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Global physical ocean data assimilation

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with inputs from various people including

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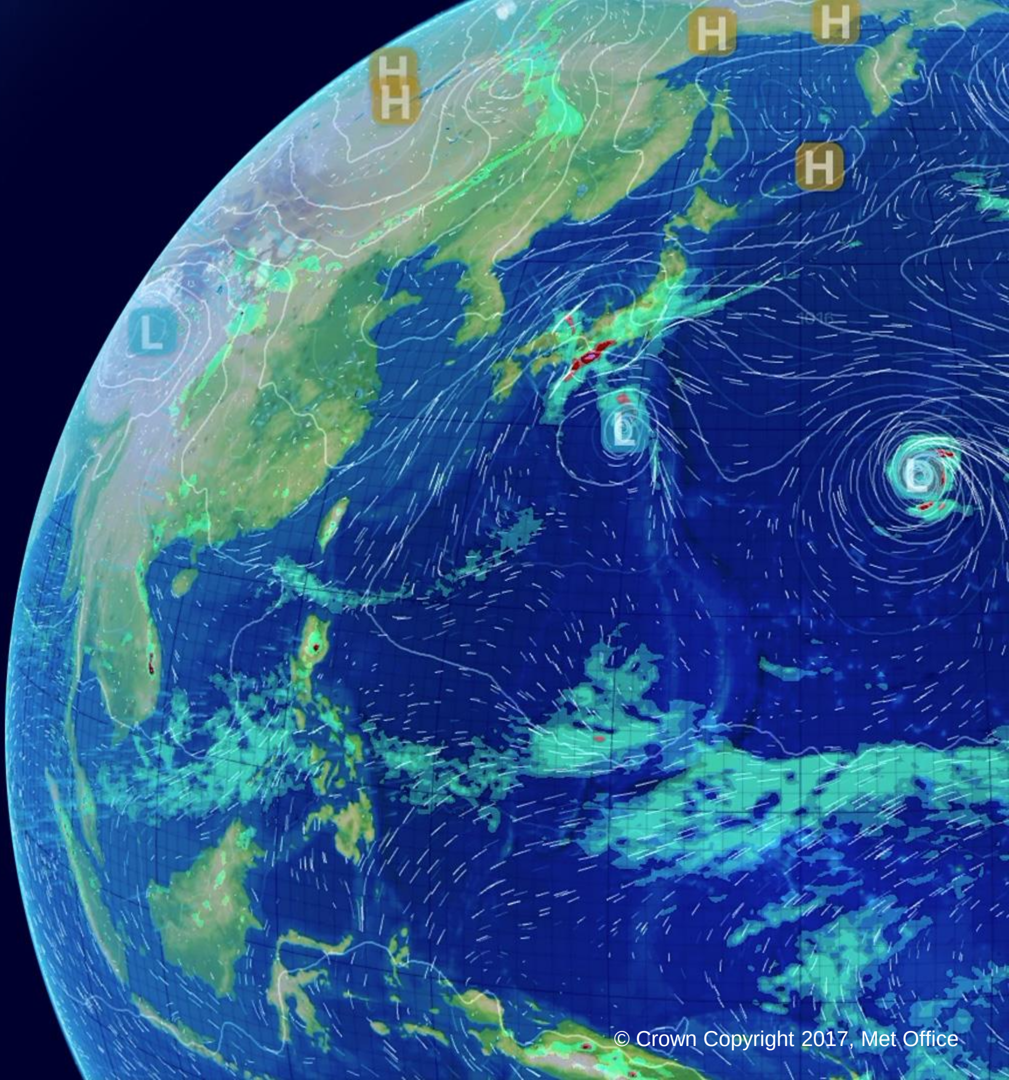
OceanPredict'19, Data Assimilation Training

Halifax, May 2019.



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1. Introduction and overview of operational global ocean data assimilation systems.

2. Observations: quality control, processing and bias correction

3. Data assimilation implementation:
    - The importance of the error covariances.
    - Initializing the model forecast.
    - Dealing with model bias.

4. Examples of on-going developments.

1. Introduction

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Introduction

- Our knowledge about the current/past state of the ocean and sea-ice is based on:

    - Numerical models based on our understanding of the physics.
    - Direct observations from in situ platforms
    - Indirect observations from space

- All of these pieces of information contain errors and sampling issues:

    - ***Models*** represent the ocean on certain spatial scales (depending on resolution), and contain errors due to:
        - Errors in surface atmospheric forcing.
        - Errors in the parameterisation of unresolved physics.
        - Errors in the numerical formulation.

    - ***Observations*** contain errors and measure the ocean on different spatial scales (to each other and to the model).

- Data assimilation aims to combine the model with the different observations in an optimal way, taking into account their respective uncertainties.

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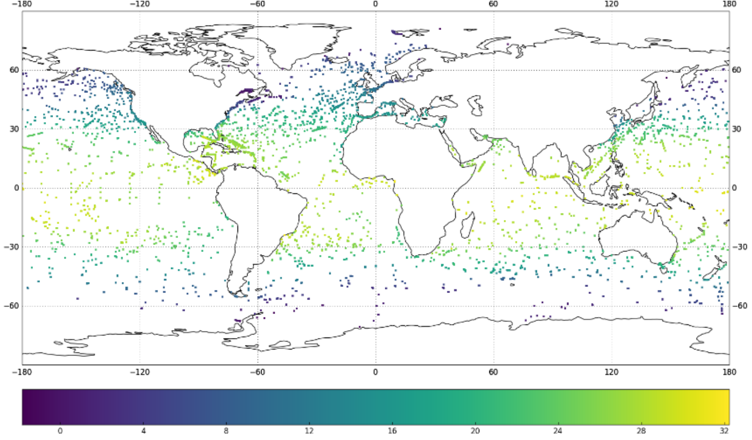
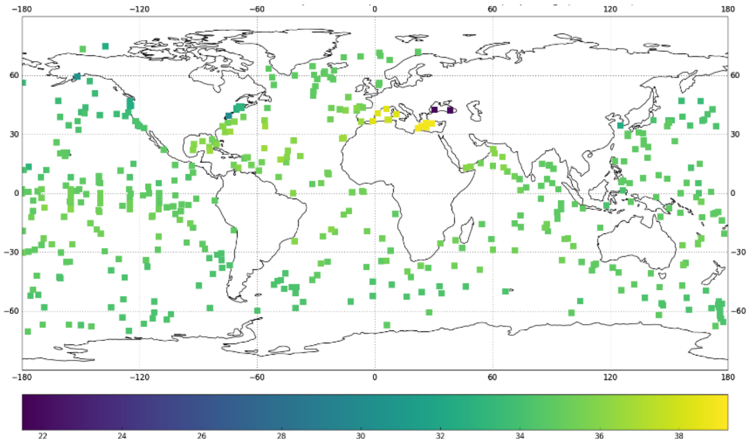
In situ observations are sparse

***In situ* measurements valid for one day on 14th Jan 2019.**

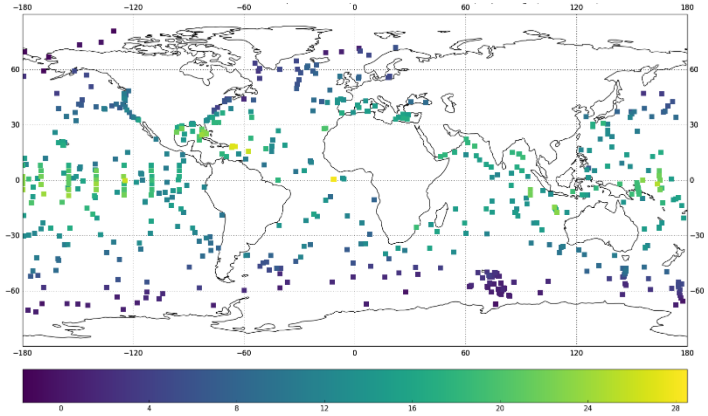


In situ SST data (ships, moored and drifting buoys)



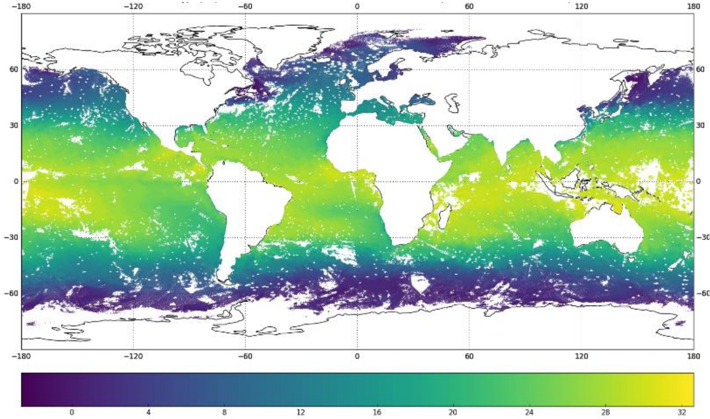
Salinity profiles (Argo, moored buoys, CTDs, gliders)

Each profile has many vertical observations (mostly to maximum of 2000m depth).

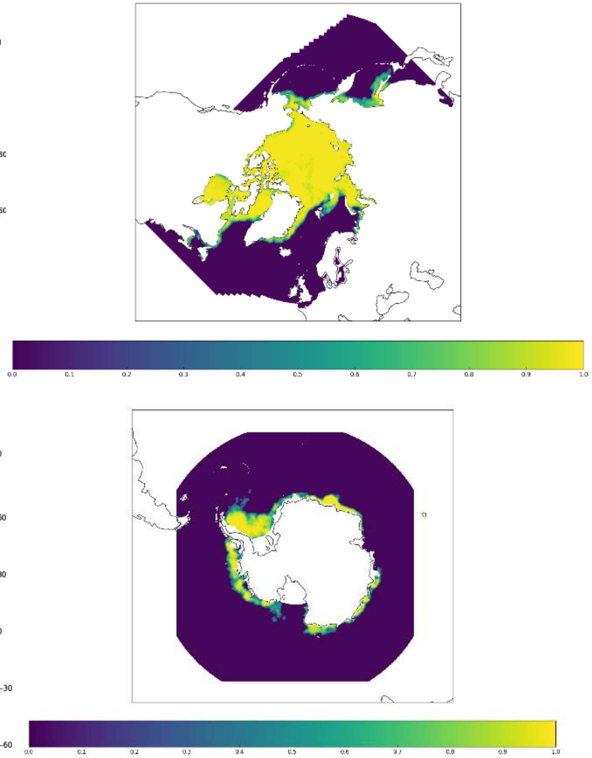


Temperature profiles (Argo, moored buoys, XBTs, CTDs, marine mammals, gliders)

Satellite observations are less sparse but still do not sample all the time/space scales we’re interested in, and don’t measure the sub-surface ocean directly.

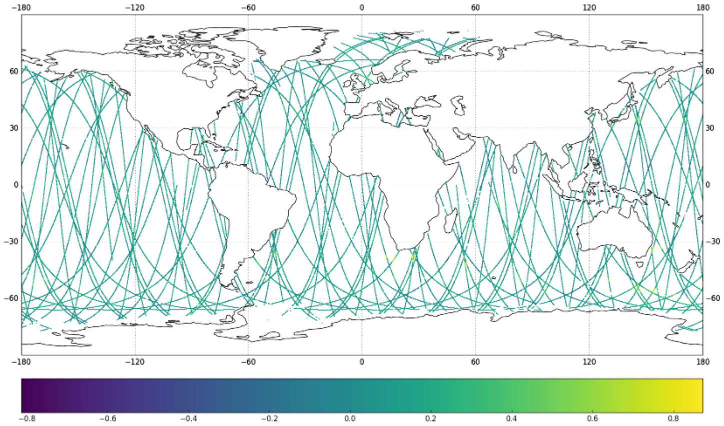


Satellite SST data
(NOAA/AVHRR, MetOp/AVHRR, AMSR2, VIIRS-G)



Satellite sea-ice concentration data
(SSMI/S)

Satellite measurements valid for one day on 14th Jan 2019.



Satellite altimeter SSH data
(Jason-3, Sentinel-3, Cryosat, Altika)

Global data assimilation systems in GOV/OceanPredict

As previously described, data assimilation aims to combine the model with the observations in an optimal way. Various methods used to do this as described in previous presentation. Also see Moore et al., 2019.

The present generation of ***operational global*** DA systems can be categorized as using:

- **3DVar** (UK [Met Office], Europe [ECMWF], USA [NRL/NCEP], Japan [MRI/JMA], India [INCOIS])
- **EnOI/SEEK**, ensemble methods with a static ensemble (France [Mercator Ocean], Canada [ECCC], Australia [BoM/CSIRO])

Most of these systems are used to produce ***near real-time operational*** analyses and forecasts, as well as ***historical reanalyses***.

One other approach used for reanalysis is that of the ECCO group which use a long time-window 4DVar approach.

Operational systems have different time windows for the data assimilation ranging from 7 days down to 1 day.

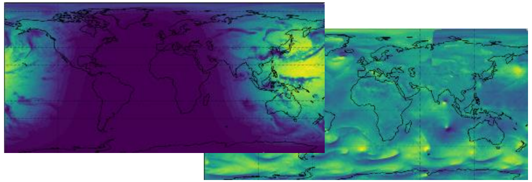
- Longer time window allows more observations in order to get a more consistent analysis over all the observations.
- Shorter time window provides information closer to real time, and allows the solution to fit higher frequency processes.

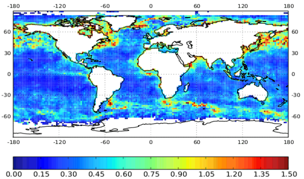
In this presentation, the examples come mainly from the FOAM system in the UK Met Office (which has a 1-day time-window).

Information about global systems available from https://www.godae-oceanview.org/science/ocean-forecasting-systems/national-reports

Overview of an operational data assimilation system







Observation database

Atmospheric forcing

Product generation and dissemination

Verification, assessment and monitoring

Observation quality control and pre-processing

Forcing extraction and processing

Model run for observation operator

Data assimilation procedure

Model run to add in increments

Model forecast

Observations and model counterparts

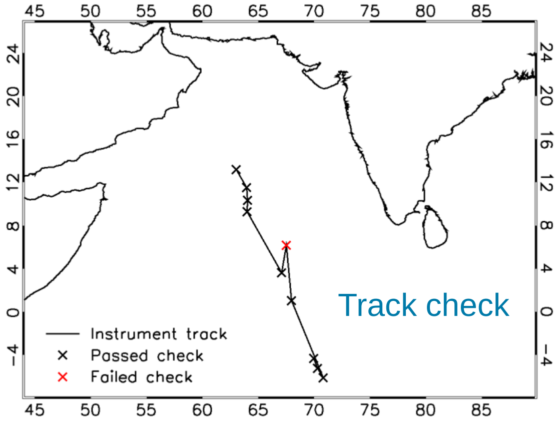
Increments

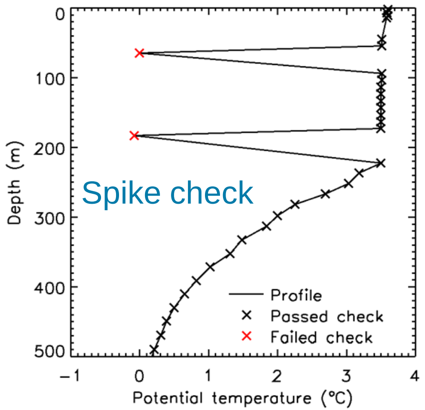
2. Observations: quality control, processing and bias correction

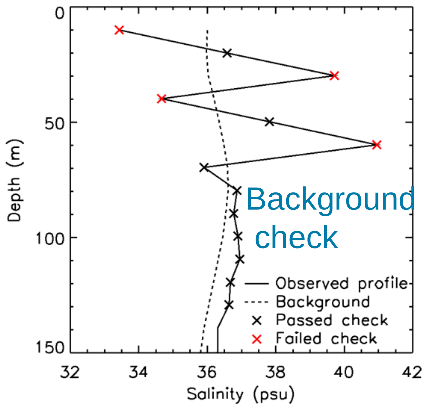
Observation quality control and pre-processing

Quality control checks:

- Use QC flags from data providers.
- Gross checks for “reasonable” values, e.g. temperature is not below freezing, salinity is not negative, …
- Compare observation with a short-range model forecast, using information about their respective errors.
- For profile data other checks include track checks, spike checks, stability checks, …





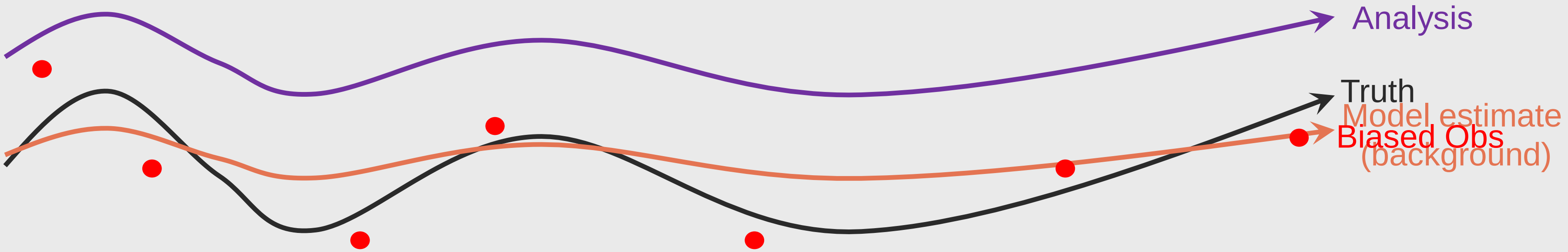


Other pre-processing tasks include:

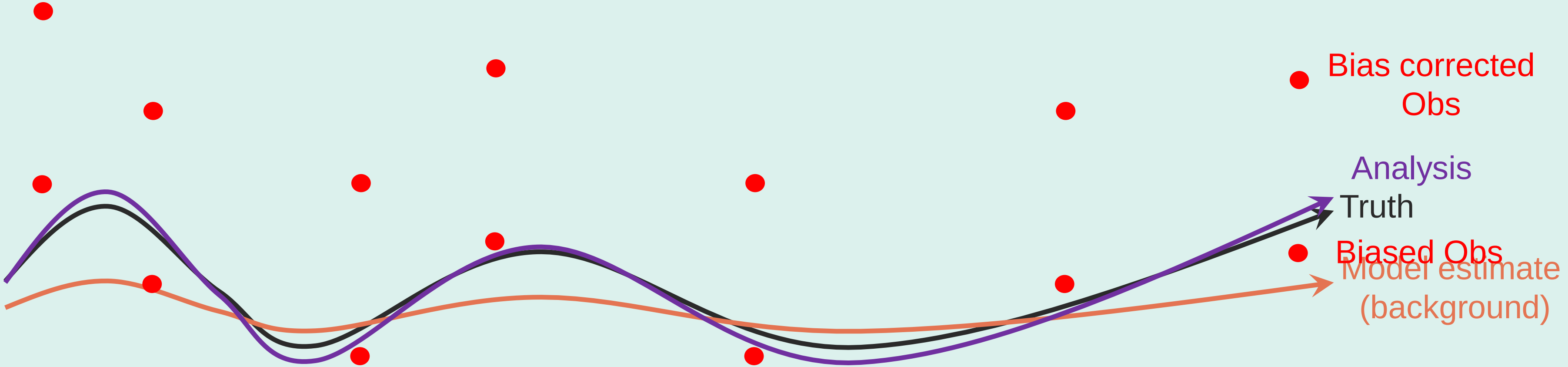
- Super-obbing (averaging) or thinning so that the observation density is not much larger than the model grid.
- For SST data, convert skin measurements to sub-skin, remove obs affected by diurnal warming.

Observation bias correction schematic

As normally written, data assimilation algorithms assume unbiased observations.
If this assumption does not hold, this happens:



If we account for the bias:

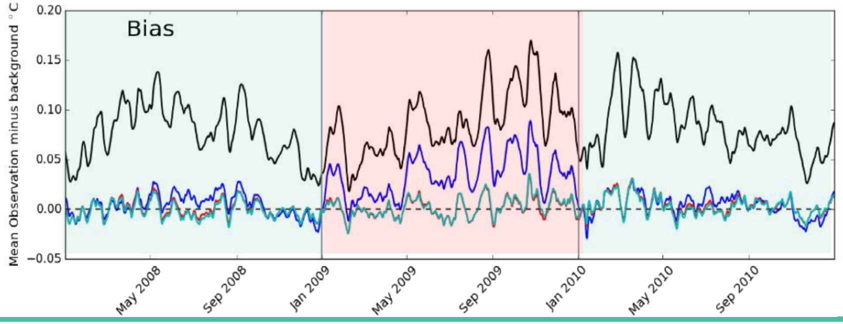


Observation bias correction

For satellite SST data:

- Each satellite has biases due partly to retrieval errors which are weather-dependent and some satellites are calibrated differently to others.
- There are reference datasets (e.g. drifters, (A)ATSR) which allow us to “observe” the bias by comparing each satellites with the reference data (with specified space/time match-up criteria).
- The “observations-minus-forecast” also give information about the average difference between the model and the observations. If we assume the model to be un-biased on certain time/space scales then these can give us information about the observations bias.
- Extra terms can be added into the data assimilation procedure such that spatially/temporally varying bias estimates can be made.

With the global FOAM system, While et al. (2019), apply a bias correction to remove biases in the AMSRE satellite.



Black -> no bias correction
Blue -> bias correction using only reference data
Cyan -> bias correction using reference data and mean innovations

For satellite SLA data, there is a need to add in a mean dynamic topography (MDT) to be able to compare to the model’s SSH field.
The MDT contains errors (mainly on small spatial scales), which introduces a bias into the observations of SSH (SLA+MDT). A method to estimate these biases in the MDT during the data assimilation process is described by Lea et al., 2008.

3. Data assimilation implementation

3DVar data assimilation

Here we use 3DVar to illustrate some aspects of data assimilation.

The standard incremental 3DVar cost function penalises:

(1) the difference between the analysis and the background (forecast), and

(2) the difference between the analysis and the observations.

$$J(\delta\mathbf{x}) = \overbrace{1/2(\delta\mathbf{x}^{\mathrm{T}}\mathbf{B}^{-1}\delta\mathbf{x})}^{(1)} + \overbrace{1/2((\mathbf{d}-\mathbf{H}\delta\mathbf{x})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{d}-\mathbf{H}\delta\mathbf{x}))}^{(2)}$$

- The vector **δx** is the difference between the analysis and the model forecast, also known as the ***increments***.
- The matrix **B** is the background error covariance matrix which is the size of the model state squared, i.e. the covariance between each variable at each grid point and all other variables at all other grid points. It is too large to estimate explicitly all the elements of **B** and we couldn't store them even if we could estimate them.
- **d** is the difference between the observations and the model background interpolated to the observation locations, also known as the ***innovations***.
- **R** is the observation error covariance matrix.
- **H** is the linearised observation operator which transforms from model to observation space.

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Importance of the error covariance specifications

At the minimum of the cost function, the analysis can be written as:

$$\boldsymbol{x}^a = \boldsymbol{x}^f + \underbrace{\mathbf{BH}^T[\mathbf{HBH}^T + \mathbf{R}]^{-1}}_{\mathbf{K}}[\boldsymbol{y} - h(\boldsymbol{x}^f)]$$

The weight given to the observations is determined by the magnitudes of the background error covariances (**B**) and observation error covariances (**R**).

In the scalar case (one observation and one model grid point and variable):

- if **B** >> **R** then $\mathbf{K} \approx \mathbf{1}$ and the resulting analysis will be $\boldsymbol{x}^a = \boldsymbol{y}$
- if **B** << **R** then $\mathbf{K} \rightarrow \mathbf{0}$ and the resulting analysis will be $\boldsymbol{x}^a = \boldsymbol{x}^f$

So, ignoring spatial and inter-variable correlations, the relative size of the error covariances determines how much weight is given to the observations.

Observation error covariances

Observation errors consist of measurement + representation error (Janjić et al., 2018).

- Measurement errors are obviously platform specific. For some platforms (e.g. satellite SST data) the data producers provide per-observation estimates of these.
- Representation errors depend on the difference between the spatial/temporal sampling of the observations, and the model grid resolution (and processes represented).

Observation error covariances are usually assumed to be uncorrelated (spatially and between platforms).

This is not true, particularly for satellite data, but it is very difficult to efficiently represent these correlations.

Methods used to mitigate against this include:

- Inflate errors to account for un-represented correlations to avoid over-fitting.
- Sub-sampling or super-obbing (averaging) to reduce spatial correlations.

Some work is starting to move towards representation of spatial correlations in **R** (e.g. Guillet et al., Ruggiero et al.).

Background error covariances

Background error covariances are correlated spatially and between variables. They therefore determine how the observation information is spread in the model (spatially and between variables).

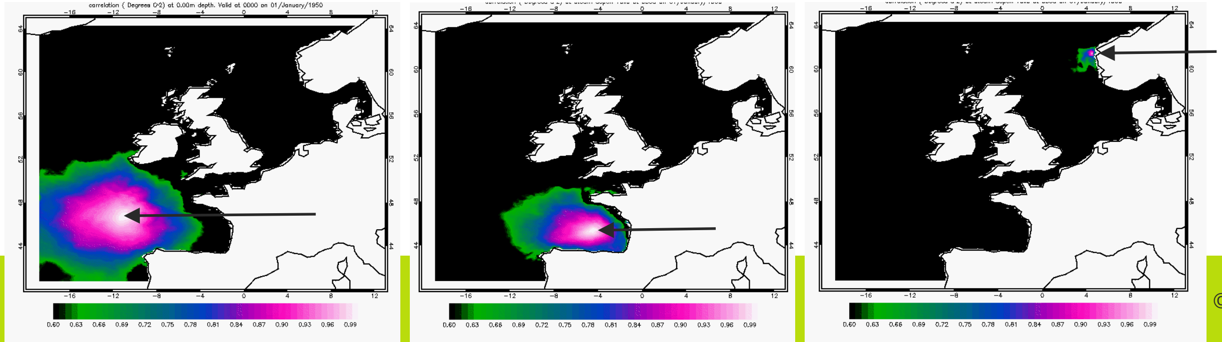
B is very large, particularly in global systems. The state vector has $n=O(10^9)$ elements for 1/12° global system and the number of elements in **B** is the size of n^2.

- Not enough information to estimate **B** exactly, and not possible to explicitly represent it in the data assimilation systems.

Various methods for reducing the size of **B** in practice, and this is one of the main differences between the different DA algorithms.

- Variational methods tend to parameterize **B** (see examples on the following slides) with the parameters calculated statistically from outputs of previous reanalyses.
- Ensemble methods use an ensemble of model runs to estimate **B**, but the small size of the ensemble leads to sampling issues so that localization and inflation methods are necessary.

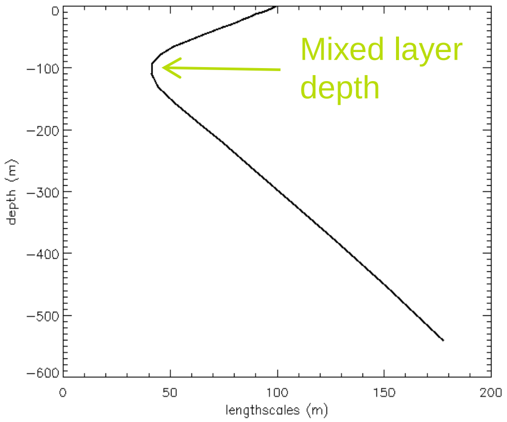
Horizontal error correlation structures can vary considerably in time and location. Dynamic and bathymetric features can affect the correlations.



Background error covariances in NEMOVAR

• We specify the univariate parts of **B** (e.g. temperature-temperature covariances) as:
  - a set of error variances (the diagonal elements of **B**).
  - a set of horizontal correlation scales to spread information horizontally.
  - a set of vertical correlation scales to spread information vertically.

Vertical correlation length scales



• The multivariate parts of **B** are specified using linearised physical balance relationships:
  - T-S water mass properties from the background model state are used to spread information from T to S.
  - The equation of state is used to estimate density changes from T & S.
  - Hydrostatic balance is used to spread information from density to SSH.
  - Geostrophic balance is used to spread information to velocity.
  - The adjoints of all these relationships are also used so that information is spread the other way.

• Sea ice is treated separately (as univariate) at the moment.

Weaver et al., 2005.

Applying the increments

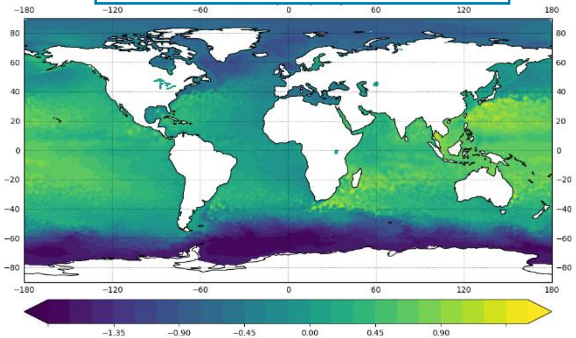
Most systems use Incremental Analysis Updates (IAU; Bloom, 1996) to add in the increments.

Simple idea:

- Want to avoid large shocks to the model.
- Slowly add the increments into the model by adding a fraction of them at each time-step during the model run.
- This method is better than nudging towards an analysis or direct initialisation.

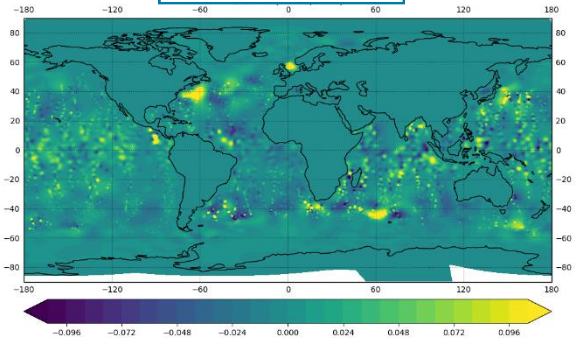
More sophisticated methods can be used, e.g. adaptive initialisation (Sandery et al., 2011).

Model sea surface height (m)

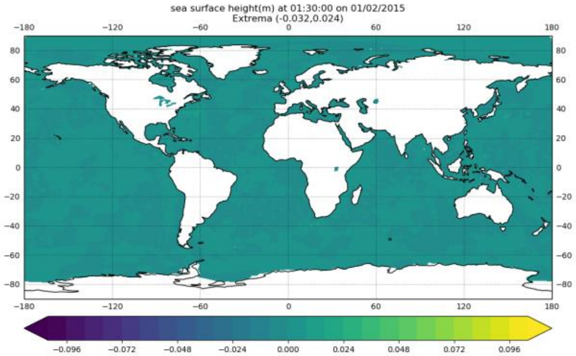


-1.8 1.4

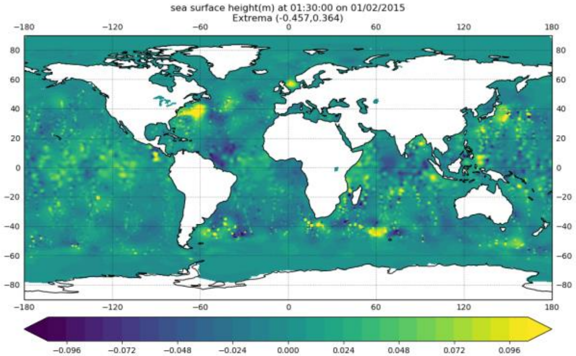
SSH increments



-0.1 0.1



Model f/c –minus- iau

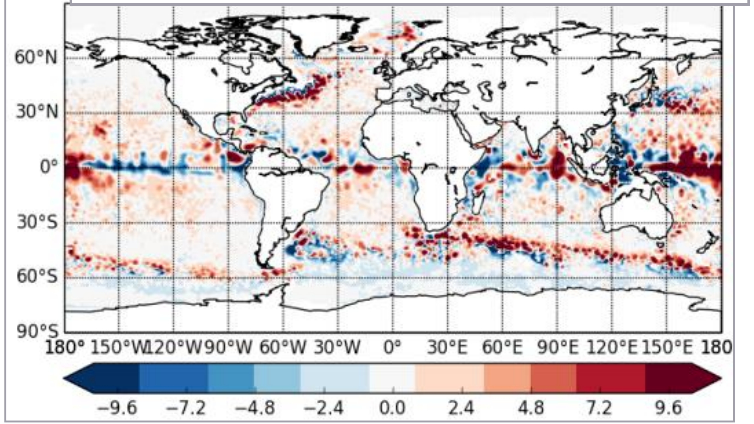


Model f/c –minus- direct initialisation

Model biases

Model biases can be estimated from the time-averaged increments.

Time-average T increments, integrated over top 500m



Dipoles in the ***western boundary currents*** and ACC
⇒ Assimilation acting to tighten the fronts
⇒ Model not able to sustain the observed frontal structures.

Large equatorial biases due to imbalances between the wind forcing and sub-surface pressure gradients
⇒ Assimilation continually adjusting the sub-surface in the same way
⇒ Generation of spurious vertical circulations.

Methods exist to correct for model biases during the data assimilation process (e.g. Balmaseda et al., 2007).

- Many groups apply a large-scale bias correction to temperature and salinity, e.g. ECMWF, Mercator.
- Some groups also apply a bias correction to deal with the large biases near the equator (e.g. Bell et al., 2004), which can generate spurious vertical circulations, and also impact on coupled physical-biogeochemical models.

4. Examples of on-going developments

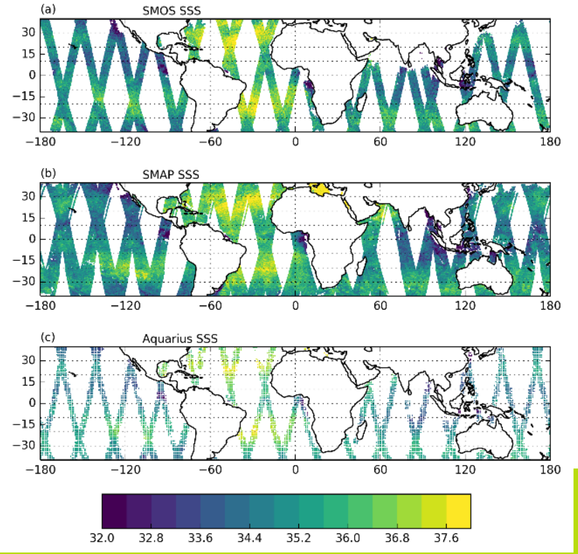
Recent/on-going developments

1. Other observation data sources:
   - ***Satellite SSS data from SMOS and SMAP.***
   - Preparing for wide swath altimeters, e.g. SWOT
   - Improving use of data from gliders
   - Velocity (from surface drifters or HF radar), and up-coming data from e.g. SKIM or SEASTAR.

2. Using “errors-of-the-day” from an evolving ensemble system in the specification of **B**.
   - Some groups are pursuing pure ensemble methods (Mercator Ocean, BoM): EnKF, LETKF
   - *Others are developing* ***hybrid ensemble/variational methods*** (Met Office, ECMWF).

Assimilation of satellite SSS data

- **Satellite SSS** DA (SMOS/SMAP/Aquarius) tested as part of ESA SMOS-NINO15 project. [Martin et al. 2019]
- Overall small, consistent, positive impact on SSS compared to Argo data, particularly in tropical Pacific.
- Also improvements to SST and SLA.
- Still work to be done before suitable for operational implementation.



Red => reduction in RMSE

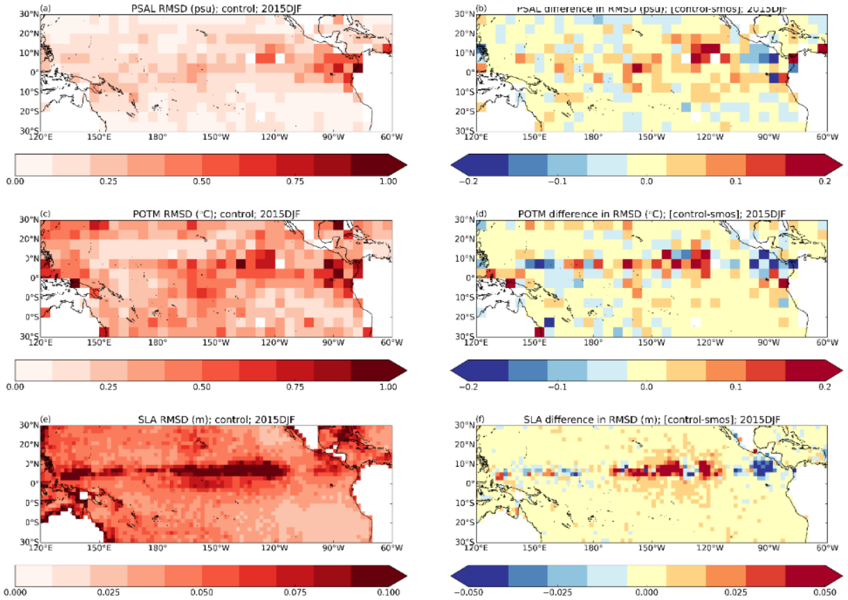
Control RMSE

SMOS impact on RMSE

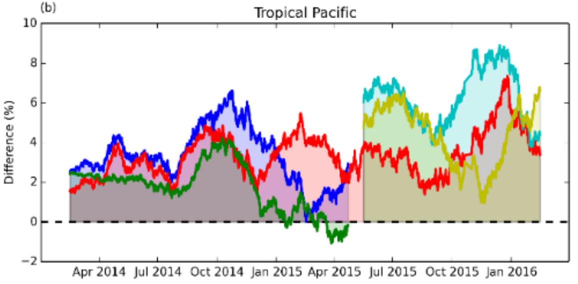
SSS

SST

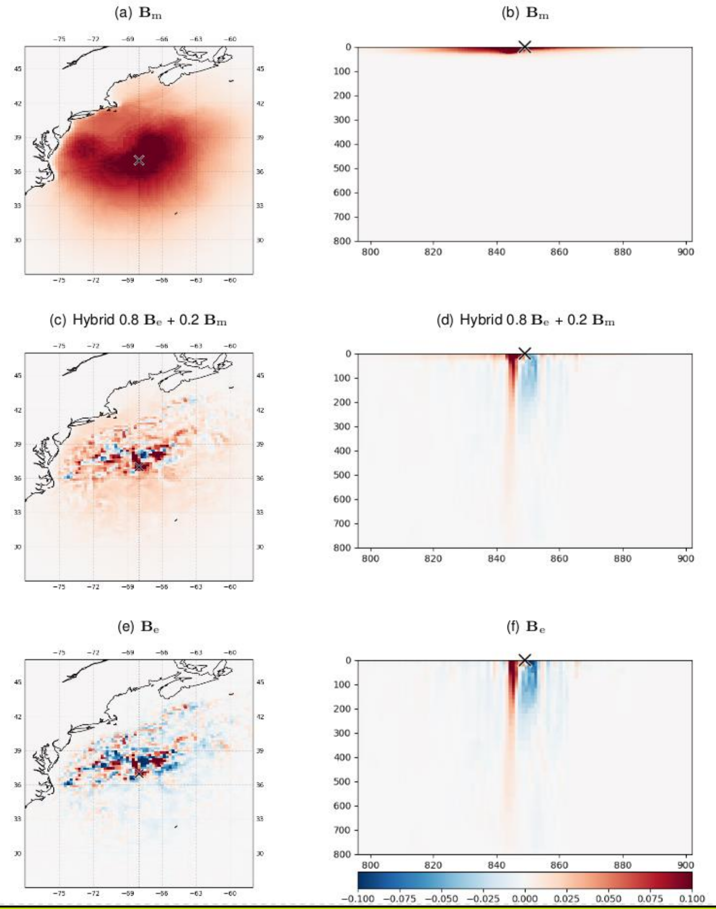
SLA



% reduction in RMSE of near-surface S compared to Argo.
Red: SMOS
Cyan: SMOS+SMAP

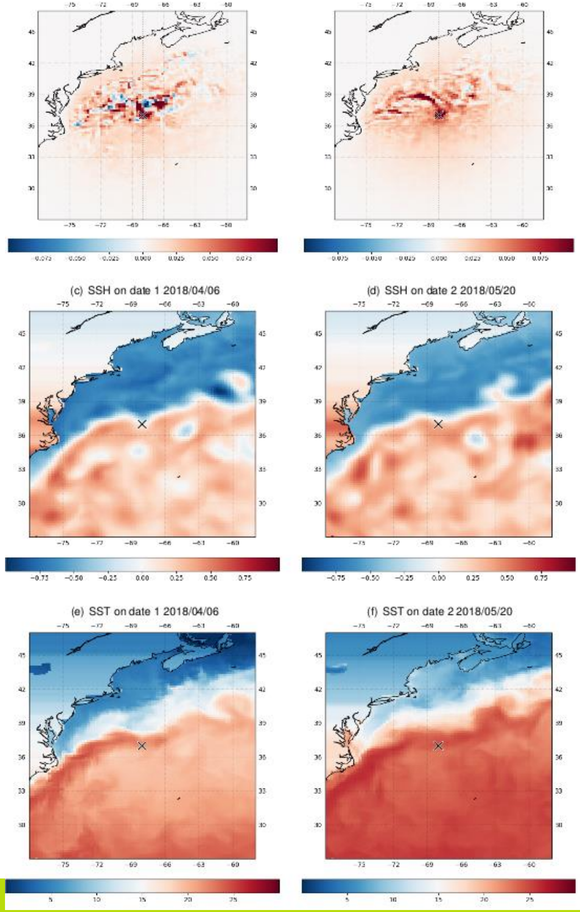


Hybrid ensemble/variational data assimilation

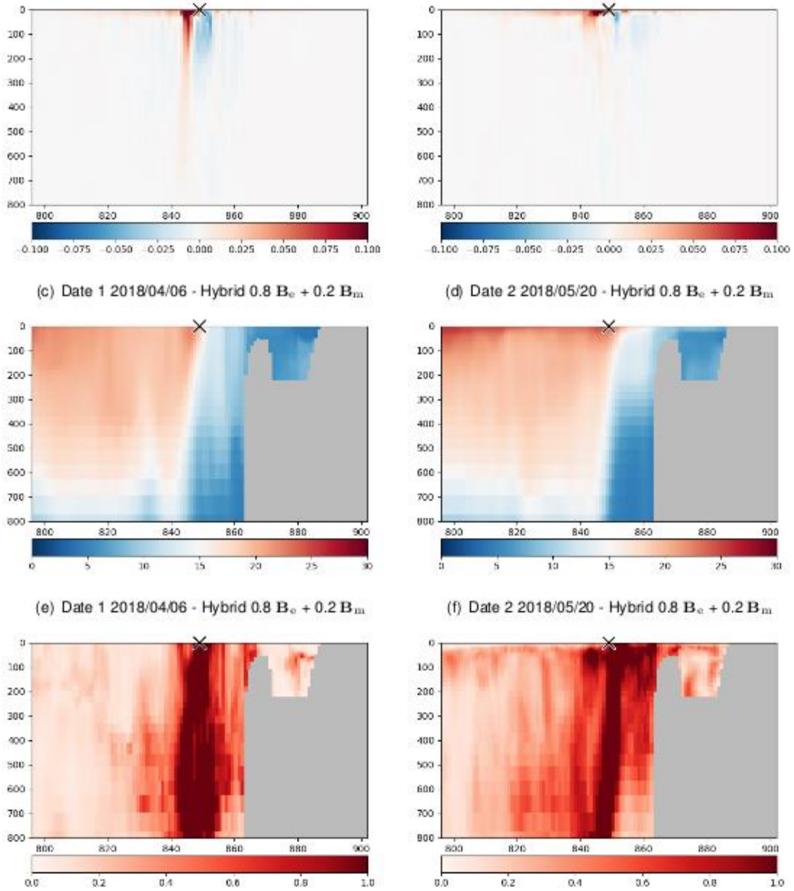


- One SST observation in the Gulf Stream
- Standard NEMOVAR projects the information vertically based on the background mixed layer depth.
- Large localisation scales here of 4° just to illustrate the method. These need estimating/tuning.
- The pure ensemble uses the observation to adjust the location of the front.
- The hybrid retains some larger scale correction based on the standard NEMOVAR system, but still makes changes based on the ensemble.

Hybrid ensemble/variational data assimilation



- One SST observation in the same location in the Gulf Stream.
- Two different dates (6th April and 20th May 2018).
- On the second date, the location of the Gulf Stream front has changed, so the ensemble error covariances produce quite a different increment.



Summary

- Most operational global systems use 3DVar or static-ensemble methods and are developing more advanced methods which make use of evolving ensemble information.

- Observation quality control, pre-processing and bias correction very important part of operational and reanalysis systems.

- The error covariance specifications are crucial for the quality of the analysis.

- Need to deal with model biases, and make sure the increments are retained by the model.

- Algorithms and implementation being continually developed and applied with increased model resolutions, new observing systems and with increased supercomputer resources.

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Thank you for listening. Questions?

Extra slides

Hybrid ensemble/variational data assimilation

- If we have an ensemble system, the ensemble provides extra information about the forecast error covariances on each day.

$$\mathbf{X} = \frac{1}{\sqrt{N_\mathrm{e} - 1}}(\epsilon_1 \ldots \epsilon_{N_e}) \qquad \mathbf{B_e} = \mathbf{X}\mathbf{X}^\mathrm{T}$$

where the ε_i are the difference between the state in the i^{th} member and the ensemble mean.

- However, the ensemble is usually only of limited size [O(10-100)] and much much smaller than the dimension of the state.
- This leads to sampling errors if the ensemble were to be used directly to specify **B** in the data assimilation.
- There are ways to reduce sampling errors by localising the spatial influence of the ensemble near each observation. However, this means that dynamical balances aren't maintained, and that observations can only have limited spatial influence (which isn't good for sparse observing systems).

$$\mathbf{B}_\mathrm{e} = \mathbf{C}_L \circ \mathbf{X}\mathbf{X}^\mathrm{T}$$

- A way to allow data assimilation schemes to gain the benefits of the robustness of the existing *modelled* $\mathbf{B_m}$, and the benefits of the errors-of-the-day from the *ensemble-based* $\mathbf{B_e}$ is to linearly combine them in the variational cost function and use the existing variational infrastructure to minimise the new cost function.

$$\mathbf{B}_\mathrm{h} = \beta_\mathrm{m}^2 \mathbf{B}_\mathrm{m} + \beta_\mathrm{e}^2 \mathbf{B}_\mathrm{e}$$

Standard 3DVar data assimilation

- In the NEMOVAR system the **B** matrix is decomposed in the following way:

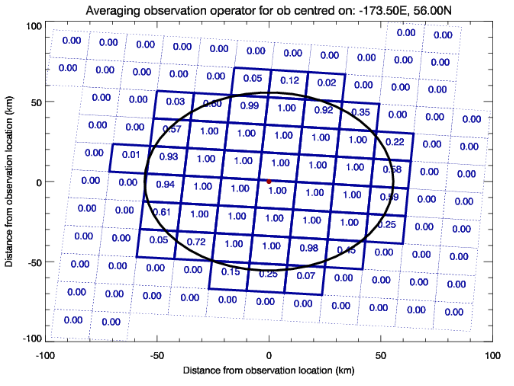
$$\mathbf{B}_{\mathrm{m}} = \mathbf{K}_{\mathrm{b}}\mathbf{D}_{\mathrm{m}}^{1/2}\mathbf{C}_{\mathrm{m}}\mathbf{D}_{\mathrm{m}}^{1/2}\mathbf{K}_{\mathrm{b}}^{T}$$

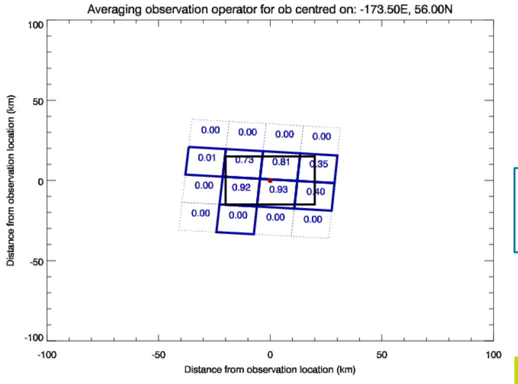
- The off-diagonal elements of **B** (determined by the correlations **C**) are modelled by assuming a functional form: a combination of 2 Gaussian functions each with their own length-scales where one is the first baroclinic Rossby radius and the second is 400km. An *implicit diffusion operator* is used to efficiently model these spatial correlations.
- We specify the diagonal elements (variances, **D**) as spatially and seasonally varying estimates based on previous reanalyses at the surface. The sub-surface error variances of temperature are parameterised based on the vertical temperature gradients (which change from day-to-day and depending on location).
- Physically-based multi-variate relationships **(K)** are specified to transfer information between variables in **B** so that the resulting increments (δx) are dynamically balanced. These are based on geostrophic and hydrostatic balances.

Observation operators

- We use, maintain and develop the central NEMO observation operator (tangent linear and adjoint code in NEMOVAR):
  - It can deal with **temporally and spatially varying vertical coordinates**.
  - Bilinear horizontal interpolation and various vertical interpolation options.
  - **Efficient grid search** to locate observations on the ORCA grids.
  - Deals with time-average observations, e.g. daily average moored buoy data.
  - The current version does not deal with TEOS-10 T/S variables (conservative temperature and absolute salinity), so this will need to be added soon.
  - Recently added an **averaging operator** which can deal with rectangular or radial footprints with the footprint size specified in degrees or metres. Useful for e.g. Microwave SST data, satellite SSS data; particularly useful as models move to higher resolution.

Radial footprint 1° diameter at 56°N, 173.5°E





Rectangular footprint 40km x 30km at 56°N, 173.5°E