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Implementing the EnKF into NorESM

by

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Abstract

The 5th assessment of the IPCC, scheduled for 2014, will partly be dedicated to evaluating the feasibility of decadal-scale climate predictions. Skillful predictions on inter-annual to decadal timescales will fill the present scientific and mitigation gaps between the established fields of seasonal forecasting and future climate change projection. We intend to study the capability of the Ensemble Kalman Filter to assimilate satellite data (at first sea surface temperature) within the Norwegian Earth System Model (NorESM). The Ensemble Kalman Filter is a state of the art multivariate data assimilation method able to handle non-linear forecasting application and provide the uncertainty of the prediction. First, a reduced and uncoupled version of NorESM is used to identify the most responsive parameters of the ocean model, and analyze for how long the benefit of the assimilation remain once observations are no longer assimilated. This manuscript details the technical implementation of the method and practical information for further use or development.

1 Introduction

Prediction from inter-annual to decadal timescales are targeted for the 5^{th} assessment of the IPCC, scheduled for 2014. It is expected that on such time-scale, the realism of the initial state is important. Indeed, *Smith et al.* (2007); *Keenlyside et al.* (2008); *Pohlmann et al.* (2009) improve their prediction using a simple data assimilation method to correct the initial state. It is expected that a more advanced data assimilation method can yield larger benefit, in particular because of the multivariate properties of the update and of its capability to handle non-linearity (*Lisæter et al.*, 2003).

The Ensemble Kalman Filter (EnKF; *Evensen*, 2003) is a state of the art multivariate data assimilation method able to handle non-linear forecasting application and provide an uncertainty of the prediction. The method is used: operationally for coupled ocean-ice model in TOPAZ system (*Bertino and Lisæter*, 2008); operationally for atmospheric model (*Houtekamer and Mitchell*, 2005); to estimate soil moisture (*Reichle and Koster*, 2005) and finally for parameter estimation on Earth System Model of Intermediate Complexity (*Hargreaves et al.*, 2004; *Annan et al.*, 2005).

We intend to test the EnKF for the first time with a full Earth System Model (NorESM). The present study is a first step toward this objective and only a test configuration of NorESM is used. The ocean model is uncoupled and forced with NCEP forcing field; the ocean model part has low resolution (2.4°) and the ice dynamics is switched off because it was being modified at the time of the study in the version of Nor-ESM used. This manuscript describes the technical effort made implementing the EnKF into NorESM, then identify some parameters simulating the model error, and finally study the persistence of the benefit of assimilation once observations are no longer assimilated. It has been decomposed in different task separated in different section:

- Adapt the EnKF code for compatibility with MICOM input/output.

- Modify the physical code of MICOM in order to run perturbed ensemble runs.
- Preparation of the observations to be assimilated.
- Post-processing of the analysis files to ensure stability of the restart file.
- Compare a run assimilated for 3 years followed by a 3 years free run against a 6 years free run.
- Conclude and identify the next challenges.

2 EnKF adaptation for MICOM

The code used for assimilation corresponds to the version 2.06 of the EnKF code. Differences with the original code are minor so that future upgrade of the code can be easily applied. There are some new files:

- m_get_micom_nrens.F90: returns the number of members available in the analysis directory.
- m_pivotp_micom.F90: computes the pivot point for one observation independently of the type of grid (bipolar, tripolar)
- m_get_micom_fld.F90: reads the record from MICOM restart files.
- m_put_micom_fld.F90: dumps the assimilated variable in MICOM restart files.

As we intended to work first on surface data such as SST and altimetry, we have not work with assimilation of profiles. The latter would necessit further development, but it should not be large as the vertical structure of HYCOM and MICOM is comparable.
Possible remaining task:

- Update the version of the EnKF to its newest version (currently 2.10). The newer version of the EnKF code uses a more precautious formulation. It consists of increasing artificially the observation error when the discrepancy between the model and the observation is larger than the ensemble spread. In the latter situation, it often reveals that the system is unable to reproduce the processes observed, and one cannot expect the correlation to be realistic.
- Allow the EnKF to assimilate profiles.
- test different localisation radius, assimilation frequency, inflation parameter.

3 MICOM adaptation for ensemble run

In order to test the EnKF code, we need to get an ensemble run of MICOM files. It is convenient and more optimal (with respect to memory) to run the ensemble in a single directory. First, MICOM reads an argument as input that corresponds to ensemble size. All diagnostics made in ASCII files (e.g. denbud, salbud ...) are only dumped for the first member to avoid crashes occurring when several jobs writes on the same ASCII file. Every member reads its input into a file call limits$mem where $mem is the corresponding to the size of the ensemble. It is possible to dump monthly average for each member. On Hexagon BCCS super computer, the maximum number of job allows to run at the same time is 20. Submitting more than 20 jobs at the same time should be avoided. The script micom/code_r94/run/run.sh has been rewritten to launch a group of MICOM members. At the beginning of the script, one must specify the number of ensemble member wanted for the run (e.g. NENS=40) and how many members each pbs_job.sh is launching (e.g. NBATCH=2). To run an ensemble simulation, one needs to edit file micom/code_r94/run/limits_mal for the starting and finishing date and launch run.sh that launches automatically the ensemble run.
Remaining task: The option of launching job by packet is currently not working robustly on hexagon. This issue has been raised to the support and has proven to be caused by a combined deficiency of the machine

set-up and MICOM code that does not free memory before quitting the program. This issue is yet within the responsibility of BCCS support but not easy solution has been found yet. Running the code with NBATCH=1 is robust and no crash has been noticed.

4 Perturbation system

In the EnKF, it is assumed that when the ensemble is large enough and uncertain parameter of the forcing are perturbed, the ensemble mean provide a more accurate estimate than each member, and the ensemble spread is representative of the forecasting error. This necessits to identify the right sources of error, and to use a sufficiently large ensemble. The following model parameter and forcing are perturbed under recommendation from Mats Bentsen:

- The current model version uses atmospheric forcing prescribed from NCEP. In order to enhance variability from the atmosphere one need to perturb the fields. A lag in the date of the forcing fields used is introduced. Note that the lag is set at the beginning of the run and kept unchanged during the model integration in order to ensure continuity of the sequence of forcing fields used. The lag is an integer chosen randomly (uniform distribution) between $\pm$ 40 days.
- The background vertical diffusion accounts for unresolved turbulent mixing. It is currently set to 0.14 but its optimal value is unknown. The value is perturbed uniformly so that bdcm2=0.14$\pm$0.02.
- Efficiency factor for wind TKE generation rm0 is perturbed uniformly so that rm0=1.5$\pm$0.3
- The parameter c in Eden and Greatbatch (2008) is perturbed uniformly so that c=1$\pm$0.25

We have analyzed the model response to this perturbation system. Figure 1 represents the spatial distribution of the ensemble spread in December 1990 with an ensemble of 40 members started in January 1990 from climatology. The spread for temperature is larger at lower latitude and is largest at the location of the strong turbulent current, e.g. Gulf Stream, Kuroshio, Circumpolar current, and El-Ninõ. The spread of salinity is mainly located in higher latitudes where salinity becomes the controlling variable. This clearly illustrate that multivariate updates are necessary if one wish to produce improvements in high-latitude. As expected spread of ice concentration is mainly located at the ice edge. The quantitative evolution of the spread is presented in Figure 2 for each variable. There is a large variability. Temperature presents maximum in June and around December, and ice concentration (fice) in April with the maximum ice extension and salinity in September with the melting of sea ice. As the spread of fice and to a minor level salinity are constrained on a smaller area than temperature, the average estimate of the spread is smaller than for temperature.

Remaining tasks:

- The perturbations should have a Gaussian distribution (now uniform) to provide more weight to the likeliest estimate.
- For technical reason, the lag used for atmospheric forcing are constrained within the current year (i.e. within 1-365). It implies that at the beginning and at the end of the year the perturbation is not centred around the assimilation date and introduces a bias.
- It could be possible to use a more advanced technique for perturbation so that they can vary in intensity spatially or in time.
- It could be interesting to analyze the role of each perturbation separately.
- The current perturbation system does not produce any spread at the Equator. This indicates that our perturbation system is not suited there, and should be completed.
- Use the EnKF to estimate the optimal values of unknown parameters.

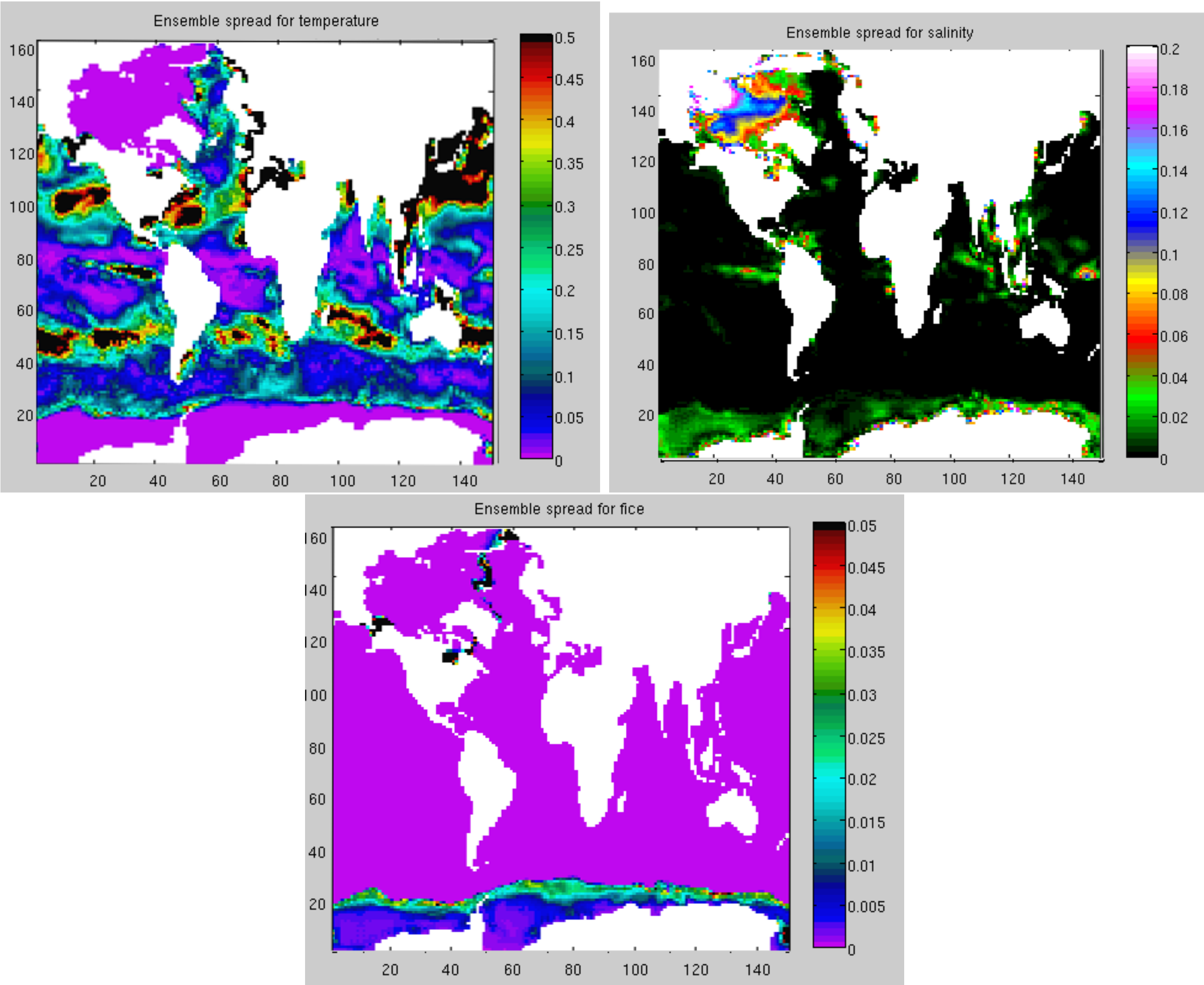


Figure 1: Ensemble spread for temperature (left), salinity (right) and ice concentration (bottom) in December 1990 computed from 40 members run with perturbations for 11 months.

5 Preparation of the observations

For simplicity and historical reasons we test first the assimilation of SST data. In view of the model resolution, we use the Reynolds SST data that provide weekly map of SST from 1981 to today with a resolution of approximately 100 km. Indeed, when the resolution of the observations is higher than that of the model, they are averaged to reach similar scale and reduce the representation error.
A script has been developed to download the data and put it in a format readable by the EnKF code. Note that only the first map of the month is retained (data is available weekly). The script is located in micom/SST_dataread/prepare_sst.sh and takes the year as input. The script must be run where the data are stored (micomassimilateSST). The final files are in ASCII format and follow the name convention: sst_$year$month.asc for the data file and a header file sst.hdr that describes the structure of the ASCII file.

A second step is necessary to interpolate the data on the model grid. For each observation, the model pivot points are computed, i.e. the model indices to which the observation belongs. The algorithms used is independent from the type of grid used (bipolar, tripolar ...). The search is adapted from the one used in MICOM. It progresses iteratively choosing the neighbouring point that minimizes the distance with the target point. The search starts from the previous pivot point kept in memory. Indeed, when the list of observation points is collocated this algorithm is very efficient. All the information necessary for the EnKF is placed in a binary file call observation.uf and a netcdf file observation.nc is created for diagnostic purpose. These files are created by the main program prep_obs. It takes as input the file infile.data that contains the name of the producer, the type of observation, the header file and the data file. Below is an example if one

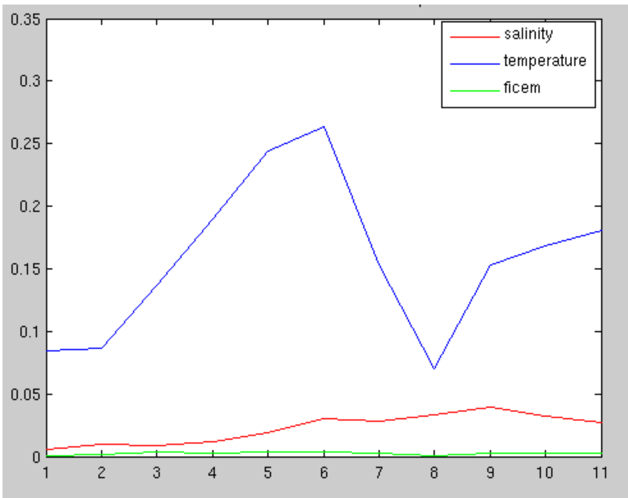


Figure 2: Ensemble spread evolution average spatially for temperature, salinity and ice concentration during 1990. (units psu, ∘ Celsius, %)

wants to assimilate Reynolds SST from January 1990:

Reynolds
SST
sst.hdr
sst_199001.asc

6 Post processing of the analysis files

The EnKF is a method that allows for multivariate updates. The multivariate changes are computed based on ensemble statistics. The EnKF code reads the file analysisfields.in that contains the name and the dimension of the variables to be corrected. The EnKF solves the analysis linearly so that the increments (i.e. the corrections applied to the forecast) are a combination of model states anomaly from the mean. If the ensemble size were infinite and variable Gaussians, the solution would be optimal. In practice, we can obtain analysis variables beyond reasonable range. A common approach is to correct a-posteriori the non-realistic values. When all MICOM variables are updated the model crashes. When only 4D (3D + time level) variables and 3D variables (2D + time level) are updated, the model restarts without any problem. The 2D variables correspond to different tracers, ice variables. One of the problems occurs when updated ice concentration is negative. A list of variables for which the assimilation is working is prepared and placed in the EnKF. micom/EnKF-MPI-TOPAZ/

A program called fixmicom post process the analysis restart files. It ensures reasonable model values and consistency between layer thickness and pressure:

- Ice concentration and thickness are positive.
- No negative dp (layer thickness). If so, it is redistributed to the neighbouring layers so that no water is lost.
- pb is recomputed from the sum of dp.
- set the two time levels equivalent for pb, dp.
- recompute: kfpla (first layer below the mix layer); "duplicated" values of pb and dp (e.g. pbu, pbv, pbu_p, pb_p,pb_mn ...)

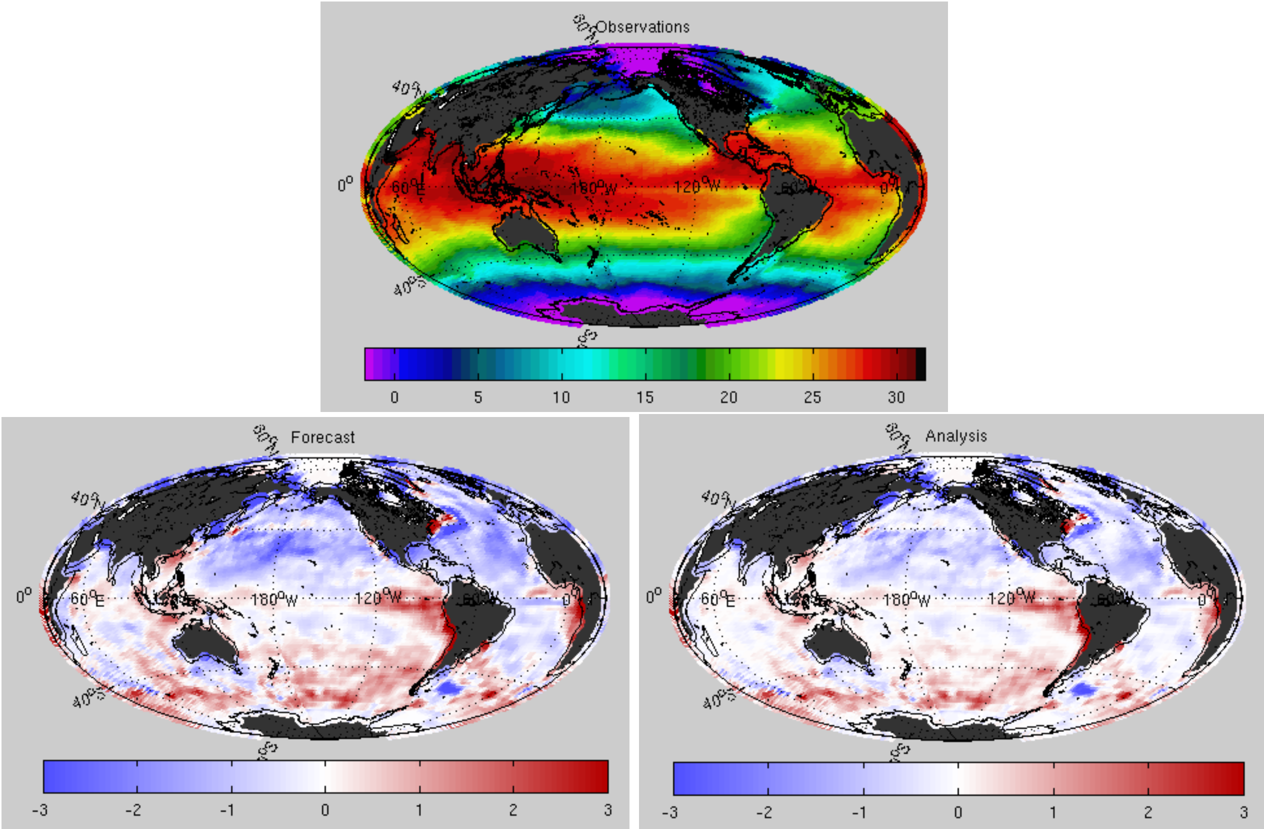


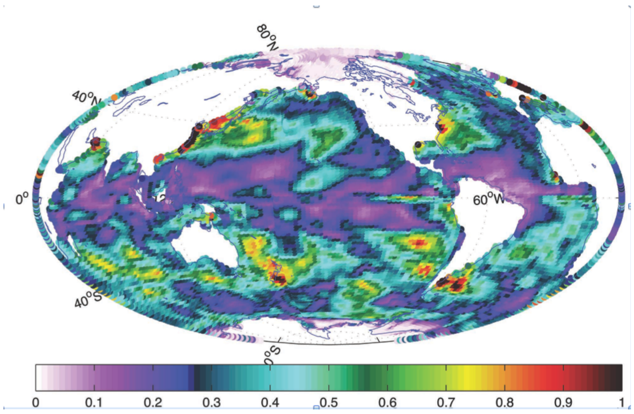
Figure 3: Example of one assimilation in April 1990: SST observation (top); model forecast minus observation (left) and model analysis minus observation (right).

Remaining task: Not all variables from the restart files are included in the analysis as it still leads to a model crash. We should identify which variables are causing the problem, but this would requires more times. The list of variables not assimilated yet is the following: tsrfm hsnwm ticem iagem tsi_tda tml_tda sml_tda alb_tda fice_tda rnfres cd_d ch_d ce_d wg2_d cd_m ch_m ce_m wg2_m rhoa frzpot mltpot.

7 Assimilation results

A main script has been created to proceed automatically this experiment. It is located in /home/nersc/fanf/micom/ma
The program automatically downloads all SST observations, and runs 40 micom members with monthly assimilation of SST over a period of 3 years (1990-1992). The ensemble forecast, analysis, and analysis diagnostics are saved in /work/fanf/$year_$month. With normal priority, the script can achieve 2 years in a day. In order to limit the amount of backup data, the main script calls the script /work/fanf/micom/Cleanup.sh that computes the ensemble average from each ensemble (analysis and forecast) and deletes the ensemble files. The last ensemble of the year is kept for restarting purposes. A year of data compressed represents 9.5 Gb. The data are saved in /migrate/fanf/Practice/$year.tar.gz

Figure 3 shows an example of assimilation in April 1990. The error is slightly reduced towards the observation. Although it is small, the effect from assimilation seems reasonable because optimal results are obtained when convergence occurs slowly. The efficiency of assimilation can vary depending on parametrisation such as localisation radius, assimilation frequency, and amplitude of the ensemble spread. The latter quantity is very useful as it provides an estimate of the model accuracy. The area where the ensemble spread is larger corresponds to area where the model is most responsive to the perturbation system. This often relates to areas where dynamics are non-linear and model most inaccurate. Figure 4 exhibits the relative good match between the model error (computed with data not yet assimilated) and the ensemble spread used as a proxy for the error. However, it seems that the ensemble spread is too small in amplitude (by a factor 3) and that the error is underestimated near the Equator. Such problems are often the result of the combined effects of



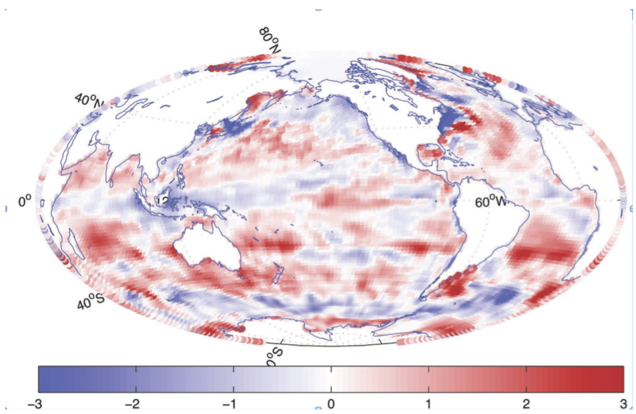


Figure 4: Ensemble spread used as a proxy for the forecast error (left). Actual forecast error computed with observation not yet assimilated (right).

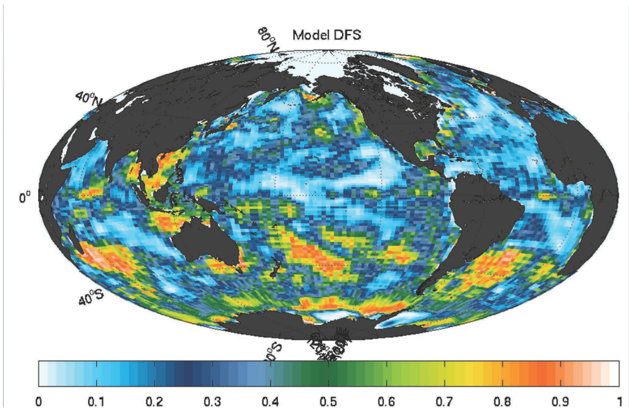


Figure 5: Degree of Freedom for signal computed in August 1990.

a too small ensemble size and an incomplete perturbation system.

It is usually difficult to quantify the multivariate impact of the assimilation as available observations covers only a small part of model variables. A common statistic used in data assimilation is the Degree of Freedom for Signal (DFS *Rodgers*, 2000). It corresponds to the trace of the Kalman gain projected on the observation space. Assuming that the proxy for the model error is perfect, it estimates the reduction of the degree of freedom resulting from assimilation. Thus, the DFS cannot exceed the ensemble size and should as a rule of thumb be about 5-10% of the ensemble size for largest update location (here between 1 and 5). In Figure 5, areas where the impact is largest are in the southern ocean in particular in the Pacific Ocean, but the impact of the assimilation seems a bit weak (rarely exceeding 1). In boreal summer time, the mix layer depths is deeper in the southern ocean and the impact from SST observations have a larger impact there.

In Figure 6 the SST RMSE from the run with assimilation is compared with a free run. The comparison is extended post assimilation period to study how long the impact remains. Between 1990 and 1993 (i.e. months 1-36 on the Figure) the assimilative run assimilates SST monthly. Between 1993 and 1995 (i.e month 37-72) boths run are continued without assimilation. The ensemble spread increases very quickly (approximately 4 months) and reaches a stable level (not shown). This indicates that we do not suffer from ensemble spread collapse that is a common cause of EnKF failure. The black line in Figure 6 represents both the RMS for forecast (prior to assimilation) and analysis state for which the error is reduced producing jumps in the curve. The latter are sharp and it seems that the benefits from assimilation are not present at next assimilation cycle (after a month). We suspect that data assimilation mainly corrects for model biases instead of correcting for the anomaly. This issue is addressed in the following paragraph. In addition to the high frequency oscillation one can notice that the error is slowly reducing compared to the free run. This is more the type of correction targeted. The most interesting and challenging period is posterior to

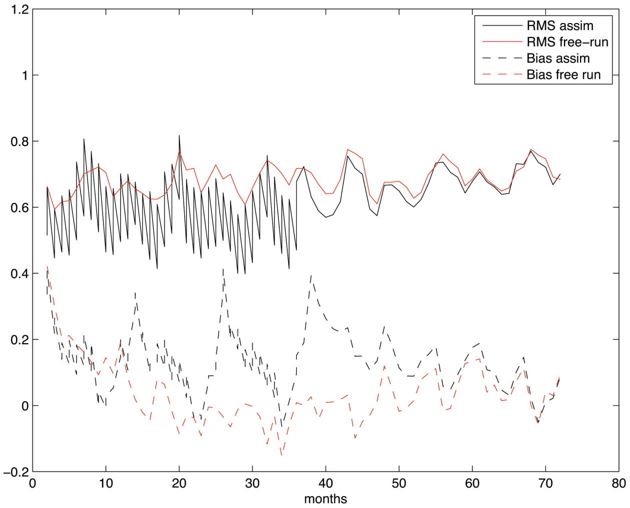


Figure 6: Comparison of a free run with an assimilated run (months 1-36) continued without assimilation (months 37-72). This experiment corresponds to the period 1990-1996.

assimilation. We have decided to continue the experiment from member 1 in order to limit the perturbation caused by the ensemble averaging. Indeed, continuing the experiment with the ensemble mean leads to instabilities that corrupt the solution. It would be interesting to test if these instabilities remain if the program fixmicom (6) was applied first. We can notice that there is some benefit from assimilation that remain posterior to the assimilation. The relative error reduction is of 7% the first year posterior to assimilation, 3% the second and just 1% the third year. One should remember that in the current set up, both simulations are forced with similar NCEP forcing, damping the discrepancies. It is possible that the benefits remain longer using a coupled atmospheric-ocean model. Figure 6 shows also the model bias with a dashed line. It seems that data assimilation has no beneficial impact on this quantity. In particular, one can also notice that at proximity of the changing year, there is a sudden increase in the bias. These jumps are most likely caused by the implementation of our perturbation system for atmospheric forcing that are biased at each change of year (see Section 4).

During the assimilation phase, we have seen that most of the error reduction induced by assimilation was no longer present at the next assimilation cycle, producing jumps in the RMSE curve of Figure 6. Such behaviour is common when data assimilation corrects for bias in a model that does not sustain changes "proposed" by assimilation. We have tried to identify the model bias in the current simulation. Figure 7 shows the histogram of SST for the model and observation. The two distributions are reasonably alike, but the model underestimates high SST values. The model resolution is yet another limitation as with coarse resolution the location of the main currents are misplaced, e.g. position of the Gulf Stream. Figure 8 represent the average of the innovations over the 3-year period. One would expect some white noise, but the plot clearly highlights the misplacement of the main currents. Instead of correcting for SST anomalies, data assimilation is repetitively trying to replace these currents. Biases in data assimilation is problematic because it limits the impact from assimilation and it can lead to repetitive updates that may amplify spurious low correlation. There are different manners to handle this problem. *Smith et al.* (2007); *Keenlyside et al.* (2008); *Pohlmann et al.* (2009) correct for the anomaly and not for the observation because their model are too far off from the observation. By this mean the model bias (Figure 8) would be zero. A more advanced way is to estimate online the model bias using the EnKF. For doing so, one just need to extend the model state with bias values that are initialised at random. After several cycle, the estimate would converge towards the parametrisation, hopefully providing best agreement with observation. So comparatively with the first approach, one estimate a spatial bias of SST but in addition allows the bias to evolve with time (e.g. seasonally). Such approach is currently used in the reanalysis of TOPAZ system.

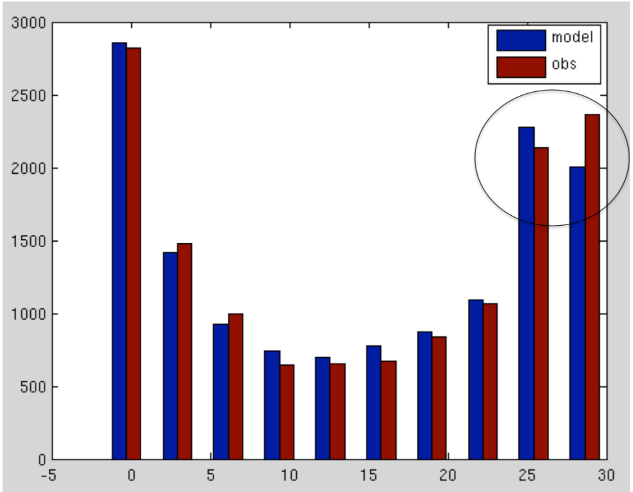


Figure 7: Histogram of SST for the model (in blue) and observations (in red) on January 1991.

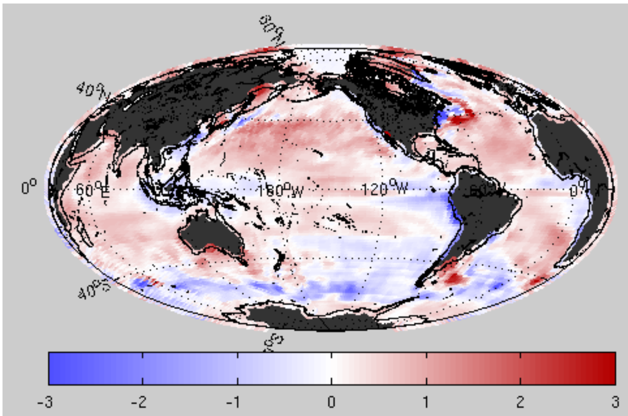


Figure 8: Spatial average of innovations (i.e. model - observation).
over the three years experiment.

8 Conclusion

The EnKF has been implemented within the framework of NorESM. The changes to the code are made so that the code can be easily updated with more recent version of EnKF. The code implemented can be easily modified to assimilate other types of measurement. A list of parameter in the ocean part of NorESM is identified to simulate the model error, but the spread in the equatorial area seems to be underestimated. As a first step towards estimating the optimal initial state for restarting the fully high resolution Earth system model, a simple test is carried out. The model is forced with NCEP forcing fields; the ocean model has coarse resolution; the ice dynamics is not activated; only SST is assimilated, and the ensemble consist of only 40 members. The system is assimilating monthly over a three years period, and continues in free run model for three more years. The accuracy is compared to a free run using similar initial state and forcing fields. It highlights that :

- Data assimilation reduces the RMS error of SST during assimilation.
- Benefits remains for approximately 2 years after observations are no longer assimilated. This corresponds to much longer period than the memory window of SST, suggesting that the multivariate changes have affected the interior water masses and energy of the system.
- The current system corrects mainly for model biases originating from the misplacement of the main currents and misrepresentation of some water masses.

The results from this first experiment are encouraging as there is room for improvement:

- The newer version of the EnKF solves the analysis with a more precautious approach: i.e. by enlarging the observation error when the observation does not fall within the ensemble spread.
- The EnKF should ignore model biases as they limits the impact from assimilation and can amplify spurious correlation.
- The forgetting factor of SST is rather small compare to other observation types and it is expected that a better realism of the initial state can be obtained assimilating also altimetry, ice concentration and ARGO profiles.
- Special care should be taken considering the variables assimilated to ensure that assimilation updates are in equilibrium with model dynamics.
- Data assimilation parameter such as localization radius, assimilation frequency, ensemble size and inflation factor should be tuned for best performance.
- Sensibility to the ensemble size should be studied.

Finally, it is expected that with higher resolution and with a fully coupled system more informations can be extracted from observations. For example correcting for mesoscale circulations contained in observations can benefit a more realistic correction. Using a coupled model would also lead to a more realistic perturbation system. But, one can also expect these changes to raise new problems as a fully coupled high-resolution system: have a much higher dimension so that the representativity of the ensemble in proportion is reduced; will be more unstable and thus more responsive to assimilation noise and the multivariate updates will become complex as the time scale between the ocean and the atmospheric part are radically different.

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