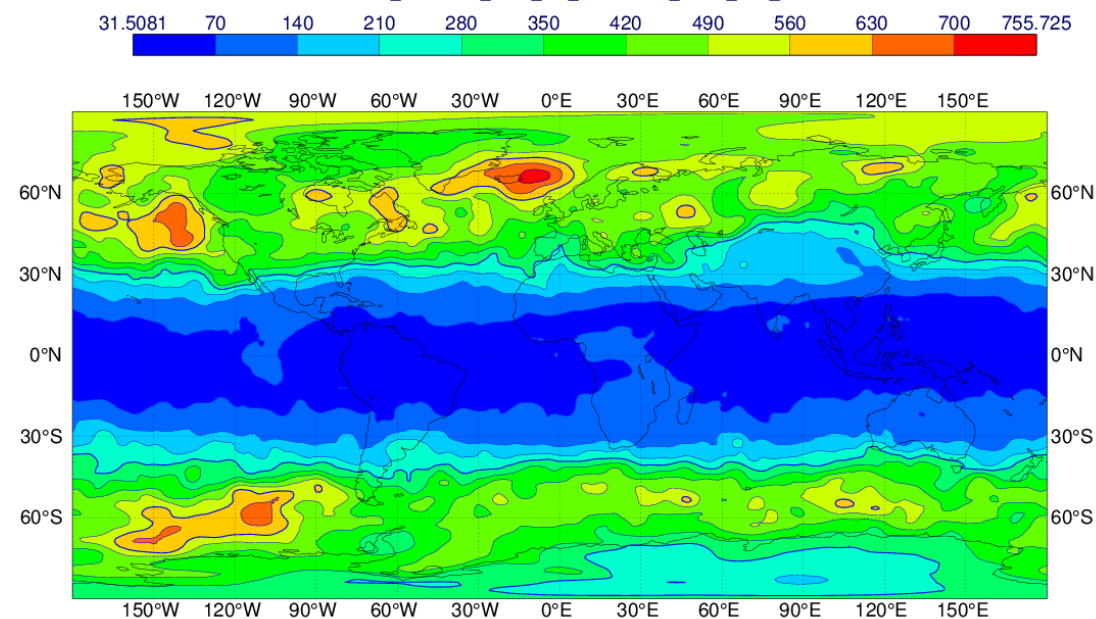
Z500hPa

Ensemble StDev and Ensemble Mean RMSE,  
averaged 2016112200 – 2017021300  
00 UTC Run

StDev T+120h

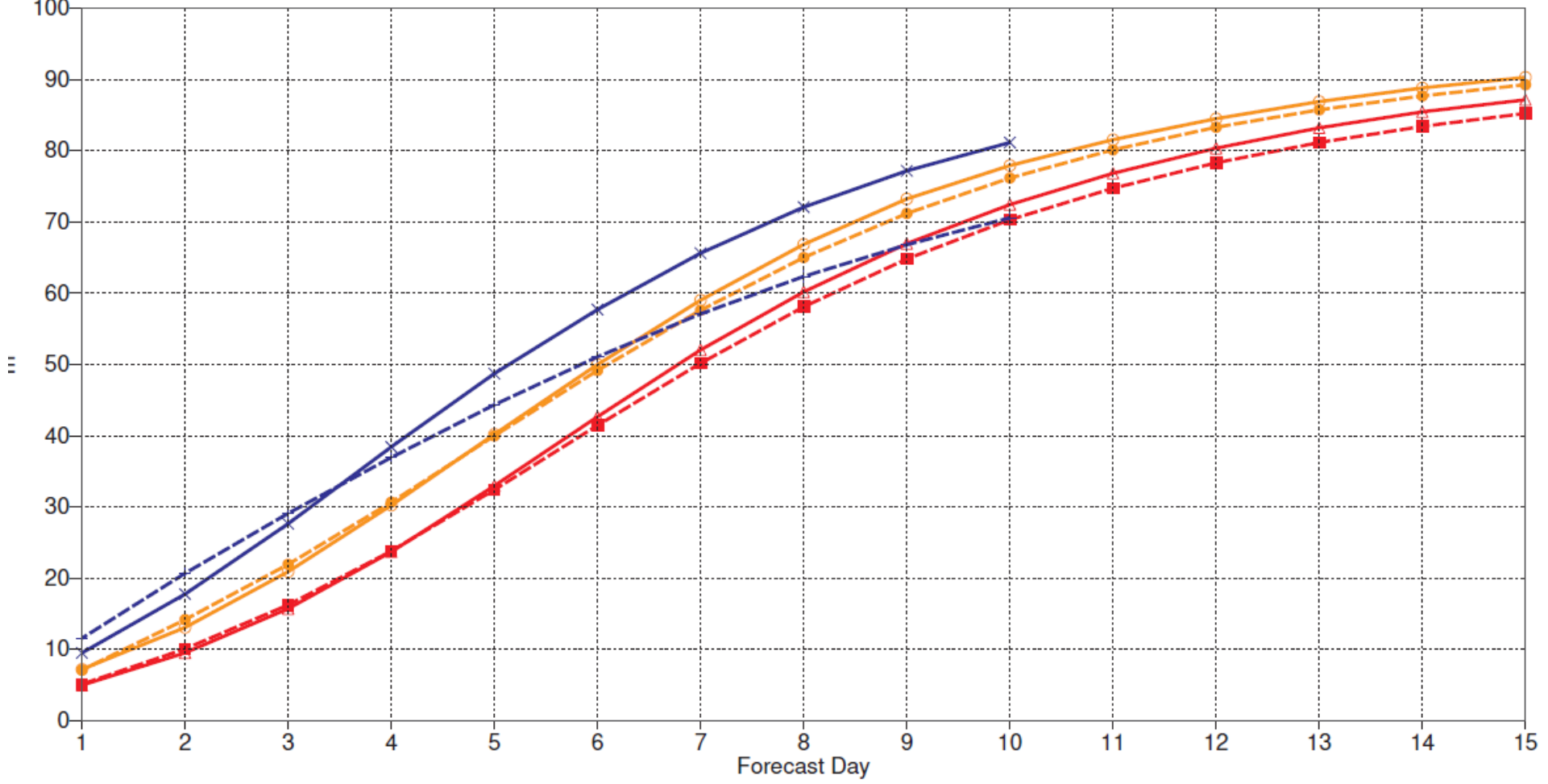


RMSE T+120h



500hPa geopotential  
 NHem Extratropics (lat 20.0 to 90.0, lon -180.0 to 180.0)  
 Date: 20010101 00UTC to 20181231 00UTC  
 oper\_an od enfo 0001  
 Mean method: standard

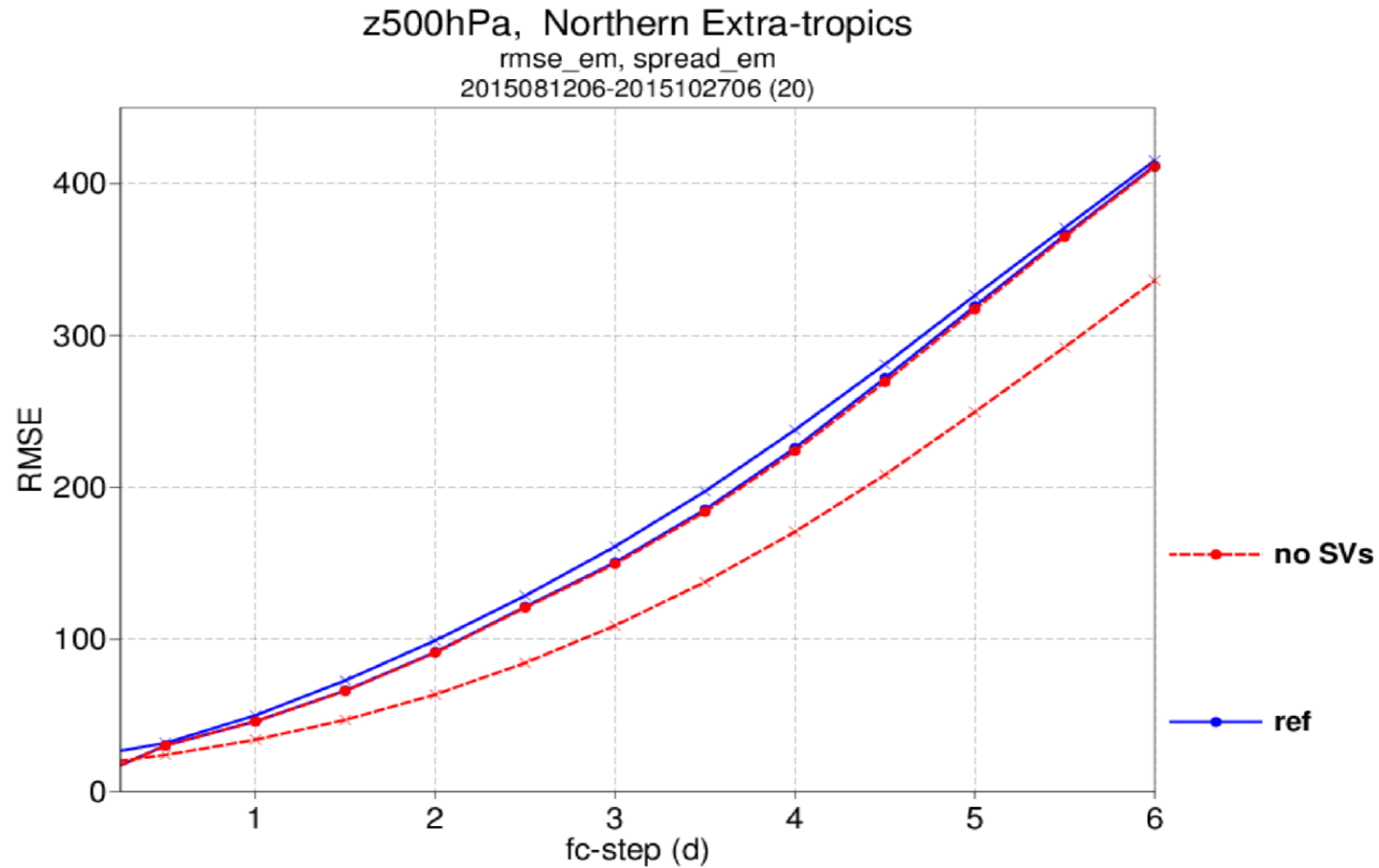
**Solid : Error**  
**Dashed : Spread**  
**2001 2008 2018**





# Why SVs?

## Impact of SVs on ENS

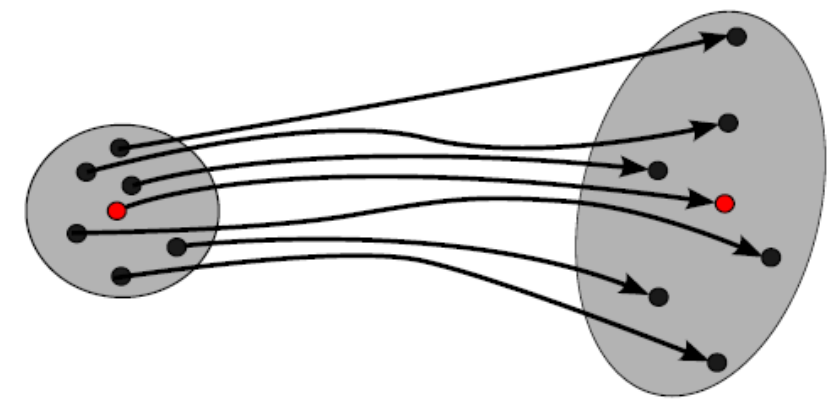


Oper like setup, TCo399, 20 Initial dates

# Singular Vector Perturbations

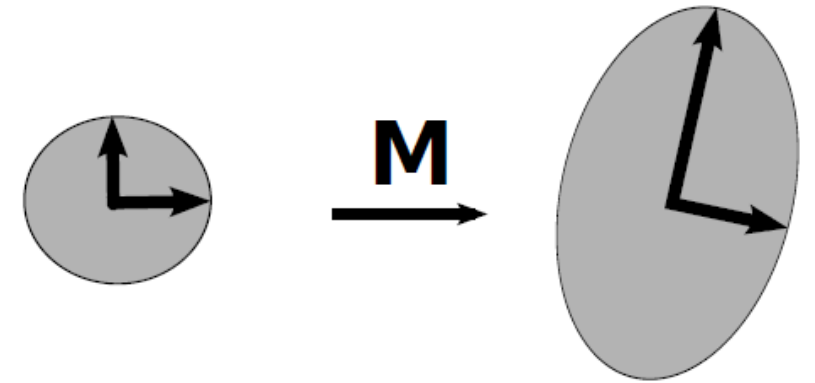
Directions of fastest growth over a finite time interval (optimisation interval)

Justification: EDA + Model Uncertainty representation produce substantial spread in the directions of the leading SVs but ensemble still under dispersive (Leutbecher and Lang, 2014, QJRM)



analysis

forecast

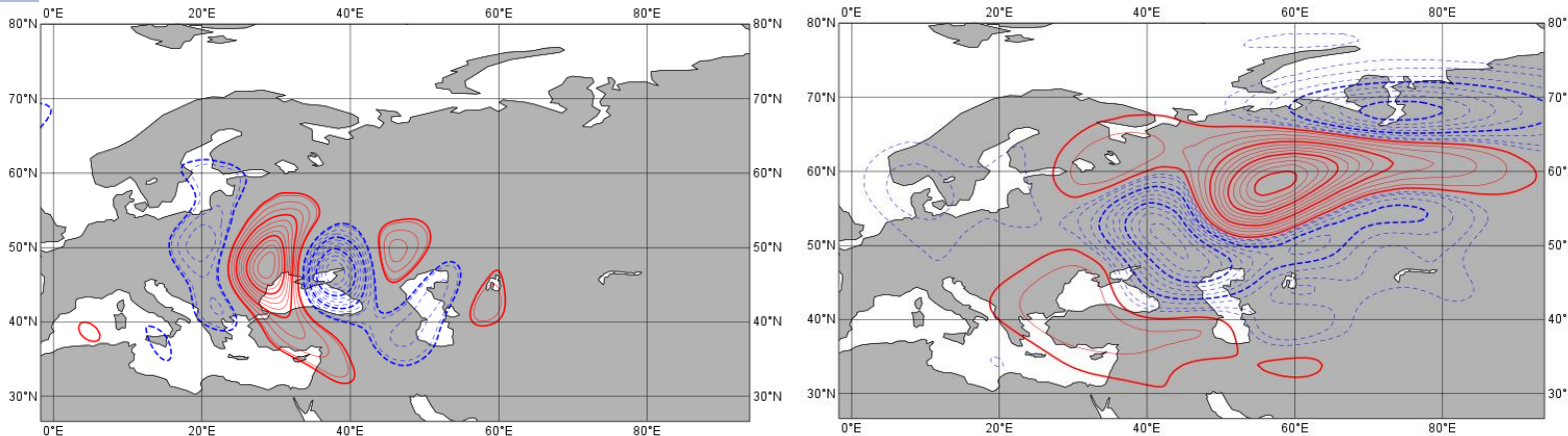


initial SVs

evolved SVs

Initial SV, T mlevel 68

evolved SV, T mlevel 49



Singular vectors are computed by solving an eigenvalue problem (e.g. Leutbecher and Palmer, 2008):

$$\mathbf{C}_0^{-1/2} \mathbf{M}^* \mathbf{P}^* \mathbf{C}_1 \mathbf{P} \mathbf{M} \mathbf{C}_0^{-1/2} \mathbf{v} = \sigma^2 \mathbf{v}$$

- $C_0$  and  $C_1$  initial and final time metrics
- $M(0, t)$  linear propagator from time 0 to t and its adjoint  $M^*$
- $P$  and  $P^*$  local projection operator and its adjoint

$$\frac{1}{2} \int_{p_0}^{p_1} \int_S \left( u^2 + v^2 + \frac{c_p}{T_r} T^2 \right) dp ds + \frac{1}{2} R_d T_r p_r \int_S (\ln p_{\text{sfc}})^2 ds$$

# Singular vectors in the operational EPS

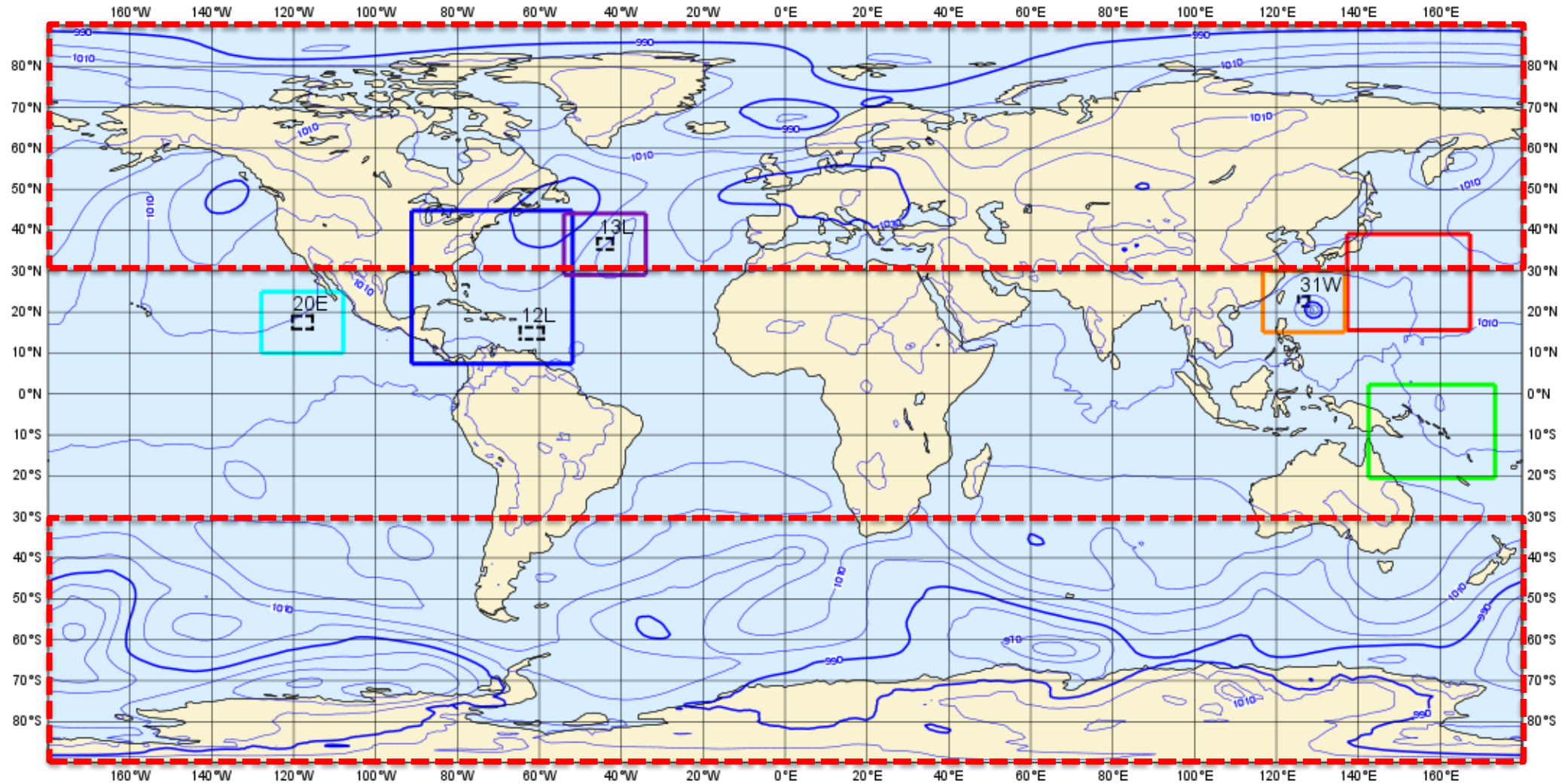
- $t_{\text{opt}} \equiv t_1 - t_0 = 48 \text{ h}$
- resolution: T42L137
- **Extra-tropics:** 50 SVs for N.-Hem. ( $30^\circ\text{N}$ – $90^\circ\text{N}$ ) + 50 SVs for S.-Hem. ( $30^\circ\text{S}$ – $90^\circ\text{S}$ ). Tangent-linear model with vertical diffusion and surface friction only.
- **Tropical cyclones:** 5 singular vectors per region targeted on active tropical depressions/cyclones. Up to 6 such regions. Tangent-linear model with representation of diabatic processes (large-scale condensation, convection, radiation, gravity-wave drag, vert. diff. and surface friction).
- **Localisation** is required to avoid that too many leading singular vectors are located in the dynamically more active winter hemisphere (Buizza 1994). Also required to obtain (more slowly growing) perturbations associated with tropical cyclones (Puri et al. 2001). In order to optimise perturbations for a specific region simply replace the propagator **M** in the equations by **PM**, where **P** denotes the projection operator which sets the state vector ( $T, u, v, \ln p_{\text{sfc}}$  in grid-point space) to zero outside the region of interest and is the identity inside it.

Now up to  
12 target  
regions!



# SV Target Areas

2018092600 | 12L 35 | 13L 43 | 20E 52 | 31W 52 |

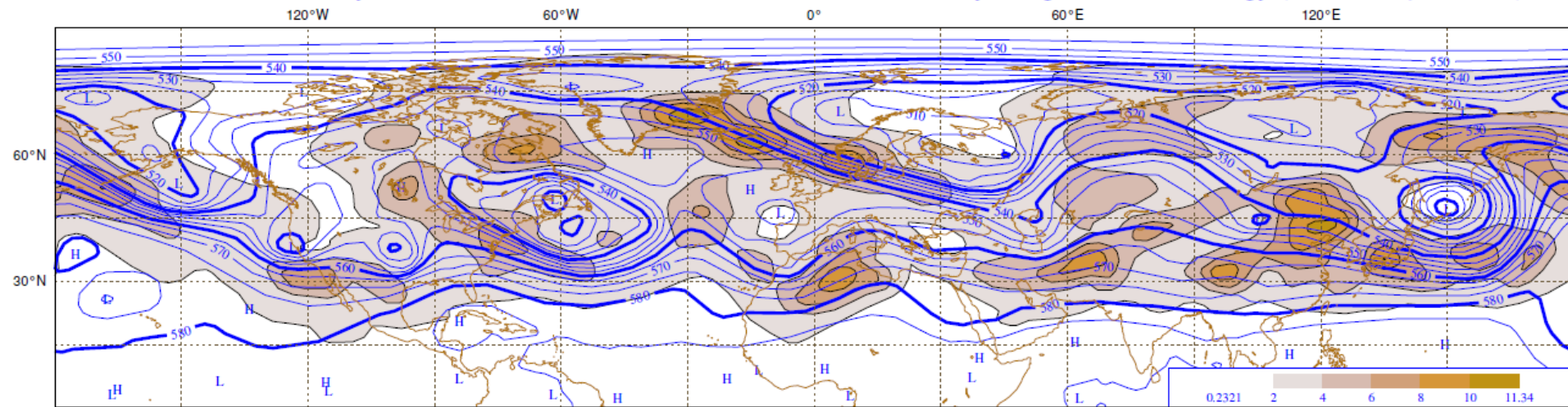


# Regional distribution of Northern Hem. SVs

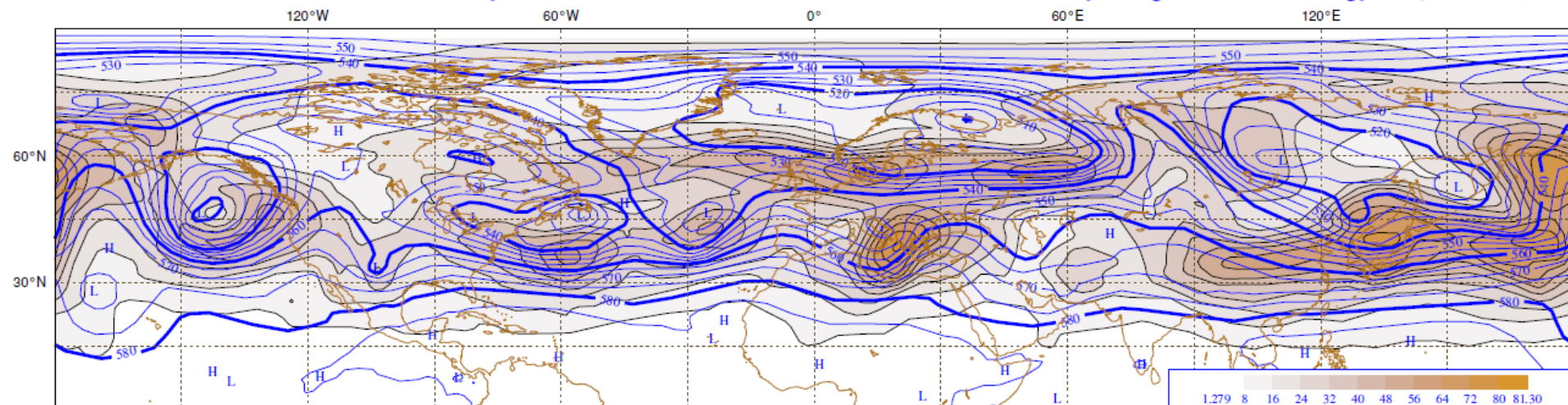
square root of vertically integrated total energy of SV 1–50 (shading)

500 hPa geopotential (contours)

initial singular vectors, 21 March 2006, 00 UTC

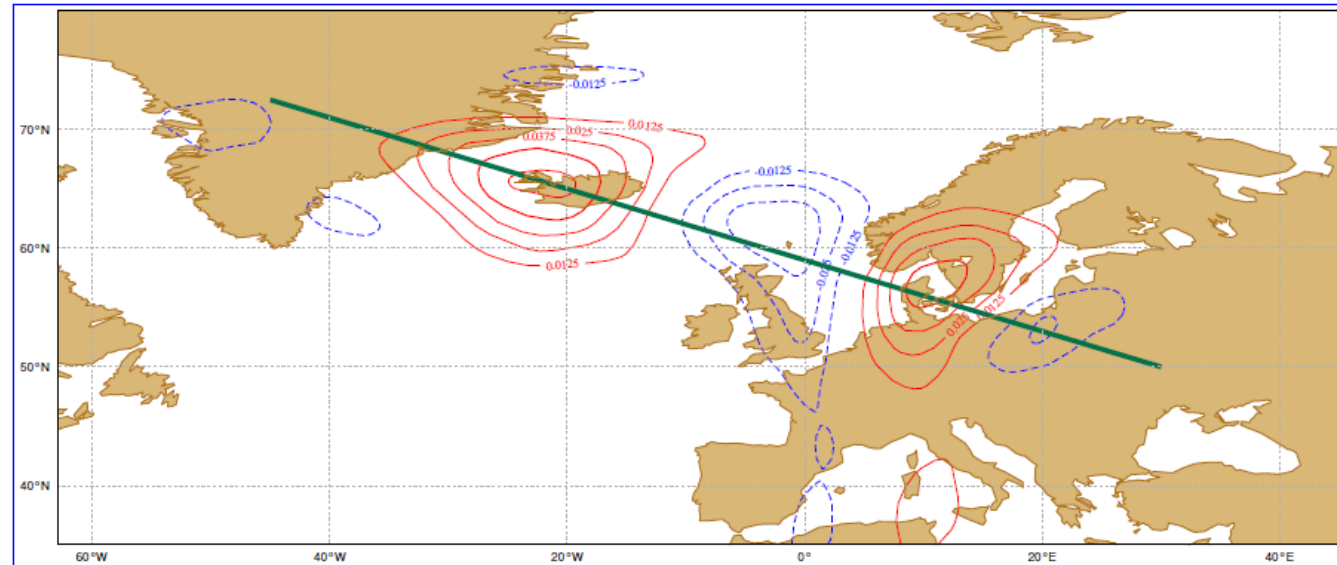


evolved singular vectors, 23 March 2006, 00 UTC

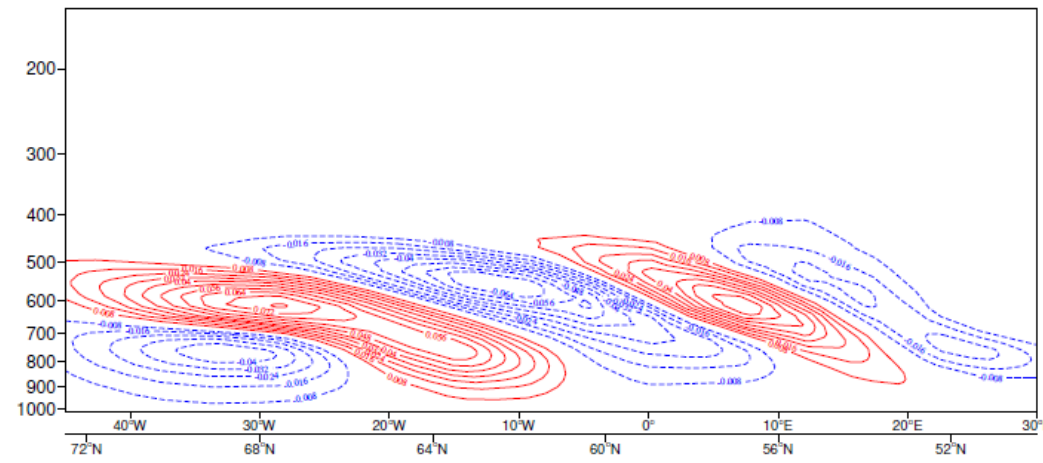


# Singular vector 5: initial time

21 March 2006, 00 UTC  
Temperature at  $\approx 700$  hPa



Cross section of temp 20060321 00 step 0 Expver 0001

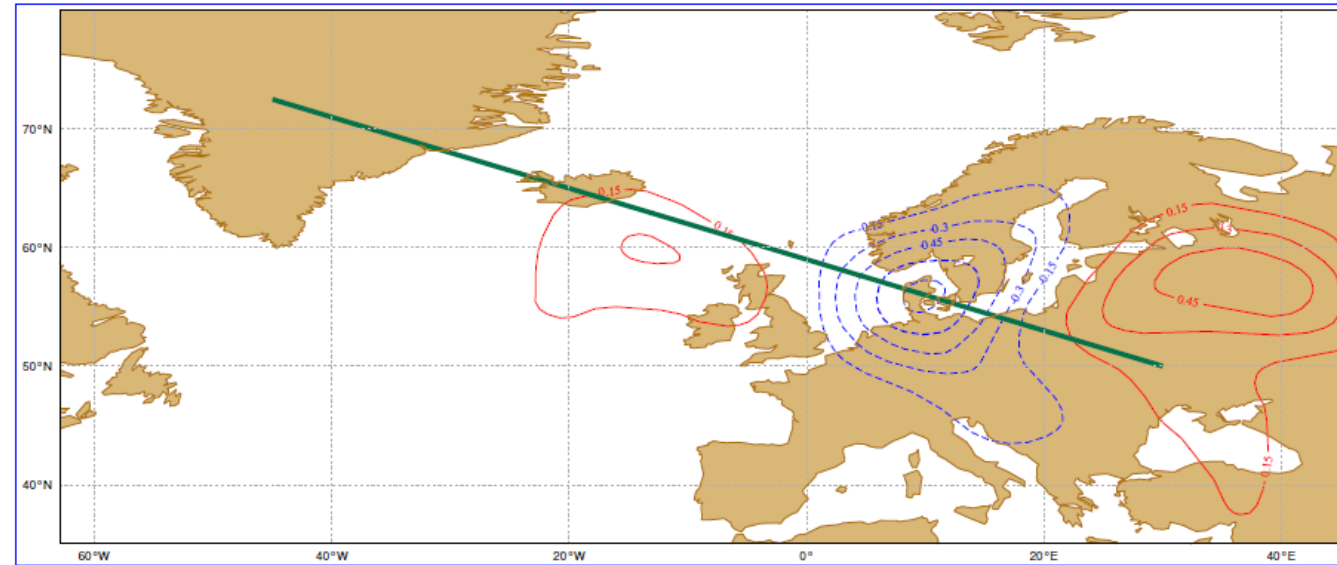




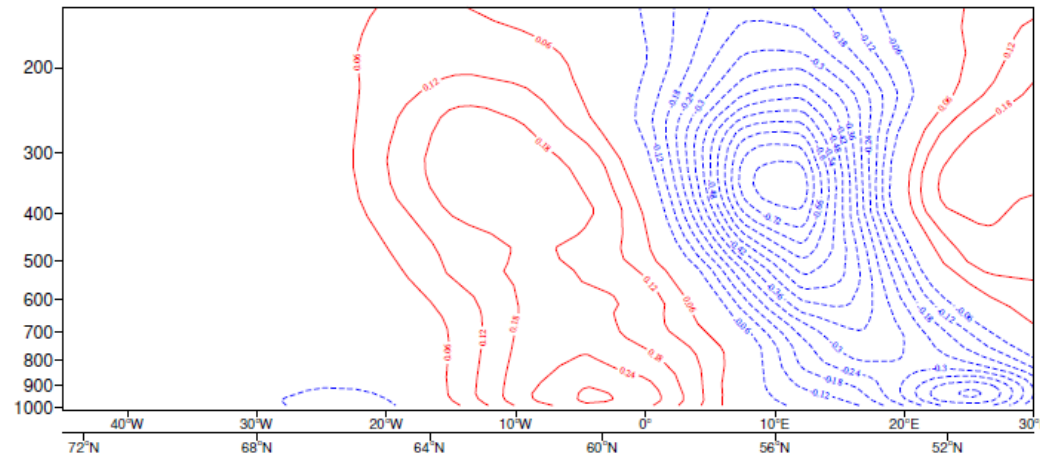
# Singular vector 5: final time

23 March 2006, 00 UTC

meridional wind component at  $\approx 300$  hPa



Cross section of v-vel 20060321 00 step 48 Expver 0001

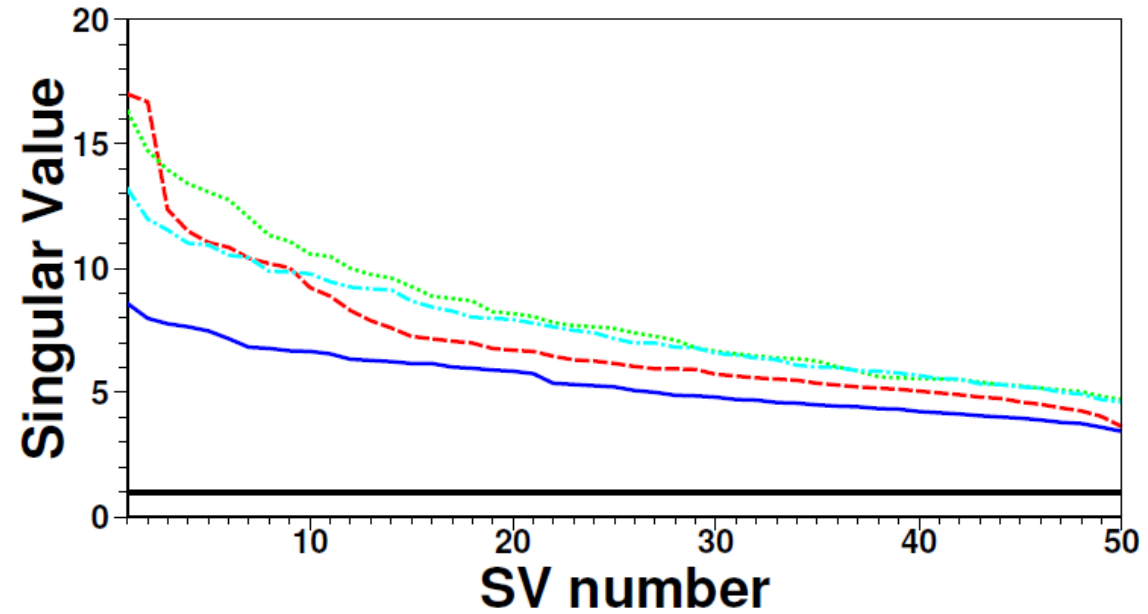




# Singular values $\sigma_j$ — extra-tropics

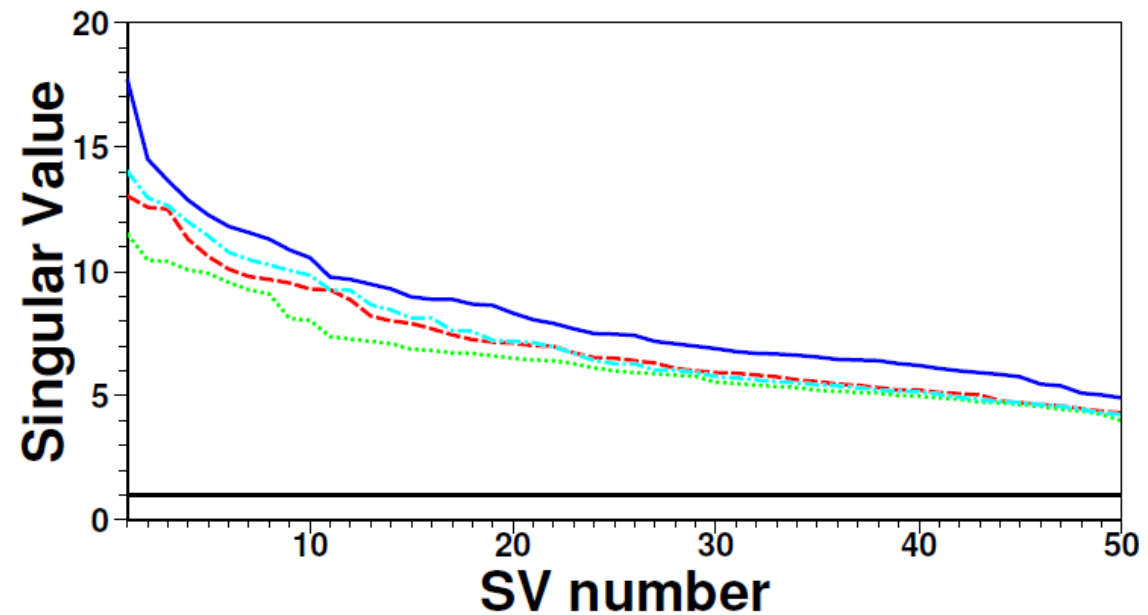
## Northern Hem.

solid: 2005070100  
dashed: 2005092100  
dotted: 2005122100  
chain-dashed: 2006032100



## Southern Hem.

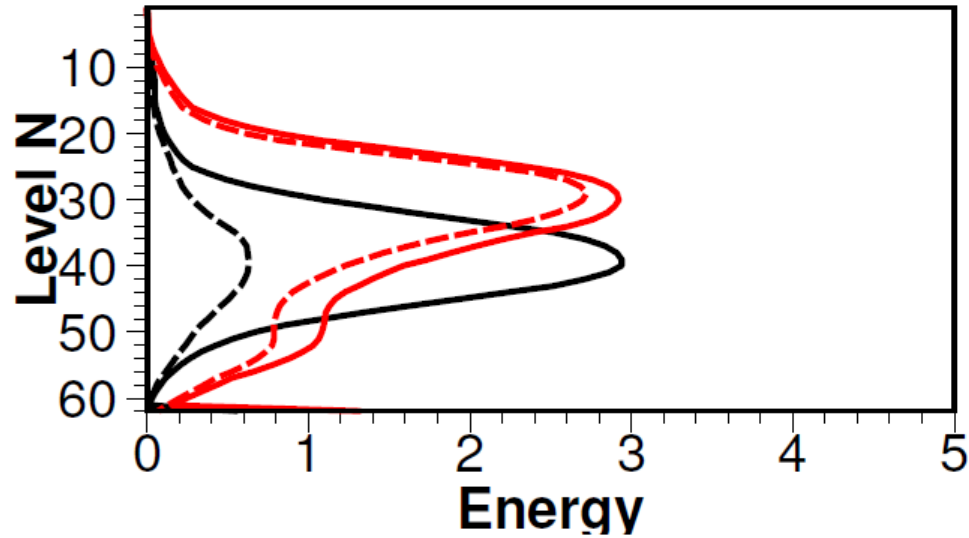
solid: 2005070100  
dashed: 2005092100  
dotted: 2005122100  
chain-dashed: 2006032100



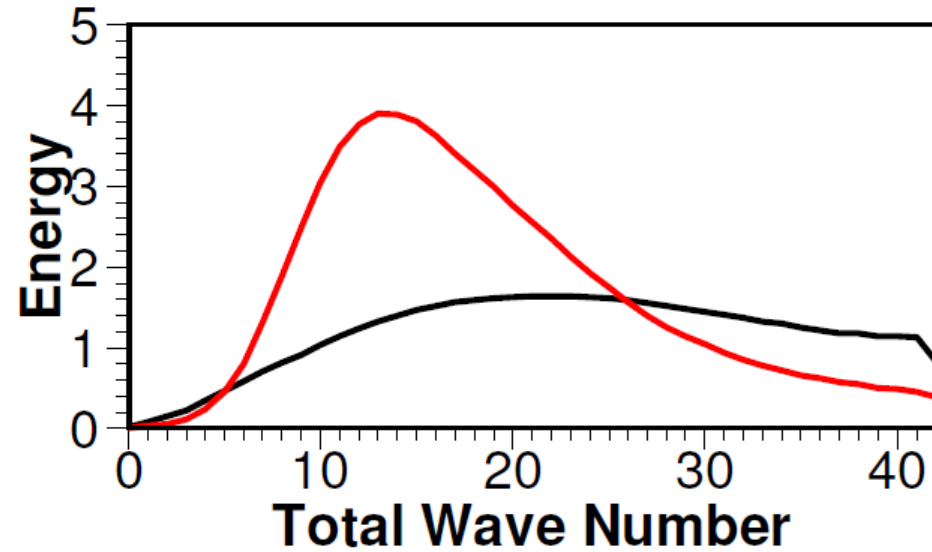
# Singular vector growth characteristics

average energy of the leading 50 singular vectors  
initial time ( $\times 50$ ), final time  $t=48$  h ( $\times 1$ )  
—: total energy; - - -: kinetic energy  
Northern hemisphere extra-tropics, 2006032100

vertical profile



spectrum



200 hPa $\leftrightarrow$ level 20	300 hPa $\leftrightarrow$ level 27
500 hPa $\leftrightarrow$ level 35	700 hPa $\leftrightarrow$ level 42
850 hPa $\leftrightarrow$ level 48	925 hPa $\leftrightarrow$ level 52

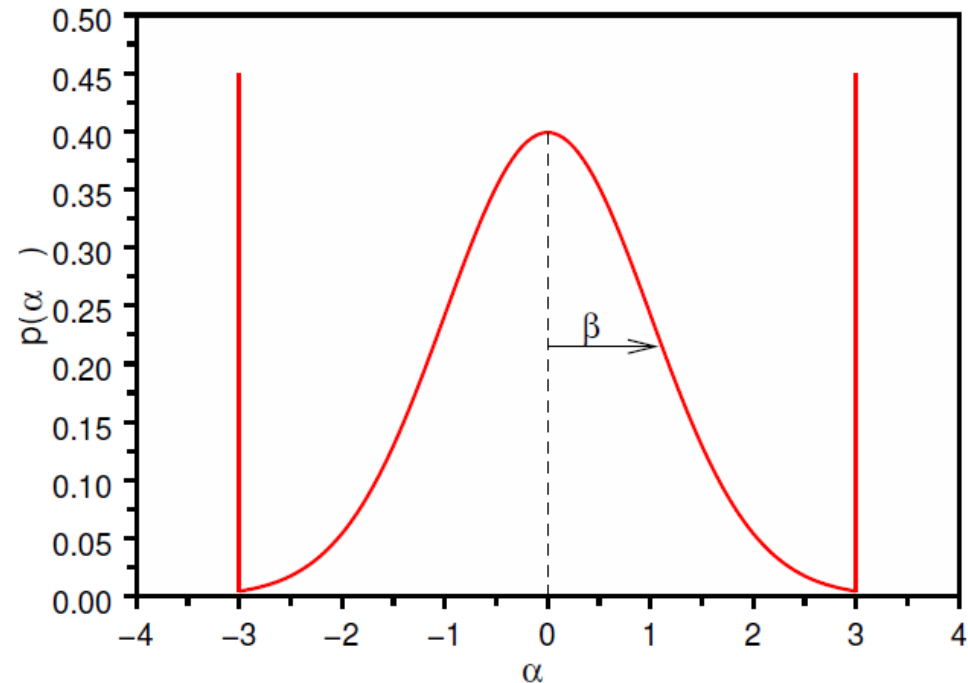
wave number	wave length
5	8000 km
10	4000 km
20	2000 km
40	1000 km

# Initial condition perturbations

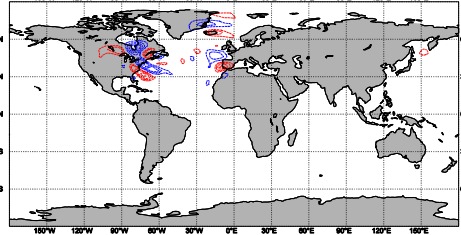
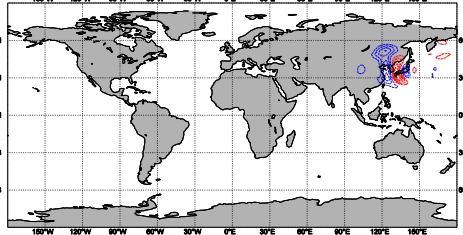
- Initial condition uncertainty is represented by a (multi-variate) Gaussian distribution in the space spanned by the leading singular vectors
- The perturbations based on a set of singular vectors  $\mathbf{v}_1, \dots, \mathbf{v}_m$  are of the form

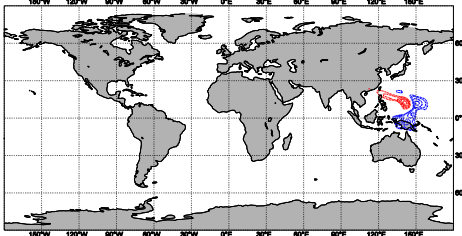
$$\mathbf{x}_j = \sum_{k=1}^m \alpha_{jk} \mathbf{v}_k \quad (5)$$

- The  $\alpha_{jk}$  are independent draws from a truncated **Gaussian distribution**.
- The Gaussian is truncated at  $\pm 3$  standard deviations to avoid numerical instabilities for extreme values.
- The width of the distribution is set so that the spread of the ensemble matches the root-mean square error in an average over many cases ( $\beta \approx 10$ ).



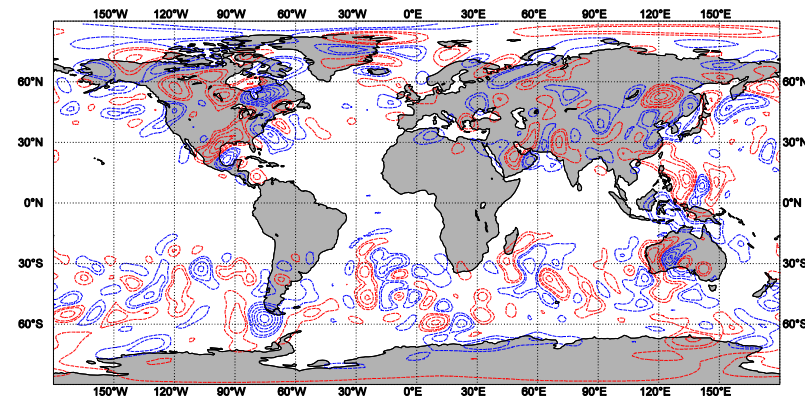
# Combine SVs to construct Perturbations:

$$\alpha_1 \times \text{SV}_1 + \alpha_2 \times \text{SV}_2 + \dots + \text{SV}_{50}$$


$$+ \alpha_{TC1} \times \text{SV}_{TC1} + \dots + \text{SV}_{TCn}$$


SVPERT 1

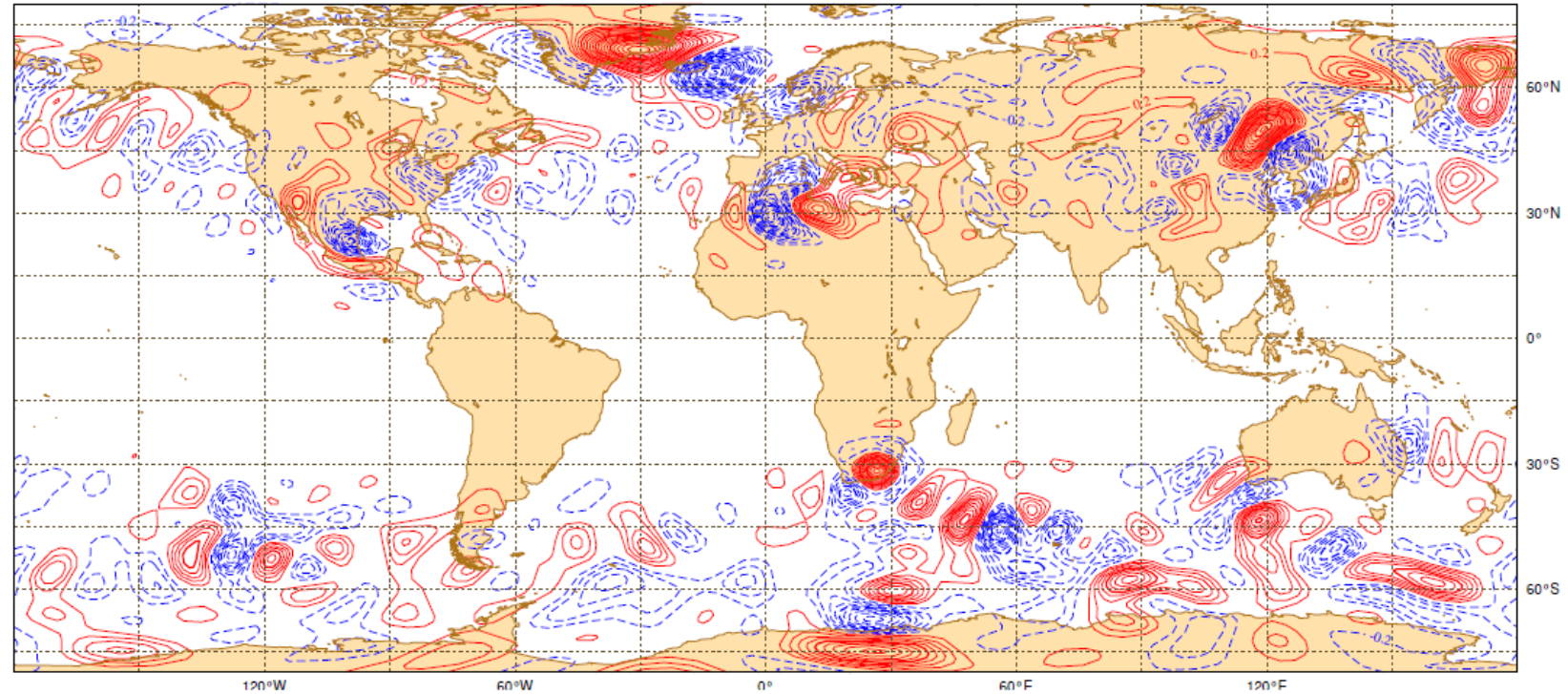
=



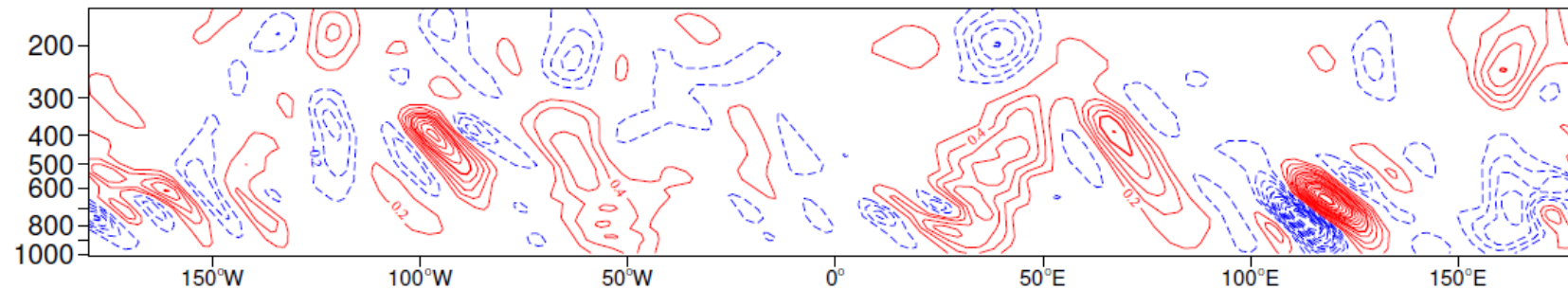


# Initial condition perturbation for member 1

Temperature (every 0.2 K); 21 March 2006, 00 UTC  
at  $\approx 700$  hPa

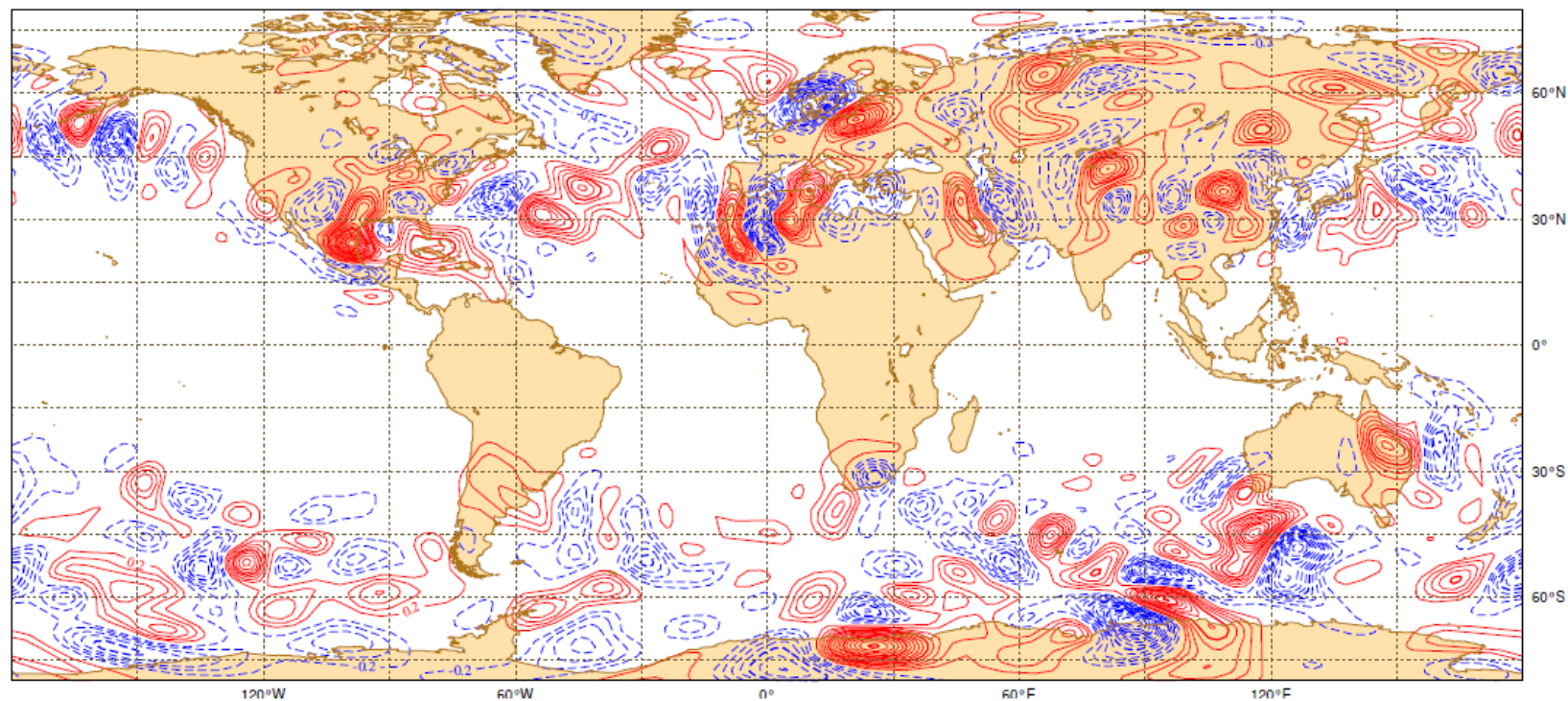


at 50°N

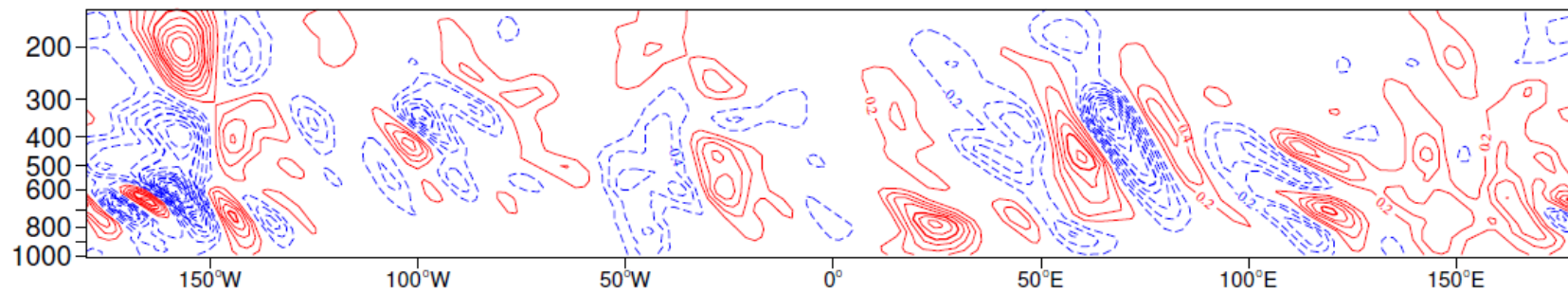


# Initial condition perturbation for member 5

Temperature (every 0.2 K); 21 March 2006, 00 UTC  
at  $\approx 700$  hPa



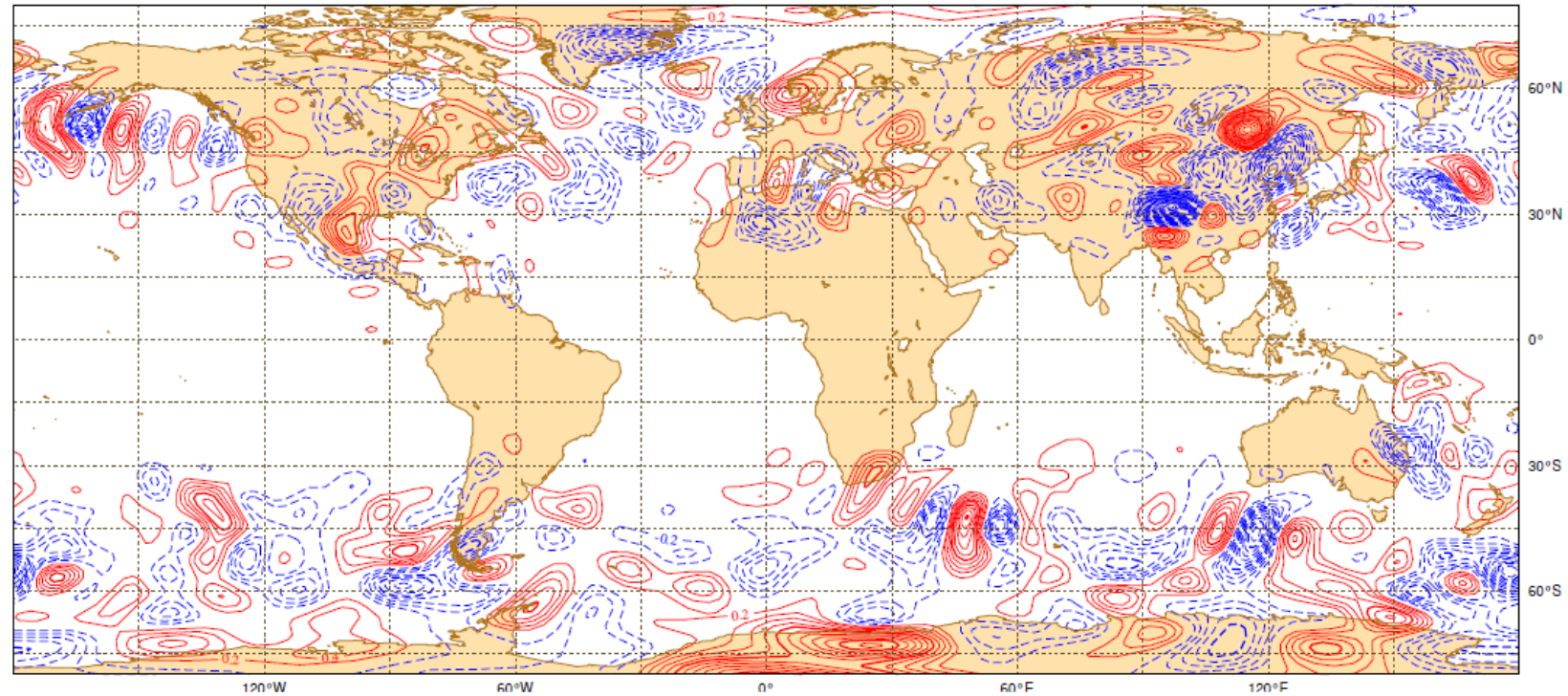
at 50°N



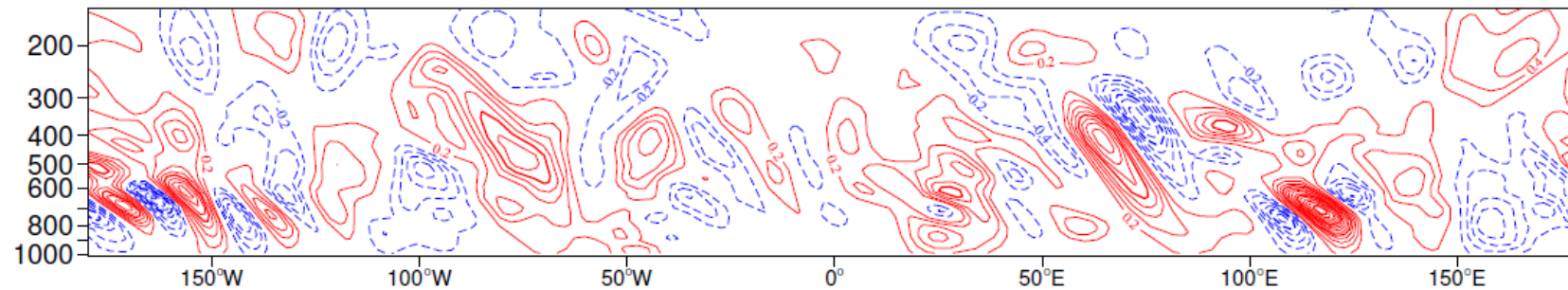


# Initial condition perturbation for member 50

Temperature (every 0.2 K); 21 March 2006, 00 UTC  
at  $\approx 700$  hPa

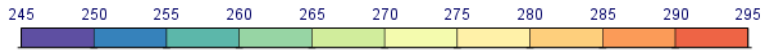


at 50°N

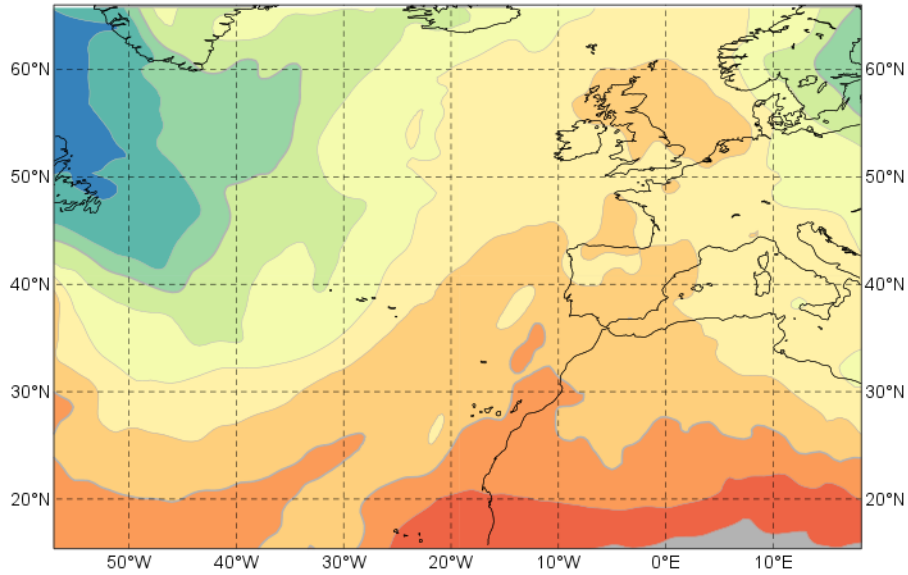


T850hPa

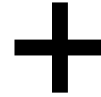
Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



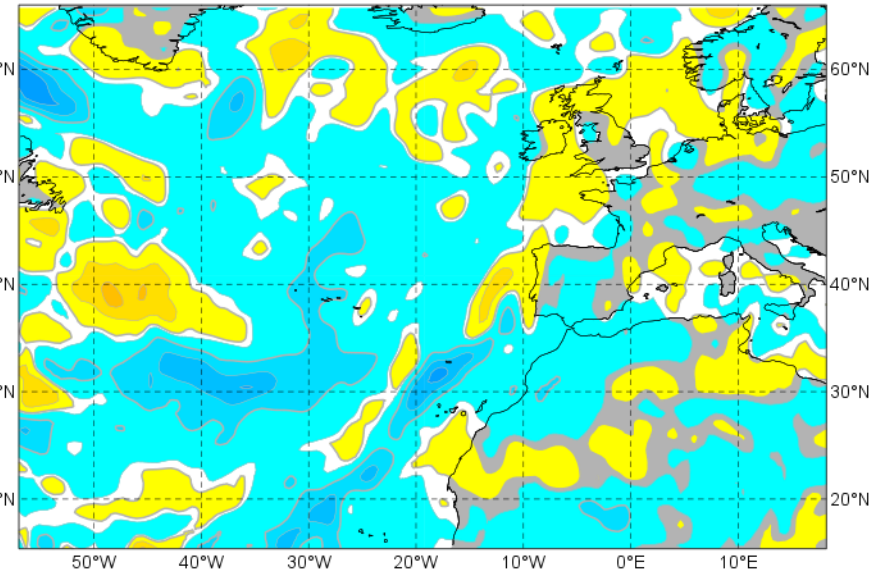
HRES  
Analysis  
00 UTC



EDA-  
Pert 3



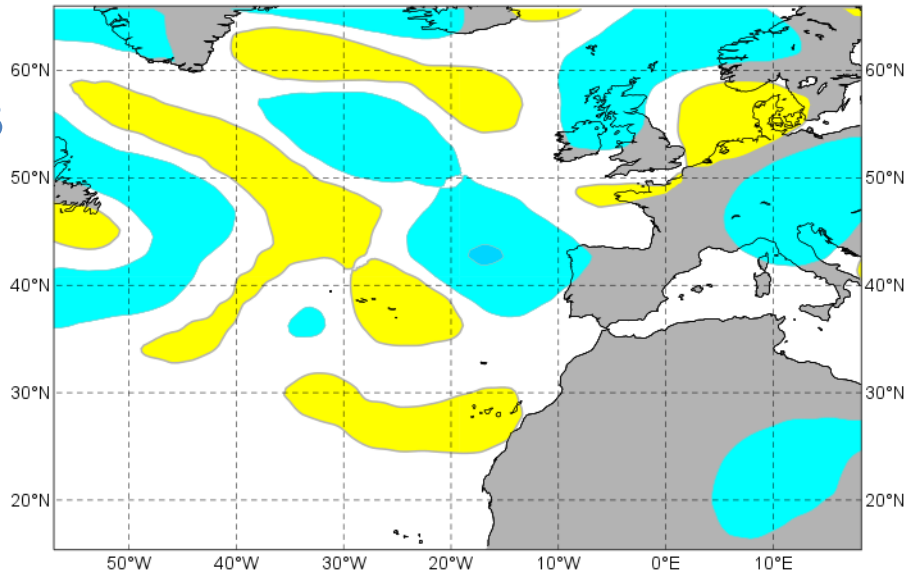
Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature



Friday 22 February 2019 00 UTC ecmf t+0 VT Friday 22 February 2019 00 UTC Model level 78 Temperature



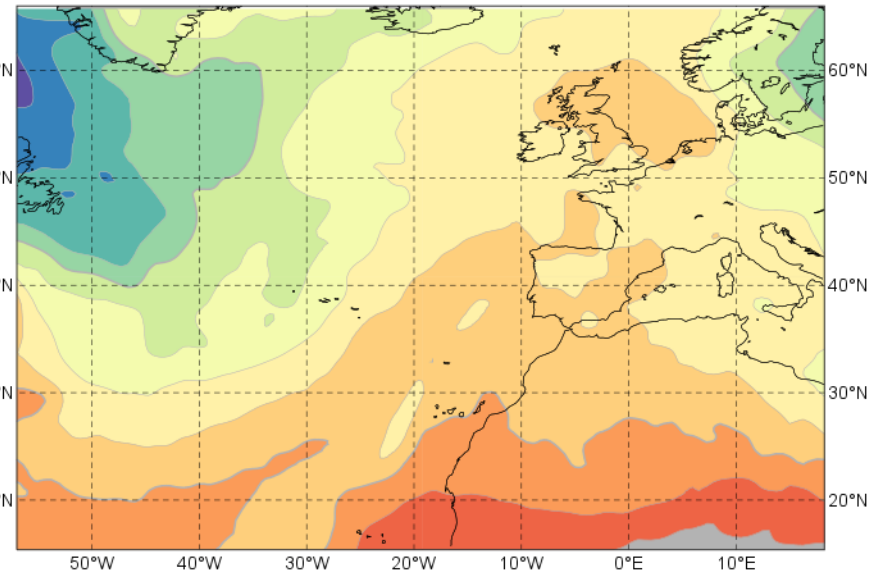
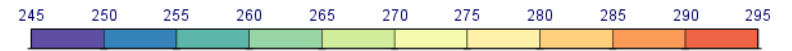
SV-  
Pert 3



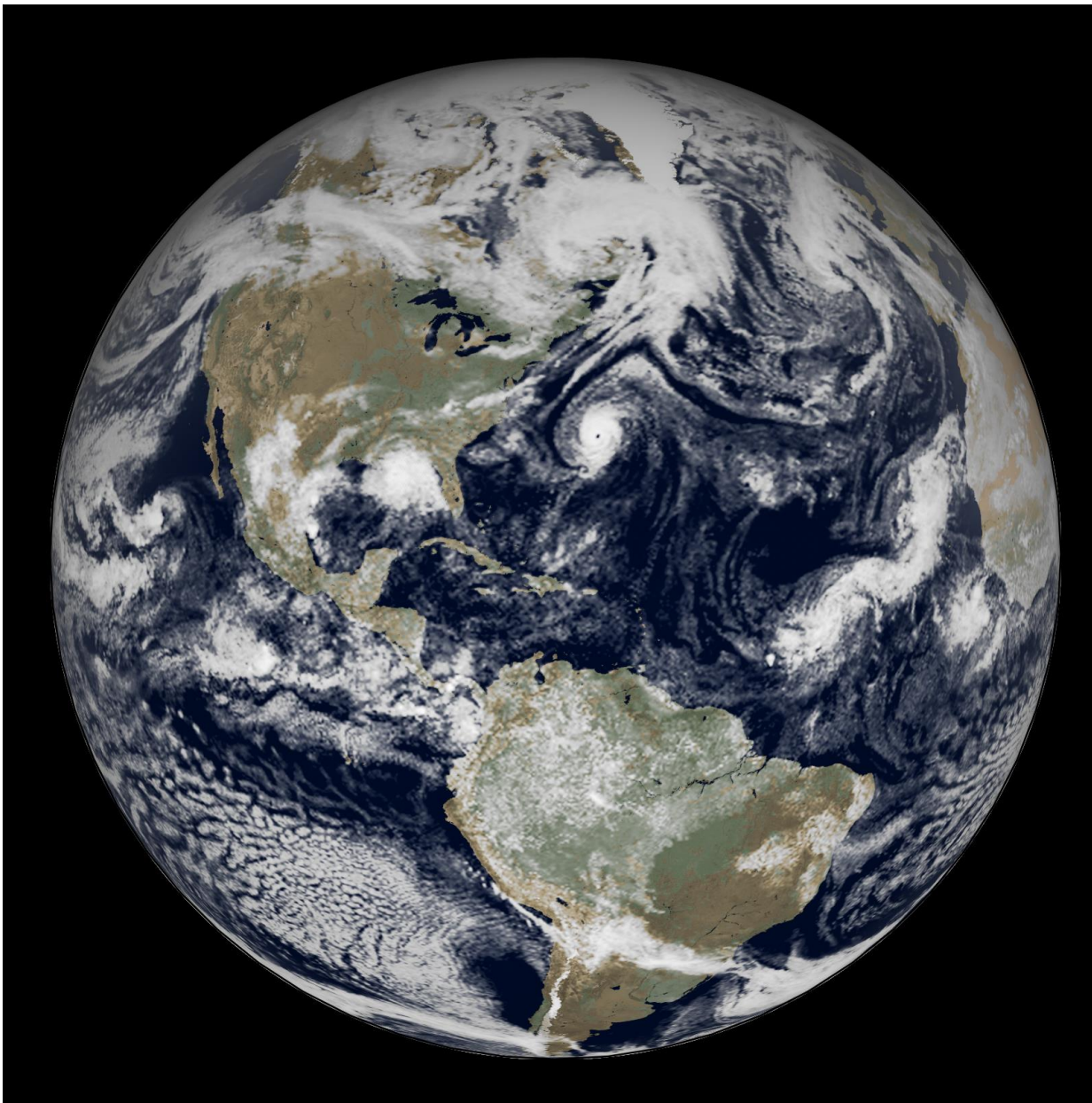
Initial  
conditions  
for ENS  
member 3



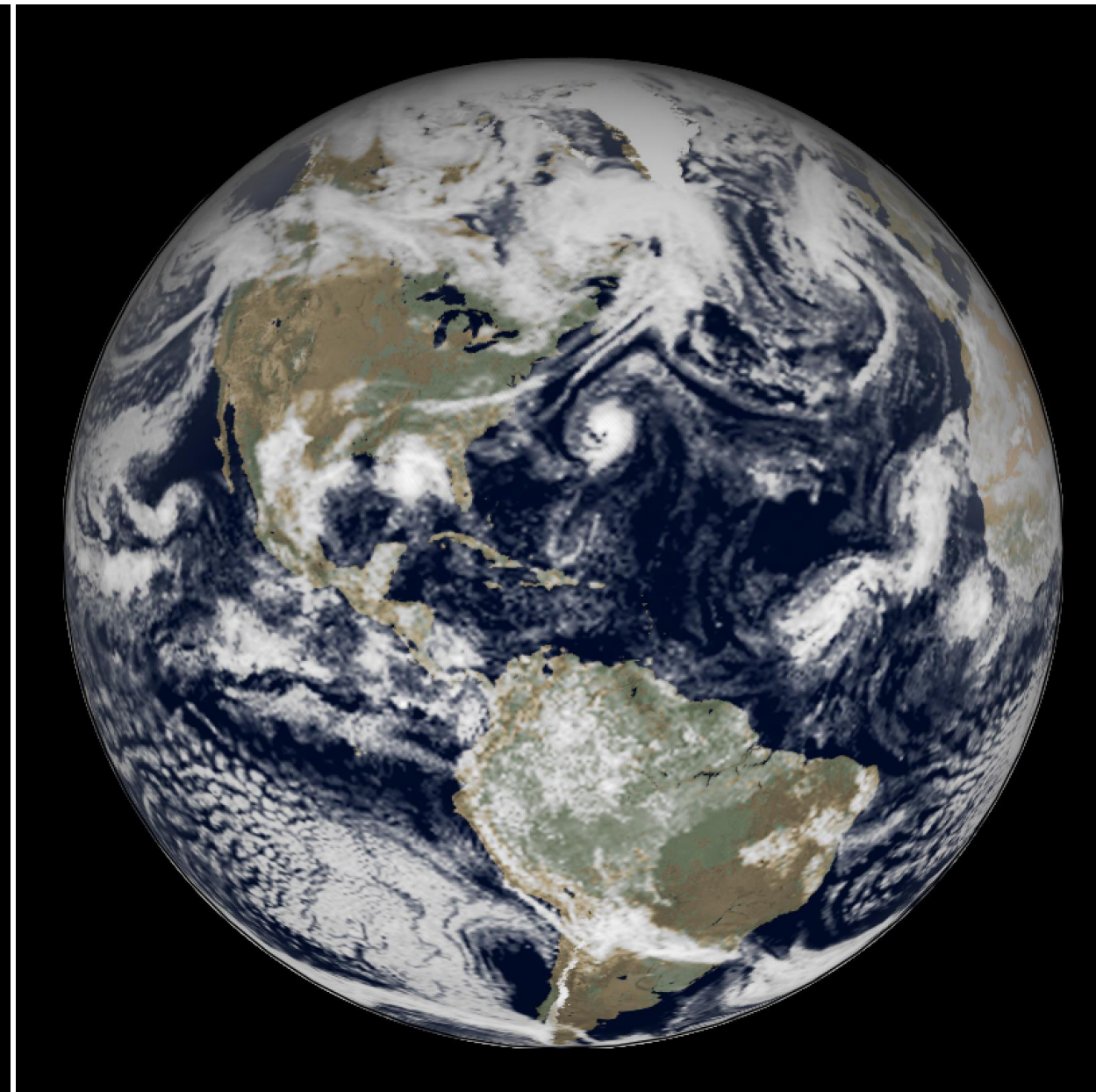
Friday 22 February 2019 00 UTC ecmf 850 hPa Temperature





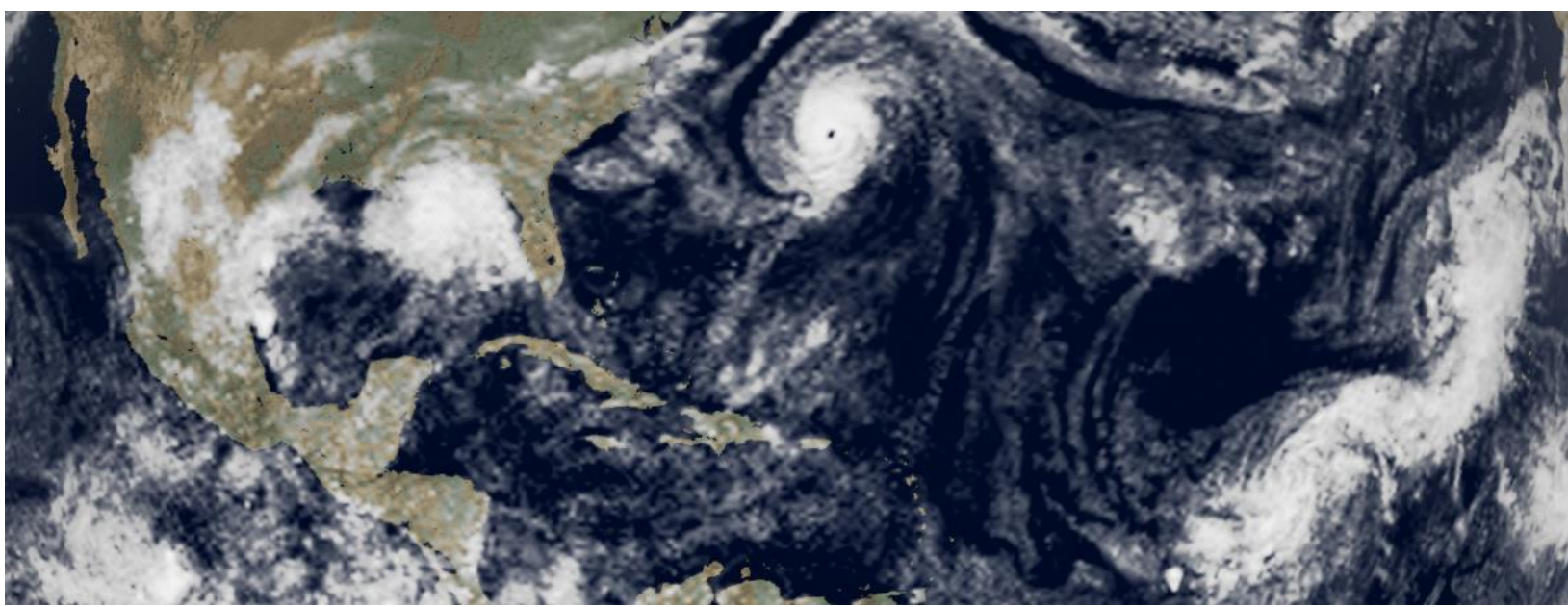


TCo1279L137



TCo639L91





TCo1279L137



TCo639L91

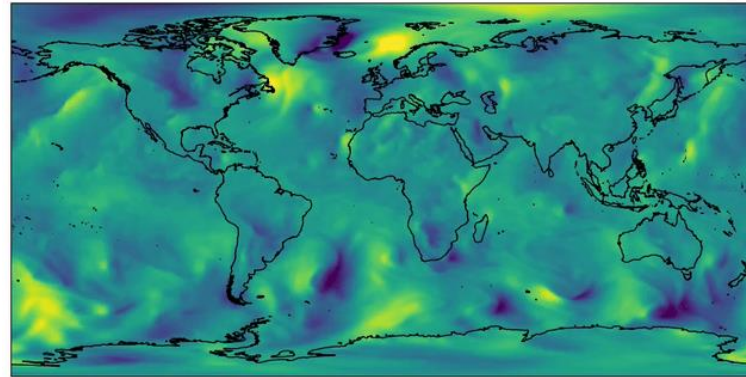
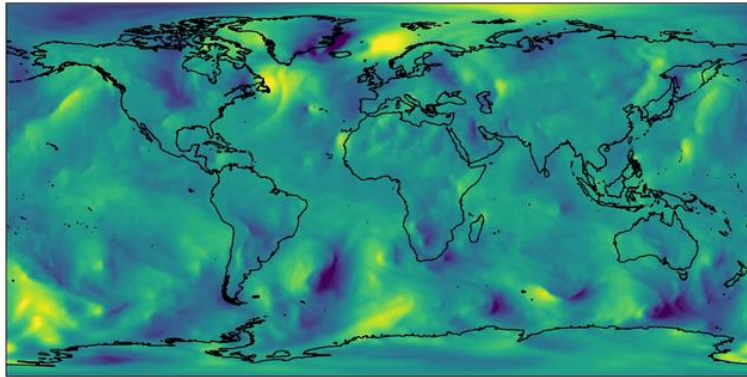
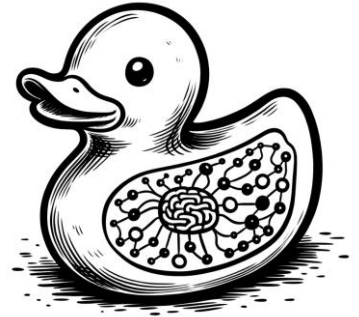
# AIFS - Artificial Intelligence Forecasting System

First implementation (~ 1deg resolution) in 2023, following Keisler 2022 and Lam et. al 2022:

- GNN architecture: Interaction Networks (Battaglia et. al 2016)
- Graph representation, hidden multi-scale mesh, edge features
- Scales to > 1000s of GPUs ; tensor parallel implementation, split model across multiple GPUs

Update beginning of 2024, update to ~ 0.25 deg:

- Attention / Transformer based GNN for encoder, decoder (Shi et al., 2021)
- Transformer backbone in processor (with sliding window, e.g. Child et al. 2019, Jiang et al. 2023)
- Trained on 64 GPUs ~ 1 Week



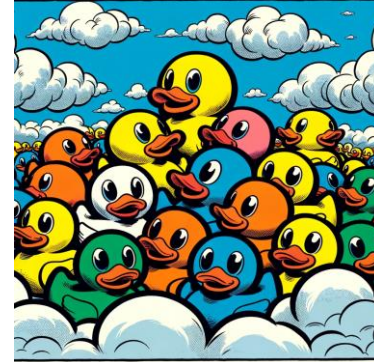
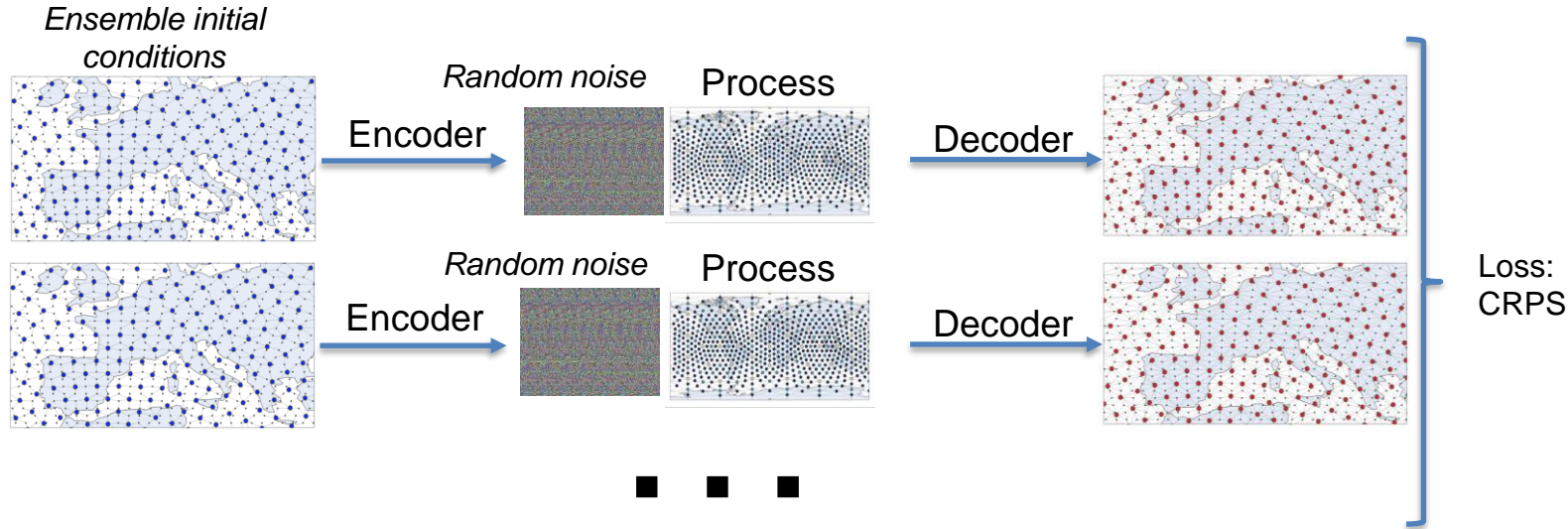
Why GNN: Encoder / Decoder: can handle arbitrary input / output grids, local and ad hoc grid refinement, changing grids etc. ; attractive for use in earth system science

See Lang, S., Alexe, M., Chantry, M., Dramsch, J., Pinault, F., Raoult, B., Clare, M. C. A., Lessig, C., Maier-Gerber, M., Magnusson, L., Bouallègue, Z. B., Nemesio, A. P., Dueben, P. D., Brown, A., Pappenberger, F., Rabier, F. (2024). AIFS - ECMWF's data-driven forecasting system. arXiv. <https://doi.org/10.48550/ARXIV.2406.01465>



# Ensemble forecasts ...

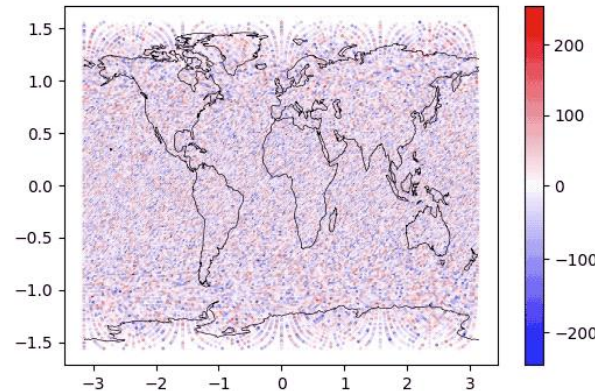
a) Instead of a MSE loss, learn an ensemble via optimizing probabilistic scores



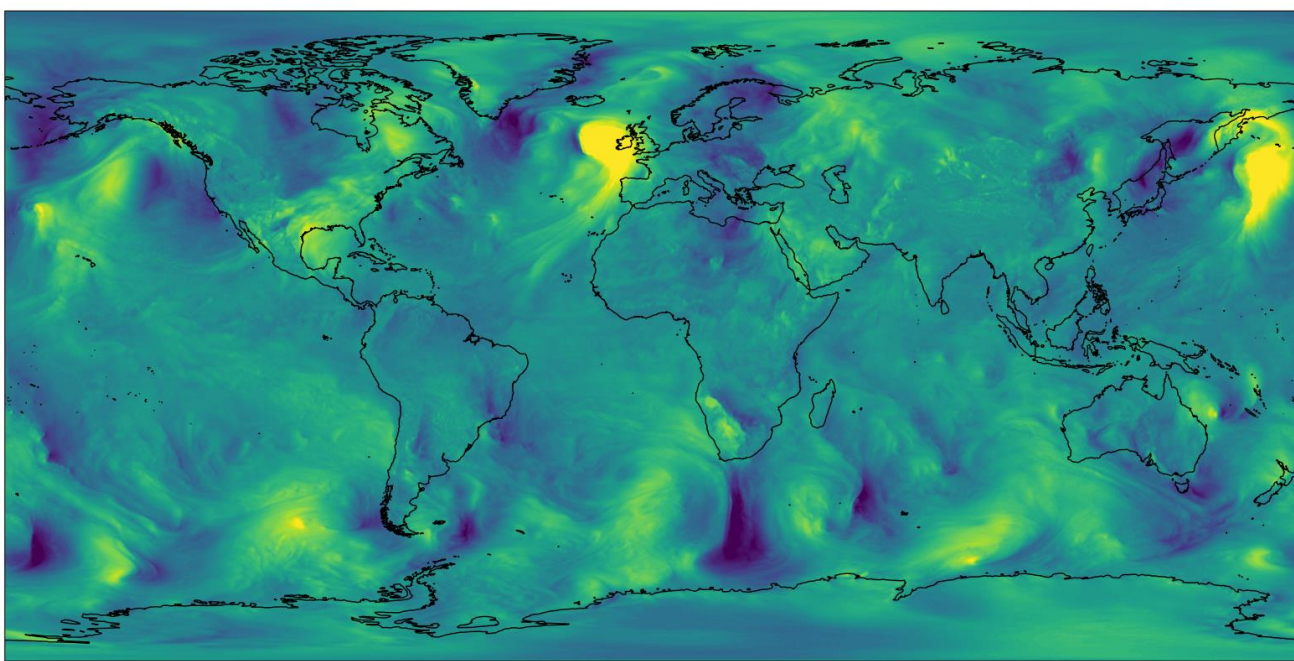
b) Create a forecast as de-noising task (diffusion training)

for example:

- Stable diffusion -> Images
- Sora -> Video
- Gencast, AIFS-Diffusion -> Weather

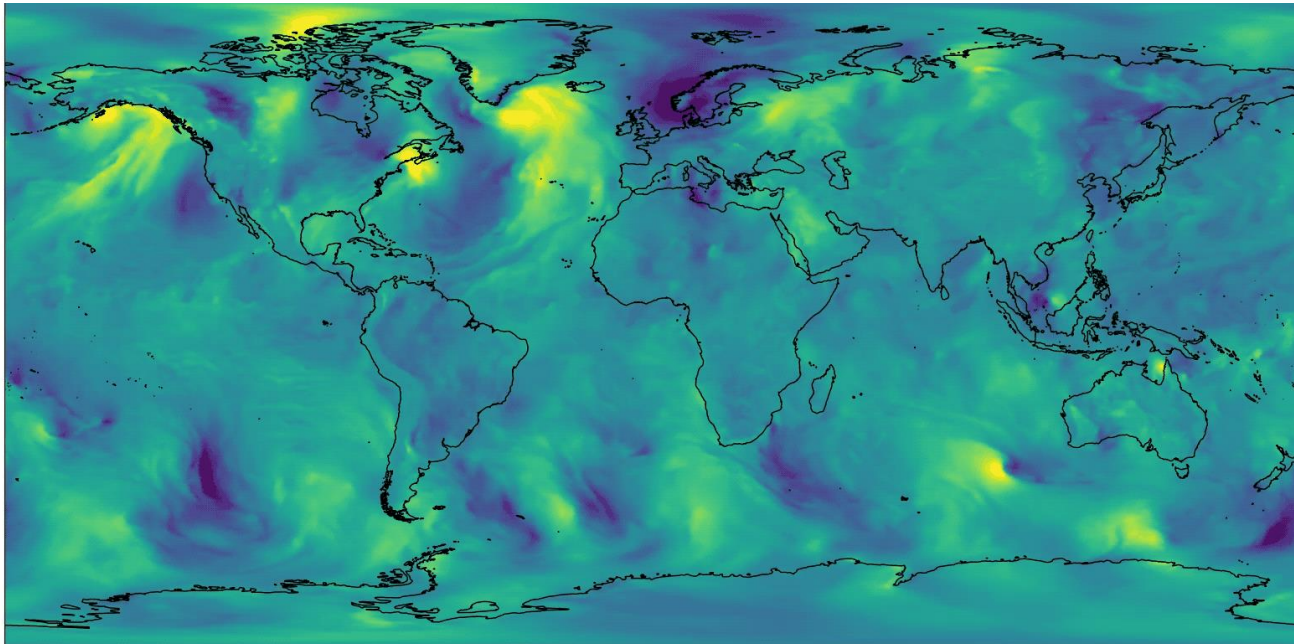


AIFS, ~ 0.25deg



Smoothing with lead time

AIFS Diffusion ~ 0.25deg



Stable statistics of forecast fields



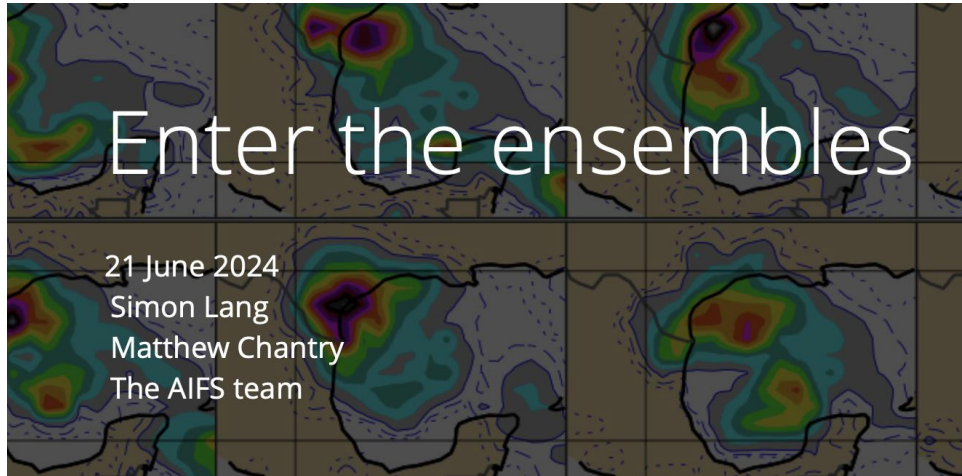
# Towards operational data-driven ensemble forecasting:

First test system running now 2x daily,

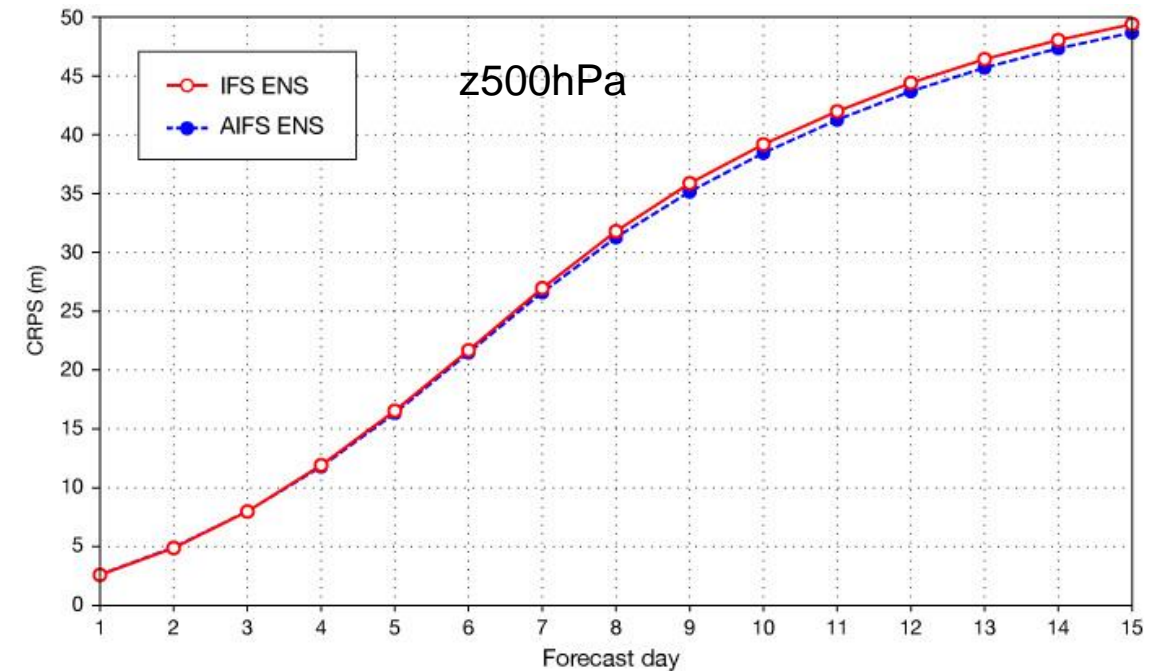
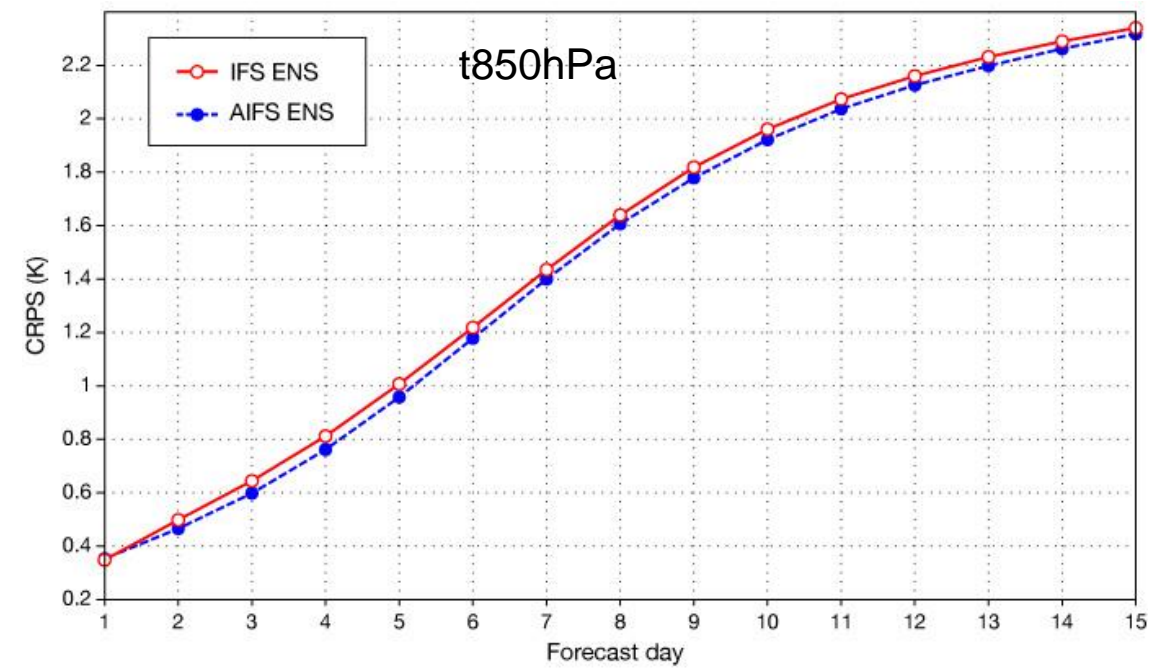
based on AIFS diffusion flavor,

Initial perturbations from operational IFS ensemble

~ 1 deg resolution, fine-tuned on oper analyses

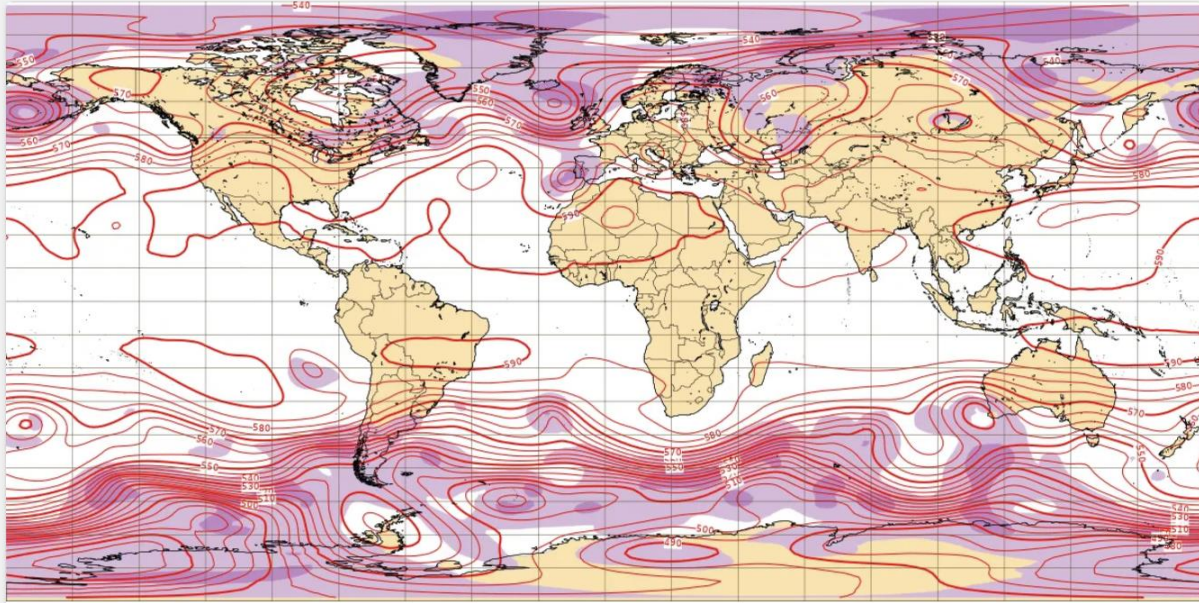


<https://www.ecmwf.int/en/about/media-centre/aifs-blog/2024/enter-ensembles>

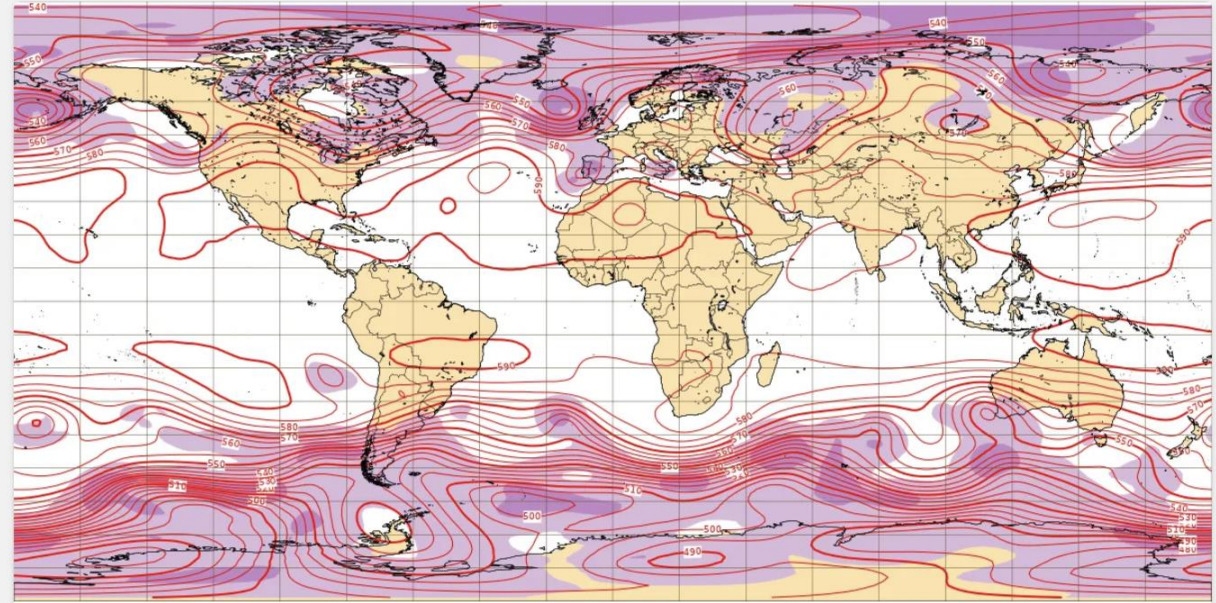




AIFS ENS Products: <https://charts.ecmwf.int>, Meteograms available



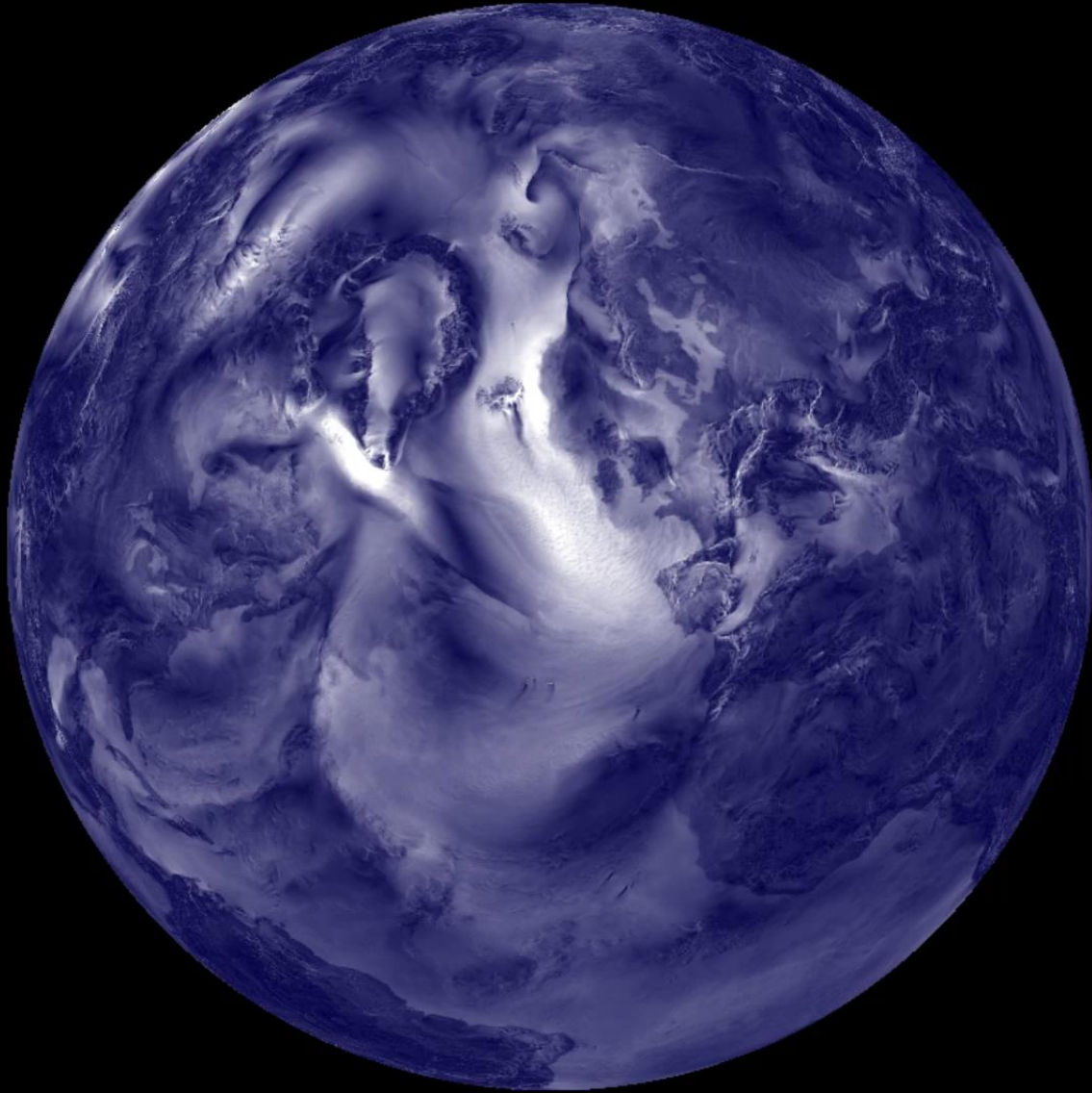
Ensemble mean and spread: 500 hPa geopotential height



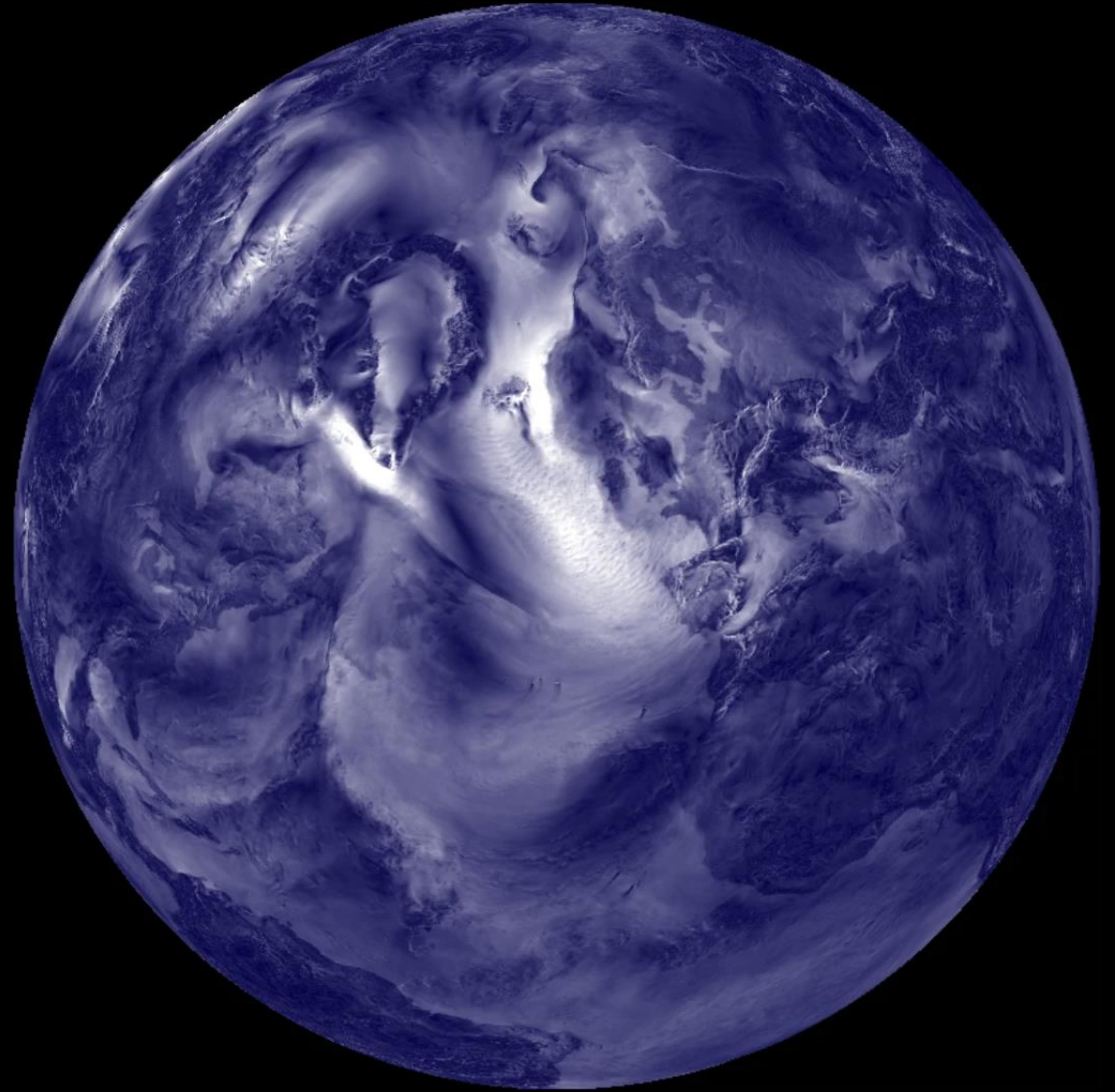
Experimental: AIFS ENS (ECMWF) ML model: Ensemble mean and spread: 500 hPa geopotential height



IFS 10m wind gusts, 2020-12-04 00 UTC 720h forecasts, 9 km spatial resolution



Control Member



Perturbed member 1

## Some References:

Buizza, R. , Leutbecher, M. and Isaksen, L. (2008), Potential use of an ensemble of analyses in the ECMWF Ensemble Prediction System. Q.J.R. Meteorol. Soc., 134: 2051-2066.

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Leutbecher, Martin and Tim N. Palmer. "Ensemble forecasting." J. Comput. Physics 227 (2008): 3515-3539.

Leutbecher, M. and Lang, S. T. (2014), On the reliability of ensemble variance in subspaces defined by singular vectors. Q.J.R. Meteorol. Soc., 140: 1453-1466.

Leutbecher, M. , Lock, S. , Ollinaho, P. , Lang, S. T., Balsamo, G. , Bechtold, P. , Bonavita, M. , Christensen, H. M., Diamantakis, M. , Dutra, E. , English, S. , Fisher, M. , Forbes, R. M., Goddard, J. , Haiden, T. , Hogan, R. J., Juricke, S. , Lawrence, H. , MacLeod, D. , Magnusson, L. , Malardel, S. , Massart, S. , Sandu, I. , Smolarkiewicz, P. K., Subramanian, A. , Vitart, F. , Wedi, N. and Weisheimer, A. (2017), Stochastic representations of model uncertainties at ECMWF: state of the art and future vision. Q.J.R. Meteorol. Soc, 143: 2315-2339.

Lang, S., Hólm, E., Bonavita, M., Trémolet, Y., A 50-member Ensemble of Data Assimilations, ECMWF Newsletter No. 158 - Winter 2018/19

Lang, S.T.K., Dawson, A., Diamantakis, M., Dueben, P., Hatfield, S., Leutbecher, M., Palmer, T., Prates, F., Roberts, C.D., Sandu, I. and N. Wedi (2021). More accuracy with less precision. Q J R Meteorol Soc, 147( 741, 4358– 4370. <https://doi.org/10.1002/qj.4181>

Lopez, P. (2020). Forecasting the Past: Views of Earth from the Moon and Beyond, Bulletin of the American Meteorological Society, 101(7), E1190-E1200.

Lam, R, Sanchez-Gonzalez A, Willson M, Wirnsberger P, Fortunato M, Pritzel A, Ravuri S, Ewalds T, Alet F, Eaton-Rosen Z and Hu W. GraphCast: Learning skillful medium-range global weather forecasting. arXiv preprint arXiv:2212.12794. 2022 Dec 24.

Lang, S., M. Rodwell, D. Schepers, 2023: IFS upgrade brings many improvements and unifies medium-range resolutions. ECMWF Newsletter 176. <https://doi.org/10.21957/slk503fs2i>

# Nonlinear Model

Consider the spatially discretised equations describing the atmospheric dynamics and physics written in this form

$$\frac{d}{dt}\mathbf{x} = F(\mathbf{x}), \quad \text{with} \quad \mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad F = \begin{bmatrix} F_1 \\ \vdots \\ F_n \end{bmatrix}$$

where  $\mathbf{x} \in \mathbb{R}^N$  denotes the  $N$ -dimensional state vector and  $F(\mathbf{x}) \in \mathbb{R}^N$  its tendency. Integrate from  $t_0$  to  $t$  gives the nonlinear model:

$$\mathbf{x}(t) = \mathcal{F}(\mathbf{x}(t_0))$$



# Tangent-linear system

Let  $\mathbf{x}_r(t)$  be a solution of

$$\frac{d}{dt}\mathbf{x} = F(\mathbf{x}), \quad (1)$$

Then the *tangent-linear system* is given by

$$\frac{d}{dt}\mathbf{x} = \mathbf{A}(\mathbf{x}_r(t)) \mathbf{x}, \quad (2)$$

where  $[\mathbf{A}(\mathbf{x})]_{jk} = (\partial F_j / \partial x_k)(\mathbf{x})$  denotes the Jacobi matrix of  $F$ .

For any solution  $\mathbf{x}$  of (2),  $\mathbf{x}_r + \varepsilon\mathbf{x}$  approximates a solution of (1) starting at  $\mathbf{x}_r(t_0) + \varepsilon\mathbf{x}(t_0)$  to first order in  $\varepsilon$ .

The (*tangent-linear*) *propagator* from  $t_0$  to  $t_1$  is the matrix  $\mathbf{M}_{[t_0,t]}$  such that  $\mathbf{M}_{[t_0,t]}\mathbf{x}_0$  is a solution of (2) for any initial perturbation  $\mathbf{x}_0$  and where  $\mathbf{M}_{[t_0,t_0]} = \mathbf{I}$ .

# Perturbation Growth

Perturbation growth is defined as:

$$\begin{aligned}\sigma^2 &= \frac{\langle \mathbf{x}(t), \mathbf{x}(t) \rangle}{\langle \mathbf{x}(t_0), \mathbf{x}(t_0) \rangle} \\ &= \frac{\langle \mathbf{M}_{[t_0,t]} \mathbf{x}(t_0), \mathbf{M}_{[t_0,t]} \mathbf{x}(t_0) \rangle}{\langle \mathbf{x}(t_0), \mathbf{x}(t_0) \rangle} \\ &= \frac{\langle \mathbf{M}_{[t_0,t]}^T \mathbf{M}_{[t_0,t]} \mathbf{x}(t_0), \mathbf{x}(t_0) \rangle}{\langle \mathbf{x}(t_0), \mathbf{x}(t_0) \rangle}\end{aligned}$$

with inner product  $\langle \cdot, \cdot \rangle$  and growth factor  $\sigma^2$ .

$\Rightarrow$  Largest growth is associated with eigenvectors of  $\mathbf{M}_{[t_0,t]}^T \mathbf{M}_{[t_0,t]}$ .  
These eigenvectors are determined by a singular value decomposition of  $\mathbf{M}_{[t_0,t]}$ .

# singular value decomposition of a matrix

Consider a matrix  $\mathbf{Q} = \begin{pmatrix} q_{11} & \cdots & q_{1n} \\ \vdots & & \vdots \\ q_{m1} & \cdots & q_{mn} \end{pmatrix} \in \mathbb{R}^{m \times n}$

Its singular value decomposition is defined as

$$\mathbf{Q} = \mathbf{U}\mathbf{S}\mathbf{V}^T, \quad (3)$$

where  $\mathbf{U}$  and  $\mathbf{V}$  are orthogonal  $m$ -by- $m$  and  $n$ -by- $n$  matrices.

Matrix  $\mathbf{S}$  is a diagonal  $m$ -by- $n$  matrix ( $s_{ij} = 0$  if  $i \neq j$ ,  $s_{jj} \equiv \sigma_j$ ). The values  $\sigma_j$  on the diagonal of  $\mathbf{S}$  are called *singular values*.

The columns  $\mathbf{u}_j$  of  $\mathbf{U}$  are referred to as *left singular vectors* and the columns  $\mathbf{v}_j$  of  $\mathbf{V}$  are referred to as *right singular vectors*.

Eq. (3) implies that

$$\mathbf{Q}\mathbf{v}_j = \sigma_j\mathbf{u}_j$$

One can show that the  $\mathbf{v}_j$  are the eigenvectors of  $\mathbf{Q}^T\mathbf{Q}$ !

see Golub and Van Loan: *Matrix Computations* for further details

## singular value decomposition of the propagator

$$\mathbf{M} = \mathbf{U}\mathbf{S}\mathbf{V}^T \quad \rightarrow \quad \mathbf{M}\mathbf{v}_j = \sigma_j\mathbf{u}_j$$

with the (initial) singular vectors  $\mathbf{v}_j$  being the eigenvectors and the squared singular values  $\sigma_j^2$  being the eigenvalues of  $\mathbf{M}^T\mathbf{M}$ . The  $\mathbf{u}_j$  are called the evolved singular vectors.

Singular vectors are optimal perturbations in the following sense.

- the ratio of the final time norm to the initial time norm is given by the singular value:

$$\frac{\|\mathbf{M}\mathbf{v}_j\|_f}{\|\mathbf{v}_j\|_i} = \sigma_j \quad (4)$$

- Singular vector  $j$  is the direction in phase space that maximises the ratio of norms in the subspace orthogonal (with respect to  $\mathbf{C}_0^{-1}$ ) to the space spanned by singular vectors  $1 \dots j-1$ .



# Norms

- The definition of singular vectors in the context of ensemble prediction involves norms (based on an inner product or metric). These are required to measure the amplitude of perturbations.

$$\langle \mathbf{x}, \mathbf{x} \rangle_C = \mathbf{x}^T \mathbf{C} \mathbf{x}$$

where  $\mathbf{C}$  is symmetric ( $\mathbf{C}^T = \mathbf{C}$ ) and positive definite ( $\mathbf{x}^T \mathbf{C} \mathbf{x} > 0$  for  $\mathbf{x} \neq 0$ ).

- For predictability applications, the appropriate choice for the **initial time norm** is the analysis error covariance metric, *i.e.* the norm that is based on the inverse of the initial error covariance matrix (or some estimate thereof).

$$\|\mathbf{x}\|_i^2 = \mathbf{x}^T \mathbf{C}_0^{-1} \mathbf{x}$$

- The **final time norm**  $\|\mathbf{x}\|_f$  is a convenient RMS measure of forecast error.
- **Total energy norm** is used both at initial and final time for the operational singular vector computations at ECMWF:

$$\|\mathbf{x}\|_E^2 = \mathbf{x}^T \mathbf{E} \mathbf{x} = \frac{1}{2} \int_{p_0}^{p_1} \int_S \left( u^2 + v^2 + \frac{c_p}{T_r} T^2 \right) dp ds + \frac{1}{2} R_d T_r p_r \int_S (\ln p_{\text{sfc}})^2 ds$$

# On the choice of the initial time norm

- The structure of singular vectors depends on the choice of the norm, in particular the initial time norm.
- An enstrophy norm at initial time penalises perturbations with small spatial scales, the initial SVs are planetary-scale structures.
- A streamfunction variance norm at initial time penalises the large scales and favours sub-synoptic scale perturbations.
- With a total energy norm at initial time, the energy spectrum of the initial SVs is “white” and best matches the spectrum of analysis error estimates from analyses differences (Palmer et al. 1998)

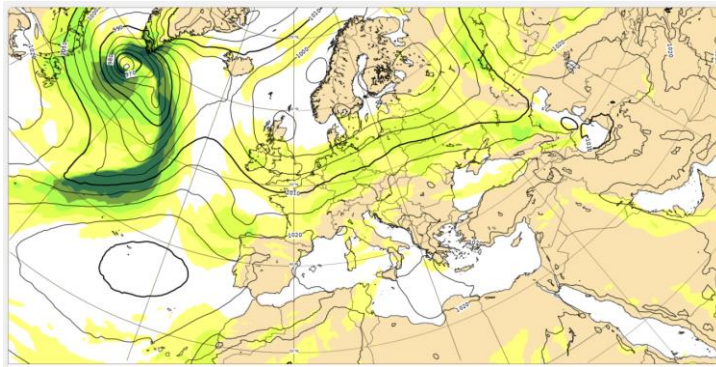
# The tangent-linear model and its adjoint

- For a numerical model with  $\sim 10^5 - 10^8$  variables it is not possible to obtain the propagator  $\mathbf{M}$  as a matrix.
- Instead *algorithmic differentiation* is used to obtain the first derivative of the numerical algorithm that represents the forecast model.  
For any initial perturbation  $\mathbf{x}$ , the evolved perturbation  $\mathbf{M}\mathbf{x}$  is obtained via an integration of the *tangent-linear model*.
- Then, the numerical algorithm representing  $\mathbf{M}^T$  the *adjoint* (transpose) of the propagator is constructed. The adjoint model is integrated backward from  $t_1$  to  $t_0$ .
- The reference solution  $\mathbf{x}_r(t)$  about which the equations are linearised is referred to as *trajectory*.
- The time interval the SVs are calculated for is called the optimization interval.

# Weather Forecasts – NWP? Data Driven?

Traditionally weather forecasts are generated by running NWP model – computer code that has been designed to represent the physical processes governing the evolution of the atmosphere. But can you produce a forecast without a NWP model?

Analysis

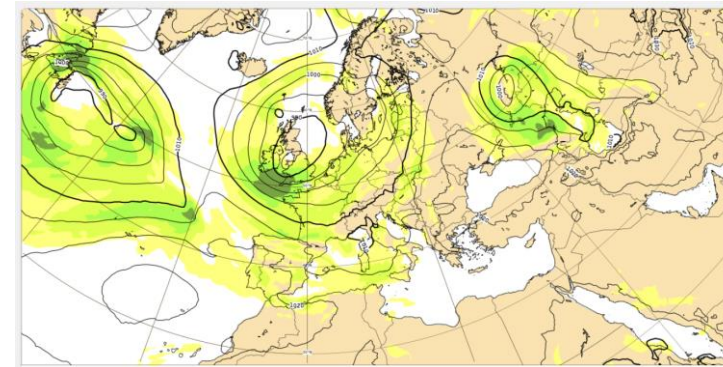


Fusion of short-range forecast with latest observations

NWP Model



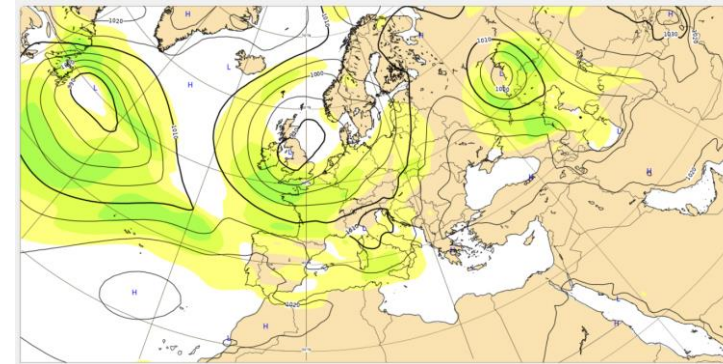
Forecast



Data Driven Model



Learned from 40 years of analyses

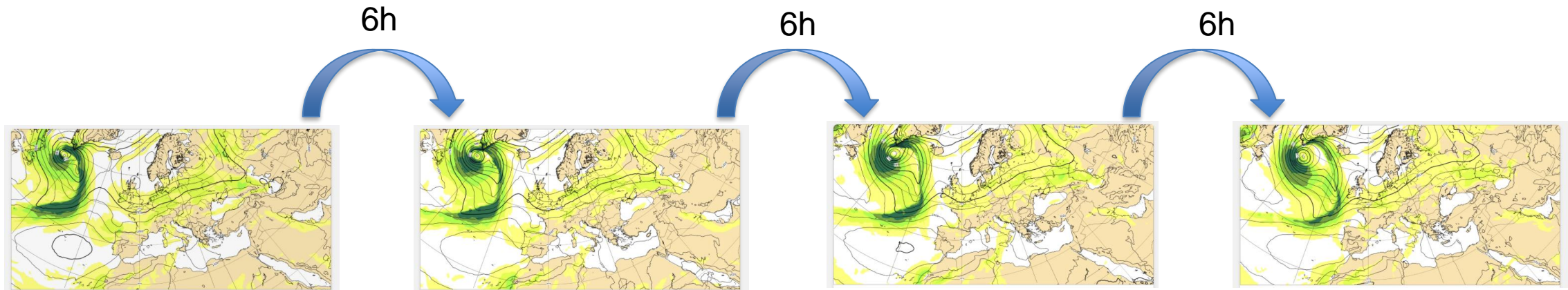




# Weather Forecasts – NWP? Data Driven?

Recent advances by tech companies and individuals show that this is possible (e.g. NVIDIA, Deepmind, Huawei, ... and others)

Here, the models learn from ca. 40 years of ERA5 re-analysis data, stepping e.g. 6h from analysis to analysis



The forecast is then autoregressively stepping 6h into the future  $x_n = f(x_{n-1}) \dots$