An Eddy-Permitting Variational Data Assimilation System for the Tropical Pacific Ocean

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Abstract

As part of the CORC (Consortium on the Ocean’s Role in Climate) consortium and the ECCO (Estimation of the Circulation and the Climate of the Ocean) consortium, a variational data assimilation system has been developed for the tropical Pacific Ocean. This system makes use of the adjoint method to adjust an eddy-permitting configuration of the MIT ocean general circulation model to observations in the tropical Pacific region. The model has a realistic configuration with parameterizations for the surface boundary layer (KPP) and open boundaries at the south and north, as well as in the Indonesian throughflow. In the assimilation method, control parameters were adjusted to fit the model to the data. The adjustable parameters include the initial temperature and salinity conditions, temperature, salinity and horizontal velocities at the open boundaries and the time-dependent surface fluxes of momentum, heat and freshwater. A decomposition of the velocities at the open boundaries into barotropic-baroclinic modes is introduced to deal with very strong sensitivities of the model sea surface height to the barotropic component. Larger viscosity and diffusivity terms are used in the adjoint model to avoid very strong sensitivities calculated in the backward run related to the nonlinear nature of our high-resolution model. Preliminary experiments in which the model was constrained with Levitus temperature and salinity data, Reynolds sea surface temperature data and Topex/Poseidon and ERS altimeter data were performed to demonstrate the controllability of this assimilation system and to study its sensitivity to the initial conditions.
1 Introduction

Estimating the circulation of the tropical ocean has long been a goal of physical oceanography. As the Southern Oscillation and its relationships to El Niño and the extratropics began to be understood (Bjerknes, 1966), more attention was focused on the tropical Pacific ocean. The spectacular global climate impacts associated with the strong 1997-98 El Niño event underscored the need for better understanding of tropical Pacific features. This event was one of the most widely discussed climate events in recent history. The great variability between El Niño events has not yet been completely understood, and leads to other questions, such as the response of the El Niño/Southern Oscillation (ENSO) to large-scale warming.

Accurate description of the spatio-temporal structure of the tropical Pacific ocean is a key step toward understanding these events and better studying the tropics currents and their interactions. The circulation of the tropical Pacific has been studied extensively in recent years using both observations and numerical models. However, to date most of these studies were limited by the small amount of available data (Durand abd Delcroix, 2000; Lagerloef et al., 1999; Vialard et al., 2001). On the other hand, numerical ocean models provide a crude approximation of reality because of the many errors in the model. The observational data set is both sparse and inhomogeneous, and one of the major challenges of data management for the effort is to combine the disparate data types and an ocean models to obtain a dynamically coherent and useful four dimensional picture of the state of the tropical Pacific Ocean (Ghil and Malanotte-Rizzoli, 1991).

High resolution tropical Pacific models require significant computing resources because of the very large basin. Consequently, simple data assimilation techniques were implemented with these models, basically based on optimal interpolation or the so-called three dimensional variational methods (Carton et al., 1996; Giese and Carton, 1999). These methods provide the analysis of the system state using the observations at a given time, without enforcing smoothness in the time dimension. At present, most of these advanced assimilation schemes are based on the adjoint method or on the Kalman filter (Wunsch, 1996). For instance, Bennett et al. (2000) used the representer method, which solves the
dual formulation of the adjoint problem, to assimilate TAO data into an intermediate coupled ocean-atmosphere model. Bonekamp et al (2001) also used the adjoint method to adjust the model wind stress over the tropical Pacific while constraining the model to temperature data profiles using a twin experiments approach. Recently, Weaver et al. (2003) successfully tested an incremental approach of the 4D-VAR assimilation problem with a primitive equation model while assimilating temperature profiles and adjusting initial conditions. Since a full implementation of the Kalman filter is not possible in practice, simplified Kalman filters with different degrees of approximations were also used to assimilate altimetric data and also TAO data in the tropical Pacific (Verron et al., 1999; Parent et al., 2003).

Most of the previous assimilation studies in the tropical Pacific use a restricted set of observations or relatively low horizontal or vertical resolutions to reduce computational burdens. We are implementing an eddy-permitting regional assimilating system for the tropical Pacific ocean. This system is nested in the ECCO global assimilation (Stammer et al., 2002; Köhl et al., 2005) which provides complete ocean products at 1° resolution from an adjoint assimilation system with the MITGCM Marshall et al. (1997). Our aim is to assimilate all data in the equatorial region into a common, dynamically consistent framework for understanding the variability of the tropical Pacific in greater detail than was possible before.

The goal of this paper is to describe the technical features of our assimilation system while focusing on the problem of variational data assimilation in a nonlinear model with widely varying sensitivities. Strong sensitivities can lead to poorly conditioned problems, and nonlinearities mean that gradient directions determined linearly are not optimal for solving the complete problem. The tropical current system is unstable to rapidly-growing perturbations which are not easily predictable or controllable by our system. We have reduced the effects of these instabilities by integrating a more viscous and diffusive model backward in time. This mismatch between adjoint and forward run is not guaranteed to succeed, but it converges well in our examples. We also use reduced cost function weights to compensate for very high sensitivities of the model solution (mainly the free surface height) to the barotropic component of the normal velocities at the open boundaries. A
complete set of analysis states and forcing fields for the tropical Pacific Ocean over a few years period is under construction and will be reported and discussed in the near future.

The paper is organized as follows. Section 2 describes the assimilation system, including the model and the assimilation method. The main characteristics of the data sets used in our study are reviewed in section 3. The assimilation experiments are described and the assimilation results are evaluated against independent data in section 4.2. Finally, concluding remarks are given in section 5.

2 The Assimilation System

2.1 The Model

The model used in this study is a general circulation model (GCM) which has been developed at the Massachusetts Institute of Technology (MIT) (Marshall et al., 1997) to support ocean general circulation studies over a broad range of scales and physical processes. It is based on the primitive (Navier-Stokes) equations on a sphere under the Boussinesq approximation. The system equations are written in z-coordinates and discretized using the centered second order finite differences approximation in a staggered “Arakawa C-grid”. The numerical code is further designed to allow for the construction of the adjoint using the automatic differentiation tool TAMC (Giering and Kaminski, 1998). Stammer et al. (2002) provided the first 2° × 2° global state estimation using this model.

The basic configuration of the model is described in Hoteit et al. (2004). It covers the entire tropical Pacific basin extending from 26°S to 26°N and from 104°E to 68°W. The bottom depth is at 6000m and the bathymetry is extracted from the global topography prepared by Smith and Sandwell (1997). The model is integrated on a 1/3° × 1/3° Mercator grid, with 39 vertical levels. The vertical resolution is spaced at 10m from the surface to 250m in depth, with spacing gradually increasing to 300m below. The model operated in a hydrostatic mode with an implicit free surface. No-slip conditions are imposed at the lateral boundaries while bottom friction is quadratic with a drag coefficient equal to 0.002.

The sub-grid scale physics is a tracer diffusive operator of second order in the vertical, with the eddy coefficients parameterized by the K-profile parameterization (KPP) mixed
layer model (Large et al., 1994). In the horizontal, diffusive and viscous operators are of second and fourth order respectively with coefficients $5 \times 10^2$ m$^2$/s and $1 \times 10^{11}$ m$^4$/s, respectively. Vertical diffusivity and viscosity are parameterized by Laplacian mixing with values $1 \times 10^{-6}$ m$^2$/s and $1 \times 10^{-4}$ m$^2$/s, respectively.

Open boundaries (OB) are set at 26oS and 26oN, as well as at four straits in the Indonesian throughflow. The OB scheme is implemented as in Zhang and Marotzke (1999). It specifies the horizontal components of the velocity on the boundary and the advection of temperature and salinity from prescribed values at the boundaries. This advection is made through a sponge layer extended 2° from the boundary in which the boundary solution smoothly tapers to the interior. Monthly mean values (centered on the 15th of each month) obtained from the ECCO global state estimate were prescribed at the grid points just outside the OB and are restored within a buffer zone of 3° over time scales linearly varying between 1 day and 40 days. The normal velocity fields across the open boundaries have been further corrected on a monthly basis: (i) to conserve the same transport at 26°N and 26°S as in the global ECCO model and (ii) to exactly balance the volume flux into the domain by the transport out in the ITF. The corrections at a boundary are added as a barotropic transport (uniformly distributed over all grid points). In the ITF, 1/2, 1/3 and 1/6 of the correction is added to the transport in the Ombai strait, Timor passage and Lombok strait, respectively.

Surface fluxes of momentum, heat, and freshwater are prescribed at the ocean-atmosphere interface. Two sets of forcing fields are used in our experiments. The first data set consists of the sea surface fields from the National Centers for Environmental Prediction (NCEP)/National Center for Atmospheric Research (NCAR) re-analysis project (Kalnay et al., 1996). This data set is available on a $1^\circ \times 1^\circ$ global grid. It contains twice-daily wind stress vectors and daily net heat flux, net short-wave radiation and water flux at the sea surface. The second forcing set is obtained from the optimized ECCO forcing fields (Stammer et al., 2004). These forcings are the NCEP forcings optimized by a variational $1^\circ \times 1^\circ$ global state estimation procedure on the same spatio-temporal distribution (Köhl et al., 2005).
Prior to data assimilation experiments, the model was integrated over 9-year period from 1992 to 2001 in a related study (Hoteit et al., 2004) for data comparison and sensitivity studies. Generally speaking, the model was shown to be able to capture much of the observed variability during the experiment period. It was therefore concluded that this model is realistic enough to be used for assimilation experiments.

2.2 The Adjoint Method

Assuming that the model is an accurate reproduction of the true ocean, the model state can in principle be brought into agreement, within error estimates, with the observations by adjusting an identifiable set of model parameters. This leads to an optimization problem of a cost function measuring the discrepancy between the model solution and data over a given period of time and constrained by the model equations subject to a set of control variables. The gradient of the cost function is used to determine descent directions toward the minimum in an iterative procedure. An efficient way to compute the gradient of the cost function is to use the adjoint method which provides the gradient by integrating the adjoint of the tangent linear model (TLM) backward in time (Wunsch, 1996).

In its general form, the objective cost function consists of a weighted model-data misfit and penalty terms on changes to the control variables relative to our knowledge of uncertainties and can be presented as

\[ J = \sum_{t=0}^{t_f} [y(t) - E(t)x(t)]^T R^{-1}(t) [y(t) - E(t)x(t)] \]

\[ + \sum_{t=0}^{t_f} |u(t) - u^b(t)|^T Q^{-1}(t) |u(t) - u^b(t)|, \]

where \( x(t) \) is the model state vector and \( u^b(t) \) a first guess of the unknown control vector \( u(t) \) at time \( t \). \( u \) may include separate components comprising errors on any set of model parameters and external forcing fields which are likely capable of controlling much of the model state. For this study we have chosen to control the initial temperature and salinity,
atmospheric forcings, and temperature, salinity and velocities at the open boundaries. The vector \( y(t) \) contains all observations available at time \( t \) and is related to the model state according to the observation operator \( E(t) \). \( R(t) \) and \( Q(t) \) are weight matrices representing the covariance of data errors and uncertainties in the background fields, respectively.

The Lagrange multiplier method was used to derive the adjoint model as described in Wunsch (1996). Details about the application are given in Stammer et al. (2002). The model is first appended to the cost function \( J \) using the Lagrange multipliers \( \mu(t) \), leading to a Lagrange function \( L \). The stationary value of \( L \) is then found by equating to zero the derivatives of \( L \) with respect to \( x, u \) and \( \mu \). This yields the so-called normal equations. Because of the complexity of the problem, the equations are solved implicitly and iteratively by employing the adjoint model to calculate the gradients of the \( J \) and then using an optimization algorithm to minimize \( J \).

2.3 Control of the Normal Velocities at the Open Boundaries

One of the benefits (or problems) of assimilating with a regional model is the possibility of treating the open boundaries as adjustable parameters. In the MITGCM, the boundary conditions require the complete specification of the state \( U, V, S \) and \( T \). Accordingly, four separate penalty terms were added to the cost function; one for each state variable (Zhang and Marotzke, 1999). Such an estimation process might however provide dynamically unbalanced open boundaries which cause deterioration in the final solution. Following Gebbie (2004), an additional term was added that penalizes the deviation from the thermal wind balance on the boundary in a 'soft constraint' approach to bring the boundaries closer to geostrophic balance. A net mass flux is still applied as a hard constraint on the adjusted velocities.

The estimation of velocities at the open boundary is often poorly conditioned when simultaneously adjusted with other control variables. The model Sea Surface height (SSH) is very sensitive to changes in the barotropic component of the normal velocities at the open boundary. This means strong sensitivity of the cost function to the velocities at
the open boundary because of the constraint term to SSH data. A mixture of strong and weak sensitivities in an optimization leads to difficult topology of the cost function manifold, severely slowing descent optimization methods. Ideally this topology would be compensated by pre-conditioning, with preconditioning by the inverse of the Hessian yielding a manifold with uniform gradients. Our system does not have an obvious simple or cost-effective method for preconditioning by an approximate Hessian. Instead, we have isolated the problematic dimensions (normal velocities) with strong sensitivities and use decreased weighting for these terms in the cost function. This is equivalent to allowing only tiny changes to the normal flow at the boundaries. This treatment is not optimal, but it has produced reasonable solutions so far, and should be relaxed as the Hessian becomes better-known.

Such a brute force approach, however, significantly decreases the weight of the baroclinic component of the normal velocities making the contribution of this component insignificant. As proposed by Gebbie (2004), the best way to deal with this problem is to decompose the normal velocity at the open boundary into baroclinic and barotropic components and then apply different weights for each component. Considering the baroclinic component as the difference between the absolute and the barotropic velocities requires an additional hard constraint: the vertical integral of the baroclinic component must be zero. To avoid a hard constraint without increasing the degrees of freedom in the controls, Gebbie (2004) removed the first layer from the baroclinic component. However, as we noticed in our numerical experiments, this results in an unrealistic vertical shear between first and the lower layers.

In order to avoid such unrealistic baroclinic structure, we adopted a normal mode decomposition to the velocities normal to the boundaries. Following Pedlosky (1987) quasi-geostrophic normal modes are the solution of the vertical Sturm-Liouville problem

\[(h_k)_{zz} + \frac{N^2}{C_k^2} h_k = 0\]  \hspace{1cm} (2)

with \(z\) the vertical coordinate, \(h_k\) the \(k^{th}\) vertical mode, \(N(z)\) is the buoyancy frequency given by \(N^2 = -g \rho_z / \rho_0 \) (\(g\) is the gravity constant, \(\rho\) the density profile, and \(\rho_0\) the
reference density), and $C_k$ the phase speed of long gravity waves with mode $k$. Here, we only use it as an orthogonal decomposition in the adjoint model to separate the barotropic and the baroclinic components, and it is not required for the forward model.

This decomposition depends on water depth and stratification and the number of modes is equal to the number of layers. In order to apply it to our primitive equation model with realistic topography, a different barotropic-baroclinic decomposition operator for each location should be determined according to the local depth and stratification. To keep the decomposition simple we assume a linear density profile whereby the decompositions depend only on local water depth. In summary, first a decomposition is computed for each number of layers $n$ (between 1 and $nr$). Then the velocity vector in each point along the open boundaries is decomposed into barotropic-baroclinic modes using the decomposition operator that corresponds to the number of water layers in this column.

2.4 Dealing with Large Adjoint Sensitivities

The use of the adjoint method for data assimilation with nonlinear models can be problematic. When the model is strongly nonlinear, the cost function becomes non-convex, implying the existence of multiple local minima (Li, 1998; Pires et al., 1996). This would prevent significant improvements in the cost function with a gradient descent optimization algorithm, since these algorithms are only designed to converge toward local minima. The choice of the initial guess for the adjusted variables then becomes crucial. This problem has been investigated by Pires et al. (1996) for the control of the initial conditions. They propose starting with assimilation over a short period, where the linear approximation still holds, and then gradually increase the length of the assimilation window while starting each longer optimization from the adjusted initial conditions determined in the shorter period. The aim was to maintain the initial conditions in the basin of the absolute minima, where the cost function is expected to be convex. Although this method was shown to improve the performance of the adjoint method, its usefulness over long time spans can be questioned since the number of local minima grows exponentially with the length of the assimilation window (Swanson et al., 1998). In this case, the cost function becomes far too irregular to allow any decrease with a gradient descent algorithm (Köhler and Wille-
brand, 2002). The method also depends on the existence of sufficient information early in the assimilation period to estimate the complete control parameters.

The presence of multiple local minima is often associated with large gradients of the cost function. This was seen in our assimilation experiments; after only a few \((2 - 3)\) months, the adjoint solution of our model was showing irregular 'spots' of very high sensitivity (Figure 1) which first appeared in the western basin of the tropical Pacific before spreading to a large area centered on the equator. These small-scale but strong gradients indicate the presence of many small-amplitude but tightly packed extrema. Similar patterns in the adjoint solution were also reported in several recent papers (Tanguay et al., 1995; Janiskova et al., 1999; Lea et al., 2002; Zhu et al., 2002). Sensitivities grow exponentially without limit because the adjoint model lacks nonlinear interactions that could otherwise slow or stop the exponential growth once the perturbations reach finite amplitude (Zhu et al., 2002). Strong sensitivities have been associated with positive Lyapunov exponents which characterize the limits of predictability of the model (Köhl and Willebrand, 2002). Likewise, the sensitivities obtained from the adjoint model become unrealistic when the time integration is too long and the corresponding tangent linear fails to describe the nonlinear perturbations (Lea et al., 2002; Zhu et al., 2002). Although this problem is not present at a given time for sufficiently small initial perturbations, this is not very useful for ocean applications since the size of the perturbations should be of the same order as the size of uncertainties (Errico and Reader, 1999).

It is important to note that although the tangent linear and adjoint models may be correct, the range of validity of the linearization is smaller than the uncertainty in the control parameters when the model is integrated beyond a month or two. Therefore, the large gradients do not provide any useful information for the optimization of the cost function or for sensitivity studies over long periods (the actual length depends on the system under study). If these instabilities are not damped, then the assimilation can be only carried out within periods where the model is weakly nonlinear, so the adjoint sensitivities are useful over finite size optimization steps. For our model, this range is of the order of a few months. We cannot accept these limits because we aim at optimizing the
atmospheric forcing fields, which can require months to years of integration time before the the effects of the errors in the forcing fields are visible above the noise in the observations. This happens both because the size of the effect at the surface increases and because the effects penetrate to greater depths where the signal-to-noise ratio is better. Surface forcing can take years to affect the ocean below the surface mixed layer, particularly outside the equatorial waveguide. One should also note that although this problem involves large sensitivities, it can not be treated as in section 2.3, since the unstable (sensitive) modes of the adjoint change with time and with each iteration.

To extend the limits of the adjoint method, Lea et al. (2002) recently proposed averaging the sensitivities of several adjoint runs in order to filter the effect of secondary minima. Such an “ensemble adjoint approach” may quickly become computationally unaffordable for long assimilation periods, since this might require a large number of adjoint runs to filter out very large sensitivities. Another approach which became popular recently consists of replacing the original unstable adjoint model by the adjoint of a modified stable tangent linear model. The latter is a simplification of the original model and is usually obtained by omitting highly unstable modes from the tangent linear model. This is similar to performing the optimization in a smooth subspace, which means loss of accuracy due to the omission of strongly nonlinear variations, generally related to small-scale phenomena. This is necessary, however, in order to optimize the cost function over long assimilation periods. For instance, Köhl and Willebrand (2002) successfully optimized the cost function of their highly nonlinear variational assimilation problem by constructing an adjoint model of the mean state that was integrated on a coarser grid employing larger mixing than the forward model. Moreover, considering only statistical quantities additionally regularizes the topology of the cost function. Recently, Zhu et al. (2002) stabilized the adjoint associated with the Mellor-Yamada turbulence closure model by disabling the dynamical terms that were the main sources of instability.

We first examined the nonlinearities in our tropical Pacific model by carrying out several forward runs to compute second derivatives of the model state with respect to various control variables using finite differencing in control parameter space. The second derivative is an indication of the nonlinearity in the sensitivity. To compute the differences
we performed three forward runs in which the zonal wind stress was perturbed as follows

(R1) A forward run with reference wind stress.

(R2) The same run as R1 but with a constant \( \epsilon ps > 0 \) perturbation on the wind stress.

(R3) The same run but with \(-\epsilon ps\) as constant perturbation on the wind stress.

The second derivatives of the sea surface height with respect to this constant (in space and time) zonal wind stress perturbation were obtained by adding the R2 and R3 solutions and subtracting twice the R1 solution. Figure 1 plots the evolution in time of the resulting second derivatives in the leftmost column. The evolution in time of the gradient of the cost functions with regard to the zonal wind stress as obtained from the adjoint model is shown in the rightmost column. It can be seen that the model SSH sensitivity is nearly linear during the first month. Some nonlinearities start to appear in the western Pacific as well as in the central Pacific near the equator after only 40 days. Then they spread over the domain and become stronger as the integration time increases. The right panel suggests that the adjoint model is stable as long as the forward model is weakly nonlinear. The appearance of large adjoint sensitivities is consistent with the timing and the locations of the model nonlinearities. As suggested by Köhl and Willebrand (2002), the existence of secondary minima that prevent the convergence of the adjoint method can be also diagnosed from an exponential increase of the norm of the adjoint variables. Figure 2 plots the (natural logarithm of the) Euclidian-norms of the adjoint variables and shows a nearly exponential growth. This means the variables of the tangent linear model will also grow exponentially. Very similar behavior was seen in other experiments with less simple perturbations and/or other control variables (not shown here). These experiments suggest that our tropical Pacific model integration is significantly nonlinear beyond a few months if the viscosities and diffusivities are set at realistic values. This would limit the length of the assimilation period in our system to 2-3 months.

Next, we examined the norm of the adjoint variables by performing the same adjoint run but using larger viscosity and diffusivity terms. Comparing to the run with the regular viscosity and diffusivity (Figure 3), the norm of the adjoint solution seems to be stabilized
when the viscosity and diffusivity were set to $3 \times 10^{12} m^4/s$ and $1.5 \times 10^4 m^2/s$ (30 times the original values), respectively. To assess the disappearance of the adjoint unbounded sensitivities, we performed the same forward runs as before but using the higher viscosity and diffusivity terms. These runs confirmed that the viscous model remains almost linear with these parameters and confirms the results of the backward run. In short, at high viscosity and diffusivity, the model becomes almost linear, at least during the first 12 months, stabilizing the adjoint over substantially longer periods.

Based on these experiments, we ran the backward (adjoint) model with 30 times higher viscosity and diffusivity values than were used in the forward run in our iteration. This extended the limit of our adjoint-based assimilation system while retaining the realism of the forward model runs with the original viscosity and diffusivity terms. Figure 3 plots the gradients of the cost function with regard to the heat flux as obtained from the adjoint model for several values of the viscosity and diffusivity parameters. It can be seen that the use of larger values of these parameters smooths the adjoint output while preserving the large scale patterns. The extra damping entails an approximation which amounts to discarding some ‘uncontrollable’ small-scale intrinsic variability, but makes it feasible to carry out the assimilation over longer periods. This approach is similar to Köhl and Willebrand (2002) but it is simpler to implement, although it is more demanding in computing resources. Furthermore, it can be easily generalized for a multi-scale approach if small-scales are of interest by gradually decreasing the values of the viscosity and diffusivity parameters while running the assimilation over shorter periods, starting each time from the previous adjusted solution. In addition, once a satisfactory solution is obtained using the damped adjoint, the damping could be reduced and the descent restarted in the hope that the estimated state from the more viscous run is within the linear range of a less-viscous model. However, similar to the Pires et al. (1996) method, this option most likely will only work well in an identical twin setup where model data differences can be reduced orders of magnitude.
3 Description of the Data Sets

The tropical Pacific Ocean is one of the most observed region of the global ocean and several data sets are available. These can be used to improve the estimates or as independent cross-validation. This section describes the data sets we used for this study.

Altimetry Data

The assimilation used sea surface height (SSH) provided by the TOPEX/Poseidon (T/P) mission. To eliminate errors associated with uncertainties in the geoid, the mean and time-varying components of the SSH data were considered separately. The one year T/P mean SSH minus the EGM96 geoid (Lemoine et al., 1997) has been used to constrain the mean model SSH during the assimilation. For the time-varying component, daily T/P data which have been obtained from NASA’s PO-DAAC at JPL and processed as described by Stammer and Wunsch (1994) were sampled on the model grid.

Sub-surface Data

The Tropical Atmosphere and Ocean (TAO) buoy array provides time series of current and temperature data at multiple locations across the equatorial Pacific (McPhaden et al., 1998). The TAO array consists of approximately 70 deep-ocean moorings spanning the equatorial Pacific Ocean between 8°S and 8°N and down to 500m. Sixth moorings located on the equator also carry upward-looking Acoustic Doppler Current Profilers (ADCP) to measure upper-ocean currents between 10m and 250m. In addition, Expendable Bathythermographs temperature (XBT’s) data from voluntary observing ships are available on 18 specific lines that cross the equator at different longitudes. A detailed description of these data can be found in McPhaden et al. (1998).

Analyzed Data

Although ocean climatologies are not usually considered “observations”, they are a collection of observations and they can be used to constrain the model solution. Here, the Levitus climatology of monthly mean temperature and salinity (Levitus and Boyer, 1994), the Reynolds monthly SST (Reynolds and Smith, 1994) were used. The Levitus
climatology is based on historical hydrographic data that are merged and spatially averaged. The Reynolds optimum interpolation (OI) SST analyses are produced on a one-degree grid using buoy and ship data as well as satellite SST data. All these data were interpolated subsequently onto the model grid first horizontally and then afterwards vertically using linear interpolation procedures.

To test the assimilation system at first, only TOPEX SSH, Reynolds SST and Levitus temperature and salinity data were assimilated in our model. The rest of the data sets were used as independent observations to test the estimates of the assimilation system following a cross-validation approach. As a final goal, we aim to include all data sets in the assimilation system.

4 Assimilation Experiments

4.1 Setup

To evaluate the performance of the system and to study its sensitivity to different setups, we carried out several experiments over one-year assimilation period starting from January 1st, 1998. As stated before, the model was constrained by along-track SSH fields from T/P, to monthly Reynolds SST, and to monthly subsurface Levitus S and T climatology. The control variables consists of the initial conditions, the atmospheric forcing fields adjusted every two days, and boundary conditions which were adjusted every week. Data and model errors were prescribed only on the diagonal of the error covariance matrices and are the same as used by Köhl et al. (2005) in the global ECCO state estimation. They have been approximated by the error profiles for temperature and salinity taken from Levitus data and by 3.5 cm for the SSH T/P data. Prior errors for the wind stress are provided as standard deviation of the differences between NCEP and QuickSCAT scatterometer wind fields. One-third of the local standard deviation of the NCEP forcing was used as the prior error for the net heat and freshwater fluxes. For the boundary conditions, Levitus errors were prescribed for $S$ and $T$ and the standard deviation of the ECCO velocities at the boundaries for $U$ and $V$. The baroclinic mode of the normal
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Table 1: Table summarizing the assimilation runs.

velocities at the boundary was weighted by the standard deviation of the same mode of the ECCO velocities. The weight for the barotropic mode was empirically set to a small value.

The descent directions toward the minimum were iteratively determined using the Quasi-Newton M1QN3 algorithm which has been developed by Gilbert and Le Maréchal (1989). After thirty iterations the rate of cost function decrease was relatively small and the differences between the model and the observations were reduced to about the levels of expected error for most of the data. We started the optimization procedure using either Levitus climatology or ECCO analyses as the initial conditions, NCEP or ECCO analyses for the atmospheric forcing fields, and ECCO analyses for the open boundaries. Three assimilation runs were performed as summarized in Table 1 and compared to the model run with the starting guess for the control parameters (which will be called the “reference run”).

4.2 Assimilation Results

4.2.1 Evaluation of the assimilation system

First we discuss the convergence properties for the total cost function and the individual cost function terms for the assimilated data obtained from the three assimilation runs NCEP-LEVic, ECCO-LEVic and ECCO-ECCOic. The results as function of the number of iterations are shown in Figure 4. As expected, the initial total cost functions is smallest when the assimilation starts from the ECCO forcing, suggesting that these forcing fields optimized on a coarse $1^\circ \times 1^\circ$ grid have good skills for SSH and SST in higher resolution models. Using Levitus as an initial guess for the initial conditions also provides a better initial cost function since the associated terms account for the biggest values in the total
cost function. The decrease in the total cost function is greatest during the first iterations, particularly for the NCEP-LEVic run. However, after only 5 iterations, the overall performance of the NCEP-LEVic run, as measured by the cost function, is as good as the run starting from the ECCO forcing. Furthermore, the cost function seems to stabilize at the same level for both runs. The convergence rate of the ECCO-ECCOic run is rather slow and the optimization is shown to not be able to adjust some residuals presented in the ECCO initial conditions after 30 iterations. For LEVic, after 30 iterations, the total cost function is reduced by more than 50% starting from ECCO forcing, and 75% if starting from NCEP forcing. Overall, similar conclusions can be made from the individual cost terms, although the convergence of the salinity term is slower than the other data terms. Now, we focus on the results of the ECCO-LEVic run.

The temporal and spatial distribution of the contributions for the individual data terms to the cost function from the ECCO-LEVic run are plotted in Figure 5. The curves have been normalized by expected error, so 1 indicates that the assimilation solution fits the data within the specified errors. For the temperature, the monthly cost function is small in January, since the assimilation starts from the same data field, and then increases over time as the model drifts from Levitus. The assimilation successfully reduces the drift and brings the model closer to the observations over the entire assimilation period. The daily SSH cost term has a “U” shape and again the assimilation is also able to control and improve its skill over the entire assimilation period. Concerning the spatial contributions to the cost function, it is shown for the salinity term only that the model/data misfit is reduced over the entire tropical Pacific domain. The results are very similar for the other data cost terms. Finally, the improvements made to the cost function after the 20th iteration are rather small and they tend to be balanced by the increase of the cost function terms for the control variables.

To assess the fit to the assimilated observations, we first compared a zonal cross-section of the mean temperature field at the equator from the reference and the assimilation runs to the Levitus field (left panel of Figure 6). The model thermocline obtained from the reference run is shown to be shallower than in the data in the western part of the Pacific and deeper in the eastern part. The assimilation successfully corrects the structure of
the thermocline and significantly improves the temperature field even in the deep layers. The variability of the SSH from the model (with and without assimilation) was also compared to the grided AVISO SSH variability. As illustrated in the maps of the SSH standard deviation from these solutions (right panel of Figure 6), the spatial structures of the assimilated SSH is clearly in better agreement with the analyzed AVISO variability than the variability of the reference run. The unrealistically strong variability over the NECC area is completely removed and shifted to the eastern Pacific. The variability of the assimilated field, however, is still rather weak in the western Pacific near the open boundaries. The assimilation is also shown to introduce small-scale features to the SSH field, particularly along the equator.

As a final evaluation of the overall behavior of the assimilation system, we also compared (not shown here) the optimized state to independent observations which have not been used in the assimilation system. Comparison with XBTs data surprisingly shows that the reference run is in better agreement with the XBTs data than the assimilation run, particularly at the EUC area. Comparing the assimilation/XBTs differences with the Levitus one, we found that the errors in the assimilation solution are mostly due to the errors in the assimilated Levitus climatology, which is expected to be large in 1998's El-Niño event. This is not a weakness of the assimilation system, but only suggests that we are overfitting Levitus and shows that the assimilation system can fit the data. Levitus needs therefore to be downweighted in our cost function. These results were consistent with a comparison of the mean zonal currents with the TAO measurements along the equator. Overall, the free-run is behaving better, particularly in the western Pacific where the assimilation was trying to deepens the thermocline while weakening the strength of the EUC.

4.2.2 Adjustments to the control variables

Here we compare the mean adjustments to the heat flux, the zonal wind stress (Figure 7), and the temperature and the normal velocity at the southern open boundary (Figure 8) as obtained from the separate assimilation runs NCEP-LEVic and ECCO-LEVic.

Starting from NCEP or ECCO analysis, the optimization is shown to reach very similar
solutions for the wind stress after 30 iterations with strong adjustments on both sides of the equator probably related to the overturning circulation. This is however not true for the heat (and fresh water) flux, although the adjustments seem to have similar structures, with less heat over the cold tongue and more heat over the subtropical gyres, but not the same magnitudes; almost 5 times larger when the optimization starts from ECCO. This result can be somewhat expected since the wind stress drives most equatorial circulation. The sensitivities with respect to the wind were therefore the largest and the optimization first adjusted this control variable. After roughly 25 iterations, the cost function terms for the other control variables started to increase, once the large structures of the wind adjustments were set. More iterations are probably needed for the stabilization of the heat and fresh water fluxes. Another reason for the slow convergence to the heat flux is the relatively short assimilation window since the impact of this flux on the tropical circulations takes several years to emerge.

Finally, the adjustments to the southern boundaries are shown to converge toward similar solutions as can be seen from Figure 8. The decomposition of the normal velocities into barotropic and baroclinic modes (as described by section 2.3) efficiently solved the problem of huge sensitivities with respect to the barotropic component allowing the adjustments of the velocities with the rest of the control variables.

5 Discussion

In this paper we have introduced an eddy-permitting four-dimensional adjoint data assimilation system for the tropical Pacific Ocean that is nested into the global ECCO assimilation approach. The implementation of this system was not simple due to two difficulties; the control of the normal velocities at the open boundaries and the nonlinearity of the model. Although both problems involve very large gradients, they are different. The first is primarily a conditioning problem while the second is related to the use of a linear optimization algorithm for the optimization of a nonlinear cost function. A generalization of the modes decomposition used in QG models was introduced to deal with the first problem in order to down-weight only the barotropic component in the optimization. Higher viscosity and diffusivity terms were used in the adjoint model to damp high sen-
sivities associated with the local minima allowing the optimization of the cost function over year-long assimilation periods.

Several experiments were performed over a one year period in 1998 to evaluate the performance of the assimilation system while constraining the model to altimetry SSH, Reynolds SST and Levitus S and T. This system was shown to be very efficient in improving the model fit to these data as well as to provide reliable estimates for the control variables. It was also found to be weakly sensitive to initial guesses, providing similar final solutions. The system was however overfitting Levitus climatology because of the use of relatively large weights (small errors) for these data in the optimization, making the comparison with independent observations less favorable for the assimilation. More appropriate weights for the assimilated data are therefore required. Recently, other data (as TAO-ARGO array, XBTs, ARGO and Drifters) were included in the assimilation system and experiments are currently underway to determine the best weights as well as the appropriate assimilation frequency for these data. The use of non-diagonal error covariance matrices for the control variables is also under development which should smooth the adjustments to these variables. Such covariances are particularly needed for the forcing fields in case of assimilation of in-situ data. This improved assimilation system will be used to construct a set of analysis states and adjusted forcing fields for the tropical Pacific Ocean over several years.

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