Ocean Data Assimilation

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1 Introduction

The seminar covers a number of different applications where ocean data assimilation is important, in particular the topics of (i) Operational oceanography, (ii) Ocean data synthesis/reanalysis, and (iii) Seasonal-decadal forecasting. In covering these applications we look at the assimilation of several different ocean data sets, in particular, (a) sea level anomalies from satellite altimeters, (b) Geoid information from the ESA-GOCE mission, and (c) In situ temperature and salinity profile data giving information on the subsurface ocean. The lecture will also touch on several important advanced problems in ocean data assimilation science of relevance to these data sets, including (1) Treatment of Observational bias, (2) the importance of state dependent covariances and (3) the need to develop methods suitable for data assimilation into fully coupled atmosphere-ocean models. In Operational oceanography the main task is to produce short term forecasts (usually out to 1 or 2 weeks ahead, comparable with the availability of medium range meteorological predictions used for forcing) of the near surface currents and ocean temperatures. Although operational oceanography centres, such as the Met Office in the UK, run global and basin scale ocean models at various resolutions constrained by satellite and in situ data assimilation, most of the user requirements are for high resolution shelf and coastal models which are run nested within the larger models, and which currently use very little data assimilation. In particular there is potential to develop the use of altimeter data in coastal model systems. In the following section we look at two particular aspects of the Altimeter data assimilation problem, the vertical projection of the altimeter data to influence the subsurface ocean, and the treatment of the uncertain Geoid as an observation bias problem in altimeter data assimilation.

2 Altimeter Data Assimilation

2.1 Vertical projection of altimeter data

The sea level changes measured by altimetry must be projected onto the baroclinic and barotropic modes of the ocean circulation model during assimilation. Figure 1 shows correlations between sea level anomalies and deep density anomalies in an early version of the US east coast model (Mellor and Ezer 1991). Such correlations can only be determined from long model runs and may thus be inaccurate and prone to reflect model biases. It may be necessary to make such covariances dependent on (x,y,t) and also potentially state dependent eg. on the presence of El Nino conditions if in the Pacific, all of which make the assimilation procedure more costly and data intensive. Cooper and Haines (1996) proposed making sea level anomalies proportional to vertical thermocline displacements, closing the problem by assuming no change to the deep pressure. This greatly simplifies the problem of determining model state variables from the altimeter measured sea level and variations on this system are now widely used operationally eg. at Met Office and ECMWF. Equation 1 summarises the key relations between sea level, thermocline displacements and changes in the local density profile.

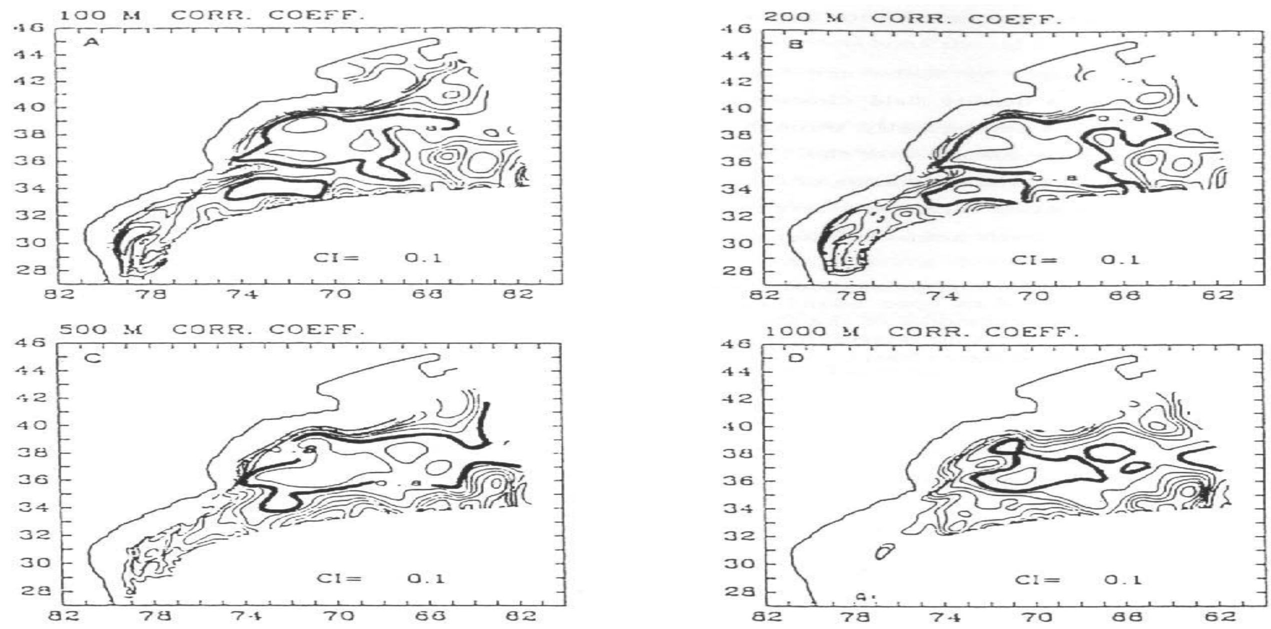

Figure 1: Correlation coefficient between density variations at different depths, and sea surface height variations, in an early version of the US East Coast forecasting model, from Mellor and Ezer (1991). The high correlations (>0.8 bold contour) were used for projecting surface height data to depth for altimeter assimilation.

$$\rho_0 g \delta\eta = -g \int_{-H}^{0} \Delta\rho dz; \quad where \quad \Delta\rho = \frac{\partial\rho}{\partial z}\Delta h \tag{1}$$

The density changes $\Delta\rho$ for any given sea level increment $\delta\eta$ depend on the local stratification and are thus state dependent. The method has the additional attraction of conserving Lagrangian water mass properties and volumes on isopycnal surfaces (water masses are merely displaced). This allows complementary data sets such as in situ water profile measurements to contribute separate information within a combined assimilation system. Such a state dependent derivation of model variables from sea level is an example of the use of ”balancing increments”, Derber and Wu (1998), Weaver et al (2005) who show how such schemes can be built into Variational or Kalman filter frameworks. In the altimeter assimilation case the unbalanced increments would consist of changes in stratification which do not change the total dynamic height of the water column, or changes in the T,S properties which would not change the density of the water column. Such changes would be undetectable in sea level measurements and thus properly subject to determination from a separate data stream i.e. in situ data.

Figure 2 shows application of this altimeter assimilation scheme applied sequentially in an ideal twin experiment in a double gyre ocean model. Figure 3 shows a similar twin experiment with a full ocean GCM, the OCCAM model (Webb et al 1997) run at 1/4 degree global resolution. The deep pressure and Geostrophic velocity fields (the streamfunction fields in the double gyre model) tend to improve immediately upon assimilating sea level (surface streamfunction) information, and diverge between assimilation times. In contrast the water properties of temperature, salinity and density, (e.g. potential vorticity in the double gyre model) improve between assimilation times as they are advected by the better velocity fields. In Figure 3 water properties, temperature errors etc, are compared at fixed depth levels and therefore show improvements at assimilation times while no change would be seen to properties on the isopycnal surfaces. It can be seen in the double gyre model that the layer 2, 3, 4 potential vorticity errors do not change at the assimilation times. These experiments demonstrate that altimeter data should allow us to improve knowledge of the deeper circulation, at least through the thermocline, and to improve the water mass distributions through advection. It should now be possible to

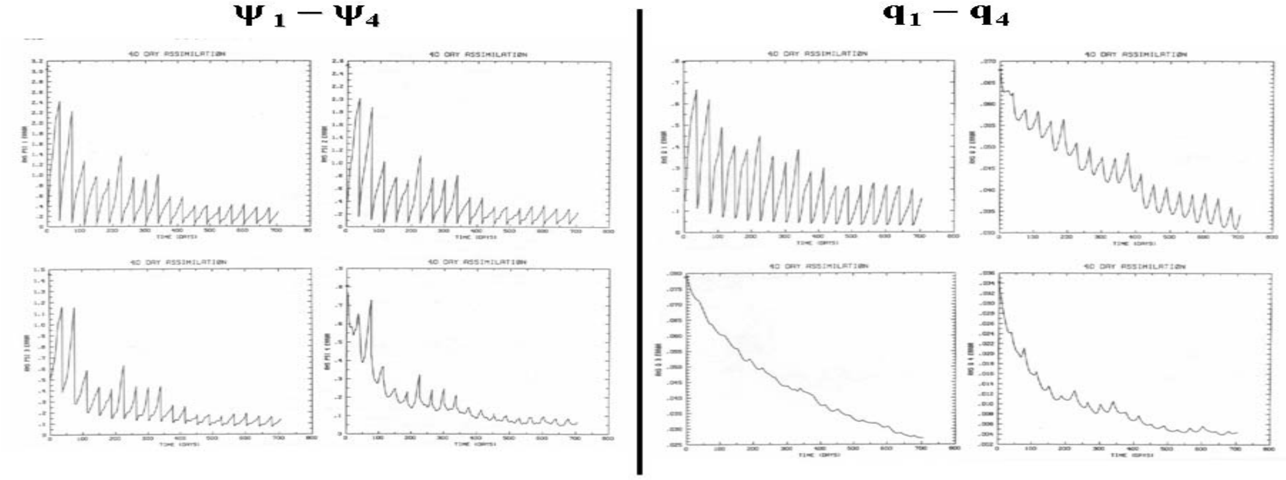

Figure 2: Timeseries of streamfunction (left) and (qg) potential vorticity (right) RMS errors from an ideal twin data assimilation experiment with a 4 layer double gyre ocean model. Assimilated data consist of the upper layer streamfunction ψ_1 (top left) every 40 days. From Haines (1991)

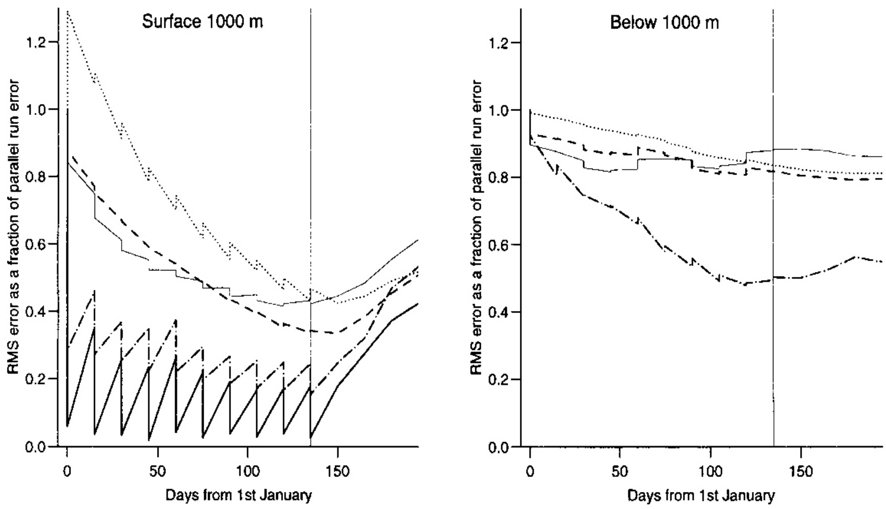

Fig. 3. As for Fig. 1 but calculated for the Gulf Stream/North Atlantic Current region. 30–80°W, 30–45°N.

Figure 3: Timeseries of sea surface height (SSH), u,v velocity and T,S, ρ errors from an identical twin experiment with the OCCAM global 1/4 degree model. Upper ocean (top 1000m) errors are on the left and deep ocean (below 1000m) are on the right. Assimilation of SSH is every 10 days. From Fox et al (2001).

show this improvement of the water properties with real altimeter data by using the newly completed network of Argo float in situ data (see later) to test for the improvement of water mass distributions, as in Figure 3.

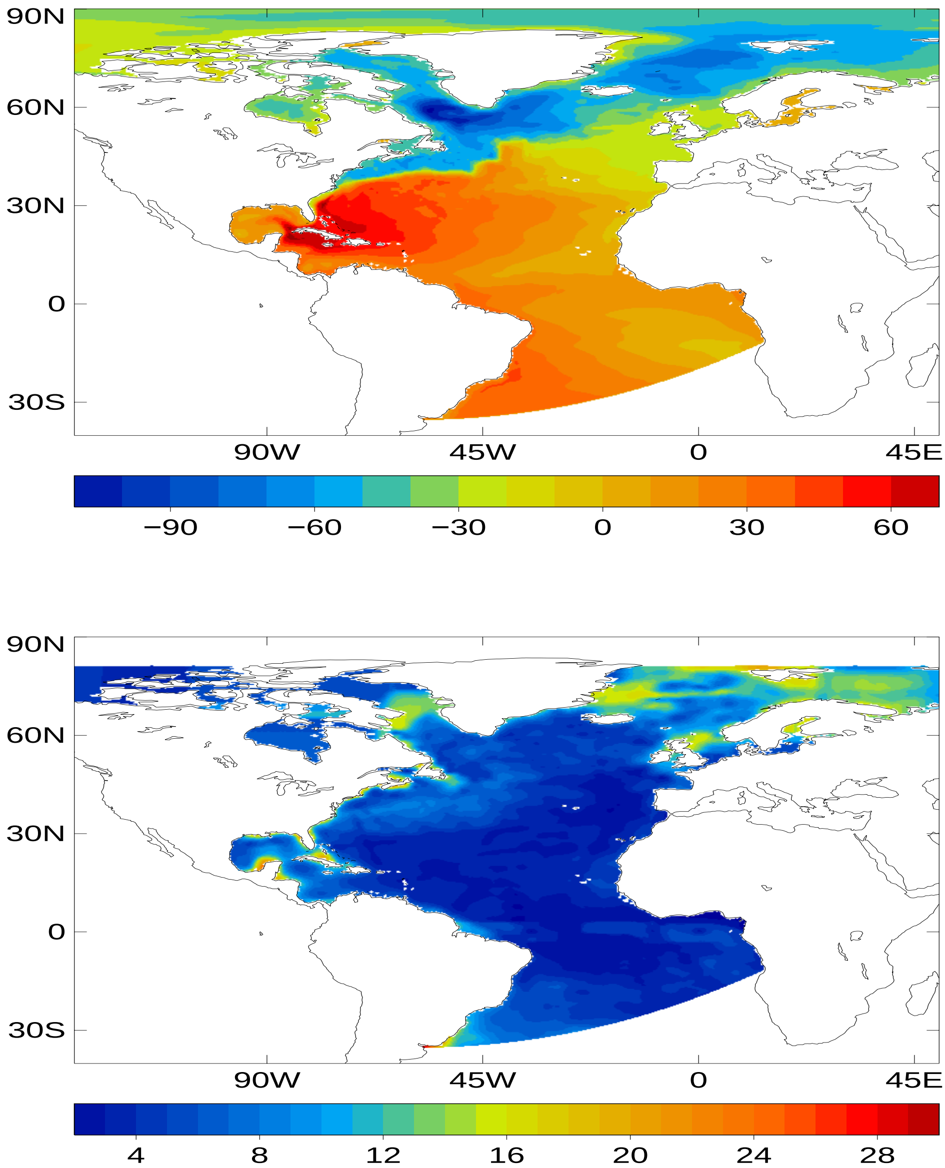

Figure 4: Top: The mean dynamic topography used in the Met Office operational oceanography FOAM model as part of the data assimilation procedure for altimeter data. Bottom: The error variance assumed to be associated with this mean dynamic topography and within which the bias scheme will allow variations. (Units cm, cm^2)

2.2 Mean sea level assimilation

The second problem for assimilating altimeter data is how to treat the mean sea level. The Dynamic topography signal that is assimilated is made up of 2 components given in Eq 2

$$\eta = < \eta > + \delta\eta \tag{2}$$

The sea level anomalies $\delta\eta$ measured by altimeters give the time dependent component of the sea level slopes, however the time-mean dynamic topography $<\eta>$ cannot be determined from altimeter data without knowledge of the Geoid slopes, as given by;

$$<\eta>= MSSH - Geoid \tag{3}$$

where MSSH is the mean sea surface height from altimetry.

The ESA GOCE mission will provide a geoid along with its covariance errors at sufficient accuracy to solve Eq 3. However the total assimilated signal will still be made up of 2 components with very different error characteristics. The mean dynamic topography component will have a considerably higher error than the altimeter anomalies, even if GOCE is a success. This uncertainty is best represented as an unknown time-constant observation bias which can be incorporated into a sequential data assimilation, scheme as in Drecourt et al (2006), Lea et al (2007). The 3dVar problem for the analysed sea level at each analysis time can (neglecting observation operators) be written as;

$$\begin{aligned} J(x,b,c) = (y-b-x)^T R^{-1}(y-b-x) + (x-x^f+c)^T B^{-1}(x-x^f+c) \\ +(b-b^f)^T O^{-1}(b-b^f) + (b)^T T^{-1}(b) + (c-c^f)^T P^{-1}(c-c^f) \end{aligned} \tag{4}$$

allowing for both observation bias b, and model bias c, components to the sea level. Observation bias is assumed to be constant in time and to have a small scale error covariance T,O, while model bias is assumed to have a larger scale error covariance P, and to represent all the detectable time varying component of the bias, eg. from the seasonal cycle. This suggests bias forecast ^{f} models given by Eq 5

$$b^f(t+1) = b^a(t); \quad and \quad c^f(t+1) = \beta c^a(t). \tag{5}$$

This scheme was implemented in the Met Office operational oceanography model FOAM in the 1/9 N Atlantic basin model for the period 2001-2005 inclusive, Drecourt et al (2006), Lea et al (2007). Figure 4 shows the mean dynamic topography used in the model (Martin et al) as well as the spatial structure of the observation bias error variance, **T**, **O**, (with a 60km covariance scale) assumed to be associated with it, (taken from 5 x Rio 2005 errors, purely as an example because the true error covariance is unknown). In contrast the model bias error variance, **P**, is assumed uniform, 2cm, with a covariance scale of 400km. This scale difference, along with the different time evolution in Eq 4, is what allows the observation and model bias errors to be separated.

Figure 5 shows time series of the mean and the standard deviation of the sea level innovations for 4 separate 5 year long experiments with and without the observational and model bias schemes applied. It can be seen that the bias terms reduce not only the innovation biases but also the standard deviations, showing that improved skill in forecasting the altimetric anomaly component of the sea level signal can be gained. Figure 6 shows the analysed mean dynamic topography bias and the mean model sea level bias identified by the scheme, illustrating the different scales and amplitudes. When the GOCE geoid is used to derive the mean dynamic topography it will be possible to use the GOCE covariance errors to condition this bias calculation properly.

3 Ocean data Synthesis / Reanalysis

The challenge for ocean synthesis or reanalysis is two-fold. First there is a need to reproduce ocean circulation and transport information, from observations which primarily consist of ocean density (temperature and salinity measurements). The second challenge is to quantify the evolution of ocean water mass volumes and properties, taking advantage of the longer timescales associated with changes in such water properties, compared with those corresponding to air-masses in the atmosphere. This longer timescale gives some hope that climatically

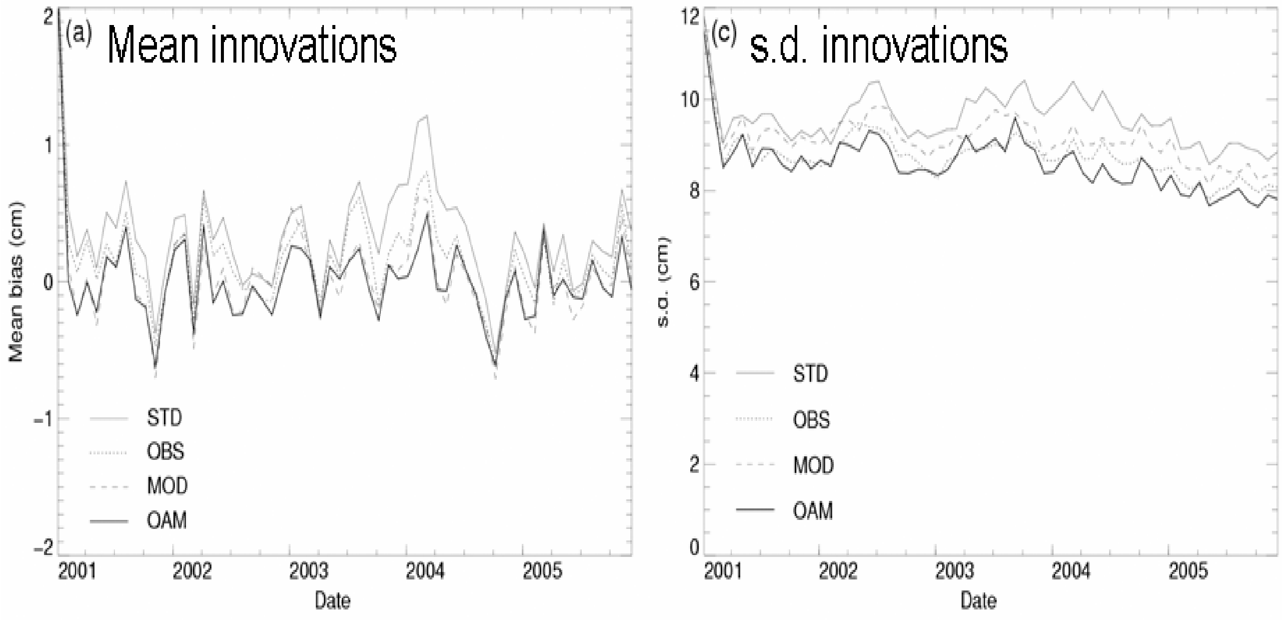

Figure 5: Left: The mean sea level innovations over the FOAM model domain from 4 altimeter assimilation experiments from 2001-2005 inclusive. STD= No bias scheme; OBS= Observation bias only; MOD= Model bias only; OAM= Both bias schemes. Right: Same experiments but for the standard deviation of the sea level innovations.

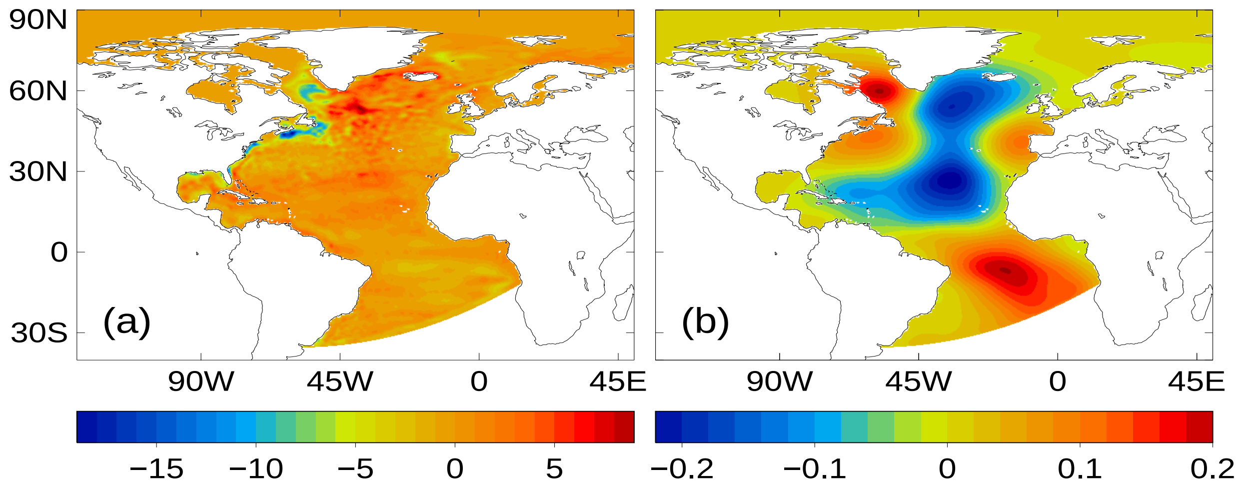

Figure 6: The mean Observation (left) and Model (right) bias fields identified by the scheme for the OAM assimilation experiments (OAM has both bias schemes applied together). The different scales of the bias correction terms can be seen. Although these fields have opposite signs at larger scales they both represent reductions of the same sign in the overall innovations. Units cm, cm/day.

relevant slowly changing signals might be identified from a good ocean data synthesis experiment, despite the sparsity of historical ocean data. A good ocean model, together with an ocean data assimilation approach that takes care to maximise the recovery of water mass information, are essential pre-requisites for a successful synthesis.

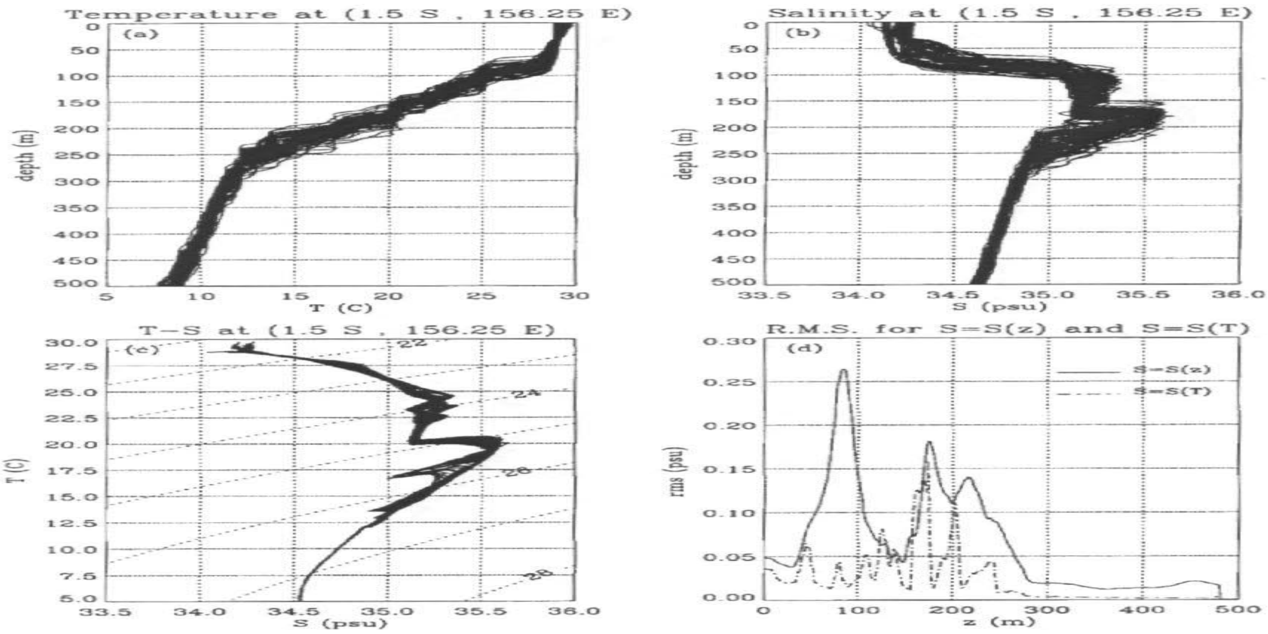

Figure 7: Comparison of Salinity variance measured in 2 different ways, based on repeated ocean profiles in the same location in the tropical Pacific. In the lower right figure S(z) shows salinity variance directly calculated from the salinity profiles at given depth levels. S(T) shows the salinity variance calculated on a set of isotherms, and then recast onto depth levels using the mean temperature profile at this location.

Temperature T, and salinity S, profiles provide observations of the physical properties of water masses, and together they also define the water density which controls pressure gradients and hence ocean circulation. Much of the historical data record is made up of T profiles alone. Figure 7 shows an example of the temporal variance of salinity S(z) compared to S(T) at one location, illustrating that much of the salinity variance in the ocean can be explained from temperature because both are Lagrangian properties affected by dynamical motions in the same way. Given this fact Haines et al (2006) have suggested that salinity data can be used to effectively recover the more subtle thermodynamic variation in water mass properties if this dynamic variability can be filtered out (because it can be recovered from the more numerous temperature measurements). For example Figure 8 shows one point correlation maps of S(z) compared with S(T) from an eddy permitting ocean model. The larger length scales associated with S(T) correlations suggests that assimilation of S(T) directly will allow larger spatial correlations to be used. This thermodynamic variability of water mass properties can also be shown to be dominated by longer timescales than most dynamical variability. These results suggest the possibility to allow a more effective use of sparse historical observations of ocean water properties in data assimilation synthesis experiments, giving a better chance of recovering and understanding climatically interesting ocean water mass signals. The equations for the application of such an assimilation method are shown in Eq 6

$$T(z) = T(z) + \Delta T(z); \quad S'(z) = S(z) + \delta S(z); \quad S(T) = S'(T) + \Delta S(T) \tag{6}$$

The gain for the assimilation of S(T) can be larger than would be the case for a conventional assimilation of S(z), by virtue of the larger length and timescales noted above, and the likely better representativity error assumptions.

Figures 9 and 10 show results from one such ocean reanalysis experiment based on the ECMWF Ocean Reanalysis System 3 (ORA3) used for seasonal forecasting, which has adopted the water mass based assimilation

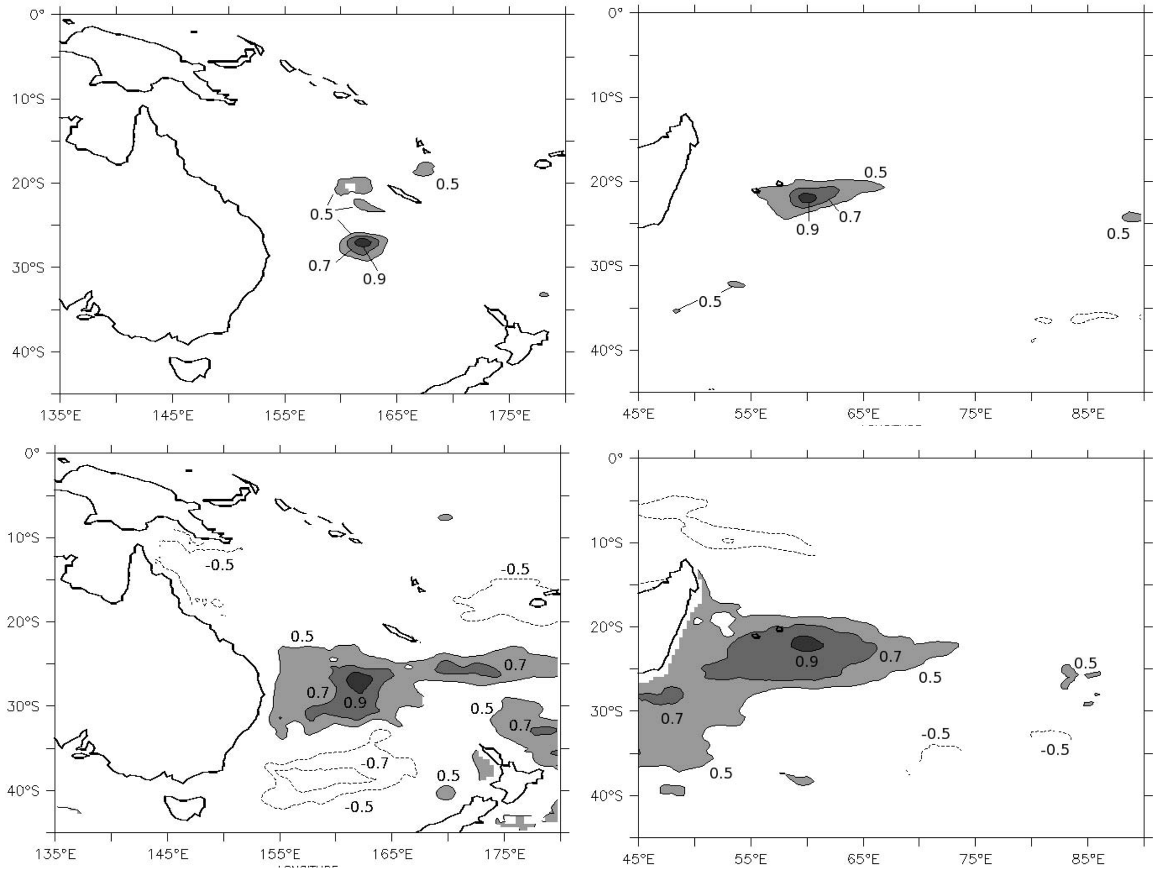

Figure 8: One point correlation maps of salinity variability at the 400m depth level (left) and on the 12C isotherm (right) (whose mean depth is 400m at the locations chosen) at 2 locations off East Australia (top), and east of Madagascar (bottom). Based on 10 years of monthly variability in the 1/3 HadCEM eddy permitting climate model.

method described above. Figure 9 shows the successive improvement of the models ability to predict ocean temperature and salinity profiles based on previously assimilated information (observation minus background errors), from experiments with no assimilation, with only temperature profile data assimilated, and with both temperature and salinity profile data assimilated. The second figure 10 shows the recovery of Atlantic MOC strength at 26N over a 40 year period, in comparison with snapshot observations from Bryden et al (2005). It is seen that the ORA3 experiment does a very good job of recovering the MOC transports where they were directly inferred (red dots), and thus give some confidence in the continuous record of the MOC obtained from 1960 onwards.

Finally figure 11 shows results from extending this assimilation approach away from using temperature and salinity as the independent variables (the results in figure 7 show that they are not independent) to using density as the dynamical variable and spiceness on a density surface as the thermodynamic variable. Spiceness is a function of T,S which is nearly orthogonal to density. These variables are, by construction, more independent, and moving to an isopycnal framework should give an approach that will also work at higher latitudes. The figure shows a cross section through the Gulf stream during assimilation of a single profile of T,S data; with background and analysed isopycnal positions on the left, and the spiceness innovations on isopycnals on the right. The greater horizontal spreading scale for the spiceness anomalies (the water mass or thermodynamic variable) can be easily seen. Work is underway to produce a new ORA3 type 40 year ocean synthesis using a density and spiceness assimilation scheme.

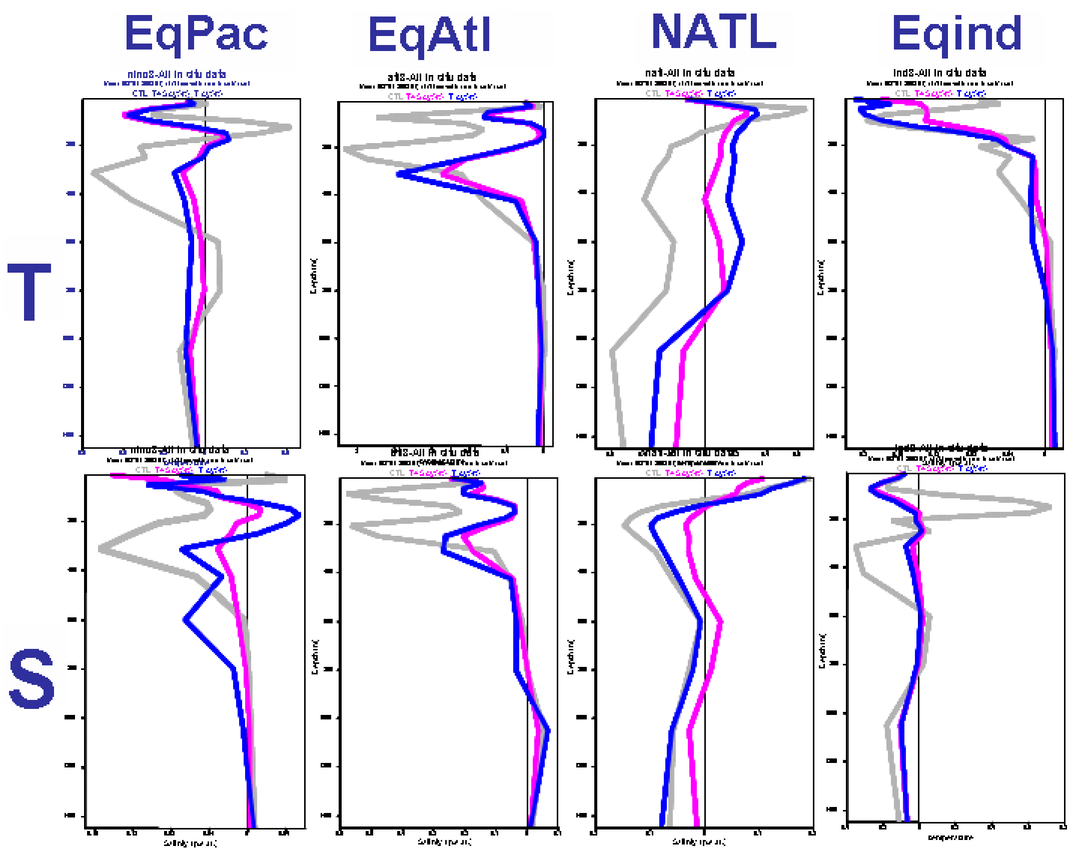

Figure 9: RMS error profiles for temperature (top) and salinity (bottom) in various ocean basins (left to right); Eq. Pacific, Eq. Atlantic, N. Atlantic and Eq. Indian. From the ECMWF ORA3 ocean reanalysis from 1991-2001. The grey, blue and pink lines show the control, T only assimilation, and T,S assimilation results respectively.

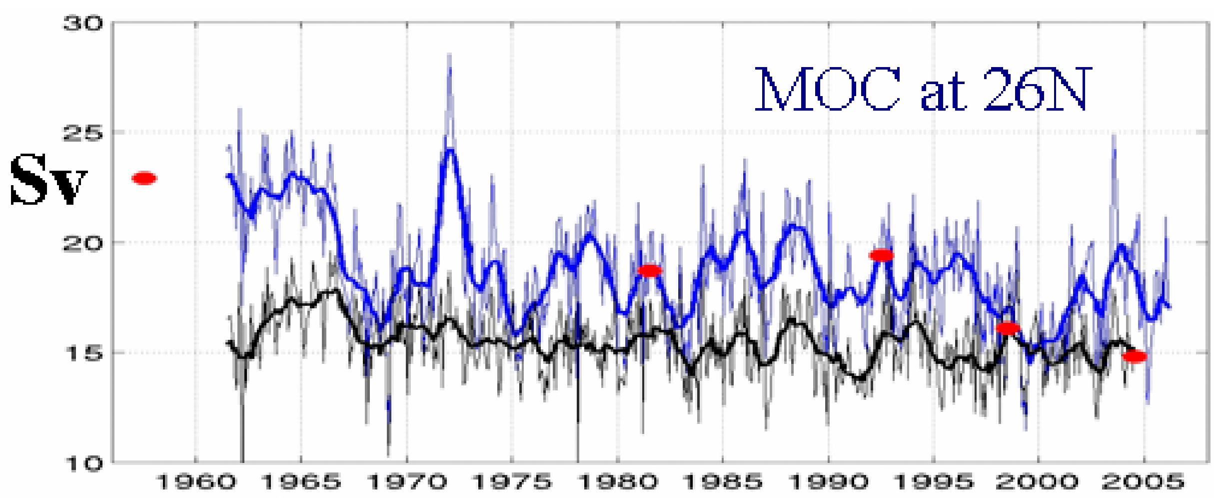

Figure 10: The timeseries of the Meridional Overturning Circulation at 26N in the Atlantic, as reproduced from the ORA3 reanalysis, blue (no assim in black). The superimposed point observations are annual mean estimates from Bryden et al 2005 based on section data. Figure based on Balmaseda et al 2007.

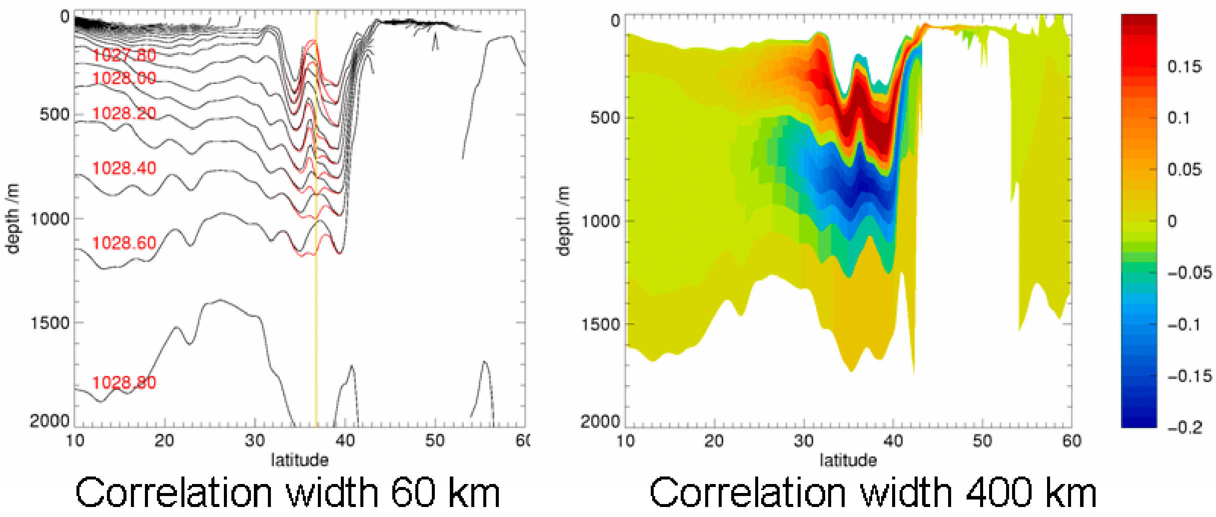

Figure 11: Isopycnal assimilation analysis from a single observation profile applied to the Met Office FOAM 1/9 N Atlantic model. The background (black) and analysed (red) isopycnal positions are shown on the left, and the spiceness innovations are shown on the right. Dan Lea Per. Comm.

4 Seasonal-Interannual prediction and Coupled data assimilation

The key requirements for seasonal-interannual, out to decadal, prediction are that it is based on ocean-atmosphere coupled modelling, and it always needs to be carried out through ensemble runs of such coupled models in order to average over the noise, introduced mainly from the highly variable and chaotic atmospheric component of the system. Ocean initial conditions are crucial to such forecasts and therefore ocean assimilation has been a large topic for the El Nino seasonal forecasting community, however other slowly evolving components of the coupled system may also be important such as soil moisture, snow cover and sea ice distributions, although much less work has gone into these aspects in a forecasting context. The ORA3 assimilation system implemented at ECMWF has already been partly described under the heading of ocean reanalysis. In seasonal forecasting mode the ocean data assimilation is performed within an ocean only model forced with analysed surface meteorology, before the ocean model is finally coupled to an atmospheric model which has similarly had independent atmospheric assimilation performed, and the two allowed to run forward freely as a coupled system.

This approach is known to have particular problems associated with shocks as the ocean and atmospheric boundary layers come into equilibrium with one another over the first hours and days of the coupled integration, which typically last out to 6 months ahead. Stockdale 1997 notes that large and rather unrealistic changes in SSTs sometimes occur in the El Nino region of the tropical Pacific within a few days. It is not clear how large a detrimental effect such initial shocks have on the coupled forecasts. An obvious solution is to seek ways of assimilating both atmosphere and ocean data directly into the coupled system prior to launching forecasts, i.e. coupled data assimilation.

The problems of coupled atmosphere-ocean data assimilation essentially arise from the mismatch in timescales of the two systems. Recently the Japan Agency for Marine Science and Technology, JAMSTEC, have had some success in developing a 4dVar scheme for their coupled model that appears to overcome this problem. Using 9 month windows overlapping with previous and successive windows by 3 months, they seek to optimise initial ocean conditions and air-sea interaction parameters in the model. The assimilated ocean data include altimeter sea-level anomalies, Reynolds SST, and in situ T,S profiles, and the atmospheric data include winds, temperature and humidity from NCEP, as well as ocean surface wind data from SSM/I. It would be impossible to match atmospheric data over such a long period as 9 months in coupled model runs so the matching operation in the adjoint of the coupled system only seeks to match running 10 day mean atmospheric fields $\bar{x}$, and in addition the atmospheric adjoint parameters λ are damped, Γ, to reduce the error growth rates, as shown in the adjoint equation below;

$$-\frac{\partial \lambda}{\partial t} = (\frac{\partial M}{\partial x})^T_{x=\bar{x}}\lambda - \Gamma\lambda + H^T R^{-1}(H\bar{x} - y) \tag{7}$$

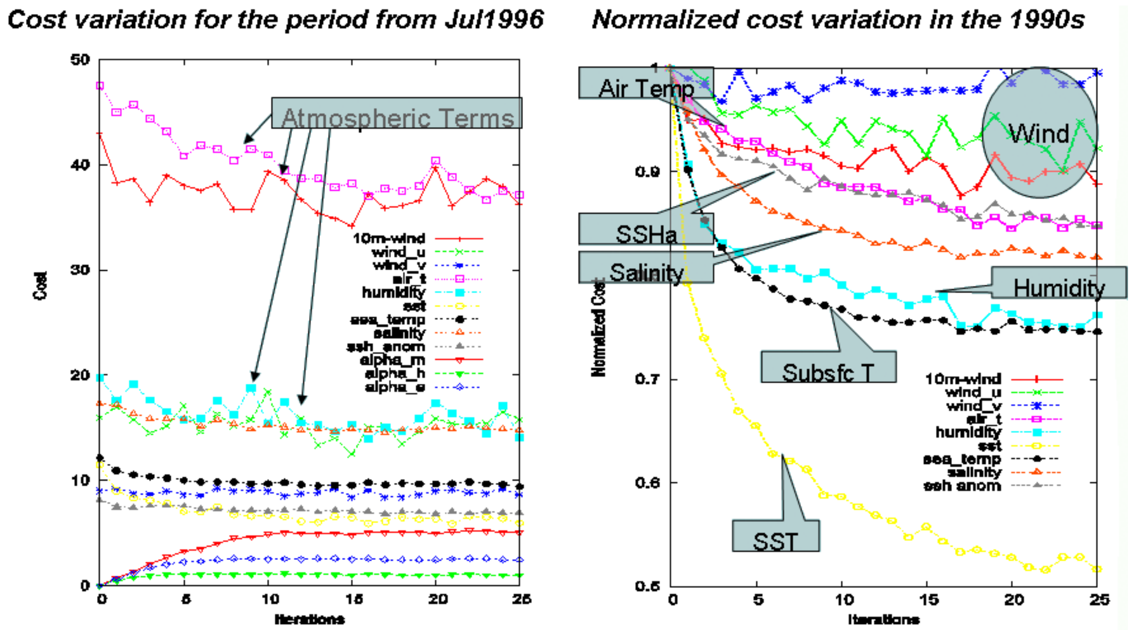

Figure 12: Cost function minimisation from the JAMSTEC coupled 4dVar system showing Left: the atmospheric state minimisation for the 9 month period beginning in July 1996; and Right: the normalised cost function minimisation for atmospheric and oceanic state variables for minimisations throughout the 1990's.

Results on the minimization of various components of the cost function (atmospheric on the left and oceanic on the right) are shown in Figure 12 The excellent reductions in the oceanic cost function component are reflected in Figure 13 which shows the overlapping 9 month Nino 3.4 values both for the first guess and the analysed 4dVar solutions, along with ensemble spread information (based on 11 ensemble members) and validation data. The excellent fit of the analysed 9 month solutions, which are free runs of the coupled model system, illustrate the success of the method. The approach therefore provides both a reanalysis framework for the oceans as well as a methodology for producing balanced initial conditions for seasonal forecasting.

At the other end of the scale of assimilation sophistication, but still based on coupled modelling throughout, is the Hadley Centre DePreSys system for interannual-decadal prediction recently published by Smith et al (2007). This is an anomaly assimilation system based on the Hadley Centre HadCM3 coupled model. Atmospheric anomaly 3D winds, temperatures, and surface pressure, every 6 hours, are calculated from ECMWF ERA15/40 data from an average period of 1979-2001. The oceanic anomaly data is calculated from a monthly gridded ocean data product developed by Ingleby and Huddleston (2007) using the same mean period as for the atmospheric data. Atmospheric and oceanic anomaly fields are projected onto the HadCM3 grid and combined with the equivalent HadCM3 model mean value from a run over the same period with varying Greenhouse gas, solar and aerosol forcing (for more details see Smith et al 2007). The assimilation system then used is crude, but is based on the coupled model at all times, consisting of running the coupled model while nudging both atmosphere and ocean fields towards the combination analysed fields described above on a very fast 6 hourly timescale. This was done for the period 1979-2001, with a series of free coupled hindcast ensemble experiments being launched regularly throughout the period.

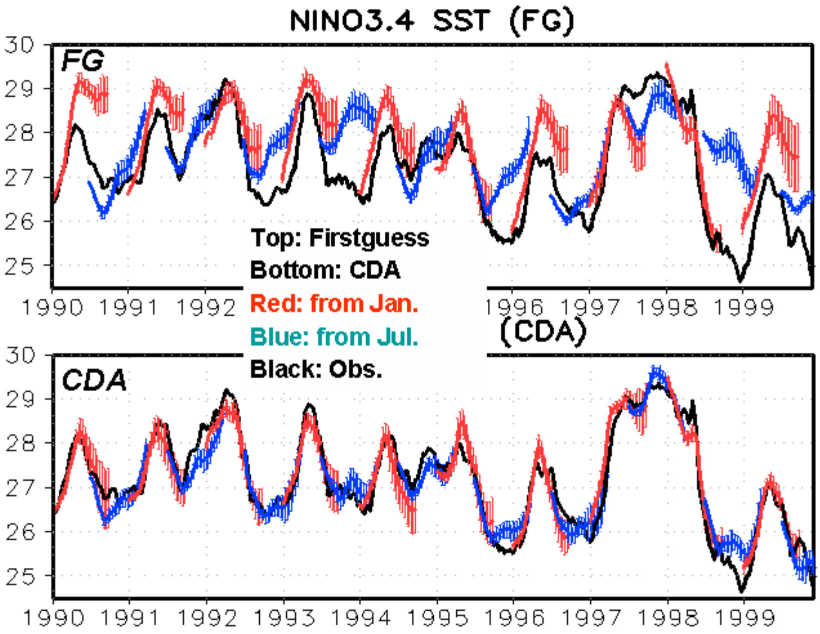

Figure 13: The impact of 4dVar assimilation on the Nino3.4 sea surface temperatures for overlapping 9 month periods. Upper panel shows the background Nino3.4 state (1st integrations) while the lower panel shows the final converged states. From the JAMSTEC coupled system.

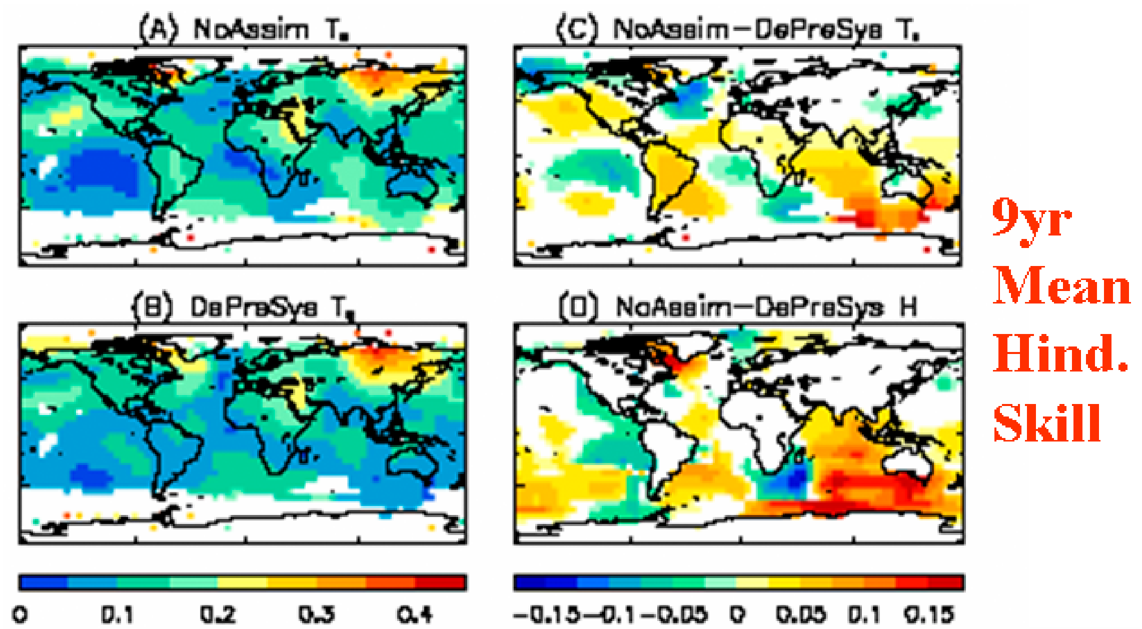

Figure 14: Impact of assimilation on 9 year hindcast mean regional surface temperature RMS errors. A,B shows the RMS errors for the system without and with data assimilation respectively. C shows the difference in RMSE A-B for surface temperature. D shows the equivalent RMSE different for upper ocean (100m) heat content. Results smoothed on a 35 degree Lat-Long scale. From Smith et al 2007.

Figure 14 shows the hindcast skill from this DePreSys system, for global surface air temperature anomalies and upper ocean heat content anomalies, as the mean skill from ensembles of 9 year hindcasts. In particular significant improvements in skill are seen between the assimilation hindcast experiments and an equivalent set with no atmosphere or ocean Assimilation.

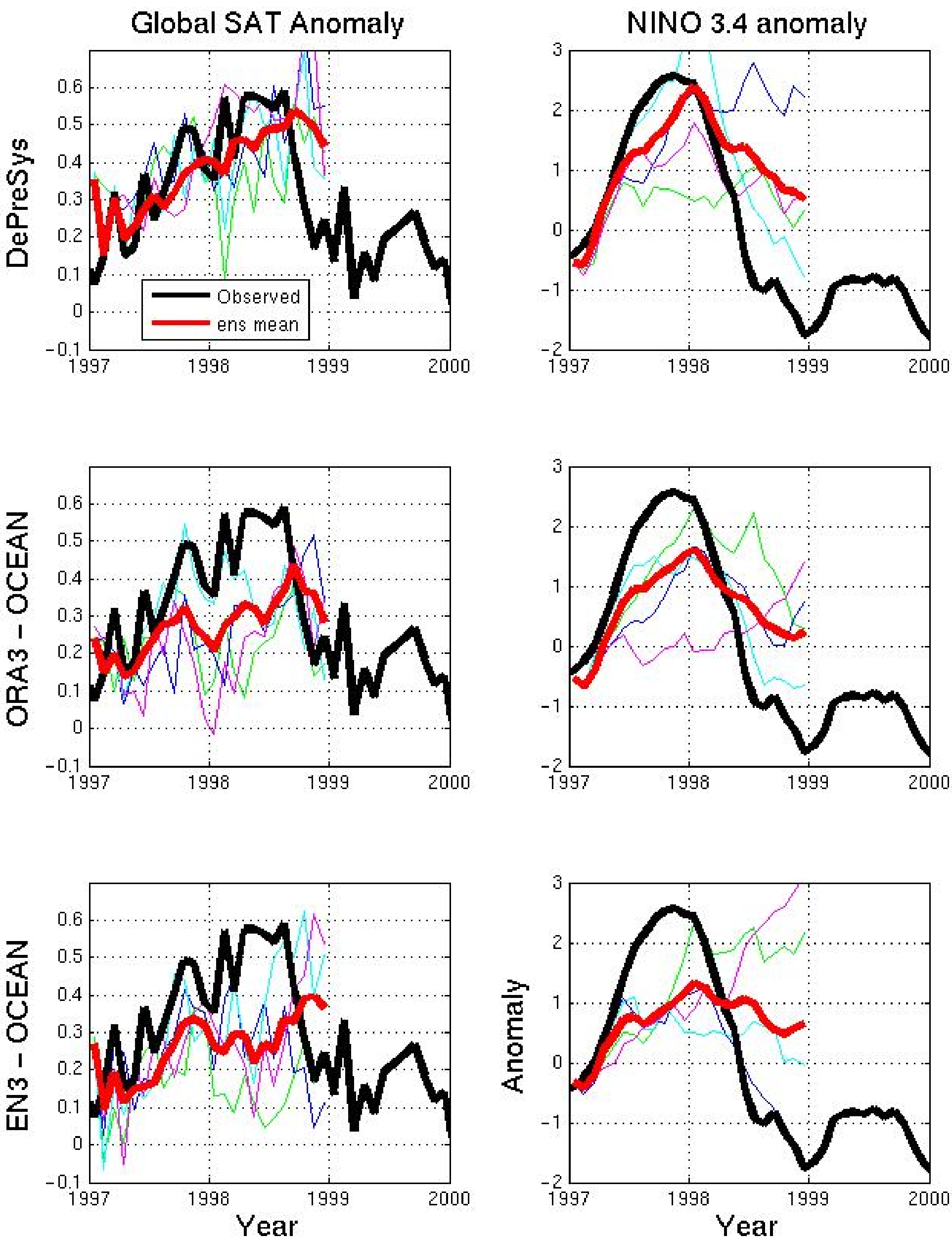

Figure 15: Hindcasts of global mean surface air temperature anomaly (left) and the Nino3.4 index (right), for the 1997 Ei Nino event. The DePreSys assimilation system is used for all the 4 member ensemble hindcasts, but with differing ocean initial conditions. Upper panels show the same DePreSys system used in Smith et al (1997). Middle panel uses the ECMWF ORA3 Ocean analysis as a basis for the ocean conditions. Lower panel uses the Ensembles3 ocean analysis for deriving the initial ocean anomalies.

This system also has demonstrable skill in seasonal prediction for example of ENSO. Figure 15 shows several hindcast ensembles of the 1997 ENSO event initialising in January 1997 and showing the response of the Global surface air temperature and the Nino 3.4 index. The different hindcasts test sensitivity to the ocean initial conditions, with experiments using the ECMWF-ORA3 ocean analysis or the Ensembles3 ocean analysis. All experiments were carried out on Reading University cluster computing resources to demonstrate the accessibility of this work in a University environment. Part of the success of DePreSys is probably due to the reduction in initial shocks resulting from the assimilation directly into the coupled system at all times, although considerably more work is required to explore the full potential of this coupled forecasting system.

5 Summary and Conclusions

Rather than go into great depth this seminar has attempted to cover a number of exciting applications and challenges of ocean data assimilation science. We have discussed the assimilation of both satellite altimeter data, which provides the most direct measure on ocean currents, and in situ profile data, which with careful treatment can be made highly complementary in their effects on the analysed ocean state. We have indicated how these oceanographic ideas can be presented in an assimilation framework based on balanced and unbalanced, or independent, state variables. This complementary use of satellite and in situ ocean data and the further separation of in situ data into dynamic and thermodynamic state information (defining the density fields and the water mass properties as a function of density) can have great benefit in deriving a climate quality ocean synthesis, making maximum use of the scarce space-time historical data sets. We have discussed the potential for assimilating ocean Geoid data from the ESA GOCE satellite (now planned for launch in April 2008) along with altimeter data, and shown how observation bias techniques may use the error covariance information from GOCE. Finally we have presented some recent results from fully coupled atmosphere-ocean data assimilation systems, and discussed their potential for improving seasonal-interannual forecasting. The potential for developing improved methods of ocean assimilation within coupled systems will be enormous if coupled models can be shown to have forecast skill for non-ENSO related phenomena.

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