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D. Mignac et al.

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

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Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Abstract

An ocean data assimilation system to assimilate Argo temperature (T) and salinity (S) profiles into HYCOM was constructed, implemented and evaluated for the first time in the Atlantic Ocean (78° S to 50° N and 98° W to 20° E). The system is based on the Ensemble Optimal Interpolation (EnOI) algorithm proposed by Xie and Zhu (2010), especially made to deal with the hybrid nature of HYCOM vertical coordinate system with multiple steps. The Argo T/S profiles were projected to the model vertical space to create pseudo-observed layer thicknesses (Δp_{obs}) which correspond to the model target densities. The first step was to assimilate Δp_{obs} considering the sub-state vector composed by the model layer thickness (Δp) and the baroclinic velocity components. After that, T and S were assimilated separately. At last, T was diagnosed below the mixed layer to preserve the density of the model isopycnal layers. Five experiments were performed from 1 January 2010 until 31 December 2012: a control run without assimilation, and four assimilation runs considering different vertical localizations of T , S and Δp . The assimilation experiments were able to significantly improve the thermohaline structure produced by the control run. They reduced the RMSD of T (S) calculated with respect to Argo independent data in 34.11 % (43.56 %) in comparison to the control run. In some regions, such as the west North Atlantic, substantial corrections in the 20°C isotherm depth and the upper ocean heat content towards climatological states were achieved. The runs with vertical localization of Δp showed positive impacts in the correction of the thermohaline structure and reduced the RMSD of T (S) from 0.993°C (0.149 psu) to 0.905°C (0.138 psu) for the whole domain with respect to the other assimilation runs.

1 Introduction

Many ocean circulation models include highly sophisticated numerical schemes and a large set of physical parameterizations. However, these are approximations of the

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Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



governing equations of the actual physical processes and, therefore, they are sources of errors or discrepancies with respect to observations. Also, errors may be produced due to inaccuracies of the initial conditions, atmospheric forcing and lateral boundary conditions (Kalnay et al., 1996; Chassignet et al., 2009). For these reasons, data assimilation methods are important scientific tools in oceanography and other fields. They combine model outputs with observational data in a mathematically optimal or sub-optimal way, and produce the so-called objective analysis with smaller errors than the model output (Daley, 1991; Kalnay, 2003). The analysis is used as the model initial condition for weather and climate forecasts (Kalnay, 2003), and more recently for ocean weather forecasts under the framework of operational oceanography (Dombrowsky et al., 2009; Chassignet et al., 2009; Schiller and Brassington, 2011). Data assimilation methods are also applied to produce long-term series of analysis for climate diagnostics studies and they contribute for a better understanding of the physical mechanisms that are responsible for the ocean variability. For example, the depth of the mixed layer and the heat content can be better represented by analyses than by model simulations without assimilation (Carton and Giese, 2008).

A major obstacle in ocean data assimilation is the relatively small number of observed ocean data available for assimilation and validation. Most of the spatial and high frequency temporal variability from the ocean surface is acquired by satellite measurements such as the sea surface height (SSH) and sea surface temperature (SST). However, these observations are available for only few decades and they are insufficient to determine the sub-surface variability (Ezer and Mellor, 1994; Chassignet et al., 2006). Therefore, the implementation of the Argo network with more than 3300 profilers freely reporting temperature and salinity data until 2000 m has transformed the in situ ocean observing system in the new millennia (Schiller and Brassington, 2011). For the first time, it is possible to have continuous measurements of the temperature, salinity and velocity of the upper ocean which makes the Argo network indispensable for any global or regional data assimilation system (Chassignet et al., 2007; Oke et al., 2008; Xie and Zhu, 2010). For example, Oke and Schiller (2007) showed that the assimilation

**Argo data
assimilation into
HYCOM with an EnOI
method in the
Atlantic Ocean**

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



of SST and SSH should be complemented with Argo profiles since the assimilation of this component plays a crucial role to improve the model thermohaline state, especially for salinity.

Among all data assimilation methods, there are the ensemble-based methods which use a set of model states to estimate the model errors (Evensen, 2003; Oke et al., 2005). One largely used is the Ensemble Optimal Interpolation (EnOI) (Oke et al., 2005) in which the ensemble members are taken from a previously done model run. This reduces the computational cost of the assimilation and makes this method suitable for operational purposes. It was already verified that the EnOI is a method that is able to effectively constrain the model towards observations. It was successfully applied to assimilate Argo data in the Pacific Ocean (Xie and Zhu, 2010), sea level anomaly (SLA) data in the South China Sea (Xie et al., 2011) and in the Gulf of Mexico (Counillon and Bertino, 2009), and SLA, SST and Argo data in the Australian region (Oke et al., 2008) and in the Indian-Pacific Ocean (Yan et al., 2010).

Considering the importance of the model in the construction of the analysis, several state-of-the-art ocean circulation models publically available should be considered in order to develop an operational ocean forecasting system with data assimilation. One choice is the HYbrid Coordinate Ocean Model (HYCOM). It is formulated in terms of target densities and employs a hybrid vertical coordinate system to combine the best features of each vertical coordinate in specific oceanic regions (Bleck, 2002). The model has fixed z levels to better represent the mixed layer, isopycnal layers to discretize the deep stratified ocean and σ levels to better reproduce the bathymetry in shallow areas. Because of the hybrid nature of the model, the best way to assimilate vertical profile data into HYCOM is still an open question. A choice of the model prognostic variables should be made a priori since only two of the state variables – temperature, salinity and potential density – are independent. Furthermore, the layer thickness, which is a key model variable, varies spatially and temporally according to the evolution of temperature, salinity and density.

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Taking into account these characteristics, Thacker and Esenkov (2002, afterward using TE) proposed a method to assimilate expendable bathythermographic (XBT) data into HYCOM with a three-dimensional variational scheme (3D-Var). In this work, the XBT profiles at z levels are converted into “observed” layer thicknesses that respect the target densities of each model layer, and the temperature and salinity of the XBTs are projected to each “observed” layer thickness previously created. Xie and Zhu (2010, afterward using XZ) used an EnOI scheme to assimilate Argo data and showed that TE approach produced significant improvements in relation to straightforward schemes, in which the variables at the model layers are interpolated to the observation profiles at z levels, and the innovation is calculated in the observational space.

Very few works have been published to evaluate the impact of in situ profile data assimilation into HYCOM with focus on the Atlantic Ocean (e.g., Thacker et al., 2004; Belyaev et al., 2012). In the present work, a data assimilation system into HYCOM was constructed, implemented and realized for the Atlantic Ocean for the first time. The data assimilation algorithm follows very closely the EnOI scheme suggested by XZ and here it is described. The present system was developed under the efforts of the Brazilian Oceanographic Modeling and Observation Network (REMO) to be a component of an operational ocean forecasting system for the Atlantic Ocean (www.rederemo.org) (Tanajura and Belyaev, 2009; Lima et al., 2013; Tanajura et al., 2013). In this paper, the focus is on the impact of Argo data assimilation over the Atlantic Ocean and on a sensitivity study of the analysis run considering different vertical localizations of the model error co-variance matrix involving temperature, salinity and especially the layer thickness. The REMO forecasting system uses a nested model approach based on HYCOM. The present work deals with the construction of large-scale analyses over almost the whole Atlantic Ocean. This domain was conceived and configured to provide reasonable boundary conditions to higher resolution grids over the South Atlantic of greater interest to REMO. In a near future, the present data assimilation methodology will be used in the Atlantic domain, and in the higher resolution grids over the Metarea V (from 35.5° S to 7° N, west of 20° W until Brazil) and sub-regions off the Brazilian coast

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



of particular interest to the Brazilian Navy and the active petroleum industry located there.

This paper is organized as follows. In Sect. 2, HYCOM and the configuration used in this study are briefly described. In Sect. 3, the EnOI scheme to assimilate Argo data is presented. Section 4 shows the design of the assimilation experiments and Sect. 5 presents their results. Section 6 contains discussions and conclusions.

2 HYCOM and its configuration

HYCOM is a primitive equation, general circulation model, which has evolved from the Miami Isopycnal Coordinate Ocean Model (MICOM) (Bleck and Smith, 1990). The main advantage of the isopycnal coordinate is its ability to maintain the properties of water masses which do not communicate directly with the mixed layer. In HYCOM, with the advection of layer thicknesses by the continuity equation, the isopycnal coordinates smoothly transit to z coordinate in the weakly stratified upper-ocean mixed layer and to terrain-following sigma-coordinate in the shallow water regions (Bleck, 2002; Chassignet et al., 2007). The freedom to adjust the vertical spacing of the coordinate surfaces in HYCOM simplifies the numerical implementation of several physical processes (e.g. mixed layer, detrainment, and convective adjustment). Also, the capability of assigning additional coordinate surfaces to the oceanic mixed layer in HYCOM allows the option of implementing sophisticated vertical mixing turbulence closure schemes (Halliwell, 2004). Hence, HYCOM is considered to be a suitable model for operational ocean forecasting systems and climate studies (Chassignet et al., 2007, 2009). In this work, the version 2.2.14 of HYCOM was used.

The model grid in the present configuration has 760×480 horizontal grid points, with a spatial resolution of 0.25° , which remains constant in longitude, but varies in latitude attaining higher resolution towards the poles. The computational model domain covered almost all the Atlantic Ocean from 78° S to 50° N and from 100° W to 20° E, excluding the Pacific Ocean and the Mediterranean Sea. The vertical domain

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



was discretized in 21 vertical layers. The chosen target potential densities were 19.50, 20.25, 21.00, 21.75, 22.50, 23.25, 24.00, 24.70, 25.28, 25.77, 26.18, 26.52, 26.80, 27.03, 27.22, 27.38, 27.52, 27.64, 27.74, 27.82, and 27.88. The first layers have a few light target density values that ensure a minimum of three fixed-depth layers near the surface of the ocean. To obtain the volumetric density in kg m^{-3} , 1000 should be added to each target density.

The vertical mixing scheme is the K-profile parameterization (KPP) (Large et al., 1994). The model bathymetry was interpolated from the Earth Topography 1 (ETOPO1) with 1 min resolution. On the lateral boundaries, relaxation to climatological temperature and salinity from Levitus (1982) was applied considering the outermost 10 grid cells and the time scale of 30 days. Constant barotropic volume fluxes were imposed: zero flux in the north; eastward flux of 110 Sv in the Drake passage; westward flux of 10 Sv in 12 grid points south of South Africa along 20° E; and eastward flux of 120 Sv from the latter region until Antarctica.

The model was initialized from the state of rest with climatological thermohaline structure and a 30 year spin-up was performed using monthly climatological forcing fields from the Comprehensive Ocean and Atmosphere Dataset (COADS) (Woodruff et al., 1987). Then, from January 1995 until December 2009, the model was forced on the ocean surface with 6 hourly atmospheric reanalysis 1 by the National Centers for Environmental Prediction/National Centers for Atmospheric Research (NCEP/NCAR) (Kalnay et al., 1996), including precipitation, wind speed at 10 m, short and long-wave radiation fluxes at the surface, air temperature and humidity at 2 m. The result of this simulation was used as initial condition to the Argo data assimilation experiments starting on 1 January 2010.

Figure 1 shows the mean state of temperature and salinity simulated by HYCOM from 1 January 1997 until 31 December 2008 and its comparison with the World Ocean Atlas 2009 Climatology (WOA09) along 25° W for the upper 1000 m. In general, the pattern of the simulated temperature and salinity is similar to the WOA09 climatology, particularly in the South Atlantic, which is the main target area for REMO. In the

North Atlantic large differences are seen between 25° N and 50° N below 400 m. The Mediterranean Water (MW) is more saline, warmer and found further north in comparison with WOA09. Moreover, the simulated temperature is higher than WOA09 in the upper 300 m of the equatorial region, while the values of high-salinity cores in the subtropical gyres are smaller than the values found in the climatology. It is expected that assimilation of Argo data will improve the model state and reduce the existing differences in the thermohaline structure with respect to the WOA09 climatology.

3 The data assimilation scheme

The analysis (\mathbf{X}^a) according to the EnOI scheme is given by the formula (Evensen, 2003):

$$\mathbf{X}^a = \mathbf{X}^b + \mathbf{K}(\mathbf{Y} - \mathbf{H}\mathbf{X}^b) \quad (1)$$

where $\mathbf{X}^b \in \mathbb{R}^N$ is the model background state or the prior, \mathbf{K} is the gain matrix, \mathbf{Y} is the vector of observations, $\mathbf{Y} \in \mathbb{R}^{N_{\text{OBS}}}$, and $\mathbf{H}\mathbf{X}^b$ is the projection of the prior onto the observational space by the observational operator \mathbf{H} . The term $(\mathbf{Y} - \mathbf{H}\mathbf{X}^b)$ is called the innovation vector and the term $\mathbf{K}(\mathbf{Y} - \mathbf{H}\mathbf{X}^b)$ is the analysis increment. The gain matrix \mathbf{K} is calculated from the equation:

$$\mathbf{K} = \alpha(\sigma \circ \mathbf{B})\mathbf{H}^T[\alpha\mathbf{H}(\sigma \circ \mathbf{B})\mathbf{H}^T + \mathbf{R}]^{-1} \quad (2)$$

where \mathbf{B} is the co-variance matrix of the model errors and \mathbf{R} is the diagonal variance matrix of the observational error. The term $\alpha \in (0, 1]$ is a scalar that can tune the magnitude of the analysis increment and σ denotes the localization operator applied over \mathbf{B} by a Schur product represented by the symbol \circ . The Eq. (2) is used by many data assimilation schemes such as the Optimal Interpolation, the Ensemble Kalman Filter (EnKF) or the EnOI. In the EnOI scheme, \mathbf{B} is estimated from the equation:

$$\mathbf{B} = \frac{\mathbf{A}'\mathbf{A}'^T}{(M - 1)} \quad (3)$$

where $\mathbf{A}' = [A'^1 A'^2, \dots, A'^M]$, $A'^k = (\mathbf{X}^k - \frac{1}{M} \sum_{m=1}^M \mathbf{X}^m)$, $\mathbf{X}^k \in \mathbb{R}^N$, is the model state vector of the k th ensemble member, $k = 1, M$, and $M = 132$ is the number of ensemble members used in all assimilation steps in this study. This ensemble of model anomalies can be taken from a long-term model run (Evensen, 2003) or a spin-up run (Oke et al., 2008) in order to capture the model variability at certain scales. Thus, even being stationary in time, this ensemble of model anomalies allows describing the spatial correlations and the anisotropic nature of ocean circulation, keeping the analysis dynamically consistent and substantially reducing the computational cost. Details on how the \mathbf{B} matrix was calculated here regarding the high frequency variability of the model are described below.

3.1 Calculation of the innovation vector

Basically, there are two ways to calculate the innovation vector. The first one projects the model state vector into the observational space. In this case, the temperature, salinity and layer thicknesses of HYCOM are projected into the vertical levels of the Argo profiles, which provide almost vertically continuous measurements of temperature and salinity, ranging from near surface until 2000 m. This procedure makes the \mathbf{H} operator to be complex and non-linear. Since the Eq. (1) is linear, the use of a non-linear operator may cause problems in the linear analysis update and may contribute to a sub-optimal assimilation performance (Xie and Zhu, 2010). A second way to calculate the innovation follows the strategy adopted by TE and by XZ for HYCOM, and it is used in the present work. In this approach, temperature (T) and salinity (S) data profiles at z levels are projected into the model vertical space to create pseudo-observed layer thicknesses ($\Delta\rho_{\text{obs}}$). This is done following the hybrid nature of the model's layers: each layer is required to have a minimum thickness and, after that requirement is satisfied, it should be as close as possible to its specified target value of potential density. Thus, each Argo profile is processed as follows. Based on a pair of profiles of potential temperature and salinity, the profile of potential density can be calculated by

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



an equation of state for seawater (Brydon et al., 1999). The estimated surface density from the Argo profile is compared to the top layer target density to decide whether any sufficiently low-density water was observed. If not, the minimum thickness is assigned to the layer and the question is repeated to the layer below. Once water with the target density is encountered, the remainder of the potential density profile can be partitioned, so that layer averages correspond to target densities until the maximum depth of the Argo profile is reached.

Figure 2 shows the vertical profiles of potential temperature, salinity and potential density in the observational space at z level and the new and synthetic observation defined at model layers for an Argo float located at 4.04° N and 23° W on 1 January 2010. In Fig. 2, each Δp_{obs} respects the target densities of the model as soon as the first target density is found in the potential density profile of the Argo data. Also, the averages for all the observational variables are computed for each layer, as shown by the discretized profiles of potential temperature and salinity in the model layers. The step functions of T , S , and Δp_{obs} are the data that will be actually assimilated by the EnOI scheme.

3.2 The modified EnOI to assimilate profile data into HYCOM

After the observation is defined in the HYCOM layers, the “observed” layer thicknesses are assimilated in a first step by Eqs. (1) and (2), and the analysis update is carried out for the model control state vector $(\Delta p_i, U_i, V_i)$; $i = 1, \dots, nz$, where Δp_i , U_i , V_i are the layer thicknesses and the baroclinic velocity components, respectively, defined at the nz model layers for a single time step. To avoid that the analysed layer thicknesses become occasionally negative, a computationally efficient scheme based on Sakov et al. (2012) is used in this work. In this process, if the thickness of a layer becomes negative, it is reset to zero and the thickness deficit is added to the neighbouring layers. The layers are traversed twice, once from top to bottom, and a second time from bottom to top. Finally, the sum of the layer thicknesses should be equal to the initial bottom pressure (or local depth).

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



In the next step, temperature and salinity are assimilated separately and in a univariate way also according to Eqs. (1) and (2), but now with the previously adjusted layer thicknesses. Finally, T or S is diagnosed below the mixed layer by the seawater equation of state. According to TE, “Within the context of HYCOM, when correcting temperature, it is necessary to decide whether to move interfaces, keeping potential densities of the layers unchanged, or to correct the densities, leaving the interfaces unchanged”. Therefore, when the assimilation of layer thicknesses is performed, the potential density should be kept constant in the ocean simulated with isopycnal coordinates. Considering that most of the T corrections in the experiments of XZ were due to changes in the layer thicknesses by the assimilation of $\Delta\rho_{\text{obs}}$, T was chosen to be diagnosed below the mixed layer in the present work, instead of S .

3.3 Generation of a running ensemble

Many works show how sensible the EnOI and EnKF schemes are to the ensemble size (Mitchell et al., 2002; Evensen, 2003; Oke et al., 2007). In the EnOI scheme, the propagation of the observational information is highly dependent on the size and the quality of the ensemble, because the final analysis can be regarded as a combination of the ensemble anomalies whose relative weight is determined by the co-variances. In this work, 132 ensemble members were used. They were selected from the model free run for each assimilation day, regarding the intra-seasonal variability and the high frequency model dynamics. This number of ensemble members was chosen after few sensitivity experiments considering a reasonable representation of the model's anomalies without high computational cost and is in agreement with the numbers used in recent works (e.g. Counillon and Bertino, 2009; Xie and Zhu, 2010; Xie et al., 2011).

The long-term model run that was used to select the ensemble members corresponded to the 12 year period from 1 January 1997 until 31 December 2008. For each assimilation step, a different model co-variance matrix was calculated. Considering the assimilation day, 11 ensemble members for each year of the 12 year period were selected around the date of the corresponding assimilation day. For instance, to perform

assimilation on 15 March 2010, 11 members centred on 15 March of each year from 1997 to 2008 were taken with 8 days apart, which gives a time window of 80 days for each year. However, the computational code developed here is flexible to use another number of ensemble members and to select different intervals between each ensemble member.

3.4 Localization

The localization technique is a feasible solution to reduce the effect of the sampling error in the ensemble-based methods, especially when the ensemble size is small (Hamill et al., 2001; Oke et al., 2007). The significance range of a measurement is a critical question in assimilation. In the present case, it should be unreasonable that a measurement in the Gulf Stream contributes to resolving the mesoscale features of the circulation of the Brazilian Current. Therefore, the localization aims to delete long-distance correlations that may appear in the gain matrix and to limit the influence of a single observation by the Kalman update equation within a fixed region around the observation location. However, a drawback of the localization is that it can break-down the geostrophic balance. Oke et al. (2007) show that localization conserves the geostrophic balance when the radius of the localization is equal to or larger than the radius of decorrelation, which is the scale in which the correlations become negligible.

For many EnKF and EnOI schemes, localization is only applied in the horizontal direction (Oke et al., 2008; Sakov et al., 2012). However, some works have already investigated the vertical localization and its impact on the analysis, such as in XZ. They presented a vertical localization scheme for T and S when assimilating Argo profiles into HYCOM. Here, localization in the vertical direction is also investigated, but differently from XZ, the focus is on Δp .

The operator $\sigma \circ$ in Eq. (2) defines the implementation of the localization by a Schur product, i.e., a product between elements with the same index in the arrays. The notation $\sigma \circ \mathbf{B}$ denotes the Schur product of a correlation matrix σ with the \mathbf{B} matrix, and this approach is used in many works (Oke et al., 2007, 2008; Xie and Zhu, 2010). Here,

the localization operator is separated into a horizontal component (σ_h) and a vertical component (σ_v), and it is defined as $\sigma = \sigma_h \sigma_v$.

3.4.1 Horizontal localization

In order to define the horizontal correlation matrix σ_h , a fifth-order function is used as in Gaspari and Cohn (1999):

$$\sigma_h(l_{ij}, L) = \begin{cases} -\frac{1}{4} \left(\frac{l_{ij}}{L}\right)^5 + \frac{1}{2} \left(\frac{l_{ij}}{L}\right)^4 + \frac{5}{8} \left(\frac{l_{ij}}{L}\right)^3 - \frac{5}{3} \left(\frac{l_{ij}}{L}\right)^2 + 1, & 0 \leq l_{ij} \leq L \\ \frac{1}{12} \left(\frac{l_{ij}}{L}\right)^5 - \frac{1}{2} \left(\frac{l_{ij}}{L}\right)^4 + \frac{5}{8} \left(\frac{l_{ij}}{L}\right)^3 + \frac{5}{3} \left(\frac{l_{ij}}{L}\right)^2 - 5 \left(\frac{l_{ij}}{L}\right) + 4 - \frac{2}{3} \left(\frac{l_{ij}}{L}\right)^{-1}, & L < l_{ij} \leq 2L \\ 0, & l_{ij} > 2L \end{cases} \quad (4)$$

In this function, l_{ij} is defined as the Euclidean distance between any two arbitrary points in the horizontal space and L is the horizontal scale of influence defined as 150 km for all the assimilated variables. It is similar to a Gaussian function in physical space but more compact. The correlation function σ_h forces the model error co-variance matrix \mathbf{B} to decrease to zero when l_{ij} reaches 300 km. Thus, the radius of localization is defined as 300 km.

3.4.2 Vertical localization

Concerning the vertical localization, XZ found considerable off-diagonal correlations values for temperature and salinity between different HYCOM layers. However, there was no significant impact in the analysis when those co-variances were filtered and no significant differences in the experiments with and without vertical localization were reported. However, in the present work, the vertical localization of co-variances between the layer thicknesses was investigated. They showed considerable off-diagonal correlations of above 0.4 or below -0.4 from the 7th layer until the bottom (Fig. 3). In

the formulation of the vertical localization operator, the “vertical distance” between the layers was measured by the water column stratification, rather than by the Euclidian distance. Thus, in order to define the correlation matrix σ_v , the following function was used:

$$\sigma_{v(i,j)} = \exp \left[-(\Delta\rho_{(i,j)}/L_\rho)^2 \right] \quad (5)$$

where $\Delta\rho_{(i,j)}$ is the density difference between the HYCOM layers i and j , and L_ρ is a vertical scale factor defined as 0.5 kg m^{-3} according to XZ. As it is shown by Fig. 3, when applying the vertical localization, the elements few entries away from the diagonal in the co-variance matrix are almost cancelled, but the correlations between the adjacent layers remain.

3.5 Observational errors

Since the observations that are actually assimilated are defined in the model vertical space, the observational errors of T and S in the model layers are calculated as a function of the depth D in meters, respectively, as in XZ:

$$\text{SD}_T(D) = 0.05 + 0.45 \exp(-0.002D) \quad (6)$$

$$\text{SD}_S(D) = 0.02 + 0.10 \exp(-0.008D) \quad (7)$$

The standard deviations of the observational errors of T vary in the vertical from 0.5°C in the surface until 0.05°C in the deep ocean. For S , they vary from 0.12 psu to 0.02 psu . According to Eqs. (6) and (7), the observational errors are assumed Gaussian with zero mean and uncorrelated.

In case of layer thickness, according to TE, the standard deviation of $\Delta\rho_{\text{obs}}$ is calculated depending on the oceanic region. For example, in the mixed layer, the layer thickness is assigned to the minimum layer thickness allowed by the model configuration, and the standard deviation is defined as $0.05\Delta\rho_k$, where $\Delta\rho_k$ represents the layer

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

thickness at the k th layer calculated from the observed profiles. In the isopycnal layers, the standard deviation is defined by the formula:

$$SD(\Delta p_k) = \max \left\{ 0.5 \delta p_k, \max \left[0.05 \Delta p_k, \Delta p_k \left(0.05 + (0.5 - 0.05) \frac{sd_{\sigma(k)}}{SD_{\sigma(k)}} \right) \right] \right\} \quad (8)$$

where δp_k is the minimum layer thickness specified by the model configuration for the k th layer, $sd_{\sigma(k)}$ is the minimum standard deviation of the potential density defined as 0.001 kg m^{-3} , and $SD_{\sigma(k)}$ is the standard deviation of the potential density from observations. The later should be small when the potential density from the “observed” layer thickness has a close value to its target density.

4 Assimilation experiments

4.1 Argo data and quality control

The Argo data employed in the assimilation were collected from a global data center (available at ftp://ftp.ifremer.fr/ifremer/argo/geo/atlantic_ocean/). All those observations were required to step into a data quality control procedure (DQC), which is an essential part to any oceanic data assimilation system since spurious data can compromise the analysis quality and introduce artificial trends in the assimilation results (Yan and Zhu, 2010). The DQC used in this work was developed by REMO together with the Brazilian Navy and tests the date, the location, and the temperature and salinity of each Argo profile previously collected. The validation of T and S profiles was made according to all criteria and references established by the Global Temperature–Salinity Pilot Program from the Intergovernmental Oceanographic Commission (IOC, 1990) and from the database of the National Oceanographic Data Center (NODC).

From January 2010 to December 2012, 47 999 valid Argo profiles were assimilated into HYCOM in the Atlantic Ocean. These profilers covered almost the entire model domain, and were especially dense in the North Atlantic, as shown in Fig. 4.

4.2 Configuration and evaluation of the assimilation experiments

Five integrations were performed from 1 January 2010 until 31 December 2012 to evaluate the impact of the Argo data assimilation and the vertical localization in the correction of the ocean state and circulation. The first one was a control run without assimilation (CTL). The other runs were assimilation runs, namely: (i) assimilation without vertical localization (ASSIM), (ii) assimilation with vertical localization of layer thickness (VLOCDP), (iii) assimilation with vertical localization of temperature and salinity (VLOCTS), and (iv) assimilation with vertical localization of all the assimilated variables (VLOCDPTS). In all the experiments with data assimilation, a 3 day observational window was considered in order to select all the valid profiles collected 3 days before the assimilation step. The interval between each assimilation step was also 3 days and the scalar α was defined as 0.3.

The Argo daily data was also used to validate the results of the experiments in a daily basis, despite the fact that assimilation was performed at each 3 days only. However, the prior state was always considered in the evaluation of the assimilation runs. The prior is the model state immediately before the assimilation step. Considering each assimilation cycle, the ocean states at 24 h, 48 h and 72 h after assimilation were assessed in the assimilation runs. Therefore, the validation of the prior is done with independent data, since all the Argo profiles employed in the validation were used only in the next assimilation cycle. This procedure is analogous to the evaluation of forecasts. Moreover, 16 fixed moorings from the Prediction and Research Moored Array in the Tropical Atlantic (PIRATA) were used as another independent dataset for validation. Their locations are represented by red dots in Fig. 4. Also, the domain was split into 12 sub-regions from a to l, as shown in Fig. 4, in order to evaluate the regional impact of the assimilation. These sub-regions and their coordinates were selected taking into account the spatial distribution of the mean kinetic energy and the mean standard deviations of SSH, SST and sea surface salinity (SSS) from 1997 until 2008. The numbers of Argo profiles used to validate the experiments in the 12 sub-regions a, b, . . . , m and

OSD

11, 1733–1781, 2014

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



I were 3085, 2352, 2522, 540, 1463, 2750, 2475, 1849, 1560, 1597, 2536 and 3067, respectively.

Outputs from the HYCOM-Navy Coupled Ocean Data Assimilation (HYCOM + NCODA) (Chassignet et al., 2007, 2009) system available in z levels and fields from the Ocean Surface Current Analyses – Real Time (OSCAR) (Johnson et al., 2007) were employed to compare the velocity fields produced by the assimilation runs. Also, the WOA09 was used to evaluate the mean state of T , S and heat content of the upper 300 m (HC300) of the experiments.

5 Results

5.1 Comparison of mean states

The first comparison is conducted with the WOA09 climatology along 25° W for the upper 1000 m (Fig. 5). It was already verified that the free model run mean from 1997 until 2008 showed substantial differences with respect to the WOA09 climatology (Fig. 1). According to Chen et al. (2000), ocean circulation models can naturally present large and systematic biases in T and S due to their initialization and configuration. This is also shown by the control run, particularly in the North Atlantic. For example, to simulate the MW in the Atlantic, relaxation of T and S in the boundary condition is imposed without mass flux. Also, no mass flux is allowed in the northern boundary at 50° N. As mentioned above, the main purpose of this grid is to provide boundary conditions for another higher resolution grid focusing on the Metarea V. It was already expected that the control run would have larger biases around the middle latitude band in the North Atlantic due to the model configuration. However, even with these limitations, the assimilation schemes are able to substantially reduce these differences and correct the ocean state towards WOA09. For example, the positive temperature bias up to 3° C and the negative salinity bias up to 0.4 psu in the upper 300 m of the control run are not produced in any assimilation run. Moreover, all the discrepancies found in the MW are

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



remarkably diminished in the data assimilation runs, which are able to decrease the differences in 0.6 psu and more than 2 °C towards WOA09 between 20° N and 40° N in the sub-surface, especially bellow 400 m. This correction is very effective in the VLOCDP and VLOCDPTS runs, which adopt the vertical localization of Δp . The VLOCDPTS run is able to more efficiently improve the mean T and S states in the North Atlantic along the entire water column by further reducing the differences of 1 °C and 0.1 psu found in the other assimilation runs with respect to WOA09. Also, at 300 m near 25° S, only the VLOCDPTS run decreases the differences towards WOA09 from more than 3 °C to almost 1 °C, while the ASSIM and VLOCTS runs are not able to reduce these differences with respect to the control run. But, south of 30° S, the improvements of T and S in the VLOCDPTS are considerably smaller than those obtained by the other assimilation runs.

Near 50° S, the control run is not representing very well the formation of the Antarctic Intermediate Water Mass (AIWM). The experiments with data assimilation can correct in 2°C and 0.3 psu the negative biases showed by the control run, except for the experiment VLOCDPTS. Since it is a region of water mass formation, it seems that the vertical correlations between model layers are very important in order to represent this physical process. In the experiments with vertical localization of $\Delta\rho$, much of this information between layers is lost (Fig. 3), and the experiment VLOCDPTS was not efficient to improve the model state for this region in particular.

In order to investigate how stratification was modified by Argo data assimilation in the upper 300 m, Fig. 6 shows the meridional section along 25° W of the mean potential density and the position of the layers interfaces for the experiments CTL, ASSIM and VLOCPTS. In general, as already shown in Fig. 5, the assimilation runs tend to decrease the temperature and increase the salinity in the upper 300 m, driving the model towards WOA09. This is associated with a general increase of the mean potential density in the sub-surface in all the assimilation experiments, especially between 30° S and 30° N. This raise of the potential density can reach more than 0.5 kg m^{-3} near the equator and in the subtropical gyres. According to Bleck (2002), the implementation

of the isopycnal vertical coordinate in HYCOM follows the theoretical formulation that each isopycnal layer will move to be as close as possible to its target density. Therefore, in the assimilation experiments the deeper layers will move towards the surface to encompass the density increase produced by the T and S increments and satisfy their target densities. For example, near the equator and in the subtropical gyre of the South Atlantic, there is a displacement of 25 m or more of the deeper layer interfaces towards the surface. In the North Atlantic, this displacement is even larger and it can reach 150 m, as can be seen by the behaviour of the white dashed line in Fig. 6 that represents the interface between the 11th and 12th layer. Large et al. (1997) showed that the warm temperature bias near the equator is a common feature of coarse-resolution models and it is related to weak zonal currents and weak zonal slopes of the isotherms. However, all the data assimilation experiments are able to force the present low resolution model to stack the layer interfaces in the upper 300 m and correct the model bias of temperature and salinity not only in the equator, but in all latitudes, especially between 30° S and 30° N.

The depth of the 20 °C isotherm is also evaluated for the experiments and the WOA09 climatology in two longitudinal sections, one along the equator and the other along 30° N (Fig. 7). In the WOA09, the depth of 20 °C isotherm along equator is about 120 m in the west side, and it gets shallower in the east side with a value of almost 50 m. The control run is clearly warmer than WOA09 in the upper ocean with temperatures higher than 28 °C in the first 100 m, so that the position of 20 °C isotherm is deeper, especially in the east side of the section with values close to 100 m. All the assimilation experiments reduce the warm bias in the upper ocean and the depth of 20 °C isotherm is lifted to a shallower position in much better agreement with the WOA09 climatology. In the North Atlantic, the control run has even a stronger bias of more than 4 °C in the upper 300 m. Hence, the depth of 20 °C isotherm of the control run is deeper than WOA09, attaining more than 300 m in the west side of the section. Again, the experiments with data assimilation are able to significantly reduce the warm bias by moving the position of 20 °C isotherm more than 150 m towards the surface. This agrees very

**Argo data
assimilation into
HYCOM with an EnOI
method in the
Atlantic Ocean**

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



well with the large displacement of the layer interfaces in the North Atlantic shown in Fig. 6, and also with the WOA09 climatology. Along 30° N, between 75° W and 65° W and between 40° W and 25° W, the experiment VLOCPDTS is able to bring the 20°C isotherm up to 50 m closer to the surface in comparison with the other runs without the vertical localization of layer thickness. On other hand, the experiment VLOCDPTS is the only assimilation experiment that does not represent very well the upwelling in the east margin of the Atlantic ocean at 30° N in Fig. 7.

To further assess the impact of the assimilation in the upper ocean thermal structure, the spatial distribution of the HC300 between 50° S and 50° N is presented in Fig. 8 for the WOA09 together with the differences (model mean minus WOA09) for each run. In general, the control run has a larger HC300 in comparison with the WOA09 climatology. Vast areas of the North and South Atlantic have more than 50 MJ m⁻² of HC300 excess than the climatology. The largest differences are attained in the Gulf Stream region (about 400 MJ m⁻²), since it is displaced northward with respect to observations, and in the southwest Atlantic around 4° S, associated with a misrepresentation of the Brazil–Malvinas confluence. When Argo data is assimilated, the model temperature is constrained towards WOA09 and there is a strong impact on the HC300. All the assimilation experiments decrease the HC300 difference with respect to WOA09 in more than 150 MJ m⁻² for large areas of the subtropical North Atlantic and 50 MJ m⁻² in the equatorial and South Atlantic. However, large differences still remain in the simulated Gulf Stream region. No Argo data was available in this region – to the north of the observed Gulf Stream – to constrain the model (Fig. 4), so that the assimilation runs could not correct this discrepancy. Also, no SST and SSH was assimilated and the assimilation of Argo only could not completely modify this important circulation feature.

5.2 Comparison with Argo profilers and PIRATA moorings

The root mean square deviation (RMSD) is calculated in a daily basis against Argo and PIRATA observations to objectively evaluate the temperature and salinity produced by the experiments. This comparison is done with independent data, since the 24 h, the

48 h and the 72 h simulations after each analysis cycle is assessed. The 72 h simulations correspond to the prior or background states used in the assimilation steps.

The depth averaged RMSD of T and S until 2000 m against the Argo profilers in the model domain from 1 January 2010 until 31 December 2012 is shown in Fig. 9. The RMSDs of the ASSIM and VLOCDPTS runs are substantially reduced from 1.75 °C and 0.30 psu in the beginning of the runs to 1 °C and 0.14 psu by the end of the runs. In Fig. 9, the only assimilation runs presented are the ASSIM and VLOCDPTS, since the other two assimilation runs produced similar curves. The first year of integration has the greatest RMSD reduction for the assimilation experiments. From the second year on, especially in the last year, the RMSD reduction is smaller and the RMSD values tend to oscillate around a stable mean. This indicates that the assimilation experiments would be now ready to run with higher values of α in order to constrain the model even closer to the observations. Here, α is equal to 0.3. This small value was chosen to avoid abrupt changes in the model state and numerical instability considering the relatively large discrepancies between the model background and observations in certain regions.

The VLOCDPTS run produces smaller RMSDs than the ASSIM run. The RMSD of the VLOCDPTS is about 86 % (69 %) of the ASSIM RMSD for temperature (salinity). However, this improvement is mainly due to the vertical localization of the layer thickness. It was found that when applying the vertical localization of the layer thickness, the number of grid points with negative Δp after assimilation and before the post-processing was extremely reduced. In the 365 assimilation steps from 1 January 2010 until 31 December 2012, more than 235 000 grid points with negative Δp were generated and needed post-processing in the ASSIM run. This number was decreased to less than 80 000 in the VLOCDP and VLOCDPTS runs, which means a reduction of 66 %. The improvement caused by the vertical localization of Δp , rather than the vertical localization of T and S , will be discussed in detail below.

The vertical profiles of the mean RMSD of all runs against Argo and PIRATA data over the whole model domain is presented in Fig. 10. The largest temperature and salinity RMSD of the control run are attained in the top 700 m with respect to Argo

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



data and in the top 200 m with respect to PIRATA data. This is associated to difficulties that models have to represent the thermocline and pycnocline regions of sharp vertical gradients (Oke and Schiller, 2007; Xie and Zhu, 2010). When Argo data are assimilated, the vertical thermohaline structure is very much improved. With respect to Argo data, the experiment ASSIM decreases the RMSD of the control run in the top 600 m from 2°C to 1.3°C and from almost 0.4 psu to 0.19 psu. Regarding PIRATA data, the experiment ASSIM reduces up to 1°C and 0.13 psu the RMSD values of the control run in the first 120 m. Gains with the vertical localization of $\Delta\rho$ are seen from 200 m to 800 m and from 1200 m until 2000 m. In these ranges, the experiment VLOCDPTS is able to decrease even more the RMSD in 0.15°C and 0.025 psu with respect to the other assimilation runs. The vertical localization of only T and S had almost no positive impacts in the RMSD, and contributed to slightly degrade S near the surface when the runs are compared to PIRATA data.

The vertical localization of T and S was also studied by XZ and they also did not find any impact in their assimilation experiments. However, the vertical localization of $\Delta\rho$ seems to be a good approach to better improve the model state, especially when correlations of the ensemble members come from a free model run that contains large discrepancies in certain regions in comparison with climatology and observations. Since the co-variance matrix of the model errors in the EnOI scheme is calculated by many snapshots of the model state, the performance of the assimilation is quite dependent on the accuracy of the error co-variances (Oke et al., 2005; Xie and Zhu, 2010). Due to the inaccuracies of the ensemble members used in this work, many vertical correlations might not be well represented, especially between distant layers. Thus, since the vertical localization of layers thickness mostly keeps the correlations between adjacent layers, this strategy avoids the generation of many grid points with negative $\Delta\rho$ during the assimilation process and makes this approach a safer way to produce a more physically consistent and reliable analysis. Also, the vertical localization of layer thickness does change the state of T and S much more than the vertical localization of T and S .

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



This reinforces the fact that the corrections of the model layer thicknesses are essential to adjust the values of T and S of the model layers, as stated by TE.

To investigate the spatial distribution of the RMSD of T and S with respect to Argo data until 2000 m, Table 1 contains the deviations for all the 12 sub-regions previously defined in Fig. 4. In the control run, the largest RMSDs of T and S are attained in the sub-regions a, b and d with values greater than 1.6°C and 0.27 psu . All those sub-regions are found in the North Atlantic, where the model has the largest differences in comparison with the WOA09 climatology and with Argo observations. This is particularly clear for sub-region a corresponding to the Gulf Stream region with RMSD of 2.3°C , and for sub-region d in the Gulf of Mexico with RMSD of 0.368 psu . It should be reinforced that this grid configuration was prepared to provide boundary conditions for a higher resolution grid focusing on the Metarea V. Hence, the control run is better adjusted with smaller RMDs in the South Atlantic than in the North Atlantic as shown in Table 1. The maximum RMSD in the South Atlantic is attained in the sub-region i corresponding to Brazil–Malvinas confluence with values of 1.29°C and 0.207 psu . For all the sub-regions, the different EnOI runs are able to reduce the RMSD values of T and S in comparison with the control run. The greatest impact of data assimilation is in the North Atlantic, where approximately 60 % of the assimilated Argo profiles are found and where the control run has its largest RMSDs. For example, the experiment ASSIM decreases the RMSD of the control run about 1°C in the sub-regions a and b, and more than 0.17 psu for the sub-regions b, c and d. In the Gulf of Mexico, this reduction is up to 0.2 psu . On other hand, the RMSD reductions by the ASSIM run in the South Atlantic are only about 0.2°C and 0.04 psu . Even with the large impact of the Argo data assimilation, some regions still remain with large RMSDs. This is the case of Gulf Stream, the Gulf of Mexico and the Brazil–Malvinas confluence in the sub-regions a, d and i, respectively, where the experiments still have RMSDs greater than 1°C and 0.145 psu . These are regions of strong gradients, variability and mesoscale eddy activity. The Gulf Stream is highly influenced by mesoscale circulation and the growth of baroclinic instability after its separation from the North American coast (Robinson et al., 1989; Spall

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

and Robinson, 1990; Lee and Mellor, 2003). Also, the Brazil–Malvinas confluence is characterized by a weak and warm southward Brazil Current meeting a strong, cold and less saline northward Malvinas Current, which results in large contrasts in stratification and strong eddy activity (Gordon, 1989; Garzoli and Garrafo, 1989; Goni et al., 1996). Thus, the large RMSD still found in the assimilation runs in these regions can be due to lack of data, inaccuracies in the ensemble members, and limitation of the model resolution to solve the mesoscale circulation patterns. Similarly, XZ found that the assimilation of Argo profiles did not capture the mesoscale activities in the Pacific Ocean due to the coarse model resolution, and the Kuroshio System remained with large RMSDs in their assimilation run.

In Table 1, the assimilation experiments with the best performances are the ones with vertical localization of layer thickness. This is particularly clear in the sub-regions a, b and c, where the experiments VLOCDPTS and VLOCDP are able to reduce the RMSD values up to 0.12 °C and 0.018 psu with respect to the ASSIM and VLOCTS runs. These 3 sub-regions are located in the North Atlantic, where the model free run has its largest bias in comparison with WOA09 (Fig. 1). They are sub-regions where the ensemble vertical correlations might not be well represented. Therefore, relaxing the vertical constraints by vertical localization should improve the model state. Small gains can also be seen in the South Atlantic when applying the vertical localization of layer thickness, for example, in the sub-region h corresponding to the Brazilian Current. The only regions where the experiments VLOCDP and VLOCDPTS are just a little bit worse than the experiment ASSIM is the Gulf of Mexico, sub-region d, for salinity, and the sub-regions j and k in the mid-latitudes close to the AIWM formation. In general, the pairs of experiments ASSIM and VLOCTS, and VLOCDP and VLOCDPTS produced similar results in all sub-regions, and the strategies with vertical localization of layer thickness attained smaller RMSDs of T and S . It corroborates to conclude that the vertical localization of Δp was more important than the vertical localization of T and S for the present experiments.

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



5.3 Adjustment of the altimetry and velocity fields

As it was shown above, the EnOI scheme used in this work adjusts the baroclinic velocity fields via their co-variance with layer thickness in the analysis increments. This is a physically consistent adjustment, since the horizontal velocity fields are dominated by the slope of the isopycnal layers, which will be responsible to generate the pressure gradient force. XZ showed that around of the assimilated Argo profiles in the mid-latitudes, cyclonic and anti-cyclonic circulations were developed, consistent with the large local modifications of the model layer thicknesses and geostrophy. This is due to the nature of the co-variances, which come from an ensemble of model states and allow describing the anisotropic patterns of the circulation (Oke et al., 2005, 2008; Xie and Zhu, 2010). Figure 11 shows the analysis increment of layer thickness and the circulation originated in the 12th layer around an Argo profile located in the mid-latitudes of the North Atlantic in 1 January 2010 regarding the experiments ASSIM and VLOCDP. The experiment ASSIM robustly induces thinning of layer thickness up to 200 m, and then a stronger and more anisotropic cyclonic pattern is imposed with velocities increments reaching 0.5 m s^{-1} . Both experiments develop a cyclonic circulation around this mid-latitude Argo profile, which is coherent with the negative analysis increment of layer thickness and the negative SSH increment also shown in Fig. 11. Thus, the geostrophic balance was preserved in both experiments. Since the experiment VLOCDP has limited influence between distant layers, the analysis increments are smoothed and smaller velocity increments of about 0.1 m s^{-1} are produced. The cyclonic gyre is better represented in the VLOCDP and VLOCDPTS (not shown) run, which shows a more negative and more continuous increment of SSH than the ASSIM run. The analysis constructed by this increment may be more suitable to initialize a model than the analysis by the ASSIM strategy considering the present background state and ensemble members. However, further adjustment of the velocity fields is made by the model itself along the integration to balance the analysis increments after assimilation of Δp , T and S .

The trend of SSH reduction by Argo data assimilation in the present experiments is confirmed in Fig. 12. It shows the 30 day SSH running mean of all experiments considering the model domain between 50° S and 50° N. From the beginning of the integration until December 2012, SSH is reduced from 0.22 m to 0.12 m in the experiments AS-SIM and VLOCTS, which is compatible with the largest impact found in the first year of assimilation in Fig. 9. The VLOCDP and VLOCDPTS runs produce a larger reduction from 0.22 m to 0.08 m. From this period on, the SSH of all assimilation experiments stabilize around these values and different SSH means are achieved in the experiments with and without vertical localization of layer thickness, but with variability very close to the control run. The diagnostic model SSH varies due to the barotropic pressure mode and especially due to the deviations in temperature and salinity caused by changes in the structure of the layer thicknesses (Chin et al., 2002). Hence, this lower SSH mean in the assimilation experiments reflects the new thermohaline state and stratification achieved when Argo data are assimilated. The thermal expansion of seawater constitutes a very important component of SSH and then the reduction of the temperature and the heat content in the assimilation experiments contribute remarkably to the SSH decrease. For example, the heat content is very well and positively correlated with SSH (Chambers et al., 1998; Willis et al., 2004; Dong et al., 2007). In this work, mean correlation values of 0.802, 0.815 and 0.812 between the HC and SSH are found for the experiments CTL, ASSIM and VLOCDPTS, respectively. When comparing the monthly means of all the experiments with the WOA09 monthly means over the entire domain (not shown), the experiments VLOCDP and VLOCDPTS are able to decrease the HC in more 7 MJ m⁻² towards the climatology. This could explain why there is a larger decrease of the mean SSH in the experiments with vertical localization of layer thickness.

In order to evaluate how the local changes in layer thickness, SSH and velocity fields affect the large-scale circulation, the zonal velocity along 25° W in the upper 300 m for all the experiments and HYCOM + NCODA analysis is shown in Fig. 13. Some observed features are clearly represented in the HYCOM + NCODA analysis, such as the South Atlantic Current (SAC) southward 40° S, the branches of the westward South

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Equatorial Current (SEC), the eastward Equatorial under Current (EUC) and the North Equatorial Countercurrent (NECC). Modifications with respect to the control run were imposed by assimilation. However, some can be considered improvements towards the HYCOM + NCODA analysis, and some cannot. For example, there is a strong zonal current in the control run up to 0.6 m s^{-1} between 30° N and 40° N associated with the Gulf Stream recirculation path, which is much more intense than in the HYCOM + NCODA analysis. This zonal current is reduced to $0.1\text{--}0.2 \text{ m s}^{-1}$ in the experiment VLOCTS and VLOCDPTS. However, it is simulated further south in comparison with HYCOM + NCODA analysis, especially in the VLOCTS run. In the experiment ASSIM, this recirculation path is even weaker and merges in the broader eastward flow. Also, in all assimilation experiments the EUC velocity decreases from 0.6 m s^{-1} to 0.4 m s^{-1} and gets closer to the magnitude of the HYCOM + NCODA analysis, but the shape of its core remain the same as in the control run and not as elongated as in the HYCOM + NCODA analysis. On the other hand, all data assimilation runs constrain the SAC near the surface, while it reaches more than 300 m in the HYCOM + NCODA analysis. Finally, assimilation is not able to reduce the magnitude of the SEC and to increase the intensity of the NECC simulated by the control run.

Using the same EnOI scheme employed in this work, XZ also did not find significant impacts in the velocity field when assimilating Argo profiles. For instance, they showed that Argo data assimilation makes the undercurrent in the Equatorial Pacific Ocean too broad with an intensification of the eastward current to greater depths. In the present work, similar results are obtained, since there is no clear signal about the impact of the Argo data assimilation as found in the thermohaline structure. The discrepancies of the model free run and its variability with respect to climatology and observations are an important limitation for the assimilation to produce the correct analysis increments, particularly for the large-scale circulation. For this reason, many works point out that the model biases should be considered during the assimilation process (Reynolds et al., 1996; Dee and Silva, 1998; Bell et al., 2004; Dee, 2005; Xie and Zhu, 2010). In addition to the comparison with the HYCOM + NCODA analysis, the surface velocity fields

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



of the assimilation runs were compared to the OSCAR fields. Again, the results did not provide a clear signal about the impact of Argo data assimilation in the surface currents. The RMSD of U and V with respect to OSCAR were reduced in less than 5 % in comparison to the control run.

6 Conclusions and discussion

In this work, an EnOI scheme to assimilate Argo data into HYCOM was successfully constructed and implemented. The first results were evaluated against observations and analyses over the Atlantic Ocean. The EnOI scheme was based mostly on the work of XZ. A key variable in the assimilation algorithm was the “observed” model layer thickness, Δp_{obs} , constructed from the Argo temperature (T) and salinity (S) profiles, according to TE. First, Δp_{obs} was assimilated and the analysis state vector considered not only the model layers thickness, but also the baroclinic velocities. This procedure is physically consistent, since the horizontal velocities fields are dominated by the difference between the layers depth, which will be the responsible to originate the pressure gradient force. After that, with the previously adjusted model layer thicknesses, T and S were assimilated in separate steps. At last, T was diagnosed below the mixed layer through the seawater equation of state following the best results found in XZ. Thus, this EnOI scheme respects the hybrid nature of HYCOM vertical coordinate system and allows restructuring the isopycnal layer thicknesses and velocities with the assimilation of Δp_{obs} . Also, a sensitivity study was performed considering different vertical localizations of the model error co-variance matrix, involving the variables T , S and especially Δp . Five integrations were realized from 1 January 2010 until 31 December 2012. The study of the impact of the vertical localization of Δp was an original contribution of this work.

The thermohaline structure of the experiments with assimilation was significantly improved until 2000 m, maximum depth of the Argo data. The RMSDs with respect to Argo observations in the assimilation runs were reduced in at least 34.11 % (43.56 %)

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



for T (S), regarding the control run over the whole domain. Spatially, the RMSD of T and S decreased for all the 12 selected sub-regions of the domain with remarkable corrections in the depth of the 20 °C isotherm and heat content in upper 300 m towards WOA09, particularly in the North Atlantic. Also, the reorganization of the isopycnal layers by the assimilation of Δp_{obs} has provided a large reduction of the diagnosed SSH model, reflecting the new thermohaline state achieved by Argo data assimilation. Indeed, the correction of layer thickness played a role in correcting the model thermohaline structure and stratification, as stated in previous data assimilation works with HYCOM (Thacker and Esenkov, 2002; Chin et al., 2002; Thacker et al., 2004; Xie and Zhu, 2010).

The vertical localization of T and S did not produce any significant impact in the assimilation experiments, which is consistent with the results found in XZ. However, the experiments VLOCDP and VLOCDPTS with vertical localization of Δp were able to decrease the RMSD of T (S) from 0.993 °C (0.149 psu) to 0.905 °C (0.138 psu) in the whole model domain with respect to the other assimilation runs. This improvement was especially seen in the North Atlantic, where the ensemble members and background had their largest biases with respect to observations and climatology. The experiments with vertical localization of Δp decreased in 66 % the number of grid points with negative Δp generated during the assimilation process by constraining the vertical co-variances between distant layers, and then reducing the degrees of freedom offered by the ensemble members. This result reinforces how important the quality of the ensemble members is in order to improve the performance of the assimilation, particularly in the EnOI scheme, in which the ensemble is stationary in time and it does not evolve with the model integration (Evensen, 2003; Oke et al., 2005, 2008). In future works with EnOI, the quality of the ensemble members should be taken into account. For example, long reanalysis with Argo data assimilation should be performed first to provide new and better ensemble members and, therefore, improve the accuracy of the model error co-variance to be employed in a new assimilation run. If more accurate

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

ensemble members are employed, it is expected that the strong vertical localization of Δp will not lead to improvements in the analysis.

Despite the evidences that the assimilation experiments caused a strong SSH reduction in the model domain and that the analysis increments of Δp and velocities were locally consistent, there was not a clear improvement in the large-scale circulation. The assimilation schemes were simply bias-blind here. The model biases should be considered in future studies to better analyze the impact of Argo data assimilation in the large-scale circulation. According to Oke and Schiller (2007), the role of Argo data assimilation is to mainly constrain the thermohaline structure of the model, especially for salinity, and this was obtained in the present work. To constrain the SST and T in the mixed layer, the assimilation of SST should be performed, and to correct the upper mesoscale circulation, the assimilation of SLA is needed.

The present work was a key-step towards two major directions. First, it was the basis for the future implementation of assimilation in the other REMO higher resolution grids. For the current domain with 760×480 horizontal grid points, the Argo data assimilation code took around 12 min of CPU of a 32 2 GHz processors to assimilate approximately 150 Argo T/S profiles. Therefore, it can be easily used in operational mode. Second, it served as the backbone to construct the assimilation code for along-track satellite altimetry data and SST analyses that will form the REMO Ocean Data Assimilation System into HYCOM (RODAS_H) for operational and research purposes (Tanajura et al., 2014).

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Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



References

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Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

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Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

- Johnson, E. S., Bonjean, F., Lagerloef, G. S. E., Gunn, J. T., and Mitchum, G. T.: Validation and error analysis of OSCAR sea surface currents, *J. Atmos. Ocean. Tech.*, 24, 688–701, 2007.
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Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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**Argo data
assimilation into
HYCOM with an EnOI
method in the
Atlantic Ocean**

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Table 1. RMSD of temperature ($^{\circ}\text{C}$) and salinity (psu) until 2000 m with respect to Argo data for the prior state of each experiment from 1 January 2010 until 31 December 2012. The calculations were performed for the whole model domain (100°W – 20°E , 78°S – 50°N) and for each one of the 12 sub-regions previously defined in Fig. 4.

	RMSD									
	CTL		ASSIM		VLOCDPTS		VLOCDP		VLOCTS	
	T ($^{\circ}\text{C}$)	S (psu)	T ($^{\circ}\text{C}$)	S (psu)	T ($^{\circ}\text{C}$)	S (psu)	T ($^{\circ}\text{C}$)	S (psu)	T ($^{\circ}\text{C}$)	S (psu)
A	2.302	0.279	1.300	0.166	1.180	0.148	1.153	0.147	1.268	0.157
B	1.722	0.283	0.728	0.113	0.647	0.107	0.674	0.110	0.707	0.109
C	1.214	0.287	0.813	0.116	0.665	0.112	0.652	0.111	0.815	0.142
D	1.663	0.368	1.089	0.160	0.995	0.175	1.016	0.170	1.034	0.175
E	0.972	0.227	0.678	0.119	0.655	0.115	0.633	0.114	0.662	0.119
F	1.177	0.163	0.761	0.097	0.729	0.094	0.729	0.094	0.765	0.098
G	1.139	0.161	0.800	0.107	0.759	0.105	0.759	0.105	0.764	0.106
H	0.756	0.166	0.633	0.125	0.550	0.115	0.554	0.109	0.651	0.132
I	1.290	0.207	1.048	0.179	1.035	0.179	1.038	0.178	1.036	0.180
J	0.920	0.158	0.670	0.124	0.700	0.127	0.709	0.129	0.673	0.124
K	0.845	0.151	0.594	0.106	0.596	0.113	0.599	0.112	0.638	0.110
L	0.786	0.140	0.575	0.090	0.549	0.082	0.548	0.079	0.595	0.092
ALL	1.507	0.264	0.993	0.149	0.905	0.139	0.915	0.138	0.972	0.147

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

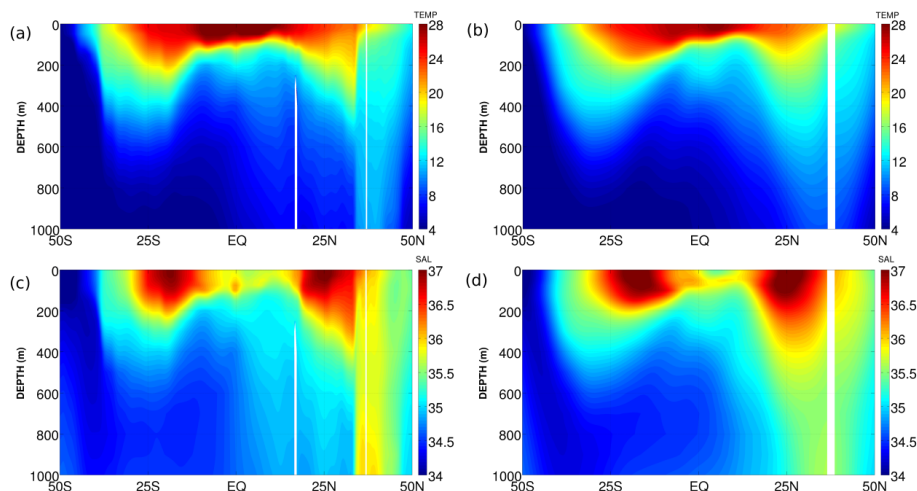


Figure 1. Mean temperature ($^{\circ}\text{C}$) and salinity (psu) in the upper 1000 m along 25°W for **(a)** averaged simulated temperature from January 1997 until December 2008, **(b)** climatological temperature from WOA09, **(c)** averaged simulated salinity from January 1997 until December 2008, and **(d)** climatological salinity from WOA09.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

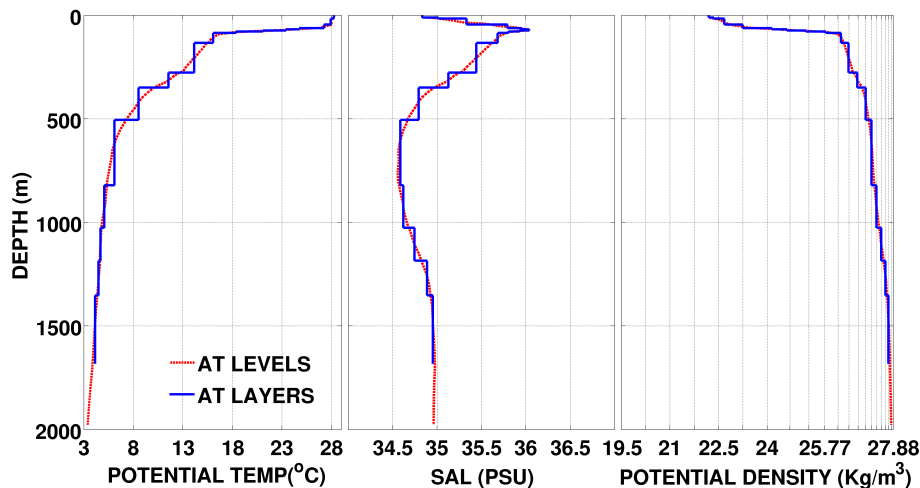


Figure 2. z level profile of potential temperature ($^{\circ}\text{C}$), salinity (psu) and potential density (kg m^{-3}) from an Argo float located at 4.04°N and 23°W on 1 January 2010 plotted against its approximation for HYCOM as layer averages. The target densities values for each model layer are indicated by the light black dashed lines for comparison.

[Title Page](#)
[Abstract](#)
[Introduction](#)
[Conclusions](#)
[References](#)
[Tables](#)
[Figures](#)
[◀](#)
[▶](#)
[◀](#)
[▶](#)
[Back](#)
[Close](#)
[Full Screen / Esc](#)
[Printer-friendly Version](#)
[Interactive Discussion](#)

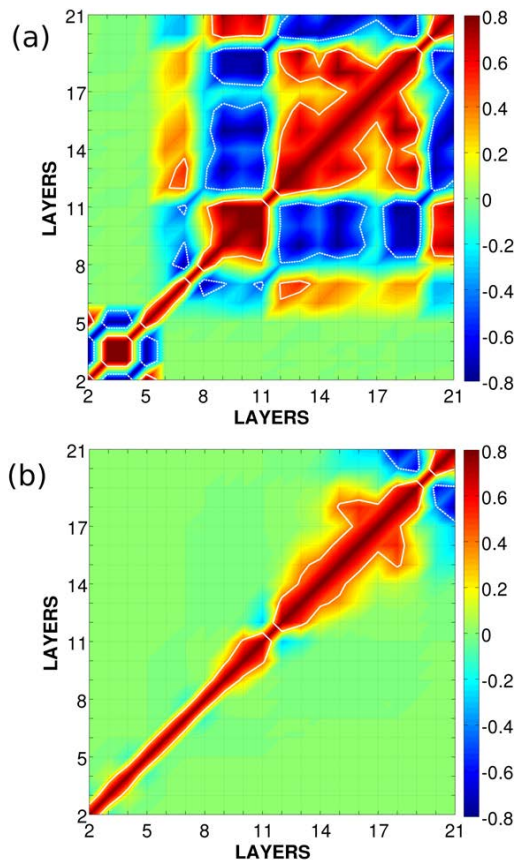


Figure 3. Vertical correlations of layer thickness between different layers at the location of an Argo float (69.95° W and 30.14° N) in the model domain: **(a)** calculated directly from the model ensembles ($M = 132$) and **(b)** after applying the vertical localization of layer thickness according to Eq. (5) and L_{ρ} defined as 0.5 kg m^{-3} . The white solid and white dashed lines denote correlations above 0.4 and below -0.4 , respectively.

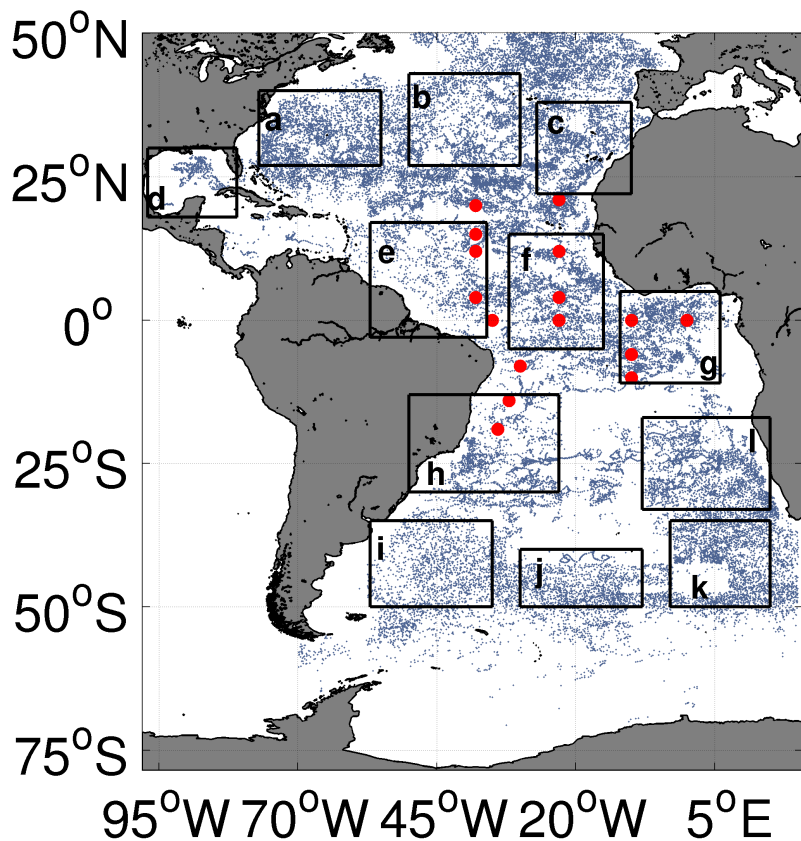


Figure 4. Locations of the 47 999 valid Argo profiles (blue dots) assimilated and also used to validate the prior state of each experiment from 2010 until 2012 in the model domain (100°W–20°E, 78°S–50°N), which excludes the Pacific Ocean and the Mediterranean Sea. The 16 fixed moorings from PIRATA used in the experiments validation are represented by red dots. The numbers of valid Argo profiles in the 12 sub-regions from a, b, m, . . . , and l were 3085, 2352, 2522, 540, 1463, 2750, 2475, 1849, 1560, 1597, 2536 and 3067, respectively.

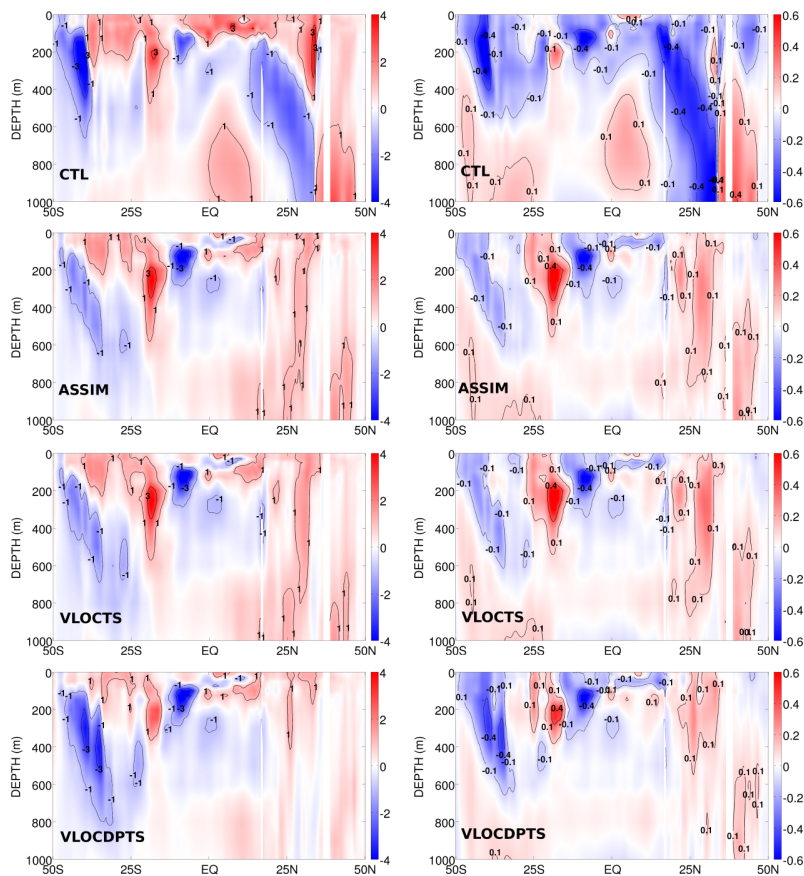


Figure 5. The model mean minus WOA09 along 25° W in the upper 1000 m for temperature (°C) in the left and salinity (psu) in the right from 1 January 2010 until 31 December 2012 according to the CTL run and the prior state of the ASSIM, VLOCTS and VLOCDPTS runs.

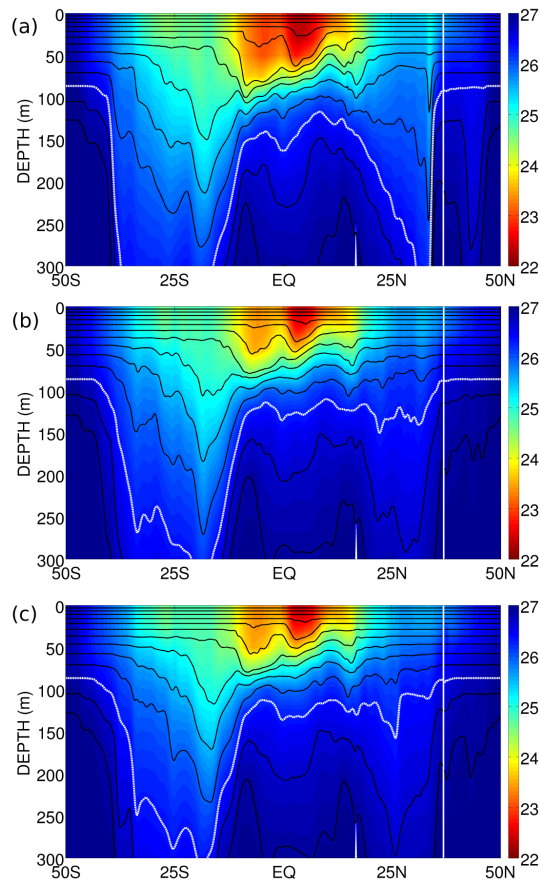


Figure 6. Potential density (kg m^{-3}) and the position of the layer interfaces along 25°W in the upper 300 m for the (a) CTL run and the prior state of the (b) ASSIM and (c) VLOCPTS runs from 1 January 2010 until 31 December 2012. The white dashed line represents the interface between the 11th ($\sigma_\theta = 26.18 \text{ kg m}^{-3}$) and 12th ($\sigma_\theta = 26.52 \text{ kg m}^{-3}$) isopycnal layer.

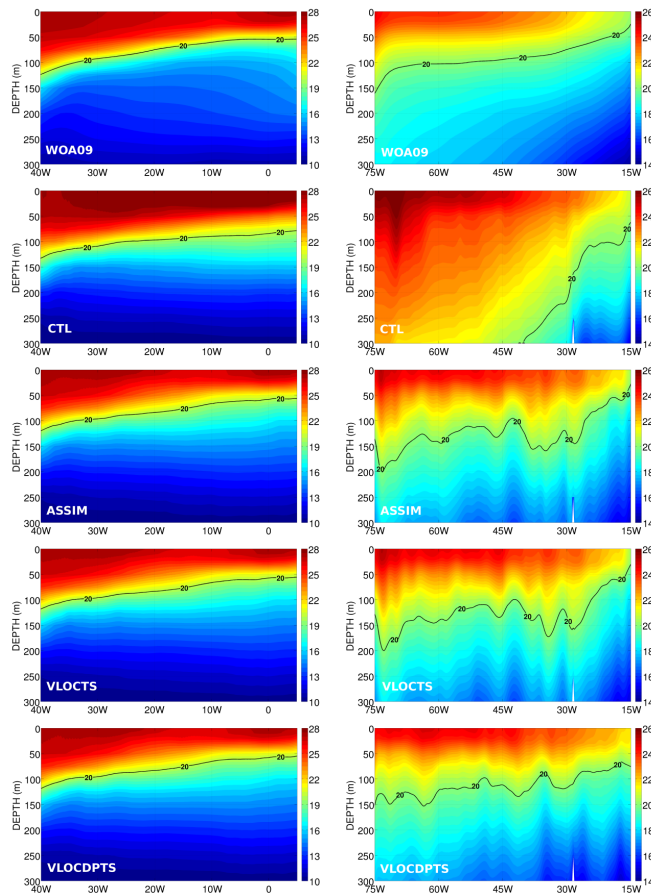


Figure 7. Temperature ($^{\circ}\text{C}$) along the equator (left) and along 30°N (right) in the upper 300 m for the WOA09 climatology, the CTL run and the prior state of the ASSIM, VLOCTS and VLOCDPTS runs from 1 January 2010 until 31 December 2012.

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

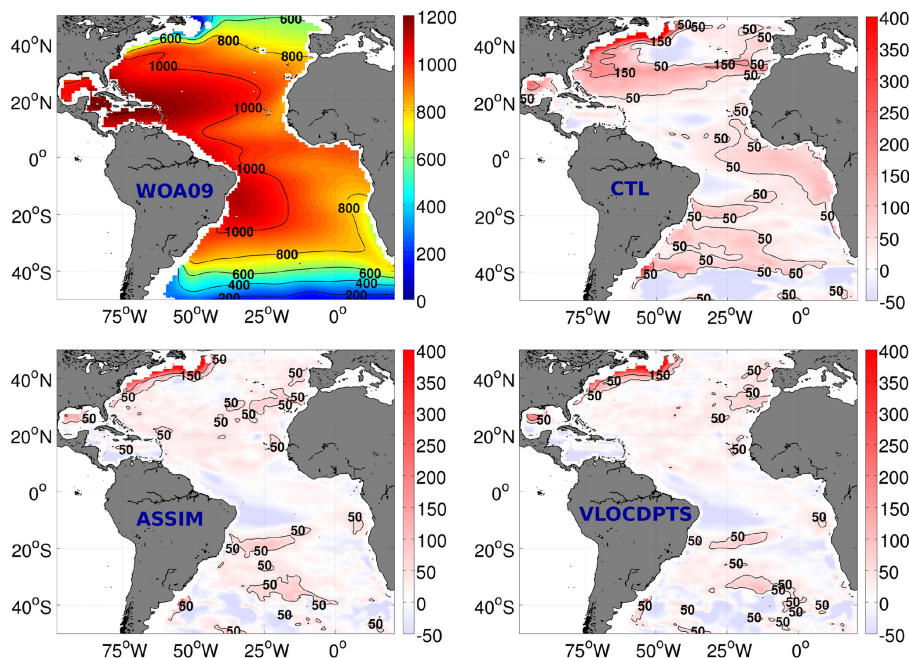


Figure 8. Heat content (MJ m^{-2}) until 300 m of the WOA09 climatology and the model mean minus WOA09 for the CTL run and the prior state of the ASSIM and VLOCDPTS runs over the period from 1 January 2010 until 31 December 2012. Shallower regions than 300 m were not considered.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

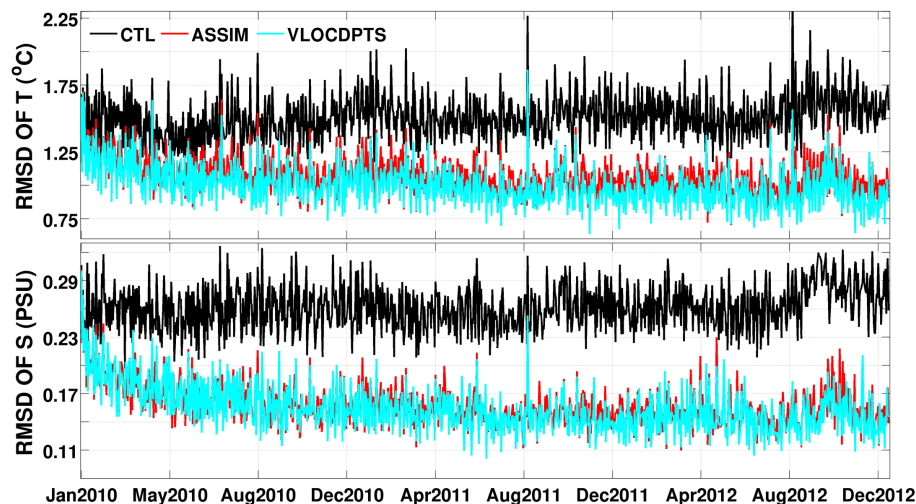


Figure 9. Depth averaged RMSD of temperature ($^{\circ}\text{C}$) and salinity (psu) until 2000 m against 47 999 Argo profilers in the model domain (100°W – 20°E , 78°S – 50°N) from 1 January 2010 until 31 December 2012 according to the control run (black) and the prior state of the experiment ASSIM (red) and VLOCDPTS (light blue).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

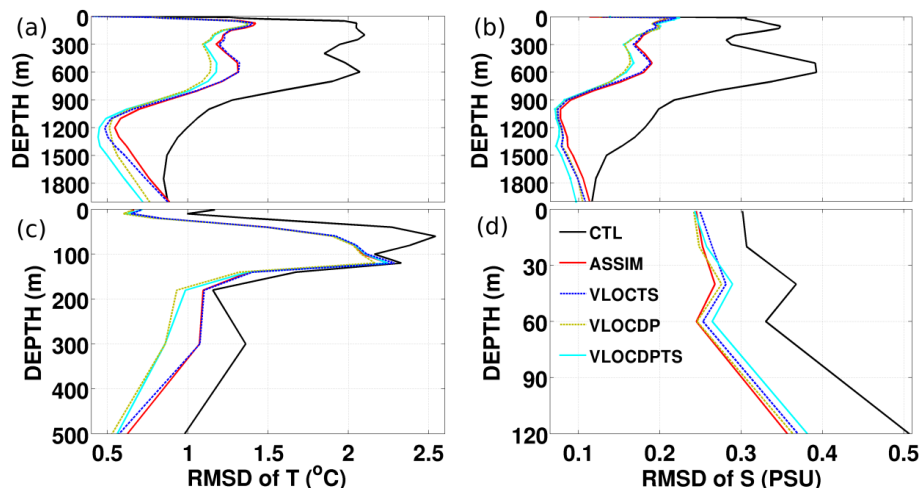


Figure 10. Vertical distribution of the RMSD of temperature ($^{\circ}\text{C}$) and salinity (psu) against 47999 Argo profilers and 16 PIRATA fixed moorings in the model domain (100°W – 20°E , 78°S – 50°N) from 1 January 2010 until 31 December 2012 according to the control run (black) and the prior state of the experiment ASSIM (red), VLOCTS (dark dashed blue), VLOCDP (dark dashed yellow) and VLOCDPTS (light blue). The figure (a) and (b) correspond to the RMSD of T and S with respect to Argo observations while the figure (c) and (d) correspond to the RMSD of T and S with respect to PIRATA data, respectively.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

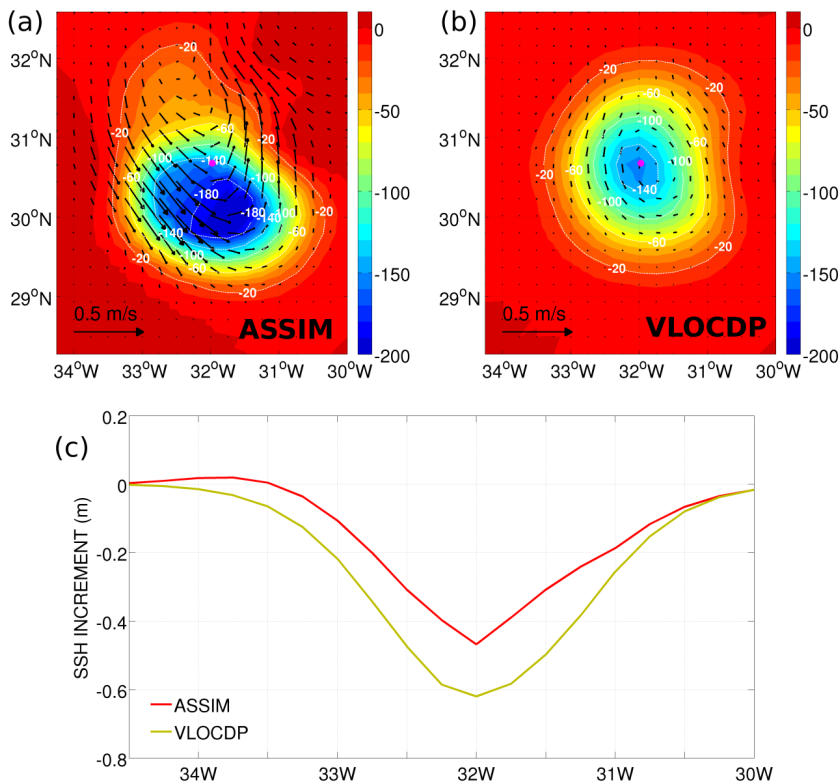


Figure 11. Analysis increments after assimilating an Argo profile located at 30.72° N and 31.98° W on 1 January 2010 of: **(a)** layer thickness (unit: m) and current components (unit: m s^{-1}) in the 12th layer for the experiment ASSIM, **(b)** layer thickness (unit: m) and current components (unit: m s^{-1}) in the 12th layer for the experiment VLOCDP and **(c)** SSH (unit: m) along 30.72° N for the experiment ASSIM (red) and VLOCDP (dark dashed yellow). The pink dot represents the location of the Argo float.

Argo data assimilation into HYCOM with an EnOI method in the Atlantic Ocean

D. Mignac et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

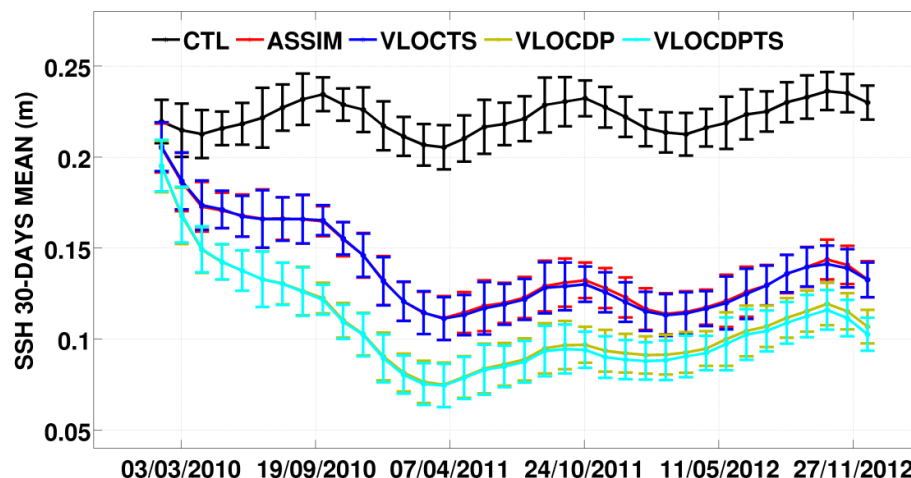


Figure 12. 30 days running SSH mean (m) of the control run (black) and the prior state of the experiment ASSIM (red), VLOCTS (dark blue), VLOCDP (dark yellow) and VLOCDPTS (light blue) from 1 January 2010 until 31 December 2012. The markers represent the 30 days running mean values of SSH while the bars correspond to the standard deviations of each run.

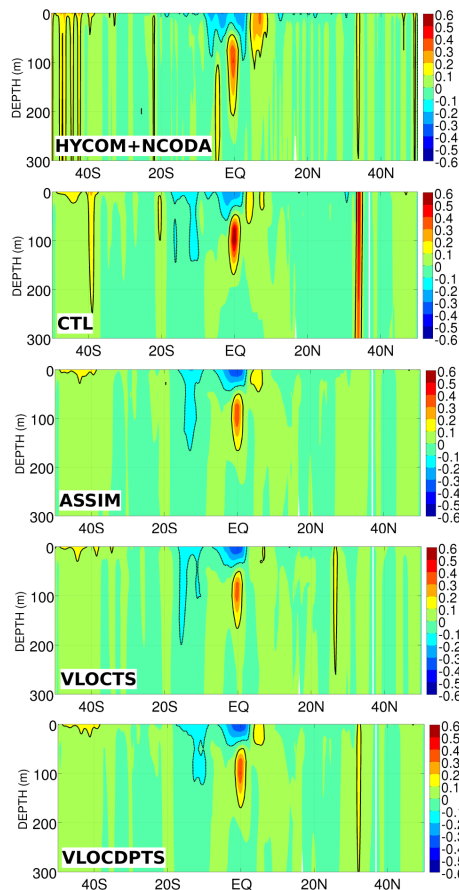


Figure 13. Zonal velocity fields (m s^{-1}) in the upper 300m along 25°W of the HYCOM+NCODA analysis, the CTL run and the prior state of the ASSIM, VLOCTS and VLOCDPTS runs from 1 January 2010 until 31 December 2012. The black solid and black dashed lines denote the contours of 0.1 m s^{-1} and -0.1 m s^{-1} , respectively.