Daily oceanographic analyses by the Mediterranean basin scale assimilation system

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Manuscript for:

Ocean Science

30 October 2006

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Abstract

This study presents the upgrade of the Optimal Interpolation scheme used in the basin scale assimilation scheme of the Mediterranean Forecasting System . The modifications include a daily analysis cycle, the assimilation of ARGO float profiles, the implementation of the geostrophic balance in the background error covariance matrix and the initialisation of the analyses. A series of numerical experiments showed that each modification had a positive impact on the accuracy of the analyses: The daily cycle improved the representation of the processes with a relatively high temporal variability, the assimilation of ARGO floats profiles significantly improved the salinity analyses quality, the geostrophically balanced background error covariances improved the accuracy of the surface elevation analyses, and the initialisation removed the barotropic adjustment in the forecast first time steps starting from the analysis.

1. Introduction

The Mediterranean Forecasting System (MFS) uses a multivariate optimal interpolation data assimilation scheme (De Mey and Benkiran 2002, Demirov et al. 2003, Dobricic et al. 2005) in order to combine a model first guess with satellite and in situ observations. Up to now, the assimilation system used in situ temperature measured by XBT (Manzella et al. 2001), satellite Sea Surface Temperature (SST) objective analyses (Buongiorno Nardelli et al., 2003) and satellite Sea Level Anomaly (SLA) observations (Le Traon et al., 2003). SST is assimilated by correcting the heat fluxes (Pinardi et al., 2003). SLA and in situ temperature observations were assimilated using the multivariate background error covariance matrix described in Dobricic et al. (2005). The analyses were produced once a week. The oceanographic model made one week long simulations, and innovations were calculated using the First Guess at Appropriate Time (FGAT) method.

The major initial improvement in the basin scale assimilation scheme was the usage of the new high resolution oceanographic model in the Mediterranean described in Tonani et al. (2006). The Mediterranean Forecasting System (Coppini et al., 2006) operational functioning was evaluated during a Targeted Operational Period (TOP) that lasted six months from September 2004 to march 2005. Immediately before and during the TOP observational period three other major modifications were introduced into the assimilation system. The first was the calculation of analyses with a daily cycle instead of weekly, the second was the modification of the background error covariance matrix in order to maintain geostrophic balance in the error covariances and the third was the assimilation of the vertical profiles of temperature and salinity by ARGO floats deployed in the Mediterranean during TOP (Poulain et al., 2006).

Each of these modifications could theoretically improve the accuracy of the ocean state estimates. The application of the daily cycle increases the frequency by which observations are

melded with model simulations. It this way the assimilation can more frequently correct background fields using observations and provide analyses which more accurately describe the evolution of fields due to physical processes with a higher temporal variability. Therefore, the forecasts starting from daily analyses could be more accurate then those starting from weekly analyses. The enforcement of the geostrophic balance in the background error covariance matrix could improve the accuracy of the multivariate corrections in the analyses. The assimilation of temperature and salinity by ARGO floats gives new information for the analyses. Especially the salinity assimilation can be important, because in the original assimilation system the salinity corrections were estimated only indirectly from the observations of temperature and SLA.

This study will describe in details the major modifications in the data assimilation scheme. It will estimate the impact of each modification on the accuracy of the analyses during the TOP observational period. This will be done by performing experiments with analyses applying different modifications during the TOP period and comparing the corresponding forecasts to the observations. Section 2 will describe the modified assimilation scheme. Section 3 will show the experimental results, and Section 4 will contain conclusions.

2. Modifications in the assimilation scheme

2.1 The Optimal Interpolation scheme

The assimilation scheme is based on the System for Ocean Forecasting and Analyses (SOFA) that is an optimal interpolation scheme (De Mey and Benkiran 2002). Demirov et al. (2003) describes the initial setup of the scheme in the Mediterranean, while the further improvements are described in Dobricic et al. (2005). The SOFA optimal interpolation is an approximation of the Kalman filter in which the analyses are the corrections of the background model estimate by observations. This can be written as:

$$\mathbf{x}_{a} = \mathbf{x}_{b} + \mathbf{K}[\mathbf{y} - H(\mathbf{x}_{b})], \tag{1}$$

where \mathbf{x}_a is the analysis state vector, \mathbf{x}_b is the background state vector or model simulation and *H* is the non-linear observational operator. The matrix **K** is defined by:

$$\mathbf{K} = \mathbf{B}\mathbf{H}^{T} \left(\mathbf{H}\mathbf{B}\mathbf{H}^{T} + \mathbf{R}\right)^{-1},\tag{2}$$

where **B** is the background error covariance matrix, **H** is the linear observational operator and **R** is the observational error covariance matrix. An assumption in SOFA is that the background error covariance matrix can be separated in horizontal and vertical components, and **B** can be written as:

$$\mathbf{B} = \mathbf{S}^T \mathbf{B}_r \mathbf{S} \,. \tag{3}$$

Here **S** contains vertical multivariate error covariances represented by EOFs, and \mathbf{B}_r contains horizontal covariances and eigenvalues of vertical EOFs:

$$\mathbf{B}_r = \mathbf{\Lambda}^{1/2} \mathbf{C} \mathbf{\Lambda}^{1/2} \,. \tag{4}$$

In Eq. (4) Λ is a diagonal matrix containing the eigenvalues of the vertical EOFs and C contains horizontal covariances modelled as Gaussian functions of distance.

In the Mediterranean the vertical EOFs are calculated from the historical model simulation for the period 1993-1997. They are calculated separately for 13 geographical regions, 20 EOFs are kept in each region and four seasons are considered

The Mediterranean Sea model set-up is based on the free surface version of the OPA 8.1 model (Roullet and Madec 2000). Its horizontal resolution is $1/16^{0}$ (~6.5km), and it has 72 levels in vertical. The detailed description of the model set-up and performance in the Mediterranean is given in Tonani et al. (2006). Surface fluxes are calculated interactively (Pinardi et al., 2003) using operational analyses of temperature, humidity, winds and cloud cover from the European Centre for the Medium range Weather Forecasting (ECMWF) available with the horizontal resolution of 0.5^{0} and 6 hours temporal resolution.

The model started the simulation on the 1st January 2002 with initial temperature and salinity obtained from the January MEDATLAS climatology (The MEDAR Group 2002). The analyses are produced starting from the 1st of January 2003 with weekly analyses until June 2004 and daily analyses afterwards. The assimilation of SLA observations uses the mean dynamic topography calculated by Rio et al (2006), based on a model estimate (Demirov et al 2003) and observations from surface drifters.

2.2 Daily assimilation cycle

Daily and weekly assimilation cycles in the basin scale system are shown in Fig. 1. All satellite observations for the previous 2 weeks are received once a week. In the assimilation with the weekly cycle 2 analyses are performed at days J-7 and J. The first analysis is made using the one week long model run which starts on the day J-14 and ends on J-7. The second analysis is made from the model run which starts from the previous analysis on the day J-7 and ends on the day J. During the model simulation misfits between the model first guess and observations are calculated using the FGAT method. In this way each week the analyses for the J-7 replaces the last analyses produced one week before. This is done because the specific quality control procedure for SLA observations produces observations with higher accuracy 2 weeks later (Le Traon et al. 2003).

In the daily cycle the model simulation which creates the background fields is one day long. Misfits are calculated using the FGAT method and the analysis is made at the end of each day. Even in this case observations for the previous 14 days arrive once a week. Therefore, the analyses for the previous 14 days are calculated starting from the day J-14. In this case there are 7 analyses that overlap with those made in the previous week (from day J-14 until day J-7).

2.3 Geostrophically adjusted error covariance matrix

The vertical EOFs are calculated from the historical model simulation in 13 regions and for each season (Dobricic et al. 2005). EOFs are quadrivariate and include surface elevation, barotropic stream function and vertical profiles of temperature and salinity from a model simulation done with the previous version of the model (Pinardi et al., 2003). This methodology produces spatially and temporally variable vertical error covariances containing the characteristic dynamical variability of the model errors in the Mediterranean. As in meteorology, we argue that vertical error correlations represented by EOFs should satisfy the geostrophic balance (e.g Daley 1991). The geostrophic balance in vertical EOFs can be estimated using the formula of Pinardi et al. (1995) which links variations of temperature and salinity in a water column with variations of the barotropic stream function and surface elevation:

$$\delta\eta = \frac{f\partial\Psi}{gh} - \frac{1}{\rho_0 h} \int_{-h}^{0} \left(\frac{\partial\rho}{\partial T} \delta T + \frac{\partial\rho}{\partial S} \delta S \right) (z+h) dz , \qquad (5)$$

where g is acceleration due to gravity, ρ_0 is the reference density, and h is the bottom constant depth. Corrections of the surface elevation, barotropic stream function, temperature and salinity arerepresented respectively by $\delta\eta$, $\partial\Psi$, δT and δS . By substituting corrections in $\partial\Psi$, δT and δS from each EOF into (5) we compute the corrections in the surface elevation $\delta\eta$ on the left side of (5). Although this relation was approximately satisfied for most of the most significant EOFs without enforcing (5), in some cases the corrections calculated from (5) was giving significantly different corrections in comparison to those calculated by EOFs (not shown). The differences appear because EOFs do not always represent physical modes of the errors which should be in approximate geostrophic balance, but only give a statistical estimate of relations between errors in the different state variables.

Therefore, we have decided to impose the geostrophic constraint given by Eq. (5) in all EOFs in order to dynamically link the errors in SLA with the errors in the barotropic stream function, temperature and salinity. Therefore, for each EOF the value for $\delta\eta$ is computed by Eq. (5) using $\delta\Psi$, δT and δS of each EOF.

After the assimilation cycle is terminated temperature, salinity, sea surface level and barotropic stream function are updated by (1). Barotropic stream function is not a prognostic variable in the free surface version of the OPA model. Therefore its correction is only used to calculate corrections of velocity components at each model level, which are prognostic variables in the model. Velocity corrections are calculated by:

$$\delta u = -\frac{1}{H_0} \frac{\partial \Psi}{\partial y}$$
 and $\delta v = \frac{1}{H_0} \frac{\partial \Psi}{\partial x}$

where H₀ is 1000m.

2.4 Assimilation of ARGO floats

The relatively large number of ARGO floats deployed in the Mediterranean by the MFSTEP (MedARGO floats, Poulain et al., 2006) gave a possibility to operationally assimilate temperature and salinity observations by ARGO floats in a multivariate mode, together with other in situ and satellite observations. In addition to the MedARGO floats the NAVOCEANO floats in the Levantine were also used. Fig. 2 shows positions of ARGO floats during the experiments described in Section 3.

2.5 Balanced initialisation

The OPA model is a free surface model in which the surface elevation is simulated using an implicit numerical scheme (Roullet and Madec, 2000). Therefore, fast gravity waves could be excited by the updated and unbalanced initial velocity field. Although the velocity corrections in the analysis contain only corrections due to the barotropic stream function, the three dimensional divergence may differ from zero in areas of variable bottom topography. This happens because the corrections in the barotropic stream function are applied under the assumption of constant bottom topography and no coastlines. As a consequence the three dimensional divergence of the velocity field along the coasts becomes different from zero.

In order to reduce the impact of the unbalanced corrections on the barotropic gravity waves, velocity corrections are filtered using the "divergence damping filter" (Talagrand 1972). However, unlike the previous applications, where it was applied on the analysis velocity field, the divergence damping filter is applied now only to the corrections of the velocity field.

The corrections in the horizontal velocity field can be filtered by successively applying the Laplacian horizontal operator:

$$\delta \mathbf{v}_{n+1} = \delta \mathbf{v}_n + a \nabla^2 \delta \mathbf{v}_n, \tag{6}$$

where δv is the correction of horizontal velocity, n indicates the iterative step in the application of the filter, and *a* is the coefficient of viscosity. Alternatively, the equation can be written as:

$$\delta \mathbf{v}_{n+1} = \delta \mathbf{v}_n + a_D \nabla D_n + a_{\mathcal{L}} \nabla \times (\boldsymbol{\zeta}_n \mathbf{k}), \tag{7}$$

where $a_D = a_{\zeta} = a$, $D = \nabla \cdot \delta \mathbf{v}$ is horizontal divergence and $\zeta = \mathbf{k} \cdot \nabla \times \delta \mathbf{v}$ horizontal vorticity of the velocity corrections. By taking the gradient of (7) it can be shown that the second term on the right side filters the divergent part of the velocity field corrections, and by taking the curl of (7) the third term filters the rotational part. Therefore by setting $a_{\zeta} \equiv 0$ only the divergence will be filtered and the vorticity will remain unchanged. This procedure is applied at each model level in order to damp the vertical velocity which would develop due to the unbalanced velocity corrections. As a consequence also the divergence of the vertically integrated velocity is filtered and the artificial barotropic waves are suppressed.

3. Evaluation of the impact of the assimilation modifications

3.1 Evaluation of analyses quality

In order to evaluate the impact of each modification on the accuracy and quality of the analyses 4 experiments are performed during the TOP period, October 1, 2004 to March 15, 2005. The reference experiment uses the assimilation system with all modifications. It uses the daily cycle, assimilates observations by ARGO floats and uses geostrophically balanced EOFs. In each of the three remaining experiments one modification at a time was not applied: the first experiment applies the weekly cycle, the second experiment does not assimilate ARGO floats, and the third

experiment applies the original EOFs which are not always in geostrophic balance. In this way it is possible to estimate the impact of each individual modification on the quality of the analyses during the period 01.10.2004-15.03.2005. The atmospheric forcing is the same in all experiments and is obtained from the ECMWF atmospheric analyses.

Fig. 3 shows the temporal variability of weekly r.m.s. of SLA misfits for all experiments. Although SLA observations are assimilated in the analyses, the r.m.s. of SLA misfits is an independent estimate of the analyses accuracy because it measures the accuracy of the background field before the SLA observations are assimilated. We can see in Fig. 3 that in the first few months there is not much difference between the experiments. However, from the beginning of December 2004 till the end of January 2005 the experiment with the original EOFs is less accurate then the reference experiment with the geostrophically balanced EOFs. Furthermore, starting from the beginning of January 2005 the experiment with the weekly cycle has a consistently higher r.m.s of SLA misfits and a lower accuracy of analyses than the reference experiment with the daily cycle. On the other hand the experiment without the assimilation of ARGO floats shows a similar performance to that of the reference experiment throughout the evaluation period. This result can be explained by the fact that there are many more SLA observations than observations by ARGO floats. They cover almost the whole Mediterranean, while in a single week ARGO floats does not influence significantly the overall accuracy of the system when compared with SLA observations in the whole Mediterranean.

Fig. 4 shows temporal evolution of the r.m.s of temperature misfits measured by ARGO floats. In this case clearly the experiment which does not assimilate data from ARGO floats has the lowest accuracy. Even the experiments with the weekly cycle or with the original EOFs seem to be slightly less accurate then the reference experiment close to the end of the evaluation period, but the differences are too small to be significant. On the other hand the temporal evolution of the r.m.s of temperature misfits measured by XBT observations (not shown) did not show any significant

impact of modifications, with all experiments having very similar r.m.s of misfits. The reason that the r.m.s of XBT temperature misfits was relatively insensitive to the assimilation of ARGO floats, could be that there was a relatively small number of XBT observations close to the ARGO observations. Furthermore, the temporal frequency of XBT observations was too low in order to show a significant impact on the daily analyses. Fig. 5 shows the temporal evolution of the r.m.s of salinity misfits measured by ARGO floats. Again, like in the case of temperature misfits, the experiment without the assimilation of ARGO floats shows the least accurate results, while the differences between other experiments seem to be too small in order to be significant.

However, sometimes even the assimilation with all modifications did not improve the accuracy of the salinity field. For example, Fig. 5 shows that a relatively large r.m.s. error in salinity at the beginning of January 2005 (Fig. 5c) is not reduced significantly by the analyses (Fig. 5a). In that period two floats were deployed in the southern Ionian Sea. Initially their salinity misfits were large and significantly influenced the r.m.s. of misfits, but after several assimilation cycles they were reduced by the assimilation system (not shown). In the absence of salinity observations the salinity field was corrected only by error covariances between surface elevation and salinity in the case of SLA observations or between temperature and salinity in the case of XBT observations. Relatively large errors in the r.m.s. of salinity misfits shown in Fig. 5 indicates that the estimate of error covariances should be improved in order to obtain a higher accuracy of salinity when direct observations are not available.

3.2 Impact of balanced initialisation

The integration of the barotropic velocity components by implicit numerical methods automatically damps all gravity waves that have a relatively small horizontal scale (Roullet and Madec 2000). As a consequence, the barotropic gravity waves developed in response to the unbalanced initial

velocity field along the coasts are dissipated in several time steps of the model integration. Therefore, the divergence damping filter will have an impact only in the first few time steps of the model integration. Fig. 6 shows the tendency of the surface elevation increment, which is proportional to the divergence of the vertically integrated velocity, after the first time step of the model integration. Without balanced initialisation the increment is very large at some places along the coast reaching amplitudes of 1m. On the other hand, after the initialisation the magnitude of the initial increment is practically negligible everywhere with the maximum value of 0.001m.

4. Discussion and conclusions

The basin scale assimilation system in the Mediterranean has been modified in order to assimilate observations with a daily frequency and to assimilate observations by ARGO floats in a multivariate mode. The EOFs representing the vertical error covariances in the background error covariance matrix were adjusted in order to enforce the geostrophic balance between temperature, salinity and barotropic streamfunction increments. The usage of the free surface model in the Mediterranean required the initialisation of the velocity increments in order to reduce the unrealistic development of barotropic gravity waves near the coasts.

The impact of each of these modifications on the accuracy of the analyses was separately estimated in a set of experiments which covered the TOP observational period. The comparison between the daily and the weekly assimilation cycle showed that the application of the daily assimilation cycle reduced the r.m.s. of SLA residuals, while it did not change significantly the r.m.s. of in situ residuals. The difference in the improvement between the r.m.s. of SLA and in situ misfits appears because SLA observations are available with a higher temporal frequency than in situ observations. Different satellite tracks often cross each other in consecutive days, while observations by each ARGO float repeat at the lower temporal frequency of 5 days or more. Therefore, daily analyses could incorporate more information from frequent observations like

satellite SLA, while they did not improve the information coming from less frequent in situ observations.

The assimilation of observations by ARGO floats significantly improved the accuracy of the analyses close to the position of ARGO floats, while the impact on the SLA residuals was small. This happened because there are many more observations of SLA then in situ profiles by ARGO floats. Therefore, the relatively small number of ARGO floats in vicinity of SLA observations cannot significantly influence the r.m.s. based on all SLA observations. The application of the geostrophic balance in vertical EOFs of the background error covariance matrix mainly has an impact on the r.m.s. of SLA but not a quantifiable effect on the profile assimilation.

Experiments showed that each modification had a positive effect on the quality of the analyses, although each modification improved analyses in a different way. In order to illustrate more clearly how each modification impacted the analyses, Fig. 7 shows the difference in the weekly averaged surface elevation field between the reference experiment and each of the three experiments at the end of the comparison period during the week 08.03.2005-15.03.2005. We can see that, in agreement with the results shown in Fig. 3, the assimilation of ARGO floats has a relatively small impact on the surface elevation field. The differences are mostly concentrated close to the position of ARGO floats shown in Fig. 2, although they can also exist remotely from ARGO observations, like in the Atlantic Ionian Stream south-east from Sicily. The differences with the experiment applying the weekly assimilation cycle is relatively small in large parts of the Algerian Current in the Western Mediterranean, the Atlantic Ionian Stream in the Ionian Sea and the Atlantic Stream in the Levantine Sea, differences are relatively large. This result indicates that the largest impact of the daily assimilation cycle is in areas where the dynamics are the most intense and have a relatively large temporal and spatial variability. The differences with the un-balanced

EOFs are spread over large parts of the Mediterranean and it seem to be connected both to the position of ARGO floats (Fig. 2) and XBT observations (not shown), and to the dynamics.

The control experiment containing all modifications had the highest accuracy of the analyses. However, sometimes the accuracy of the salinity field was not high. This problem might be due to the relatively inaccurate representation of the error covariances between surface elevation, temperature and salinity in the error background matrix. In order to improve the estimate of error covarinces in the future they will be updated with a higher temporal frequency.

Acknowledgments: This study was financed by the EU project MFSTEP (Mediterranean Forecasting System: Towards Environmental Predictions, Contract number: EVK3-CT-2002-00075).

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