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A Multivariate Treatment of Bias for Sequential Data Assimilation: Application to the Tropical Oceans

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Abstract

This paper discusses the problems arising from the presence of system bias in ocean data assimilation, taking examples from the ocean analysis systems used at ECMWF for seasonal forecasting. It is shown that the presence of system bias can be damaging for the representation of interannual variability due to the non stationary nature of the observing system. It is also shown that some of the bias in the eastern Pacific is caused by the data assimilation process, and it seems to be linked to the existence of a spurious vertical circulation.

An explicit multivariate algorithm for treatment of bias in sequential data assimilation has been formulated using the framework developed by Dee and Da Silva. The generalised scheme allows the multivariate constraints for the bias to be different from those for the state vector error covariance matrices, and in particular it encompasses the pressure gradient correction scheme of Bell *et al.* as a special case. A simple model for the time evolution of the bias is also provided.

The algorithm has been implemented in the ECMWF ocean data assimilation system. Several ocean reanalysis experiments have been conducted to evaluate the sensitivity of the results to the choice of multivariate formulations and to the choice of time parameters. Confirming previous studies, results show that the pressure correction scheme is successful in reducing the bias in temperature while also reducing the error in the velocity field. Direct bias correction of only the temperature field can consistently reduce the mean assimilation increment, but at the expense of increasing the error in the velocity field. Results also show a large sensitivity to the choice of the parameters controlling the time evolution of the bias.

1 Introduction

Data assimilation is a common practice for the generation of historical climate reanalyses that can be used in the study of climate variability (Ji *et al.* 1995, Carton *et al.* 2000b, Stammer *et al.* 2002, among others) and for the initialization of seasonal forecasts with coupled models (Behringer *et al.* 1998, Alves *et al.* 2004, Chen *et al.* 2004 to cite some examples). Although the benefits of data assimilation in reducing the uncertainty and in improving initial conditions for seasonal forecasts have been demonstrated (Alves *et al.* 2004, Vidard *et al.* 2005) the procedure itself is not without problems. In some cases the estimate of the ocean state can be degraded by the assimilation. The bias in the data assimilation system (or system bias) is one of the most serious obstacles for the reliable representation of climate variability, since the ever-changing observing system can induce spurious signals (Segschneider *et al.* 2000, Vidard *et al.* 2005), and may even be the cause of systematic error in the analysis (Bell *et al.* 2004). The problem of bias is not exclusive to the ocean, but is also present in atmospheric reanalysis (Dee 2005). In the case of the ocean the magnitude of the time-average error or bias is comparable to, or larger than, the random component, as illustrated in this paper.

The standard procedure to deal with systematic error in a data assimilation system is to augment the model state with a set of variables for the bias (Friedland 1969). Specific assumptions about the nature and time evolution of the systematic error are needed. Following these ideas, Dee and Da Silva (1998) (DdS in what follows) developed an algorithm for the online estimation and correction of the bias in sequential data assimilation. It was succesfully applied by Dee and Todling (2000) to the global assimilation of humidity observations in the Goddard Earth Observing System (GEOS) data assimilation system. The general algorithm was too costly for multivariate bias estimation in a global system, since it required an extra assimilation step to estimate the bias. A simplified version of the algorithm that avoids this extra step was first applied by Radakovitch *et al.* (2001) to land-surface temperature assimilation. For a comprehensive review of bias correction algorithms see Dee (2005).

Bell *et al.* (2004) (BMN in what follows) use the simplified DdS algorithm, but only for the on-line estimation of subsurface temperature bias in the tropical oceans. However, in the BMN scheme the bias correction is not applied directly to the temperature field. Instead, it is applied as a correction to the pressure gradient. The BMN method was also applied by Huddelston *et al.* (2005) to diagnose errors in the wind stress forcing. The ideas of the pressure correction have also been developed in parallel outside the field of data assimilation by Sheng *et al.* (2001), and have been successfully applied to the correction of the Gulf stream in eddy-permitting models (Eden *et al.* 2004).

The simplified DdS algorithm requires proportionality between the bias and state error covariance matrices. This is not the case in the BMN scheme, which uses different control variables for the bias and state vector. In this paper we develop an explicit multivariate formulation of the simplified DdS scheme and relax some of the unnecessary constraints. The BMN pressure correction scheme can be considered as a specific choice of multivariate formulation.

The DdS bias correction algorithm requires the prescription of a model for the time evolution of the bias. The simplest and most widely-used model is that of constant bias. Dee and Todling (2002) discuss this assumption, pointing out the pitfall that a constant bias allows a single observation to influence the bias estimation indefinitely. The introduction of a memory term may thus be desirable. Moreover, the systematic error may not be constant in time: it may be flow dependent (i.e. depend on the diurnal or seasonal cycle), or it may be associated with the non stationary errors of the external forcing (such as discontinuities in the atmospheric analysis system that provides the surface fluxes). Radakovitch *et al.* (2001) introduced a model for the bias where the diurnal cycle is prescribed as a harmonic function. Chepurin *et al.* (2005) formulated a comprehensive model for bias evolution that consists of the online estimation of the multiplicative coefficients associated with given patterns of spatial variability. Although quite general and elegant, the method relies heavily on the robustness and stationarity of the prescribed spatial patterns, and its application to historical reanalysis of the global ocean may be premature (for instance, the patterns of error of subsurface temperature in the southern hemisphere would be difficult to obtain from past records). In this paper we choose a simpler model for the time evolution of the bias term that allows us to discuss the sensitivity of the solution to the prescribed parameters.

The work presented in this paper evaluates the sensitivity of the ocean analysis system to the multivariate formulation of the bias covariance matrix and to the model for its time evolution. The emphasis is on the equatorial oceans, in particular the Pacific ocean. In section 2, the outstanding problems arising from bias in the system are illustrated with examples from the ECMWF operational ocean analysis systems. Section 3 introduces a generalized algorithm for treatment of system bias, based on DdS. The formulation allows the balance relationships in the bias error covariance matrix to be different from those in the state error covariance matrix. It also allows for slow time evolution of the system bias. The sensitivity to the multivariate formulation and to the time evolution is discussed in section 4. A summary and conclusions are offered in section 5.

2 Bias in the ECMWF ocean analyses systems

2.1 ECMWF operational ocean data assimilation systems

ECMWF has had an operational ocean analysis since 1996 as part of the seasonal forecasting system. In January 2001, the data assimilation component of the original operational system (System 1 or S1 in what follows) was upgraded together with other components in the seasonal forecasting suite. We refer to this second operational analysis as System2 (S2), and at the time of writing is the current operational system. The operational system consists of real-time as well as historical ocean analyses, the latter being used as initial conditions for the hindcasts to calibrate the seasonal forecast system. A description of the two successive ocean analysis systems is given in Anderson *et al.* (2003), Balmaseda (2004) and Alves *et al.* (2004). Here we just offer some concise information.

The background state for the data assimilation is produced by an ocean model forced by analyzed surface fluxes of momentum, heat and fresh water. The ocean model is based on HOPE (Hamburg Ocean Primitive Equation model) version 2 (Wolff et al. 1997). The ocean data assimilation scheme is an Optimum Interpolation (OI) scheme, and in the results presented here only subsurface temperature data are assimilated. The original system (S1) was univariate, while S2 includes balance constraints to update salinity and velocity, following the schemes proposed by Troccoli *et al.* (2002) and Burgers *et al.* (2002) respectively.

Originally, the temperature data came from the GTSPP (Global Temperature Salinity Profiling Project) at NODC (National Oceanographic Data Center). These include data from XBTs, mooring data from TAO, PIRATA and TRITON, and more recently from the ARGO floats. Since 2004, the observations are taken directly from the Global Telecommunication System (GTS). An analysis is performed every 10 days, using observations which span a window five days either side of the model background. There is no temperature assimilation in the top model level; instead the model SST is relaxed to analyzed SST (Reynolds *et al.* 2002) with a relaxation time-scale of 3 days.

In this section we will consider four sets of analysis: the operational analyses, called $ASSIM\_S1$ and $ASSIM\_S2$ for systems S1 and S2 respectively, and the corresponding control analyses ($CNTL\_S1$ and $CNTL\_S2$) without data assimilation. Forcing fields from ERA 15 (Gibson *et al.*, 1997) are used until 1993, and fluxes from the operational atmospheric analysis after that. ERA 40 (Uppala *et al.*, 2005) was not available at the time of operational implementation of S2, but fluxes from ERA 40 will be used in the experiments described in section 4.

2.2 Errors in the mean state

Figure 1a shows a vertical profile of the 1987-2001 mean difference between the analyses and the observations averaged over the Niño 3 area. The solid line corresponds to $ASSIM\_S2$ and the dotted line $CNTL\_S2$. Below 200 metres, $ASSIM\_S2$ is much less biased than $CNTL\_S2$. In the upper 200 meters both analyses are biased with respect to the observations, although in the opposite direction: the analysis without data assimilation is too cold with respect to the observations, while the analysis with data assimilation is too warm. This suggests that the data assimilation procedure is a source of error.

To assess the impact of the data assimilation it is important to use independent data such as the velocity data provided by the TAO moorings. Figure 1b shows the average zonal velocity at mooring location 110°W. The grey line represents the observations from TAO. The velocities from $ASSIM\_S2$ and $CNTL\_S2$ are represented by the solid and dotted lines respectively. The maximum value of the undercurrent is better reproduced by $ASSIM\_S2$ than by $CNTL\_S2$, which produces weaker-than-observed currents. However, in the assimilation, the undercurrent is too broad, and does not have a sharp maximum centered around the thermocline as in observations. Although the large values of the zonal velocity beneath the thermocline may not seem particularly worrying, they are associated with quite a large spurious downwelling circulation that will be the subject of further discussion in section 4. The point made here is that the zonal current can be compared with observations, whilst the vertical velocity is difficult to measure. The degradation of the equatorial currents during the assimilation of temperature data is a common feature in other assimilation systems (Burgers *et al.* 2002, Vialard *et al.* 2003, Balmaseda 2004, Huddleston *et al.* 2004, Ricci *et al.* 2005), although it seems to be absent in 4D-Var analyses (Weaver *et al.* 2003, Vialard *et al.* 2003).

BMN suggested that spurious vertical circulations induced by the assimilation may cause additional errors in the temperature field. They went further to suggest a possible positive feedback between errors induced by the data assimilation (degradation of currents) and errors in the model temperature field, that could lead to the existence of a bias in the system different from the bias in the analysis without data assimilation. The

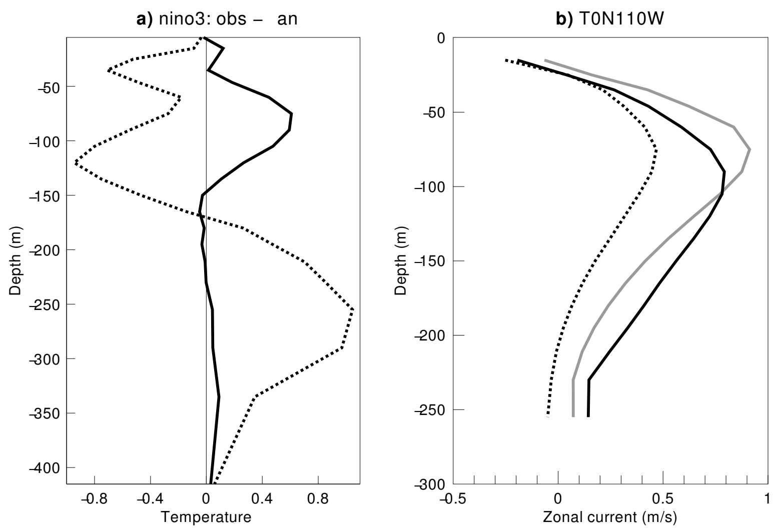


Figure 1: a) Vertical profiles of the 1987-2001 mean temperature analysis minus observation statistics averaged over the Eastern Pacific (Niño 3 area). The solid line is for the ASSIM_S2 operational ocean analysis, and the dotted line is for the CNTL_S2. The assimilation of data reverses the sign of the systematic error. b) Vertical profiles of the 1987-2002 mean zonal velocity at 110°W. The grey line represents the TAO current meter measurements. The solid line is for ASSIM_S2 and the dotted line is for CNTL_S2.

BMN method is successful in eliminating the spurious circulations induced by the data assimilation, and as a consequence, reduces the bias in the temperature field.

Figure 2 shows the time evolution of the temperature increment from *ASSIM_S*2 in the Eastern Pacific (Niño 3 area: 90°W-159°W, 5°N-5°S) at 100 m depth. The 24-month running mean of the assimilation increment, representative of the slow frequency (or systematic) component of the error, is shown in black, and the high-pass residuals, representative of the random component of the error, appear in grey. Two important features can be appreciated: a) the magnitude of the slow frequency component of error is large compared to the high frequency component and b) the systematic error is not constant in time. Particularly noticeable is the negative trend after 1998. The changes in the systematic error may be due to changes (local or remote) in the observation coverage (introduction of the TRITON moorings in the Western Pacific, for instance). They could also be due to the flow-dependent nature of the error: during the cold phase of ENSO (that started at the end of 1998) the slope of the thermocline is very pronounced, which may be difficult to simulate with a model that tends to produce a flatter-than-observed thermocline (see discussion in section 4). Or they could be caused by changes in the surface fluxes associated with changes in the atmospheric analysis. More work is needed to understand these trends, but in any case, figure 2 highlights the non stationarity of the systematic error. Ideally, a bias correction algorithm should take this into account.

2.3 Systematic error and Interannual Variability

In practice, the presence of systematic error may introduce spurious temporal variability in regions where the observation coverage is not uniform in time, which may be a serious problem when the ocean analysis is used to represent interannual variability.

Figure 3a shows the time evolution of the sea level in the equatorial Atlantic (70°W-30°E,5°N-5°S) from *ASSIM_S*1 (black line). The most striking feature is the sudden decrease in the sea level at around 1985.

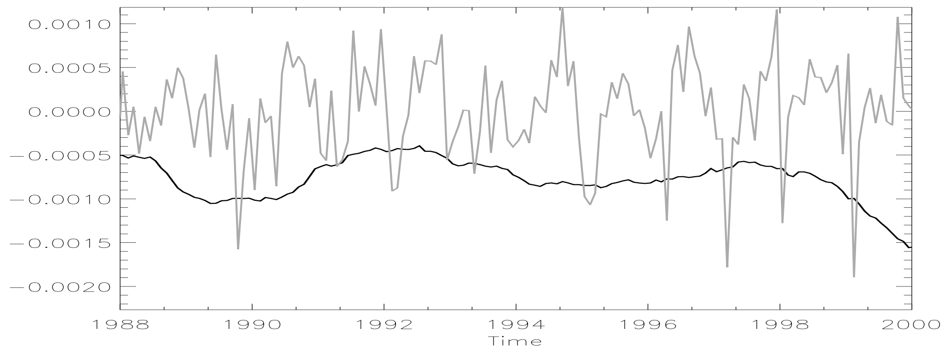


Figure 2: Time evolution of the low and high frequency components of the assimilation increment from S2 in the Niño 3 area at 100m depth. The 24-month running mean is shown in black and the high-frequency residuals are shown in grey. Units are ^{o}C/hour.

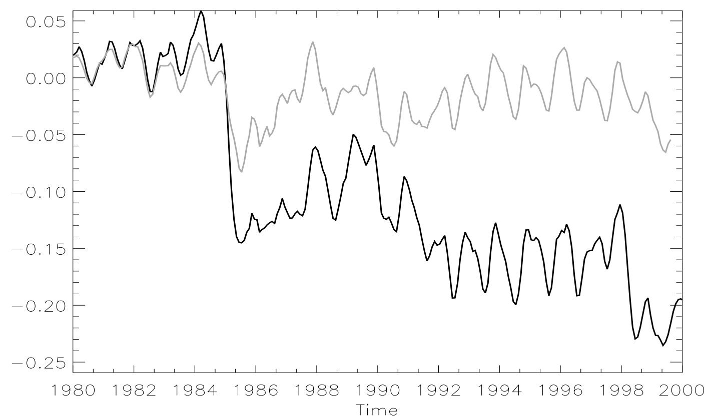
The $CNTL\_S1$ (not shown) does not exhibit any particular anomaly during that time. An inspection of the time evolution of the observations used in this analysis[1], shown in fig 3b, reveals a sudden increase in the number of observations that were assimilated at the time in the equatorial Atlantic around January 1985. Other (smaller) sea level changes apparent in the $ASSIM\_S1$ run occur when the observation coverage changed: both the increase in the number of observations at around 1992 and the appearance of PIRATA moorings around 1998 are associated with a decrease in the sea level of the equatorial Atlantic. The latter was reported by Segschneider *et al.* (2000).

The sudden jump in sea level in the $ASSIM\_S1$ run in figure 3a is a side effect of the data assimilation. The data corrects for a large error in temperature due to a very diffuse thermocline (not shown). The correction requires a large negative increment to the temperature field. Without the corresponding balance correction to the salinity field (as was the case in $S1$), the vertical stability of the water column is disrupted, and the assimilation induces spurious convection. Convection could be prevented if the temperature-salinity (T-S) relationship of water mass is preserved, which would imply updating the salinity field at the same time as the temperature (Troccoli *et al.* 2002).

The grey curve in fig 3a shows the sea level evolution after applying the T-S constraint. The abrupt jump of the sea level in 1985 is alleviated by the inclusion of the balance relationship, but changes in the sea level associated with the evolution of the observing system are still noticeable. If changes in the observing system are very sudden, it may be helpful to have an *a priori* estimate of the bias in the system, as will be discussed in section 4. The knowledge of the climate variability in the Equatorial Atlantic remains a challenge, both for ocean models and ocean data assimilation systems (Stockdale *et al.* 2005). Ocean models with typical climate resolution of 1 ° (lat/lon) are not able to simulate accurately the mean state and the interannual variability of the equatorial Atlantic. Data assimilation is not a solution yet, and often degrades the representation of the interannual variability in this area (Balmaseda 2004, Vidard *et al.* 2005).

[1]More comprehensive historical observational data sets are now available, such as that prepared as part of the ENACT project.

a)



b)

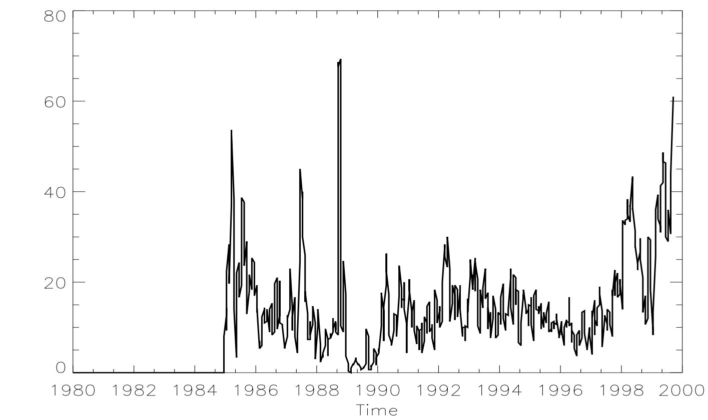


Figure 3: Time evolution of a) the sea level averaged over the equatorial Atlantic, as represented by the ASSIM_S1 (black line) ocean analysis from S1 and by an ocean analysis where conservation of water mass characteristics is imposed (grey line). b) Time evolution of the number of observations over the same region used in the analysis.

3 Bias correction algorithm

3.1 Two-step and one-step bias correction algorithms

The standard procedure to deal with systematic error in a data assimilation system is to augment the model state with a set of systematic error variables. The generic DdS bias correction algorithm for the k^{th} analysis cycle of a data assimilation system with bias $\mathbf{b}$, state vector $\mathbf{x}$ and observation vector $\mathbf{y}$ is given by

$$\begin{aligned} \mathbf{b}_k^a &= \mathbf{b}_k^f - \mathbf{L}\left[\mathbf{y}_k^o - \mathbf{H}(\mathbf{x}_k^f - \mathbf{b}_k^f)\right] \\ \mathbf{x}_k^a &= (\mathbf{x}_k^f - \mathbf{b}_k^a) + \mathbf{K}\left[\mathbf{y}_k^o - \mathbf{H}(\mathbf{x}_k^f - \mathbf{b}_k^a)\right] \end{aligned} \tag{1}$$

where the superscripts f and a refer respectively to the forecast and analysis of a given variable. The matrices $\mathbf{L}$ and $\mathbf{K}$ are the gain matrices for the bias and the state respectively, and are given by

$$\begin{aligned} \mathbf{L} &= \mathbf{P}^b\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{H}\mathbf{P}^f\mathbf{H}^T + \mathbf{R}\right]^{-1} \\ \mathbf{K} &= \mathbf{P}^f\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^f\mathbf{H}^T + \mathbf{R}\right]^{-1} \end{aligned} \tag{2}$$

where $\mathbf{P}^f$ and $\mathbf{P}^b$ are the error covariance matrices for the unbiased state and for the bias term, respectively, and $\mathbf{R}$ is the observation error covariance matrix.

Equation (1) requires two analysis steps: one for the bias estimation and a second for the state vector. Radakovitch *et al.* (2001) proposed a simplification that could be used if the bias is nearly constant in time,

$$\mathbf{b}_k^f \approx \mathbf{b}_{k-1}^a \tag{3}$$

and the bias error covariance matrix is taken to be proportional to the forecast error covariance matrix, with the proportionality constant γ small compared to one,

$$\mathbf{P}^b = \gamma\mathbf{P}^f. \tag{4}$$

If γ is small then the bias updates will be small as well, and it may be acceptable to replace $\mathbf{b}_k^a$ by $\mathbf{b}_{k-1}^a$ in (1). Then we can reverse the order of the equations in (1) to approximately obtain

$$\begin{aligned} \mathbf{x}_k^a &= (\mathbf{x}_k^f - \mathbf{b}_{k-1}^a) + \mathbf{K}\left[\mathbf{y}_k^o - \mathbf{H}(\mathbf{x}_k^f - \mathbf{b}_{k-1}^a)\right] \\ \mathbf{b}_k^a &= \mathbf{b}_{k-1}^a - \gamma\mathbf{K}\left[\mathbf{y}_k^o - \mathbf{H}(\mathbf{x}_k^f - \mathbf{b}_{k-1}^a)\right]. \end{aligned} \tag{5}$$

The algorithm described in (5) only requires one analysis step, since the second term on the right hand side of the equations is the same, and thus the bias update equation is trival to compute. This simplification is described in more detail in Dee (2005). The requirement of proportionality between the covariances matrices may be too strong. It would require the balance constraints for the bias to be the same as those for the state vector. In particular, it does not encompass naturally the BMN scheme, where the bias term acts only in the momentum equation as a correction to the pressure gradient. In the following we show that the requirement of proportionally can be safely relaxed if applied to the subspace orthogonal to the null space of $\mathbf{H}$ (observable subspace hereafter).

3.2 Decomposition into observable and non-observable subspaces

Let us now decompose the n-dimensional state space into two orthogonal subspaces of dimensions p and $q = n - p$ that we call the observable and the null subspace. Vector $\mathbf{x}$, matrix $\mathbf{K}$, and symmetric matrix $\mathbf{P}$, of dimensions $nx1$, nxp and nxn respectively can be written

$$\begin{aligned} \mathbf{x} &= \mathbf{x}_{\|} + \mathbf{x}_{\perp} \\ \mathbf{K} &= \mathbf{K}_{\|} + \mathbf{K}_{\perp} \\ \mathbf{P} &= \mathbf{P}_{\|\|} + \mathbf{P}_{\perp\|} + \mathbf{P}^T_{\perp\|} + \mathbf{P}_{\perp\perp} \end{aligned} \tag{6}$$

where subscript $\|$ represents the image of operator $\mathbf{H}$, or observable subspace, and subscript $\perp$ represents the null subspace of operator $\mathbf{H}$. Let $\mathbf{T}_o$ be the projector operator from the state vector space onto the observable subspace, defined such that

$$\begin{aligned} \mathbf{x}_{\|} &= \mathbf{T}_o\mathbf{x} \\ \mathbf{H}\mathbf{x}_{\|} &= \mathbf{H}\mathbf{x} \\ \mathbf{H}\mathbf{x}_{\perp} &= 0. \end{aligned} \tag{7}$$

With naming convention, operators $\mathbf{L}$ and $\mathbf{K}$ in (2) can be written

$$\begin{aligned} \mathbf{L}_{\|} &= \mathbf{P^b}_{\|\|}\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^b_{\|\|}\mathbf{H}^T + \mathbf{H}\mathbf{P}^f_{\|\|}\mathbf{H}^T + \mathbf{R}\right]^{-1} \\ \mathbf{L}_{\perp} &= \mathbf{P^b}_{\perp\|}\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^b_{\|\|}\mathbf{H}^T + \mathbf{H}\mathbf{P}^f_{\|\|}\mathbf{H}^T + \mathbf{R}\right]^{-1} \\ \mathbf{K}_{\|} &= \mathbf{P}^f_{\|\|}\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^f_{\|\|}\mathbf{H}^T + \mathbf{R}\right]^{-1} \\ \mathbf{K}_{\perp} &= \mathbf{P}^f_{\perp\|}\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^f_{\|\|}\mathbf{H}^T + \mathbf{R}\right]^{-1} \end{aligned} \tag{8}$$

and the analysis equations (1) can be written for the observable and non observable subspace separately as follows:

$$\begin{aligned} \mathbf{b}^a_{\|k} &= \mathbf{b}^f_{\|k} - \mathbf{L}_{\|}\mathbf{d}_k \\ \mathbf{x}^a_{\|k} &= (\mathbf{x}^f_{\|k} - \mathbf{b}^a_{\|k}) + \mathbf{K}_{\|}\mathbf{d}_k \end{aligned} \tag{9}$$

$$\begin{aligned} \mathbf{b}^a_{\perp k} &= \mathbf{b}^f_{\perp k} - \mathbf{L}_{\perp}\mathbf{d}_k \\ \mathbf{x}^a_{\perp k} &= (\mathbf{x}^f_{\perp k} - \mathbf{b}^a_{\perp k}) + \mathbf{K}_o\mathbf{d}_k, \end{aligned} \tag{10}$$

where $\mathbf{d}_k$ represents the innovation vector, a vector of the observable subspace defined as:

$$\mathbf{d}_k = \mathbf{y}^o_k - \mathbf{H}(\mathbf{x}^f_{\|k} - \mathbf{b}^a_{\|k}). \tag{11}$$

3.3 A generalized two-step bias correction algorithm

The algorithm can be further generalized by allowing the bias and state vector to have different vector components. Let us define an operator $\mathbf{T}_x$ from the bias space with image in the state vector space such that:

$$\mathbf{b}_x = \mathbf{T}_x\mathbf{b}. \tag{12}$$

To simplify the expressions we introduce the variable $\tilde{\mathbf{d}}$ to represent the approximated unbiased innovation vector:

$$\tilde{\mathbf{d}}_k = \mathbf{y}_k^o - \mathbf{H}(\mathbf{x}_k^f - \mathbf{b}_{xk}^f), \tag{13}$$

and the variable $\mathbf{w}$ to represent the approximately unbiased state vector

$$\mathbf{w}_k^f = \mathbf{x}_k^f - \mathbf{b}_{xk}^f. \tag{14}$$

If the bias and state gain matrices are proportional in the observable subspace,

$$\mathbf{L}_{\|} = \gamma \mathbf{K}_{\|}; \quad \gamma << 1 \tag{15}$$

and the bias evolves slowly in time as required in eq 3, then the two-step algorithm in eq 1 can also be approximated by a one-step algorithm as follows:

$$\begin{aligned} \mathbf{x}_k^a &= \mathbf{w}_k^f + \mathbf{K}\tilde{\mathbf{d}}_k \\ \mathbf{b}_{\|k}^a &= \mathbf{b}_{\|k}^f - \gamma \mathbf{K}_{\|}\tilde{\mathbf{d}}_k \\ \mathbf{b}_k^a &= F(\mathbf{b}_{\|k}^a) \end{aligned} \tag{16}$$

In (16), F is an operator acting over the component of the bias in the observable subspace into the bias subspace, and it represents the multivariate relationship for the bias. Note that the observations in (16) only give information about the bias in the observable subspace ($\mathbf{b}_{\|}$), while the total bias vector $\mathbf{b}$ can be derived from $\mathbf{b}_{\|}$ through F. There is freedom for the choice of F, which allows the multivariate relationships for the bias to be different from those for the state vector. In this way, different balance constraints can be specified for different time scales (for instance, geostrophic balance for the short time scales and Sverdrup balance for the longer time scales). In some cases it may be convenient to use different variables for the state and for the bias, provided that there is a known transformation from one to the other. For instance, in the data assimilation system described in section 2, the observable variable was temperature (T), and the state vector consisted of the 3D temperature, salinity, velocity and sea level fields (T,S,$\vec{U}$,η). In the BMN scheme, the bias vector consists only of pressure gradient, which is derived from the T observations. In this way, expression (16) includes the BMN scheme as a particular choice of multivariate relationship.

3.4 The generalized two-step bias correction algorithm

We have seen in the previous section that the bias term evolves in time, although slowly. The hypothesis of constant bias in equation (3) could be relaxed to allow for the slow time evolution of the bias without incurring large errors. Chepurin *et al.* 2005, propose a generalized model for the time evolution for the bias that allows flow-dependent errors and seasonal cycle. Radakovitch *et al.* 2001 includes the diurnal cycle as a sinusoidal harmonic. Here we propose a less parameterised model for the time evolution of the bias. The rational behind this simplification is to avoid having to fit a large number of degrees of freedom with a reduced number of observations, while still giving some flexibility. The model for the time evolution of the bias is the following:

$$\begin{aligned} \mathbf{b}_k^f &= \bar{\mathbf{b}} + \mathbf{b}'^f_k \\ \mathbf{b}'^f_k &= \alpha \mathbf{b}'^a_{k-1} \end{aligned} \tag{17}$$

The total bias is represented as the sum of two terms: a prescribed bias term $\bar{\mathbf{b}}$, estimated *a priori*, and a departure $\mathbf{b}'_k$ from $\bar{\mathbf{b}}$. Only the departure $\mathbf{b}'_k$ is estimated with the on-line algorithm. The term $\mathbf{b}'^f$ has finite memory given by the factor α. The introduction of the memory term will limit the influence in time of isolated or sporadic observations. It is a way of accounting for the uncertainty in the estimation of the bias term, which is proportional to the age of the observations and it also has the potential to allow for time dependent bias. A side effect is that values of α less than one will underestimate the magnitude of the bias. To compensate for that, the constant term $\bar{\mathbf{b}}$ is introduced in (17).

The term $\bar{\mathbf{b}}$ is not affected by the on-line estimation and has to be estimated *a priori*, preferably with independent information. If there is not enough information for independent estimation, it can always be set to zero. Apart from compensating for the damping effects of the memory term, the inclusion of the *a priori* bias term offers other practical advantages. It has the potential to prevent abrupt changes in the analysis associated with the appearance of observing systems (note that the bias estimated online may prevent discontinuities due to the disappearance of observing systems, but it does not necessary help with changes due to the appearance of new observing systems). The prescribed term could also represent well-known systematic errors of faster time scale than that allowed by the longer memory term of the online estimation, such as the seasonal cycle (the seasonal cycle is not easy to represent by a limited number of harmonics). Finally, the a-priori estimation may give information about other variables or balanced relationships not easy to estimate through the on-line procedure. For instance, the bias in the T, S and mean sea level could be estimated independently using geoid information from satellite gravity missions such as GRACE, together with some climatology of the hydrography, while the bias estimated on-line would act only on pressure.

Combining equations (16) and (17), the final expression used in the estimation of the bias would be:

$$
\begin{aligned}
\mathbf{w}_k^f &= \mathbf{x}_k^f - (\bar{\mathbf{b}}_{xk} + \alpha \mathbf{b}'^a_{xk-1}) \\
\mathbf{x}_k^a &= \mathbf{w}_k^f + \mathbf{K}\tilde{\mathbf{d}}_k \\
\mathbf{b}'^{\mathbf{a}}_{\|\mathbf{k}} &= \alpha \mathbf{b}'^a_{\|k-1} - \gamma \mathbf{K}_{\|} \tilde{\mathbf{d}}_k \\
\mathbf{b}_k^a &= \bar{\mathbf{b}}_k + F(\mathbf{b}'^a_{ok})
\end{aligned}
\tag{18}
$$

In (18) it is clear that the estimation of the bias will depend on the values of parameters α and γ that control the time evolution and the amplitude of the bias, on the estimation of $\bar{\mathbf{b}}$ and on the prescription of F. In the following section we conduct a set of experiments to evaluate the sensitivity of the solution to these factors.

4 Sensitivity experiments

4.1 Experimental setup

For the sensitivity experiments we use an up-to-date version of the data assimilation system described in section 2. The observations come from the more comprehensive and quality-controlled data set produced as part of the ENACT project (Ingleby and Huddleston 2004). The forcing fields are derived from ERA 40, with the modifications in the fresh water introduced by Troccoli and Kallberg (2004). The version of the ocean model is the same as for S2, but at lower resolution (2 x 2 degrees lat/lon with equatorial refinement). All the experiments start from the same spin up and span the period January 1987 - December 2001. Only subsurface temperature data are assimilated, but salinity and currents are updated through the multivariate relationships described in section 2.

Table 1 shows the summary of the different experiments. Experiment E_0 was conducted as a control, with standard assimilation and no bias correction. Then, a set of 3 experiments was conducted to test the sensitivity

Experiment	time-decay $\sim \alpha^{-1}$	γ	$\mathbf{F}(\mathbf{T},\mathbf{S},\mathbf{P})$	$\bar{\mathbf{b}}(\mathbf{T},\mathbf{S},\mathbf{P})$
E_0		0	(0,0,0)	(0,0,0)
E_inf	infinite ($\alpha = 1$)	0.3	(0,0,P)	(0,0,0)
E_2Y	2 Years	0.3	(0,0,P)	(0,0,0)
E_2Yslow	2 Years	0.1	(0,0,P)	(0,0,0)
E_2Yslow_T	2 Years	0.1	(T,0,0)	(0,0,0)
E_2Yslow_TS	2 Years	0.1	(T,S,0)	(0,0,0)
E_2Yslow_$\bar{b}$	2 Years	0.1	(0,0,P)	(T,S,0)

Table 1: Summary of experiments conducted

to the parameters controlling the time evolution and amplitude of the bias (α and γ). In these experiments F was chosen to simulate the BMN scheme, i.e. the information from the temperature observations is used to correct the pressure gradient, but no explicit correction is made to the temperature field. In experiment E_inf, α is set to 1., so the observations will influence the bias estimate indefinitely. The value of γ is initially set to 0.3. In experiment E_2Y, γ is still 0.3, but the value of α is equivalent to a time-decay of 2 years. In experiment E_2Yslow the time-decay is 2 years, but γ is decreased to 0.1, so that the bias is updated more slowly (see equation (18)). In all of these experiments $\bar{\mathbf{b}}$ is zero.

To test the sensitivity to the multivariate formulation, another experiment E_2Yslow_T was conducted, with the same time parameters as E_2Yslow but with F such that only the temperature field is corrected, without modification to the pressure gradient. Similarly, in experiment E_2Yslow_TS the temperature and salinity fields are corrected.

Finally, experiment E_2Yslow_$\bar{b}$ was used to evaluate the importance of the prescribed bias. The term $\bar{\mathbf{b}}$ contained modifications to the temperature and salinity fields, and zero correction to the pressure gradient. The term was derived from a climatological model run, where the ocean model was forced by climatological ERA 40 fluxes and relaxed to the WOA98 climatology (Levitus *et al.* 1998) with a time scale of 3 years. The $\bar{\mathbf{b}}$ was estimated as the annual mean of the corrections due to the WOA98.

4.2 Sensitivity to the multivariate formulation

Figure 4 shows the 1987-2001 average of a longitude-depth section of the assimilation increments along the equator from experiments E_0, E_2Yslow_T and E_2Yslow (panels a, b and c respectively). The mean increment in fig 4a has a large-scale dipolar structure, as if the data assimilation were correcting the slope of the thermocline, making it deeper in the western Pacific and shallower in the eastern Pacific. This kind of error could appear if the equatorial winds were too weak, although it may be due to other mechanisms. In section 2, it was suggested that the negative increment in the Eastern Pacific is in fact induced by the assimilation process. In the experiments E_2Yslow_T and E_2Yslow, where the bias has been corrected online, the resulting mean increment is smaller (the mean increment is not expected to be removed entirely since α is less than 1). The reduction of the mean increment in temperature is expected from the mathematical consistency of the bias correction algorithm. However, the smaller mean increment does not guarantee a better analysis.

For a more impartial test of the performance of the bias correction algorithms we need to look at independent variables. Figure 5 shows an equatorial cross-section of the vertical velocity for the same three experiments shown in figure 4. The spurious vertical circulation in the Eastern Pacific associated with the degradation of the zonal current discussed in section 2 is evident in panel a. Correcting the bias in temperature only degrades it even further (fig 5b). The behaviour is similar to (and consistent with) that observed in experiments where the

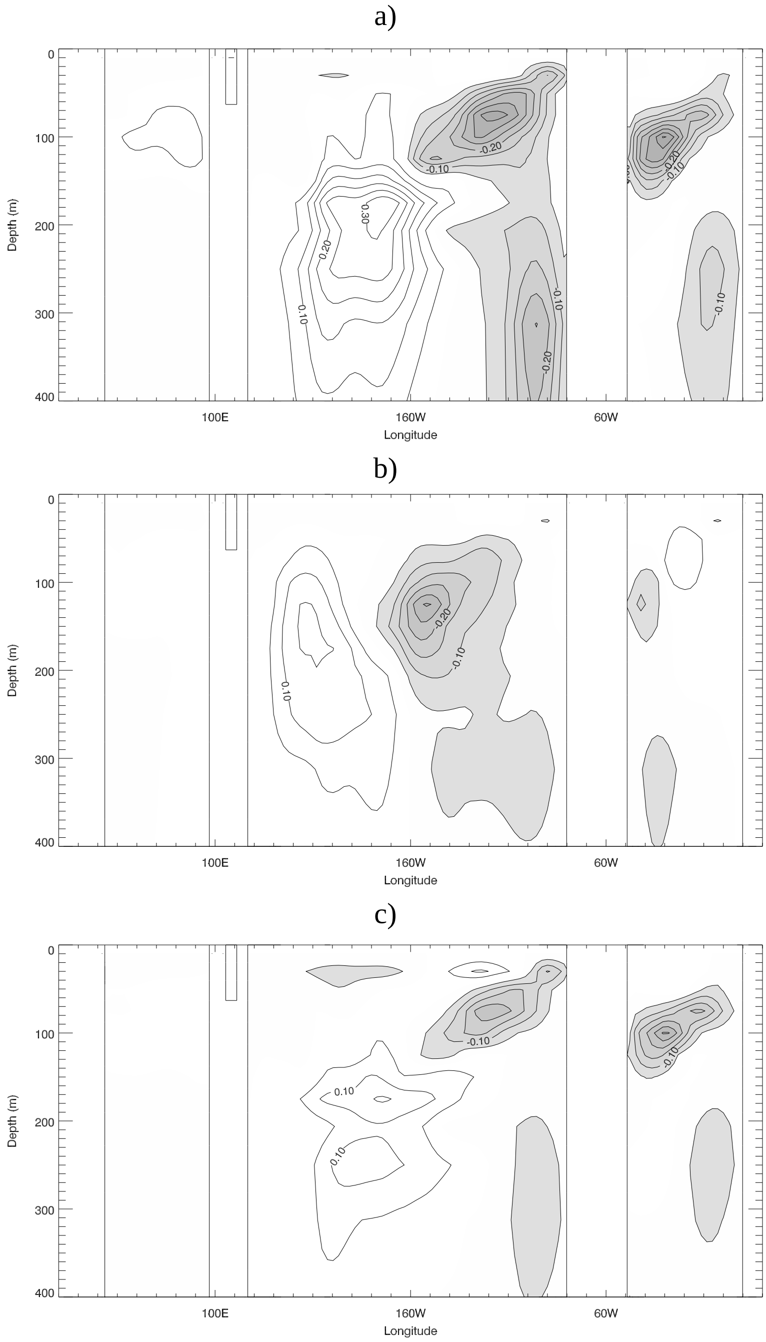


Figure 4: Equatorial longitude-depth section of mean assimilation temperature increment for experiments (a) E_0, (b) E_2Yslow_T and (c) E_2Yslow. Contours every 0.5°C/10-days. The mean corresponds to the time average during the period 1987-2001.

weight given to the observations is increased: the equatorial currents are systematically degraded (not shown). Ultimately, if a bias correction algorithm is used, the observations are indirectly given more weight, since they are allowed to influence the estimate twice (and for longer time).

In the experiment where the bias is treated by applying a correction to the pressure gradient using the BMN scheme (fig 5c), the spurious circulation does not appear. This result illustrates large sensitivity of the results to the choice of multivariate relationship. As pointed out by Burgers *et al.* (2002), the systematic error may have its origins in the momentum equation (resulting from inaccuracies in the wind field and in the vertical mixing of momentum among others). If so, the error should be "adiabatic", since it is due to the wrong redistribution of heat. The BMN is a way of imposing adiabaticity in the assimilation of temperature data, by assuming that the error arises entirely from an incorrect value in the pressure gradient terms, and using the temperature increments given by the assimilation to derive a correction to the pressure gradient.

It can be argued that in experiment E_2Yslow_T, where the bias acts only on temperature, no balance corrections are made to salinity, with the potential of disrupting the water mass characteristics. (Ricci *et al.* (2005) show that the impact of salinity on the velocity field is not neglegible). In experiment E_2Yslow_TS, the salinity field is updated using a gain matrix proportional to the gain matrix of the state vector, which represents the T-S preservation scheme of Troccoli *et al.* (2002). Results (not shown) were very poor, with very visible trends in salinity and sea level. A possible reason for the poor results may lie in the nonlinear nature of the T-S relationship: the bias in S obtained by accumulating the salinity increments of the independent analysis cycles is not the same as if the nonlinear T-S relationship is computed using the bias in T. This result also highlights the separation of the bias correction into observable and non-observable subspaces. In fact it implies that applying the proportionality criteria in (4) beyond the observable subspace is not appropriate. The preservation of water mass characteristics can still be used as a constraint for the bias term, but further work is needed for its correct implementation.

4.3 Sensitivity to the time evolution

Figure 6 shows results from experiments conducted to evaluate the sensitivity to the time evolution of the bias term. In the left column, the time evolution of the estimated temperature bias over the region Niño 3 at three different depths is shown. The time evolution of the 24-month running mean of the temperature increment in shown in the right column, together with the value of the mean assimilation increment (ticks on the right y-axis). Because of the 24-month running mean, the time axis in these graphs is limited to the period 1989-2000. The black solid line is for experiment E_2Yslow, the grey solid is for experiment E_inf and the grey dashed line is for experiment E_2Y. For reference, the thin black line shows the value that the bias would have had in experiment E_0, had it been estimated using the same parameters as in E_2Yslow (remember that the online bias correction is not active in E_0). The resulting values and behaviour of the bias estimates are very different in the different experiments. In the following section we try to use these diagnostics to assess the quality of the resulting analysis.

One possible criterion for assessment is to require that the estimate of the bias *a posteriori* is consistent with the model prescribed *a priori* for the time evolution of the bias. For instance, if the *a priori* assumption is that the bias is constant, thn the resulting estimate should exhibit asymptotic convergence to a constant value, after reaching which the innovation vectors should be white noise with zero mean. In general, the time average of the temperature increment should be as close as possible to zero.

At 30m depth (fig 6a), the bias in experiment E_inf (which assumes constant bias) does not converge. The bias keeps increasing with time, and the resulting value is of the opposite sign to the reference experiment E_0 but with much larger amplitude. The 24-month running mean assimilation increments (fig 6b) are mainly

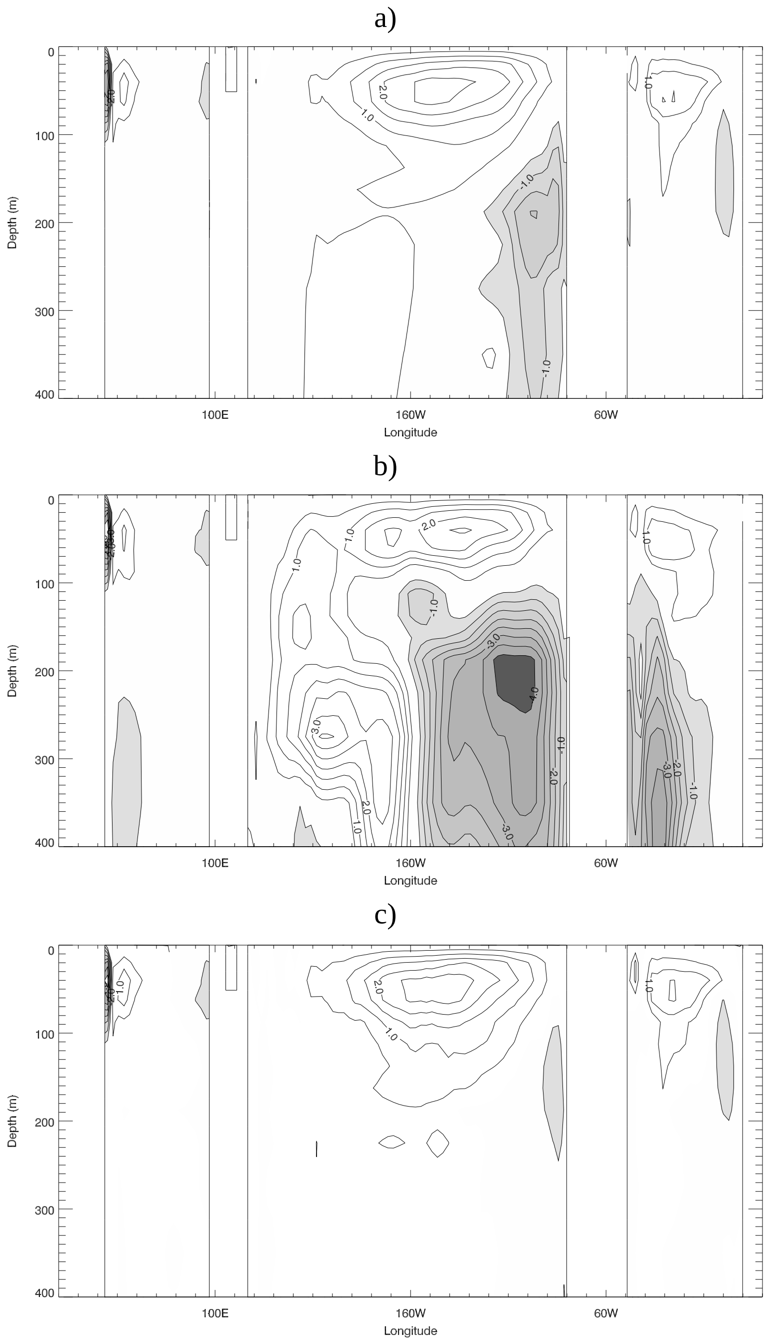


Figure 5: Equatorial longitude-depth section of the 1987-2001 average vertical velocity for the experiments (a) E_0, (b) E_2Yslow_T and (c) E_2Yslow. Contour interval is 0.5m/day

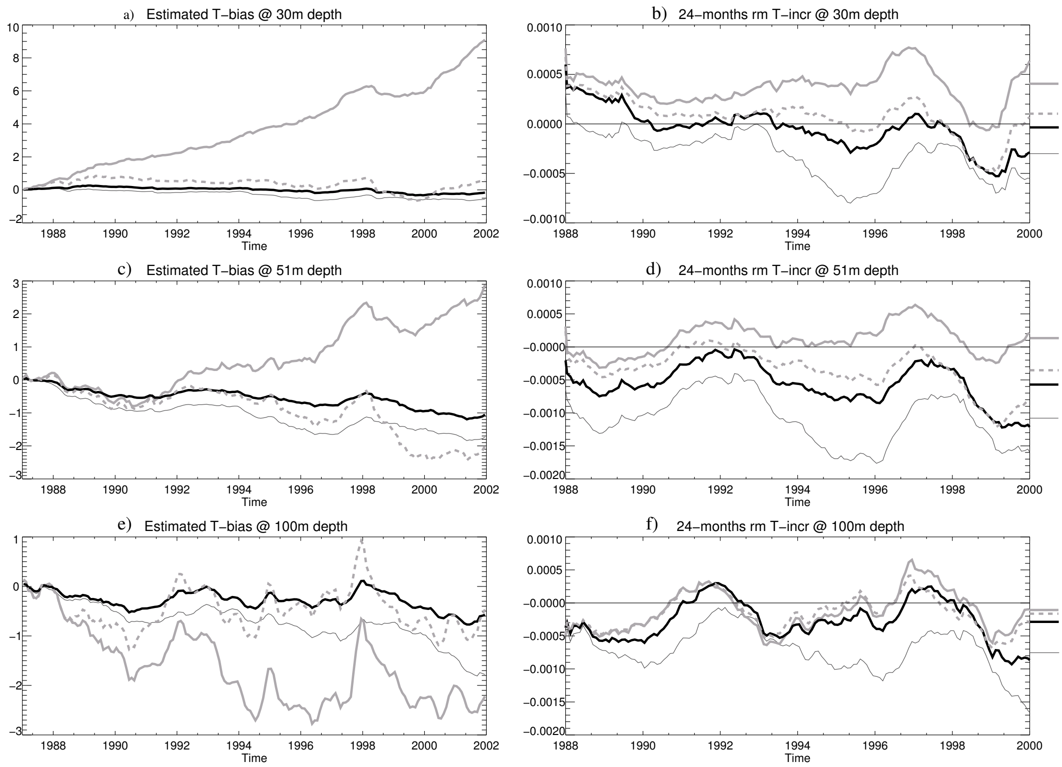


Figure 6: Time evolution of the estimated bias (left column) and 24-month running mean assimilation increment (right column) at different levels in the Niño 3 area. Values for the 1988-2001 average assimilation increment are shown on the right y-axis of the right panels. Shown are the results from experiment E_2Yslow (thick solid black line), E_inf (solid grey line), E_2Y (grey dashed line) and E_0 (thin solid back line). In the case of experiment E_0 the bias is only a diagnostic; it is not corrected interactively.

positive, and after 1996 exhibit large fluctuations in time. The value of the mean temperature increment in E_inf is positive and has the largest absolute value. The resulting velocity field is too weak compared to the observations (not shown). It can be concluded that at least for this region and level, the time evolution of bias diagnosed *aposteriori* for experiment E_inf is not consistent with model for the bias prescribed *apriori*; the bias is overcorrected, resulting in a change of sign. It is not clear at this point if the pathological behaviour of E_inf is caused by the infinite memory ($\gamma = 1$) or by the larger amplitude of the bias (which is a function of α and γ). The bias in the experiments with finite memory is more stable. The evolution of the 24-month running mean increment shows that at 30m depth both E_2Y and E_2Yslow have less bias than E_0.

At 50m depth, the behaviour of the experiments is more varied. From the point of view of the bias, experiment E_inf is still the outlier, and again it overestimates the value of the bias, although not as clearly as before. In fact, it shows the smallest absolute value of the mean increment. The sensitivity of the results to parameter the γ can now be appreciated by comparing the experiments with finite memory: E_2Yslow where γ is .1 (black line) to experiment E_2Y, where γ is 0.3 (dashed grey line). Consistent with a larger value of γ, experiment E_2Y exhibits more time variability, and clearly adapts faster to a large negative value after the change observed in 1998 (and discussed in section 2), where it remains until the end of the run. From this graph it is not easy to say if the resulting value of the bias after 1998 is correct. There is a hint that the 24-month running mean is going back to zero after 1999, which is consistent with the stabilisation of the bias. This is the experiment where the high frequency of the assimilation increments had smaller variance (not shown). Experiment E_2Yslow exhibits much smoother temporal behaviour, as expected from the smaller value of γ. The magnitude of the bias is smaller than that in experiment E_0, which reflects the positive impact of the on-line correction. The mean assimilation increment is also smaller than in E_0, but larger than in E_2Y. In the two experiments with finite memory the velocity field is improved with respect to the reference experiment E_0 (not shown).

At 100m depth, in terms of mean absolute error, the best estimator is the experiment with infinite memory. The experiment with fast update (E_2Y) follows closely, and experiment E_2Yslow underestimates the magnitude of the bias (fig 6f). Although in some areas E_inf is good, it tends to overestimate the bias, sometimes producing quite pathological behaviour, and the experiments with finite memory, as expected, tend to underestimate the bias.

There is no experiment that behaves best in all locations, which suggests that the time parameters may need to be spatially dependent. Without any further theoretical insight, the spatial distribution of parameters α and γ could be estimated empirically, together with $\bar{\mathbf{b}}$ (which appears in (18) but has not been discussed yet).

The results illustrate that the sensitivities to the time evolution of the bias are quite large, and sometimes complex behaviour can arise from the coupling between the bias and the state vector in the estimation algorithm (in equation (18) the coupling is implicit in the innovation vector $\tilde{\mathbf{d}}_\mathbf{k}$).

From these results it is clear that further work is needed to develop a satisfactory framework for treatment of time dependent bias, or more generally, for treatment of errors at different time scales. There is also a need for well defined metrics that allow us to assess the mathematical consistency and physical validity of the bias correction algorithms.

4.4 Sensitivity to the prescribed bias

In order to make good use of recently-developed and future observing systems, such as the ARGO floats, it may be desirable to have an *a priori* estimate of the bias term. Otherwise, the arrival of new information may induce discontinuities and spurious variability in the analysis of traditionally poorly observed areas. In our simple model for the evolution of the bias (Eq. 17), the *a priori* bias estimate is given by $\bar{\mathbf{b}}$.

If observations are scarce, $\bar{\mathbf{b}}$ may not be easy to estimate. By gathering all the existing observations in a climatology, such as the WOA98, it would be possible to "gain" spatial coverage by sacrificing the time dimension (and under the strong assumption that the system is stationary). This is roughly the strategy followed here to estimate the term $\bar{\mathbf{b}}$. The ocean model forced by ERA 40 climatology is nudged, with a time scale of 3 years, to the WOA98 climatology. The time scale for relaxation is an ad-hoc way of introducing uncertainty for the WOA98 estimate. There may be more optimal ways of estimating $\bar{\mathbf{b}}$, but we chose a simple one for demonstration purposes. The relaxation terms in the T and S equations are taken to provide the estimate of $\bar{\mathbf{b}}$, which would be used to correct T and S directly. There is no pressure correction in $\bar{\mathbf{b}}$ (see experiment E_2Yslow_$\bar{b}$ in Table 1).

As expected, poorly observed regions such as the Equatorial Indian Ocean are better represented if the term $\bar{\mathbf{b}}$ is introduced (in the sense that the mean assimilation increments are reduced). The Equatorial Indian Ocean is only sensitive to the $\bar{\mathbf{b}}$ term, while the on-line correction to pressure has almost no effect.

Figure 7 shows the vertical profiles of the 1987-2001 mean assimilation increments for region EQ3 in the Central-Western Pacific (150°E-190°W, 5°N-5°S) and for region EQATL in the Equatorial Atlantic. Shown are the results for experiments E_0 (solid back line), E_2Yslow (black dashed line) and E_2Yslow_$\bar{b}$ (in solid grey). In region EQ3 (left panel of fig 7), which is a relatively well observed area, the term $\bar{\mathbf{b}}$ has a visible impact on the reduction of the mean temperature increment in the upper ocean. The impact of the T and S corrections from the term $\bar{\mathbf{b}}$ is comparable to the impact of the on-line pressure correction. This suggests that the reason for error in this area, where the mixed layer is quite deep, may be a combination of diabatic and

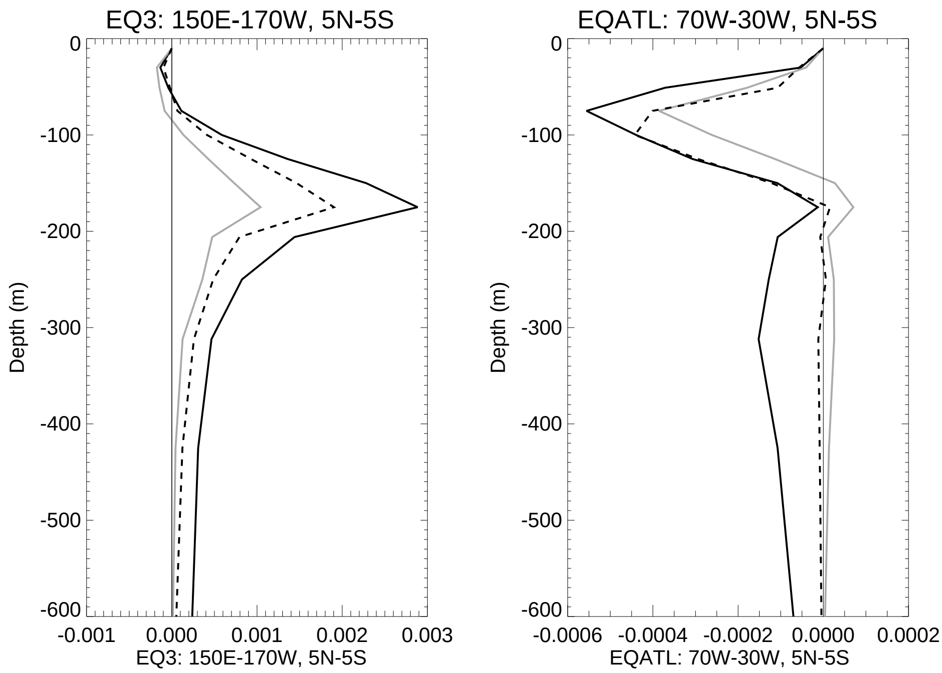


Figure 7: Vertical profiles of the 1987-2001 mean temperature assimilation increment for region EQ3 (left column) and for region EQATL (right column). Shown are the results for experiments E_0 (solid back line), E_2Yslow (black dashed line) and E_2Yslow_$\bar{b}$ (in solid grey).

adiabatic problems, and where direct corrections to the temperature and salinity equations are required as well as corrections to the pressure gradient.

The term $\bar{\mathbf{b}}$ also improves the estimate of the Equatorial Atlantic, both the mean (reduced mean assimilation increment in left panel of figure 7), and the interannual variability. The quality of the interannual variability can be measured by the correlation of the analysed sea level anomalies with those from the altimeter data. The correlation period is 1993-2001. If no bias correction is applied, the data assimilation degrades the correlation (from 0.65 in the analysis with no data assimilation to less that 0.4 in the experiment E_0). The inclusion of the on-line correction in pressure in experiment E_2Yslow slightly improves the estimate, but the correlation is still lower than the no data assimilation case. By introducing the term $\bar{\mathbf{b}}$ in experiment E_2Yslow_$\bar{b}$ the value of the correlation increases to 0.8. The higher value of the correlation due to the term $\bar{\mathbf{b}}$ is an encouraging result.

5 Summary and conclusions

The presence of bias in an ocean data assimilation scheme is a serious obstacle to the reliable representation of climate by historical ocean reanalysis. It is shown that both the ocean mean state and variability can be degraded by data assimilation in some areas. The examples have been taken from the ECMWF operational ocean analysis systems, but they are common to other ocean data assimilation systems.

In large areas of the equatorial Pacific the low frequency component of the temperature assimilation increment is large compared to the higher frequency component, which is clear evidence that the forecast error is correlated. It is also shown that the low frequency component of the error is not stationary, but exhibits considerable low frequency variability. Particularly noticeable and worth further investigation is the change in behaviour of the system after 1998, where the temperature increments around the thermocline in the Niño3 area become increasingly negative.

Consistent with other assimilation systems, comparison with TAO currents shows that the equatorial zonal velocity in the Eastern Pacific is degraded when assimilating temperature data. The degradation of the zonal velocity is associated with a spurious vertical circulation underneath the thermocline. As pointed out by BMN, the results suggest that the spurious circulation can be the cause of this systematic error: the error in the data assimilation has the opposite sign to the error in an analysis where no data have been assimilated.

Data assimilation systems affected by bias are very vulnerable to changes in the observing system. This fact was illustrated by showing the degradation of interannual variability in the Equatorial Atlantic due to the sudden changes in the observation coverage. The sustainability of observing systems is therefore vital for ongoing and future estimates of climate variability. To make optimal use of new and existing observations it is necessary to develop data assimilation algorithms that explicitly deal with bias.

In this paper we presented a modified version of the DdS 1-step algorithm for on-line estimation and correction of system bias. The modifications included an explicit multivariate formulation which allows the balance constraints for the bias to be different to those for the state vector. In this context, the correction applied to the pressure gradient proposed in the BMN scheme can be considered as a particular choice of balance relationship. Modifications have also been introduced in the equation for the time evolution of the bias, by inclusion of a memory term that allows for non-stationary bias, and a prescribed bias term that can act as a first guess. The modified bias correction algorithm has been applied to the ECMWF ocean data assimilation system, and a series of ocean reanalyses have been conducted with different multivariate constraints and time evolution. All the experiments span the period January 1987 - December 2001 and use the ENACT experimental setup.

Experiments reflect the sensitivity of the results to the choice of multivariate formulation. Direct correction of the bias in temperature (observed variable) does not lead to better analyses, and in fact can degrade the equatorial currents. However, if the bias is corrected using the BMN scheme by modifying the pressure gradient, the bias in temperature is reduced and the velocity field is improved. It is therefore important to have insight into the nature of the error. If the error in temperature is due to adiabatic processes that erroneously redistribute heat, the bias gain matrix should reflect this adiabaticity. Otherwise, it will introduce sources and sinks of heat that may eventually deteriorate the solution. Budget analysis of the assimilation statistics (Ricci *et al.* 2005) is a very valuable tool to obtain information about the nature of the error.

Although the sensitivity to the time parameters varies considerably from region to region and from level to level, experiments with finite memory tend to do better, at the expense of underestimating the size of the bias. The multivariate scheme is quite sensitive to the parameters controlling the time evolution of the bias. While stability of the univariate algorithm is mathematically guaranteed, the stability of the multivariate system is less clear. It has been shown that under the assumption of constant bias, the multivariate algorithm can lead to overestimation of the bias term. In the upper levels of the Eastern Pacific, the system fails to stabilize, producing estimates that are worse than the non-bias corrected results. From a practical point of view, underestimation of the bias is probably a safer option, unless the stability of the system is well understood.

In order to avoid discontinuities in the ocean analysis due to changing observing systems it would be desirable to have an *a priori* knowledge of the system bias, preferably obtained using independent data. The new geoid information provided by the gravity mission GRACE could be very valuable in this respect.

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