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Daily oceanographic analyses by Mediterranean Forecasting System at the basin scale

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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 the temporal variability shorter than a week, 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, 2007\(^3\)), 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 was 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 FGAT method consists in calculating misfits during the integration of the numerical model exactly at the time when observations are made. The analysis is then calculated assuming the misfits correspond to the analysis time.

The major initial improvement in the basin scale assimilation scheme was the usage of the new high resolution general circulation model in the Mediterranean described in Tonani et al. (2007)\(^2\). The Mediterranean Forecasting System (Pinardi et al., 2007\(^3\)) 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., 2007\(^4\)).

Each of these modifications could theoretically improve...

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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 than 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 Sect. 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:

\[ x_a = x_b + K [y - H(x_b)], \]  

where \( x_a \) is the analysis state vector, \( x_b \) is the background state vector or model simulation and \( H \) is the non-linear observational operator. The matrix \( K \) is defined by:

\[ K = BH^T \left( HBH^T + R \right)^{-1}, \]  

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:

\[ B = S^T B_S S. \]  

Here \( S \) contains vertical multivariate error covariances represented by EOFs, and \( B_s \) contains horizontal covariances and eigenvalues of vertical EOFs:

\[ B_s = \Lambda^{1/2} C \Lambda^{1/2}. \]  

In Eq. (4) \( \Lambda \) 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 (Demirov et al., 2003). They are calculated separately for 13 geographical regions, 20 EOFs are kept in each region and four seasons are considered (Dobricic et al., 2005).

The Mediterranean Sea model set-up is based on the free surface version of the OPA 8.1 model (Roulet and Madec, 2000). The horizontal resolution is 1/16°. This means that in the latitudinal direction the horizontal distance between points is 7 km, and in the longitudinal direction it is between 6 km at 30° N and 5 km at 44° N. The model 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 (Castelletti et al., 1998) 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° and 6 h temporal resolution.

The model started the simulation on the 1 January 2002 with initial temperature and salinity obtained from the January MEDATLAS climatology (The MEDAR Group 2002). Analyses are produced starting from the 1 January 2003 with the weekly cycle until June 2004 and the daily cycle afterwards. The SLA data are derived by the SALTO-DUACS project and two satellite altimeters are used: Jason-1 and Geosat Follow On (GFO). The assimilation of SLA observations uses the mean dynamic topography calculated by Rio et al. (2007). The estimation of the mean dynamic topography is obtained by the objective analysis which used a modelling estimate by the previous MFS general circulation ocean model with the horizontal resolution of 1/8° for the time period 1993–1997 (Demirov et al., 2003) as the background field. This background field was corrected using a combination of surface velocity observations by drifters and SLA in the period 1993–1997.

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 two 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 two 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:

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

(5)

where \( g \) is acceleration due to gravity, \( \rho_0 \) is the reference density, and \( h \) is the bottom constant depth, chosen to be 1000 m. Corrections of the surface elevation, barotropic stream function, temperature and salinity are represented respectively by \( \delta \eta \), \( \delta \Psi \), \( \delta T \) and \( \delta S \). By substituting corrections in \( \delta \Psi \), \( \delta T \) and \( \delta S \) from each EOF into Eq. (5) we compute the corrections in the surface elevation \( \delta \eta \) on the left side of Eq. (5). In most EOFs differences between the original \( \delta \eta \) and that calculated from Eq. (5) were relatively small. However, in some cases differences were significant, and sometimes values had the opposite sign (not shown). This result indicates that statistically estimated error correlations represented by EOF eigenvectors are sometimes due to ageostrophic dynamics.

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 existing \( \delta \Psi \), \( \delta T \) and \( \delta S \).

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 barotropic velocity components, deduced from the total velocity field components which are prognostic variables in the model. Barotropic velocity corrections are calculated by:

\[ \delta u_B = -\frac{1}{h} \frac{\partial \Psi}{\partial y} \quad \text{and} \quad \delta v_B = \frac{1}{h} \frac{\partial \Psi}{\partial x}, \]  

(6)
where $h$ is 1000 m. The model total velocity field is separated into its vertically integrated or barotropic component and a baroclinic part. The barotropic part is then corrected by the terms in (6) in a new estimate of the total velocity.

### 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., 2007) 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 NAV-OCEANO floats in the Levantine were also used. Figure 2 shows positions of ARGO floats during the experiments described in Sect. 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 (Roulet 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 calculated under the assumption of constant bottom topography and no coastlines. As a consequence the three dimensional divergence of the velocity field near the coasts is 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:

$$
\delta v_{n+1} = \delta v_n + a \nabla^2 \delta v_n,
$$

where $\delta v$ 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:

$$
\delta v_{n+1} = \delta v_n + a_D \nabla D_n + a_\zeta \nabla \times (\zeta_n \mathbf{k}),
$$

where $a_D=a_\zeta=a$, $D=\nabla \cdot \delta v$ is horizontal divergence and $\zeta=\mathbf{k} \cdot \nabla \times \delta v$ horizontal vorticity of the velocity corrections. By taking the gradient of (8) 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 (8) the third term filters the rotational part. Therefore by setting $a_\zeta=0$ 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 (1 October 2004–15 March 2005). In this period the MFSTEP made a relatively large number of in situ observations by ARGO floats and XBT instruments, which could be used for the evaluation of different assimilation schemes. The reference experiment uses the assimilation system with all modifications. It uses the daily cycle, it assimilates observations by ARGO floats and it 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 in the daily cycle, and the third experiment applies the original EOFs which are not always in geostrophic balance to the daily cycle. In this way it is possible to estimate the impact of each individual modification on the quality of the analyses. The atmospheric forcing is the same in all experiments and is obtained from the ECMWF atmospheric analyses.

Figure 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 SLA misfit is an estimate of the analyses accuracy because it compares model forecasts with observations before the SLA observations are assimilated. In each daily analysis there are about 150–200
SLA observations in the Mediterranean along a few tracks (Fig. 4a). Positions of tracks differ in each subsequent day (Fig. 4b) and they do not repeat since the Jason-1 and GFO satellite repeat times are longer. Therefore, in order to make the statistics robust, FGAT misfits are grouped into one week long time intervals also in the case of the daily cycle. In this way the number of misfits used for the calculation of the r.m.s. for the daily and weekly cycle experiments is identical and it is about 1000–1500 misfits/week, with tracks covering quite uniformly the Mediterranean Sea (Fig. 4b). It is important to notice that this grouping of the misfits still allows us to estimate the impact of the daily analysis scheme, because the impact of the more frequent daily updates should improve the free model run starting from the daily analyses, even when misfits are grouped weekly.

From Fig. 3 we can see that in the first few months there is not much difference between all the experiments. However, from the beginning of December 2004 till the end of January 2005 the experiment with the original EOFs is less accurate than 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 thus 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 cover only several points in the Mediterranean. Therefore, the assimilation of ARGO floats does not influence significantly the overall accuracy of the system when compared with SLA observations in the whole Mediterranean.

In order to estimate how important are the differences in results between experiments, Fig. 3 can be compared to Fig. 8 in Dobricic et al. (2005). We can see in Dobricic et al. (2005) that, in comparison to the free run of the coarse (1/8 degree resolution) model, the weekly data assimilation reduces the r.m.s. of SLA misfits by ~3cm. A similar result was obtained also for the data assimilation with the high resolution ocean model used in this study (not shown). Figure shows that in the period December 2004–January 2005 the daily cycle improved the r.m.s. of SLA misfits obtained by the weekly cycle by ~0.3 cm, i.e. by ~10% of the overall reduction due to the data assimilation. Due to the end of the TOP period and the consequent drop of the number of ship of opportunity XBTs, experiments were stopped at the end of February 2005 so that our evaluation is done with an almost uniform set of data for the whole time period. Although there is no experimental proof, we can expect that even with smaller amount of data the daily will always show improvements with respect to the weekly analysis cycle system. However, we can see from Fig. 3 that the relatively large improvement is especially limited to certain time periods of the year.

The improved r.m.s. of SLA misfits by a daily analysis system eventually could be explained by the fact that the misfits in the weekly scheme increase during the seven days long forecast or free run. However, Fig. 5 does not confirm this hypothesis, because it does not show a net increase of the r.m.s. of SLA misfits as a function of the day of the forecast. A very similar result was also obtained for the period December 2004–January 2005, when the difference between the daily and the weekly scheme was the largest (not shown). Probably, the daily scheme is more accurate because in one week many satellite tracks are positioned close or cross each other (Fig. 4b). Therefore, it seems that the more frequent assimilation of SLA observations by the daily scheme may increase the accuracy of the analyses in areas where observations are made several times during a single week.

Figure 6 shows temporal evolution of the r.m.s. of
temperature misfits computed using 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 than 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 computed using 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. Figure 7 shows the temporal evolution of the r.m.s of salinity misfits computed using 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.

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. Figure 8 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
Fig. 8. The increment of the surface elevation (cm) in the first model time step starting from the analysis on 1 October 2004. The figure shows a part of the coast where the un-initialised analysis produced particularly large oscillations of the surface elevation. The result for the un-initialised analysis is shown in the upper panel, and for the initialised analysis in the lower panel. The contour interval in the upper panel is 25 cm and in the lower panel 0.025 cm.

initialisation the increment is very large at some places along the coast reaching amplitudes of 100 cm. On the other hand, after the initialisation the magnitude of the initial increment is practically negligible everywhere with the maximum value of 0.1 cm.

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 temperature and salinity residuals. The difference in the improvement between the r.m.s. of SLA and in situ observations misfits appears because the 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 than in situ profiles by ARGO floats. Therefore, the relatively small number of ARGO floats in vicinity of SLA observations cannot significantly influence the
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. 9 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, between 8 March 2005 and 15 March 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 Mediterranean, but in areas with the relatively strong surface circulation, like the area 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 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 still not higher than in the systems with less improvements. 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. For example we can see in Fig. 6 that the vertical structure of the temperature misfits has seasonal variability with the highest errors close to the bottom of the mixed layer which forms in summer. Similarly, we may expect that also salinity errors have a large spatial variability due to the relatively complex dynamics of the surface circulation and relatively high salinity gradients between the Atlantic waters with low and Mediterranean waters with high salinity (Dobricic et al., 2005). Furthermore, the path of the Atlantic water in the Mediterranean may have a high interannual variability (e.g. Demirov and Pinardi, 2002). Therefore, in order to improve the estimate of error covariances, in the future they will be updated with a higher temporal frequency.

It is important to notice that with the optimal interpolation scheme the calculation of seven daily analyses requires a similar amount of computational time as a single weekly analysis, because the computational time mainly depends on the number of observations. On the other hand, in a three dimensional variational scheme which is defined on the model space, computational time would mainly depend on the size of the model grid which is fixed, and computationally the daily scheme would be seven times more expensive than the weekly scheme. In that case, when deciding whether to use the daily or the weekly scheme, the increase of the computational time should be considered in addition to improvements in accuracy shown in this study.

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