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Assimilating GRACE derived oceanic mass distributions with a global ocean circulation model

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Abstract

To study the sub-seasonal distribution and generation of ocean mass anomalies, Gravity Recovery and Climate Experiment (GRACE) observations of daily and monthly resolution are assimilated into a global ocean circulation model with an ensemble based Kalman-Filter technique. The satellite gravimetry observations are processed to become time-variable fields of ocean mass distribution. Error budgets for the observations and the ocean model's initial state are estimated which contain the full covariance information. The consistency of the presented approach is demonstrated by increased agreement between GRACE observations and the ocean model. Furthermore, the simulations are compared with independent observations from 54 bottom pressure recorders. The assimilation improves the agreement to high-latitude recorders by up to 2 hPa. The improvements are caused by assimilation induced changes in the atmospheric wind forcing, i.e., quantities not directly observed by GRACE. Finally, the use of the developed Kalman-Filter approach as a destriping-filter to remove artificial noise contaminating the GRACE observations is presented.

Keywords: Data assimilation, GRACE satellite gravimetry, Time variant ocean mass distribution, GRACE error estimation, Correction of atmospheric forcing

1. Introduction

In the field of oceanography, the problem of satellite observations often lies in the close entanglement of volume, mass and temperature on the one hand and mass, pressure and velocity of water parcels on the other hand. Other than altimetry which measures sea level changes that may originate in salinity, temperature, ocean dynamics or mass changes, satellite gravimetry measures mass anomalies alone.

From March 2002 on, the GRACE satellites have measured the gravity field of the Earth with unprecedented precision. To synthesize fields of mass anomalies from the GRACE spherical harmonic (Stokes) coefficients, additional post processing is necessary, e.g., to reduce the noise in the higher-degree coefficients which results in the well known stripes in the GRACE solutions. In the first years of the GRACE mission, low pass filtering with an isotropic Gaussian filter as described by Wahr et al. (1998) was the standard procedure. Since then, improvements have been made with the de-correlation

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method by Swenson and Wahr (2006) and with anisotropic filter designs (e.g., Werth et al., 2009). For smaller regions, the accuracy of these filter methods is insufficient and so called re-parameterization methods were introduced. Information of the spatial and temporal structure of the observed region is used to improve the mass anomaly fields from GRACE by using least squares (e.g., Sasgen et al., 2010; Schrama and Wouters, 2011). Recently, a GRACE product is released which uses a Kalman-Filter approach and increases the temporal resolution to daily values (Kurtenbach et al., 2012).

Oceanographic GRACE studies deal with the estimation of mass trends (e.g., Quinn and Ponte, 2010), the steric and non-steric contributions to interannual and seasonal sea level variability (e.g., Willis et al., 2008) and the derivation of the mean dynamic topography (e.g., Vianna et al., 2007). Recently, the focus shifted from trend and mean field estimation to higher frequencies (e.g., Bonin and Chambers, 2011; Quinn and Ponte, 2011). These studies note high discrepancies between modeled and observed ocean bottom pressure at monthly and sub-monthly periods and recommend to study and minimize these discrepancies by data assimilation techniques.

The assimilation of geodetic observations is frequently applied in oceanography (e.g., Wenzel and Schröter, 2007; Saynisch et al., 2011b). For gravimetry data, many model-to-observation comparisons exist (e.g., Chambers, 2006; Dobslaw and Thomas, 2007) but the assimilation of GRACE observations is a newer field of research. Köhl et al. (2012) use an adjoint assimilation method to integrate monthly gravity field data, in combination with other oceanographic observations, in a global ocean circulation model. They found that ocean bottom pressure is partly complementary to combinations of other oceanographic data sets which include altimetry but the authors note that in the assimilation context these data sets have larger prior errors. Furthermore, these combinations fail in certain regions, e.g., under the sea-ice, are restricted to the upper ocean, have a low sampling interval or a low spatial resolution. Our study takes a similar approach as Köhl et al. (2012) but because of the mentioned problems, focuses on the information contained in the GRACE measurements alone. The goal of our paper is first to understand the gain to expect from GRACE assimilation in the oceanic context and to identify connected problems, sensitivities, physical mechanism, error budgets and possible improvements by using the complementary information contained in GRACE without the superposition of error budgets and assumptions from different observation types. Consequently, to be entirely consistent, the observation error is estimated from GRACE data alone and the success of our assimilation is evaluated by comparisons with direct measurements of ocean mass, i.e., measured by bottom pressure recorders. Furthermore, since GRACE data contains significant physical signals below the monthly resolution (Bonin and Chambers, 2011; Kurtenbach et al., 2012; Quinn and Ponte, 2012; Bergmann and Dobslaw, 2012), our study extends the assimilation of Köhl et al. (2012) to high-frequency mass variability by using the GRACE observations of Kurtenbach et al. (2012) which have daily resolution. Instead of an adjoint method, our study applies an ensemble based Kalman-Filter assimilation technique and in contrast to the globally uniform observation error of 1 hPa used in Köhl et al. (2012), a globally varying observation error with full covariance information is incorporated. Despite all aforementioned progress in the processing of GRACE measurements, the mass anomalies of different GRACE centers show still significant differences (Quinn and Ponte, 2008; Sakumura et al., 2014). Because in some regions these differences are larger than the distributed formal errors, we use these differences to estimate the GRACE observation error budget.

The findings of these more fundamental assimilation experiments can be utilized afterwards for a beneficial assimilation of combinations of oceanographic observations

or for the design and motivation of future satellite gravimetry missions.

The experiment’s setup is described in Sect. 2. The description includes the ocean model (Sec. 2.1), the incorporated gravimetry data and its processing (Sec. 2.2), the assimilation method (Sec. 2.3) and the estimation of the incorporated error budgets (Sec. 2.4). In Sect. 3 the results of the GRACE assimilation are presented and discussed. We summarize the obtained results in Sect. 4.

2. Methods and Data

2.1. Ocean model

The Ocean Model for Circulation and Tides (OMCT, Thomas et al., 2001) is used in this study. Despite the model’s name, tides are switched off to be consistent with the assimilated GRACE observations (see Sec. 2.2). The applied OMCT version has a resolution of 1.875 degrees in the horizontal and 13 layers in the vertical direction. This resolution is sufficient, given the fact that the spatial resolution of the assimilated GRACE data is limited by spherical harmonic degree 40, i.e., 1000 km on the Earth’s surface. Furthermore, Bingham and Hughes (2008) suggest that ocean bottom pressure differences between eddy permitting and coarser resolution ocean models are in general small. Quinn and Ponte (2012) show that on sub-seasonal timescales and for observed variability of some hundred kilometer extent, the ocean is barotropic. The OMCT’s temporal resolution of 30 minutes is sufficient to assimilate the daily GRACE observations. The model is forced by 6-hourly ERA-Interim products (wind-stress, freshwater-flux, heat-flux) from the European Centre for Medium-Range Weather Forecasts (ECMWF, Uppala et al., 2008) and river runoff from the Land Surface Discharge Model (LSDM, Dill, 2008). The OMCT conserves mass and the correction of artificial mass change due to the Boussinesq-Approximation follows Greatbatch (1994). In this configuration, the OMCT is well suited for mass related studies in general (Dobslaw and Thomas, 2007), for the modelling of short term ocean bottom pressure variability in particular (Bergmann and Dobslaw, 2012) and is in use for the GRACE de-aliasing (Flechtner, 2007).

Two different simulations are generated with this model setup. First, the reference simulation consists of the OMCT’s reaction to the ECMWF forcing and is similar to the simulation which is used for the GRACE AOD1B-RL04 de-aliasing product (Flechtner, 2007). Second, the assimilation simulation consists of the OMCT coupled to an ensemble Kalman-Filter (see Sec. 2.3) with the constraint to reproduce observation-based daily ocean bottom pressure fields from GRACE (see Sec. 2.2).

2.2. Gravimetry observations

In this study, daily GRACE solutions from the Institute of Theoretical Geodesy (ITG) of the University of Bonn are assimilated. The ITG-GRACE solutions use a Kalman smoother approach to estimate daily gravity fields (Kurtenbach et al., 2012). The Stokes coefficients of ITG-GRACE are provided up to degree $N=40$. The observations are cut to a time window from January 2003 to August 2009. For the estimation of changes in ocean bottom pressure, non-tidal mass effects of atmosphere and ocean (i.e., the GAC product) are added back. Additionally, the degree 1 term is included as a mean annual sinusoid determined from Satellite Laser Ranging and DORIS observations (Eanes, 2000). Following Wahr et al. (1998), spectral leakage of continental signals is minimized by applying a Gaussian filtering with a half-width radius of 300

km. Fields of ocean bottom pressure changes are estimated from the Stokes coefficients ΔC_{lm} and ΔS_{lm} according to Wahr et al. (1998):

$$\Delta p_{bot}(\phi, \lambda, t) = \frac{a_E g \rho_E}{3} \sum_{l=1}^N \sum_{m=0}^l \frac{2l+1}{1+k_l} P_{lm} \sin(\phi) \cdot (\Delta C_{lm} \cos(m\lambda) + \Delta S_{lm} \sin(m\lambda)),$$

where a_E is the semi-major axis of the reference ellipsoid, ρ_E the Earth's mean density, g the mean gravitational acceleration, k_l the load Love numbers of degree l , P_{lm} the normalized associated Legendre functions of degree l and order m , ϕ the geographical latitude and λ the geographical longitude. The geographical positions are identical to the grid points of the ocean model used for the assimilation.

In addition, one year (2004) of monthly GRACE data from the Deutsches GeoForschungsZentrum (GFZ) are assimilated. The GFZ-data is described in Sec. 2.4 and is assimilated to demonstrate certain properties of our Kalman-Filter approach.

2.3. Assimilation setup

For the assimilation of GRACE observations, the Singular Evolutive Interpolative Kalman-Filter (SEIK) of Pham et al. (1998) is used. Kalman-Filters combine an observation (x^o) and a model forecast (x^m) to generate an analysis state (x^a):

$$x^a = qx^m + (1-q)x^o \quad (1)$$

Here, q is a weighting factor between zero and one. For better understanding, it is assumed that the observation's and the model's state space are the same in dimension and physical meaning (otherwise, the equations become less intuitive). After the calculation (1), the analysis state is used to generate a new model forecast for the next time when observations become available. In the Kalman-Filter formalism, the weighting factor q depends solely on the errors P and R of x^m and x^o :

$$q = \frac{R}{R+P} \quad (2)$$

As can be seen in (1) and (2), if the observation error R becomes much larger than the model error P , then $q \approx 1$ and $x^a \approx x^m$. Likewise, if $P \gg R$ then $x^a \approx x^o$. In this study, a time-invariant observation error R is assumed and derived in Sec. 2.4. In contrast to R , the model error P is assumed to show substantial dynamic behavior. Since the incorporated ocean model is nonlinear, we use an ensemble Kalman-Filter (EnKF) to propagate the model's initial error by an ensemble of model simulations $x_{i=1 \dots n}^m$:

$$P(t) = \text{var}_i(x_i^m(t)) \quad (3)$$

Here $\text{var}_i(\cdot)$ denotes the variance over the n ensemble members at a certain time t , i.e., the cross-ensemble variance. In real applications, P and R are often high-dimensional matrixes containing variances and covariances, i.e., $\mathbf{R}$ and $\mathbf{P}$. The initial model error $\mathbf{P}(t_0)$ is estimated in Sec. 2.4 and used to generate an ensemble $x_i^m(t_0)$ that fulfills equation (3) at $t = t_0$. The individual $x_i^m(t_0)$ are then propagated through time by the ocean model operator and subsequently (3) is used to estimate $\mathbf{P}(t)$. In the utilized SEIK-EnKF, all evaluations and calculations are made in a subspace $\mathbb{P}$ of the model's state space. Hereby, $\mathbb{P}$ is spanned by the leading eigenvectors of the model's error

covariance matrix $\mathbf{P}$. This means, $\mathbb{P}$ is spanned by the directions in which the model error grows strongest. Equation (3) becomes:

$$\|\mathbf{P}(t)\| = \|\text{var}_i(x_i^m(t))\| \quad (4)$$

The operator $\|\cdot\|$ projects its argument on $\mathbb{P}$ and the equation (4) describes the 2nd-order-exact sense of Pham (2001). In this sense, the cross-ensemble covariance of the initial model ensemble and the estimated model's initial error covariance $\mathbf{P}(t_0)$ are identical (see Sec. 2.4). The mean of the initial ensemble $x_i^m(t_0)$ is chosen to be identical to the initial state of the reference simulation.

The dimension of $\mathbb{P}$ is usually much smaller than the model's state space and small ensemble sizes are sufficient to propagate the model's initial error (Nerger et al., 2007). In this study, the used ensemble has 32 members and is constructed as described in Pham (2001). By evaluating the leading eigenvalues of $\mathbf{P}(t_0)$, 32 members are sufficient. More members do not improve the results.

The assimilation setup is depicted in Fig. 1. It can be seen how the ocean state ensemble is iteratively propagated through time by the OMCT model operator. The propagation is subject to the atmospheric forcings from ECMWF (grey). The forcings are interpolated from their 6 hourly resolution to the 30 minutes time step of the ocean model. To take errors in the forcing into account and consequently to allow the forcing to be adjusted by the data assimilation, a forcing ensemble layer is added to the ocean model (green). These two-dimensional fields are individual for every ocean ensemble member and are added to the prescribed forcing from ECMWF (which is the same for every ocean ensemble member). The added fields will be referenced as EnKF-ADD fields from now on. The initial cross-ensemble mean of the EnKF-ADD ensemble is zero and the cross-ensemble covariance is equal, in the 2nd-order-exact sense, to the forcing error covariance estimated in Sec. 2.4. The EnKF-ADD fields are treated as part of the ocean model's control vector and change during the model's EnKF update step (red).

The coupling of the OMCT ensemble to the SEIK-Filter is realized with the Parallel Data Assimilation Framework (PDAF, Nerger and Hiller, 2012). The update step takes place whenever GRACE observations (yellow) are available, i.e., once a model day. The update changes the ocean model state and the EnKF-ADD fields consistently. Since this study focuses on the short term mass re-distribution, the global ocean mass is removed from observed and modelled ocean bottom pressure fields (compare w. Quinn and Ponte, 2012; Köhl et al., 2012). The subtraction is realized within the SEIK observation operator during the SEIK analysis step and consequently, the spatial average of the ocean bottom pressure field is not part of the model-to-observation comparison. Temporal anomalies are likewise calculated in the observation operator and reference to the 1st January of 2003. In this paper, the Kalman-Filter's control vector consists of the two-dimensional field of sea surface height (SSH); the three dimensional fields of ocean temperature, salinity and velocity; and the two-dimensional EnKF-ADD fields, i.e., freshwater-flux and wind-stress.

Since in the SEIK-Filter, the output of the assimilation simulation is represented by the mean over an ensemble, it is necessary to quantify the influence of the cross-ensemble mean operator on the output of the simulation. Therefore, the initial ensemble states of the assimilation simulation are individually propagated through time, but without data assimilation and, as a result, with time-invariant EnKF-ADD fields. The mean over this ensemble of simulations is compared with the reference simulation. The differences are negligible. Consequently, differences between assimilation simulation

and reference simulation must be attributed to the data assimilation, i.e., the GRACE observation's information content.

2.4. Error estimation

2.4.1. Observation errors

The observation error variance and covariance information can be an important factor in the fusion of model forecast and observation in the Kalman-Filter analysis step (see Sect. 2.3). The formal errors of the single GRACE processing centers disregard the differences in the possible processing strategies and are longitude-invariant. To consider the full spatial variability of GRACE errors, one needs to go beyond the formal errors. Quinn and Ponte (2008) estimate GRACE errors by comparing GRACE data with assimilative ocean models. To avoid circular reasoning, we do not use assimilation and ocean model based estimates of GRACE errors for the assimilation of GRACE data into an ocean model. In our study, the errors of the ocean bottom pressure observations are estimated from GRACE alone.

The differences between GRACE products from different centers products show latitudinal and longitudinal variations and regionally surpass the formal errors (Sakumura et al., 2014). When spatially averaged, the differences and the formal errors become comparable in size (Quinn and Ponte, 2008). Therefore, we use these differences to estimate the GRACE observation errors. In particular, monthly Release-05 solutions from the University of Texas (CSR), the Jet Propulsion Laboratory (JPL) and the Deutsches GeoForschungsZentrum (GFZ) are used.

The data is cut to the same time period (2003-2009) as the ITG-GRACE data which is used in the assimilation experiment. To match the spatial resolution of ITG-GRACE, the monthly solutions are truncated at degree and order 40. The processing is similar to the processing of ITG-GRACE (see Sect. 2.2) and differs only in the removal of GRACE observational artifacts, i.e., the stripes. To reduce these effects in the monthly solutions, a degree- and order-dependent spatial filtering of the Stokes coefficients with a non-isotropic two-point kernel function is applied (DDK2, Kusche, 2007). Note that, an additional filtering of the ITG-GRACE coefficients is not necessary due to the intrinsic Kalman smoothing.

The monthly JPL, CSR and GFZ ocean bottom pressure estimates are used to calculate time series of pairwise differences at every geographical position of the ocean model grid. If the ocean model has M grid points this results in $3 \times M$ time series (CSR-JPL, JPL-GFZ, GFZ-CSR). By calculating the temporal variances and covariances between these time series of differences, three covariance matrices are derived. Each with the a dimension of $M \times M$.

The root-mean-square-value (RMS) over all entries of a covariance matrix is calculated to choose the largest covariance matrix. To have a conservative observation error estimate, we choose this largest matrix as the observation error covariance for the ITG-GRACE data assimilation. In this RMS-sense, the largest covariance matrix is the matrix based on the JPL-GFZ differences. The diagonal entries, i.e., the variances of the JPL-GFZ ocean bottom pressure differences are plotted in Fig. 2 (top). Apart from stripe like error patterns in the tropics, the largest errors are located in the high latitudes above 60° . This agrees with Sakumura et al. (2014) who compare the different GRACE solutions and find the highest misfits between the JPL and GFZ products, especially, in the polar areas. By comparing ocean models and GRACE observations, Chambers and Bonin (2012) also find the GRACE errors to be higher in the polar and subpolar regions. This seems to be in contrast to the formal errors distributed with the

GRACE solutions, which, due to the convergence of satellite ground tracks, decrease at the high latitudes. One reason for these high latitude misfits is the increased variance of ocean bottom pressure anomalies in the polar areas. There, the low vertical density gradients inhibit the baroclinic compensation of ocean pressure anomalies. As a result, pressure anomalies are mostly barotropic (Quinn and Ponte, 2012) and strong surface anomalies, e.g., due to wind, can reach down to the ocean bottom. The GRACE data should be cleaned from these signals prior to the gravity field modeling by subtracting the AOD1B product. Therefore, it could be that the AOD1B does not fully remove the respective signals (see also, Quinn and Ponte, 2011). Another reason is a tide-alias error in the GRACE solutions. The error results in a spurious 161 day oscillation which grows towards the poles (Steffen et al., 2009).

A main question remains: How well do these differences between the monthly solutions describe the errors of the daily ITG solution. The GRACE data we use for the error estimation differs from the GRACE data we use for the assimilation in spacial and temporal resolution as well as in the applied destriping filter. These conceptual differences influence the noise variances and the noise correlations to an unknown extent. The differences in spacial resolution can be neglected due to the consistent limiting to degree and order of 40. The noise in the monthly solutions may be smaller, due to temporal averaging, than in the daily solution. In addition, the differences between monthly solutions may underestimate the true noise because the errors in the monthly solutions could be similar and cancel out in the differences. The influence of the different destriping procedures is unclear, too. It turns out, however, that the presented assimilation technique is very robust under a broad range of observation error estimates and completely insensitive to the stripes in the GRACE data (see Sect. 3). Otherwise, the presented error estimates should only be used with great caution as observation errors for the ITG data.

Nonetheless, our errors correspond to 1-3 cm of water column equivalent and agree with the ranges and distributions in literature (Quinn and Ponte, 2008; Chambers and Bonin, 2012). In addition, our error estimates are more conservative, i.e., higher, than the formal errors and the globally homogenous value of 1 cm used in Köhl et al. (2012).

Because the coastal areas are affected by signal leakage between land and ocean, the error estimates of regions within 600 km from the coast are masked out of the assimilation process.

2.4.2. *Model error*

In the SEIK-Filter analysis step, the model error is estimated by the spread of the ocean model ensemble. The spread of the ensemble itself is a consequence of the different initial state of each ensemble member and the therefore different reactions to the atmospheric forcing. Since the forcing itself has substantial errors (e.g., Trenberth et al., 2011; Chaudhuri et al., 2013), the forcing fields are included in the assimilation process (see Sect. 2.3). The errors of the initial ocean state and the initial forcing are estimated consistently together. The first year (2003) of the reference simulation (sea surface height, temperature, salinity and velocity) is extended by the respective ERA-Interim forcings (freshwater-flux and wind-stress). The variables are detrended grid point wise. At every grid point a sinusoidal curve of annual period is fitted to the model/forcing fields and subtracted. Afterwards, the temporal covariance matrix for the year 2003 is calculated representing the non-seasonal variability. From this initial year's covariance matrix, the initial assimilation simulation ensemble and the initial EnKF-ADD ensemble is sampled (see Sect. 2.3 and Saynisch and Thomas, 2011). For freshwater-flux and wind-stress, the calculated variances, i.e., the diagonal entries of

the error covariance matrix are plotted in Fig. 3. The highest non seasonal wind-stress variances are located in the westerlies at latitudes above 50° . For the freshwater-flux, the pattern is more complex. High variances are found below 50° of latitude peaking in the thirties and the intertropical convergence zone. Note that, the covariances, i.e., the non-diagonal entries (not plotted), are also used to generate the initial EnKF-ADD ensemble.

3. Results and Discussion

3.1. Comparisons with assimilated satellite data

The time frame of the experiment is from January 2003 till August 2009. In a first evaluation, we estimate the quality of the model simulations by the relative explained variance (REV, e.g., Storch and Zwiers, 1999):

$$REV = \frac{\text{var}(x_{obs}(t)) - \text{var}(x_{obs}(t) - x_{model}(t))}{\text{var}(x_{obs}(t))},$$

where x_{obs} and x_{model} are the GRACE-based and the modelled ocean bottom pressure time series. Note that, positive values indicate reasonable explanatory power of the model with respect to the observations. Negative values indicate a failure of the model to explain the observations. In the upper panel of Fig. 4 the relative explained variance of the reference simulation is plotted. High discrepancies can be seen, e.g., in the Antarctic region, the East Pacific Rise, the Hudson Bay and the regions around Alaska. Apart from these peak values, large parts of the model ocean show a variance of the model-to-observation misfit which is at least as large as the variance of the observed signal itself. In the coastal regions, the misfits can be assigned to river discharge, glacial processes (e.g., Cazenave and Chen, 2010) and the respective land leakage (esp., Amazonas, Patagonia and Alaska). In shallow regions and regions of complex topography, the misfits originate in insufficient resolution of the ocean model (esp., Indonesia). The remaining misfits must be attributed to unrealistic model behavior. Nonetheless, a reasonable agreement can be seen in the Indian Ocean.

The assimilation of ITG-GRACE data results in a better agreement between modelled and observed mass distributions. In the middle panel of Fig. 4, the respective comparison of the assimilation simulation with the observation is plotted. The gain of relative explained variance in the assimilation simulation with respect to the reference simulation is plotted in the lower panel of Fig. 4. The large discrepancies in the Pacific Ocean and in the Southern Ocean are strongly reduced. The global mean of the explained variance rises by approximately 15 hPa^2 . For comparison, on timescales shorter than 60 days the ocean bottom pressure variances have a global mean of 4 hPa^2 but can reach up to 40 hPa^2 in the high latitudes (Quinn and Ponte, 2011). The global mean correlation between modelled and observed ocean bottom pressure increases from 0.15 in the reference simulation to 0.36 in the assimilation simulation. The increased agreement becomes most evident in the Pacific and in the North Atlantic. Parts of the central Atlantic show only a moderate explained variance or a slight worsening compared with the reference simulation. These are regions where the estimated observation errors are higher (compare lower panel of Fig. 4 with the upper panel of Fig. 2) than the cross-ensemble variance of the ocean model ensemble. This hints either to missing variability in the ocean model, including the EnKF-ADD fields, or to inconsistencies in the observation data, i.e., the observed ocean pressure is not entirely of oceanic origin in these regions. The leakage induced misfits (see e.g., Alaska

in the middle panel) remain because these regions are masked out of the assimilation process (compare Sect. 2.4).

In an assimilation experiment without the EnKF-ADD formalism, i.e., without changing the forcing, the Kalman-Filter success is poor (not shown). We conclude that the increase of explained variance in the assimilation simulation is to the larger part achieved by the EnKF-ADD fields. The temporal mean and the standard deviation of the EnKF-ADD fields are shown in Figs. 5 and 6. The standard deviation fields have the same order of magnitude, but half the size of the respective mean fields. The existence of a non-zero mean in the EnKF-ADD fields hints to an unrealistic bias in the ECMWF forcing fields. Not surprisingly, the mean patterns resemble the estimated initial error covariances (see Fig. 3). Nonetheless, the EnKF-ADD contributions change significantly in shape and strength over the time of the assimilation period, as can be seen by the variance patterns. To study the connection between EnKF-ADD fields and the assimilation's impact on ocean bottom pressure, the correlations of EnKF-ADD fields with ocean bottom pressure differences, between reference and assimilation simulation, are calculated. In Fig. 7 the correlations are plotted for the EnKF-ADD wind-stress fields. The colors show the correlation between the Kalman-Filter impact and the absolute value of the altered wind-stress. The arrows indicate a direction of the correlation. The meridional (zonal) component of the arrows is the correlation between ocean bottom pressure and meridional (zonal) wind-stress. The plot indicates that the bottom pressure changes which reduced the model-to-observation misfits in the assimilation simulation are generated by altered wind-stress. The change in wind-stress leads to changes in sea surface and thermocline height. On short time scales of up to 30 days in deep ocean regions and of up to 100 days in shallow regions, surficial changes in mass distribution are equivalent to ocean bottom pressure changes (Vinogradova et al., 2007; Bingham and Hughes, 2008; Quinn and Ponte, 2012). Considering the McCullagh formula by which Polar Motion excitations and GRACE coefficients of degree 2 and order 1 are equivalent, our findings are in agreement with Saynisch et al. (2011a), wherein the authors conclude that the mass distribution signals contained in oceanic Polar Motion observations are also generated by barotropic responses to atmospheric momentum forcing. We conclude that most of the Kalman-Filter impact on the modelled ocean bottom pressure distribution is due to a barotropic reaction to the wind-stress forcing.

In the bottom of Fig. 2, the RMS of the observation error covariances, i.e., the non-diagonal entries, that are derived from the JPL-GFZ misfits are plotted for every grid point. This plot demonstrates the contributions to the assimilation that arise from the non-diagonal entries of the observation error covariance matrix. To study the influence of the observation error covariances, the assimilation of the daily ITG-GRACE data is repeated by using only the diagonal entries of the observation error covariance matrix estimated by the JPL-GFZ differences (see Sect. 2.4). The resulting relative explained variances increase substantially and are depicted in Fig. 8 (compare with middle panel of Fig. 4). In contrast to the original ITG-GRACE assimilation, which uses the full error covariance, the observed mass anomalies of the whole Atlantic and the ACC are much closer reproduced in the diagonal-only assimilation. Only the Arctic region shows no increased reproduction compared with the reference simulation. We conclude that the spatial correlations between the observation errors are the limiting factor for the assimilation of ocean bottom pressure observations.

It is well worth noting, that the presented Kalman-Filter approach does not reproduce the stripes contained in the ITG-GRACE observations. This is partly because the SEIK-Filter does not invert the observation operator explicitly during the analysis step.

To get the analysis-increment from the observations the SEIK-Filter uses a recombination of the forecast-members. Therefore, the stripes are not reproduced because they are not in the span of the leading eigenvectors of the ocean model's cross-ensemble variance. Or stated otherwise, the cross-ensemble variance, i.e., the ocean model error, is small in these regions compared with the estimated observation errors (see Fig. 2, top).

Because in general the destriping of the GRACE solutions is based on time-invariant statistic assumptions, it would be interesting to develop an approach that is more dynamic and contains more physical information by incorporating an ocean model. Therefore, we study how much information our assimilation set-up can extract from stripe contaminated observations. Since there is no respective version of ITG-GRACE available, a version of the GFZ solution which still contains stripes (GFZ-GRACE) is used instead. The only difference in the GFZ-GRACE processing to the one described in Sect. 2.4 is that the destriping step is not applied. For better comparability with the ITG-GRACE assimilation, the monthly GFZ-GRACE solutions (destriped and non-destriped) are interpolated to daily values using a spline approach. Since the unprocessed stripes are at least three orders of magnitude larger than the previously assimilated ocean bottom pressure signal, these three orders of magnitude must be considered as observation error and the error budget has to be adapted accordingly. A matrix with entries of $1 \times 10^3 m^2$ on the diagonal and zero elsewhere is used as observation error matrix. This number is an upper bound to typical GRACE errors of 1-3 cm (Quinn and Ponte, 2008) that are increased by the three orders of magnitude which distinct typical ocean bottom pressure signals from the artificial stripes: $1 \times 10^3 m^2 > (0.03m \times 10^3)^2$. Note that, this experiment was run over the period of one year (2004) only. In the resulting GFZ-GRACE assimilation, no stripes are reproduced (not shown). The success of the GFZ-GRACE stripe assimilation is evaluated against the fully processed, i.e., destriped GRACE observations from GFZ. The relative explained variances are depicted in Fig. 9. The model-to-observation agreements grow globally in the GFZ-GRACE assimilation compared with the reference simulation. The GFZ-GRACE assimilation shows pronounced agreements throughout the whole Southern Ocean and the gain in explained variance reaches up to 80 hPa² in the Southeast-Pacific Basin. The agreements are remarkable and the method can be ranked among the already existing destriping mechanisms mentioned in Sect. 1.

3.2. Comparisons with independent ocean bottom pressure recorders

To further quantify the quality of the GRACE assimilations, we compare the model output with independent, i.e., not assimilated, observations. For this comparison, data sets of in situ ocean bottom pressure recorders are used. The data was recorded by Pressure Inverted Echo Sounders (PIES) and is provided by Macrandar et al. (2010). The recordings are quality controlled, i.e., outliers are eliminated and drifts are reduced by a quadratic fit. Tides are removed by means of the FES2004 tide model (Lyard et al., 2006). To mimic the removal of the global mean ocean bottom pressure in the Kalman-Filter, the comparisons with the ocean model simulations take only signals of 100 days and shorter into account, i.e., trends, annual and semi-annual signals are not contained in the recorder data and are, therefore, not part of the comparisons. It is important to point out that PIES recorders are not evenly distributed over the ocean (Fig. 10, top panel). Furthermore, the PIES are mostly located close to coasts or in places with complicated topographic or dynamic characteristic, e.g., in deep-sea trenches, the Fram Strait or the Drake Passage. In addition, PIES measurements are point-measurements,

but ocean model grid points represent up to ten thousand square kilometers. The RMS-differences between 100 day highpass-filtered model simulations (respectively assimilations) and the 100 day highpass-filtered in situ recorders are displayed in Fig. 10. The corresponding numbers are given in Tab. 1. The global decrease in RMS-difference due to assimilation is 0.2 hPa. The regional contributions to this value are very different. In the Pacific region the RMS-differences between ITG-GRACE assimilation and PIES do not change compared with the reference simulation. One problem is that most of the PIES are located close to the coast where the GRACE-observations are influenced by continental leakage and the assimilation is switched off (see Sect. 2.4). A second problem is that many PIES are located near islands or ridges that are not resolved in the ocean model. Furthermore, some PIES time series are not very well reproduced by the satellite GRACE observations. In Fig. 11, the time series of a PIES located in the equatorial Pacific is plotted. This particular PIES is not close to the coast, but is situated in a shallow region with complicated bathymetry and dynamic. It can be seen that ITG-GRACE data itself has little resemblance to the PIES observation. Consequently, the assimilation fails to reproduce the recorder data. In general, ocean models and satellite observations show insufficient sub-monthly variability in this equatorial region (compare also with Fig. 2 of Bonin and Chambers, 2011). In the Indian and Atlantic region, there is a slight decrease of the model-to-observation misfits of up to 0.1 hPa in the mean. In the high-latitude regions, there is a pronounced RMS-decrease of up to 1.9 hPa, i.e., a decrease of 35 % (see, e.g., PIES #7, #21). The mean RMS of the regions decrease from 4.1 hPa to 3.7 hPa in the Arctic and from 3.7 hPa to 3.3 hPa in the Southern Ocean. This pronounced impact on polar latitudes agrees with the findings of Köhl et al. (2012) and extends them to higher frequencies. In Fig. 12, the PIES #21 from the ACC region is plotted and both, ITG-GRACE and assimilation reproduce the recorder data very well. In most cases, the agreement between diagonal-only assimilation and PIES is better than between the original ITG-GRACE assimilation and PIES. In some cases, this relation is inverted. Here, overfitting occurs (e.g., PIES #45, #48). These PIES are located close to the North-American west coast where the original ITG-GRACE assimilation ignores the observations (see middle panel of Fig. 4). In contrast to this, the diagonal-only assimilation reproduces the ITG GRACE observations (see Fig. 8). The worse fit of the diagonal-only assimilation to PIES in this region hints to coastal-leakage artifacts in the ITG-GRACE data. We conclude, to avoid overfitting it is important to consider the covariances of the observation errors in the assimilation process.

In the case of the assimilation of non-destriped GFZ-GRACE data, the same global dependencies can be seen (Fig. 13, turquoise squares, see also Table 1). Note that, this experiment has a short time window of one year (2004) and the depicted RMS cover only this period. Furthermore, not all PIES have a reasonable overlap with that period. Most of the remaining model-to-PIES RMS reduce by assimilating the heavily striped GFZ-GRACE observations. The global mean RMS reduction amounts to 0.5 hPa. At least in this short experiment, the level of agreement to the PIES data is comparable but slightly (0.1 hPa) better than in the original ITG-GRACE assimilation (blue/white squares) and comparable but slightly (0.05 hPa) worse than in the diagonal-only ITG-GRACE assimilation (green squares). The better agreement of the diagonal-only ITG-GRACE assimilation is most pronounced in the Arctic Ocean (up to 0.6 hPa) where high-frequency signals play an important role (Quinn and Ponte, 2012, see also Fig. 12). Nonetheless, the benefit from the assimilation of monthly non-destriped data is remarkable. Given the very noisy observation data and the crude observation error approximation used in this particular experiment, the results show how robust

the presented EnKF formalism performs if a reasonable ocean model ensemble can be constructed.

4. Summary

Daily and monthly gravity field observations from the GRACE satellite mission are processed to derive ocean bottom pressure anomalies. These observations are assimilated with a dynamic global ocean circulation model. The daily observations are assimilated for the period 2003 to 2009. The monthly data is assimilated for the year 2004. The assimilation method is an ensemble based Kalman-Filter that operates on a small, but optimal subspace of the model's state space. Variances and covariances of the initial model state errors are estimated and incorporated into the filter. To consider errors in the atmospheric forcing, i.e., wind-stress and freshwater-flux, the Kalman-Filter is extended to employ an ensemble of individual forcings. Variances and covariances of the GRACE observation errors are estimated. The assimilation experiments are calculated with and without use of the observation error covariance information.

Compared with a reference simulation, the assimilation of GRACE data leads to increased agreement between modelled ocean bottom pressure fields and the ocean bottom pressure fields observed by GRACE. The global mean correlation rises from 0.15 to 0.36. The physical explanation for the higher correlations are found in wind-stress changes which are generated by the assimilation of GRACE data. These changes generate barotropic signals which influence the ocean bottom pressure fields.

Apart from reproducing the GRACE observations, the presented Kalman-Filter approach shows great potential in reducing the artificial stripes that contaminate GRACE observations. The assimilation of non-destriped GRACE data shows similar results as the assimilation of destriped GRACE data. The reason is the EnKF's rejection of features that lay outside the leading eigenvectors of the model's cross-ensemble variance. This is an advantage over other, e.g., adjoint, assimilation methods.

In addition, the assimilation simulations show increased agreement to independent, i.e., not assimilated observations from in situ ocean bottom pressure recorders. In our assimilation, RMS-differences reduce by up to 35 %. The improvements are most pronounced in the high latitudes. In the comparison with bottom pressure recorders, the assimilation of daily ITG solutions leads to slightly better results than the assimilation of monthly GRACE data. The reproduction of satellite and in situ ocean mass observations is limited by the observation error budget and especially, by the error's correlations. Assimilation experiments under the assumption of uncorrelated observation errors show substantially increased agreement to the assimilated satellite observations and moderate increased agreement to the independent in situ observations. The comparison to the bottom pressure recorders shows that the information contained in the observation error correlations can prevent the assimilation from overfitting.

Since in fact the GRACE observation errors are correlated and good destriping algorithms already exist, these benchmark experiments could be considered dispensable but they demonstrate the power and robustness of the applied filter technique when a reasonable model is constructed. Furthermore, the experiments show what information can be extracted from the observations if future satellite missions or coming processing techniques could decrease the observation's errors and especially their correlations. The presented assimilation framework will be improved in future studies by a dynamical approach to the error budget of the forcings and the observations. Furthermore, until the observation and processing errors become smaller, the application of localized error budgets should be considered.

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Figure 1: Schematic of this study's ensemble based Kalman-Filter configuration and time stepping.

Figure 2: Estimated error budget of the assimilated GRACE observations. Variances of the JPL-GFZ misfit (top). RMS-values of the covariances, i.e., the nondiagonal entries of the observation error covariance matrix (bottom).

Figure 3: Estimated initial error variances of the EnKF-ADD fields, i.e., the initial EnKF-ADD cross-ensemble variances. Zonal wind-stress (top), meridional wind-stress (middle) and freshwater flux (bottom).

Figure 4: Relative explained variance of the observed ITG-GRACE mass distribution as explained by the reference simulation (top), as explained by the assimilation simulation (ensemble mean, middle) and the differences, i.e., the gain in relative explained variance by the assimilation simulation (bottom). The thin black line is the zero contour line.

Figure 5: Temporal mean of the forcing corrections estimated by the Kalman-Filter. Zonal (top) and meridional (middle) EnKF-ADD wind-stress and the EnKF-ADD surface freshwater flux (bottom). The plots show ensemble means.

Figure 6: Temporal standard deviations of the forcing corrections estimated by the Kalman-Filter. Zonal (top) and meridional (middle) EnKF-ADD wind-stress and the EnKF-ADD surface freshwater flux (bottom). The plots show ensemble means.

Figure 7: Color: Correlation between EnKF induced changes in absolute wind-stress (EnKF-ADD) and EnKF induced ocean bottom pressure changes. Zonal (meridional) vector components: Correlation between EnKF induced ocean bottom pressure changes and changes in the zonal (meridional) wind-stress components. Examples for full positive ($=1$) correlation are plotted in the legend. Only vectors with absolute values corresponding to correlations of 0.8 or greater are plotted. Note: The covariance of ocean bottom pressure with the Euclidean norm of the wind-stress is smaller (or equal) than the Euclidean norm of the respective single covariances. Therefore, arrows appear also in regions where the colors indicate correlation values below 0.8.

Figure 8: Same as middle panel of Fig. 4, except for the diagonal-only assimilation. Relative explained variance of the observed ITG-GRACE mass distribution as explained by the diagonal-only assimilation (ensemble mean) where only the diagonal entries of the observation error covariance matrix are considered. The thin black line is the zero contour line.

Figure 9: Same as Fig. 4, except for the assimilation of non-destriped GFZ-GRACE data. Relative explained variance of the destriped GFZ-GRACE mass distribution as explained by the reference simulation (top), as explained by the assimilation simulation (ensemble mean, middle) and the differences, i.e., the gain in relative explained variance by the assimilation simulation (bottom). The thin black line is the zero contour line.

Figure 10: Geographical location of the utilized Pressure Inverted Echo Sounders (PIES, top) and RMS-differences for 2003-2009 between modelled ocean bottom pressure and in situ recordings by PIES (bottom). RMS-differences between PIES and reference simulation (red), between PIES and assimilation simulation (ensemble mean, blue/white) and between PIES and diagonal-only assimilation simulation (ensemble mean, green).

Figure 11: Ocean bottom pressure anomalies. In situ data from PIES #27 (DART 52403, equatorial Pacific, black). Reference simulation (red). Diagonal-only assimilation simulation (ensemble mean, green). ITG-GRACE observations (gold).

Figure 12: Ocean bottom pressure anomalies. In situ data from PIES #21 (AWI ANT13a, Southern Ocean, black). Reference simulation (red). Diagonal-only assimilation simulation (ensemble mean, green). ITG-GRACE observations (gold).

Figure 13: RMS-differences for 2004 between modelled ocean bottom pressure and in situ recordings by PIES, between PIES and reference simulation (red), between PIES and assimilation simulation (ensemble mean, blue/white), between PIES and diagonal-only assimilation simulation (ensemble mean, green) and between PIES and assimilation of non-distorted GRACE data (ensemble mean, turquoise). For the geographical location of the PIES see Fig. 10.

	Station No.	Data corresponding to 2003-2009 (Fig. 10)			Data corresponding to 2004 (Fig. 13)			
		ref	assim	diag-only	ref	assim	diag-only	GFZ-assim
Arctic Ocean	1	4.24	4.25	3.78	5.37	5.06	4.41	4.73
	2	3.92	3.91	3.20	4.80	4.35	3.82	4.38
	3	3.64	3.64	2.87	-	-	-	-
	4	4.10	4.05	4.03	-	-	-	-
	5	4.66	4.61	4.62	-	-	-	-
	mean	4.11	4.09	3.70	5.09	4.70	4.12	4.56
Southern Ocean	6	4.32	4.15	3.51	5.40	5.06	3.75	3.60
	7	5.28	4.94	3.61	-	-	-	-
	8	3.16	3.02	2.79	-	-	-	-
	9	3.66	3.56	2.73	-	-	-	-
	10	2.92	2.84	2.43	-	-	-	-
	11	2.77	2.70	2.36	3.51	2.98	2.36	2.92
	12	3.34	3.32	3.26	-	-	-	-
	13	7.25	7.23	7.29	-	-	-	-
	14	2.80	2.78	2.58	4.25	3.38	3.04	3.01
	15	2.51	2.52	2.47	3.65	2.65	2.46	2.56
	16	2.27	2.16	1.93	-	-	-	-
	17	3.18	3.18	3.20	3.78	3.68	3.79	3.62
	18	3.01	2.98	2.98	3.87	3.23	3.35	3.14
	19	4.12	4.10	4.13	5.13	4.17	4.26	4.14
	20	3.39	3.35	3.41	3.78	3.42	3.41	3.37
	21	5.40	4.12	3.51	-	-	-	-
	mean	3.71	3.56	3.26	4.17	3.57	3.30	3.30
Ind. O.	22	2.21	2.22	2.10	-	-	-	-
Pacific Ocean	23	1.71	1.73	1.75	-	-	-	-
	24	1.78	1.77	1.74	-	-	-	-
	25	1.88	1.94	1.90	1.63	1.81	1.78	1.75
	26	1.43	1.44	1.44	1.55	1.42	1.45	1.36
	27	1.85	1.84	1.86	-	-	-	-
	28	3.77	3.79	3.77	2.53	2.36	2.21	2.31
	29	3.16	3.17	3.29	3.27	3.49	3.59	3.51
	30	3.74	3.76	3.82	-	-	-	-
	31	2.07	2.03	2.03	-	-	-	-
	32	1.70	1.69	1.77	-	-	-	-
	33	1.57	1.59	1.62	-	-	-	-
	34	2.18	2.20	2.19	-	-	-	-
	35	2.04	2.05	1.94	-	-	-	-
	36	1.60	1.62	1.61	-	-	-	-
	37	3.34	3.36	3.17	-	-	-	-
	38	3.38	3.37	3.55	-	-	-	-
	39	1.81	1.80	1.86	-	-	-	-
	40	2.94	2.99	2.87	-	-	-	-
	41	1.90	1.80	1.88	-	-	-	-
	42	3.73	3.75	3.75	4.42	3.85	3.81	3.82
	43	3.56	3.59	3.63	4.38	3.84	3.72	3.87
	44	1.84	1.81	1.78	-	-	-	-
	45	1.51	1.51	1.72	2.02	1.99	1.95	1.75
	46	2.72	2.70	2.86	-	-	-	-
	47	4.25	4.24	4.19	-	-	-	-
	48	2.58	2.58	2.74	-	-	-	-
	49	3.52	3.53	3.58	-	-	-	-
	50	1.33	1.33	1.47	-	-	-	-
	51	2.71	2.72	2.72	-	-	-	-
	52	1.56	1.54	1.51	-	-	-	-
	53	1.40	1.41	1.43	-	-	-	-
	mean	2.40	2.41	2.43	2.81	2.68	2.64	2.63
Atlantic Ocean	54	1.94	1.93	1.87	-	-	-	-
	55	4.62	4.67	4.16	-	-	-	-
	56	4.82	4.84	4.81	-	-	-	-
	57	4.46	4.49	4.44	-	-	-	-
	58	2.46	2.44	2.41	-	-	-	-
	59	1.88	1.86	1.92	-	-	-	-
	60	2.39	2.38	2.35	2.55	2.10	1.95	2.05
	61	1.98	1.96	1.88	2.48	2.05	1.97	2.09
	62	2.11	2.08	2.00	2.44	2.11	2.09	2.14
	63	5.46	5.45	5.46	-	-	-	-
	mean	3.21	3.21	3.13	2.49	2.06	2.00	2.09
global	mean	3.00	2.96	2.85	3.54	3.15	2.96	3.01

Table 1: RMS-differences [hPa] between modelled ocean bottom pressure and in situ recordings by PIES.