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Mitigating temporal aliasing effects of high-frequency geophysical fluid dynamics in satellite gravimetry

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SUMMARY

Temporal aliasing errors induced by high-frequency tidal and non-tidal mass variability in the Earth system are among the three most important error sources that limit the accuracy of present-day surface mass estimates from satellite gravimetry. By means of end-to-end simulations, we demonstrate that the Kalman Smoother approach developed by Kurtenbach *et al.* effectively captures non-tidal submonthly variability, and thereby reduces temporal aliasing errors way beyond the level of simply subtracting the standard dealiasing model AOD1B. Validation against *in situ* ocean bottom pressure observations confirms that the Kalman Smoother solutions published together with the ITSG-Grace2016 monthly gravity fields contain high-frequency signal over the oceans not predicted by AOD1B. The daily gravity fields therefore reduce aliasing artefacts in the monthly gravity fields, and at the same time provide observational evidence on submonthly bottom pressure variability presently not reflected in state-of-the-art numerical ocean circulation models. It is thus recommended to include a Kalman Smoother approach into any standard GRACE processing scheme. For a hypothetical double-pair configuration currently under consideration as a future mass change mission, we find that the benefit of the Kalman Smoother is much smaller thanks to the increased number of observations taken at different inclinations, which lead to generally reduced aliasing errors and much more isotropic spatial error correlations. We also reassess the idea of pre-eliminating low-resolution daily gravity fields and find large distortions in the monthly mean gravity solution at spatial wavelengths around the cut-off-degree of the daily fields. We thus recommend further study for any satellite gravity mission concept that critically relies on such pre-elimination schemes for reaching its science objectives.

Key words: Fluid dynamics; Gravity anomalies; Satellite geodesy.

1 INTRODUCTION

Satellite gravimetry as realized with the GRACE (2002–2017; Tapley *et al.* 2019) and GRACE-FO (since 22 May 2018) missions provides unique remote sensing information on barystatic sea level variations (Reager *et al.* 2016), the mass balance of the continental ice sheets (Shepherd *et al.* 2012), and the long-term changes in global groundwater resources (Famiglietti 2014). For both missions, two spacecrafts are trailing each other in a nearly polar and circular orbit at altitudes of about 500 km, whose relative positions are precisely measured by a microwave ranging system operating in the k and ka bands. Together with auxiliary sensor data from, for example, accelerometers, star cameras and GNSS receivers, a global estimate of the Earth's gravity field is routinely calculated from just 30 d of observations. Scientific data collected during the course of both missions now allow the processing of more than 170

independent monthly gravity fields from the year 2002 until the present day.

Even after 15 yr of experience in analysing GRACE sensor data, the accuracy of those monthly gravity fields is still above the instrument error baseline predicted prior to the launch of the first mission (Kim 2000). Present-day numerical end-to-end simulations for the performance of GRACE-like gravity missions indicate that temporal aliasing errors due to high-frequency mass variability in the Earth system are among the top three error sources, together with ocean tides and accelerometer noise (Flechtner *et al.* 2016). It is important to note that whereas instrument accuracies cannot be changed after launching a satellite, the quality of background models can be improved even after the end of a mission, thereby opening opportunities to ameliorate the gravity fields from the GRACE period via reprocessing of the archived sensor data. In addition, refined analysis approaches might be considered that explicitly make use

of the latest knowledge about uncertainties in the geophysical background models applied during the gravity field estimation process. This includes not only deterministic signals, but also stochastic information about high-frequency mass variability in the Earth's geophysical fluid layers.

Signals that cannot be reconstructed directly from a time-series with 30 d sampling would cause temporal aliasing artefacts in any monthly mean solution as long as they are not accounted for. In the past, four different approaches have been developed to treat periodic and non-periodic variability at periods shorter than 60 d in the GRACE gravity field processing:

(i) Applying *a priori* background models from independent sources is the classical approach followed by numerous geodetic techniques. Background models based on observations and/or numerical models are implicitly assumed to be error-free and are thus subtracted from the observation vector. Prominent examples are the subdaily tide model applied in the estimation of daily Earth orientation parameters (Petit & Luzum 2010), or the Atmosphere and Ocean Non-Tidal De-aliasing Level-1B (AOD1B) product (Dobslaw *et al.* 2017) used for the removal of high-frequency non-tidal atmospheric and oceanic variability in both gravity field processing and precise orbit determination (Rudenko *et al.* 2017).

(ii) Co-estimation of variability at specified frequencies is possible as soon as a multiyear data record becomes available. For any orbital period, signals from a certain tidal constituent alias into a particular long-period variation where the exact frequency of the aliased signal depends on both the tidal frequency and the revisit time of the sensor. As long as alias frequencies are sufficiently well separated from each other and from otherwise distinct periodicities of geophysical variability, the original tidal signal can be unambiguously reconstructed. For example, the orbit of TOPEX/Poseidon has been specifically tailored to estimate ocean tides via that approach, and early attempts based on GRACE data were successful as well for a number of individual frequencies (Bosch *et al.* 2009; Mayer-Gürr *et al.* 2012). The co-estimation of tides is also believed to be a promising concept for gravity missions of the next generation (Hauk & Pail 2018).

(iii) The non-tidal mass redistribution on Earth varies smoothly in time, and it is fair to assume that global gravity fields of two subsequent days are thus correlated to a large extent. Those correlations can be mathematically modelled by means of a first-order Markov process, so that information from adjacent days stabilizes the solution for subsequent epochs. This approach has been introduced by Kurtenbach *et al.* (2009) and has been later extended to consider correlations forward and backward in time via a Kalman Smoother (Kurtenbach *et al.* 2012). Setting-up such constrained daily parameters in the estimation of a monthly solution is expected to reduce temporal aliasing since the high frequency signal is absorbed by the extended parameter space. The ITSG-Grace2016 series does not only provide monthly mean gravity fields, but also a series of daily snapshots obtained with this method (Mayer-Gürr *et al.* 2016).

(iv) High-frequency signals in satellite gravimetry might be also tackled with daily pre-elimination of low-resolution gravity fields. In the case of a single-pair mission as GRACE, observations from 24 hr only allow to solve for a very limited set of gravity field parameters, which would thus not provide spatial details. For the hypothetical case of two pairs of satellites flying in different orbits, however, numerical simulations suggest that the amount of data collected during a single day is sufficient to solve for the characteristic low-resolution features of the time-variable gravity field independently from day-to-day (Wiese *et al.* 2011). This approach could

Table 1. Specification of mission configurations and gravity field parameter estimation approaches considered in numerical closed-loop simulation experiments.

G	Single-pair mission with GRACE-like instrument errors
GK	G plus co-estimation of daily Kalman Smoother fields
B	G plus a second satellite pair at 70° inclination
BK	B plus co-estimation of daily Kalman Smoother fields
BW	B plus daily parameter elimination of low degrees

thus compensate for any errors in the non-tidal dealiasing models at large spatial scales and would eventually make such *a priori* models entirely dispensable (Daras & Pail 2017).

In this paper, we will reassess the presently available analysis methods for the treatment of non-tidal submonthly mass variability signals in the processing of time-variable global gravity fields. We will first report results from end-to-end simulations of the GRACE mission performance intended to reevaluate the relative importance of different error sources and the impact of a Kalman Smoother scheme on mitigating temporal aliasing (Section 2). By means of validation against *in situ* ocean bottom pressure, we will then demonstrate that the daily Kalman Smoother results published with ITSG-Grace2016 indeed contain submonthly signal over the oceans not known *a priori* from AOD1B (Section 3). The paper closes with an assessment of different processing approaches to minimize temporal aliasing for a future double-pair configuration (Section 4), and a brief summary of our findings (Section 5).

2 NUMERICAL PERFORMANCE SIMULATIONS FOR THE GRACE MISSION

The basis of our study on the impact of temporal aliasing in satellite gravimetry are closed-loop simulations, since only a numerical simulation environment allows for the unambiguous separation of individual contributions to the overall error budget of a satellite mission in a controlled way. We will, however, closely relate our simulation results to the real GRACE data analysis as applied for processing the ITSG-Grace2016 gravity field solutions. We consider in total five simulation settings with different mission characteristics and processing choices (Table 1). Throughout all simulations, we use k-band range-rate observations between the satellites with a precision of $2.8 \mu\text{m s}^{-1}$ at 10 Hz, star camera assembly white noise with 0.1 mrad, and precise orbit determination uncertainties with white noise at 3 cm per axis with 300 s sampling. We further assume accelerometer errors with $\sqrt{1 + 0.005f} \cdot 10^{-10} \text{m s}^{-2}/\sqrt{\text{Hz}}$ in along-track and radial direction, and with $\sqrt{1 + 0.1f} \cdot 10^{-9} \text{m s}^{-2}/\sqrt{\text{Hz}}$ in cross-track direction. All simulations cover 30 d and lead to a single monthly mean gravity field.

We start with a conventional GRACE mission configuration (labelled with G in the following). Integrated orbits are fitted to real GRACE orbits from January 2006 on a daily basis so that deviations do not exceed 40 m. Attitude is directly taken from the GRACE star camera data, and antenna phase centre variations are treated in the same way as in the ITSG-Grace2016 processing. Non-gravitational forcings as solar radiation pressure, albedo and drag are also configured as in ITSG-Grace2016. Normal equations are accumulated over the whole simulation period and solved for spherical harmonics of the gravity potential from degree 2 until degree and order 120. Alternatively, we use the same set of noisy observations, but additionally model residual submonthly variations in the time-variable

gravity field by means of a Kalman Smoother (GK). Here we exploit the fact that the Kalman smoother can be formulated as a least squares adjustment, to which additional parameters can be easily introduced, such as the monthly spherical harmonic coefficients.

As a possible contribution to the design of a future gravity mission, we consider a constellation of two satellite pairs operating in differently inclined orbits (B) as initially proposed by Bender *et al.* (2008). The polar pair is identical to the GRACE-like mission described above, whereas the second pair orbits with an inclination of 70° at an average height of 429 km with an initial satellite separation of 120 km. This mission layout has been identified before as a very promising setting based on a vast number of different simulation experiments (Panet *et al.* 2013; Gruber *et al.* 2014). For this double-pair configuration, we also attempt to model the residual sub-monthly variability with a Kalman Smoother (BK). Alternatively, we consider pre-elimination of daily low-degree coefficients (BW). Pre-elimination of daily parameters introduces daily gravity field parameters into the monthly gravity field recovery. Monthly and daily parameters are linearly dependent, which means that gravity field signal can be freely shifted between these parameter groups. The result is a rank deficiency, which entails that the adjustment problem has no unique solution. The daily pre-elimination approach uses a two-step estimation scheme to avoid this rank deficiency, but this neglects correlations between daily and parts of the monthly gravity field parameters. On the other hand, while the approach in the ITSG-Grace2016 processing is similar, all correlations are taken into account, that is all parameters are estimated together in a single least squares adjustment, and the rank deficiency is resolved by the introduction of a constraint, which is designed to prevent monthly gravity field signal to be absorbed by the daily solutions. Results for the double-pair mission will be presented in Section 4.

For each of those five settings, we apply three different sets of errors in the background models for gravitational forces (Table 2). We consider static gravity field errors (S) by replacing GOCO05s (Mayer-Gürr 2015) with EGM96 (Lemoine *et al.* 1998). Synthetic high-resolution time-variable gravity field changes are taken from the updated Earth System Model from the European Space Agency (ESA-ESM; Dobsław *et al.* 2015). The non-tidal time-variable synthetic gravity from ESA-ESM is frequently denoted AOHIS because it includes mass variability in the atmosphere (A), oceans (O), terrestrial hydrosphere (H), continental ice sheets and mountain glaciers (I) as well as solid Earth deformations (S). In ESA-ESM AOHIS coefficients the oceanic part from OMCT is replaced by the MPIOM STORM experiment (von Storch *et al.* 2012) for degrees and orders above 60 to also include meso-scale ocean circulation processes that are not well represented in OMCT. For the retrieval step, we assume realistically perturbed *a priori* knowledge about the large-scale atmospheric and oceanic (AO) mass variability by means of the so-called DEAL coefficients from ESA-ESM, which do not include the meso-scale variability from MPIOM STORM. In other words, DEAL represents a standard OMCT-like ocean model that does not simulate mesoscale variability coming from MPIOM STORM. They are moreover augmented with the random error component AOerr that represents the spread between present-day state-of-the-art ocean and atmosphere models as described in detail by Dobsław *et al.* (2016). The effects of ocean tides (T) are considered from the differences between FES2014b (Carrere *et al.* 2015) and EOT11a (Savcenko & Bosch 2012) for all tidal constituents applied in the ITSG-Grace2016 data processing.

The retrieved global gravity fields from the simulations are subtracted from the synthetic time-variable gravity model ESA-ESM to

get true errors, which can be either expressed in terms of power spectral densities (PSD) of the range-rate residuals or in terms of degree variances (Fig. 1). For the GRACE simulation that only considers errors in the static gravity field (G-S), we note an almost perfect resemblance with the so-called GRACE baseline errors published well before the launch of the mission by Kim (2000). Moreover, the uncertainty estimates derived from a variance component estimation are very well aligned to the true errors introduced into the closed-loop simulation, thereby confirming the reliability of the ITSG-Grace2016 error estimation approach. When additionally considering errors in non-tidal atmosphere and ocean mass variability and oceanic tides (G-SAOT), true errors increase substantially and align very well to the errors estimated for the actual GRACE monthly solution for January 2006 as published in ITSG-Grace2016, indicating that our error assumptions introduced into the simulations are indeed very well justified.

When errors from the ocean tide model are excluded (G-SAO), we note a reduction of errors with respect to ITSG-Grace2016 in particular at the lowest degrees for both true and estimated errors (Fig. 2). When additionally estimating daily Kalman Smoother fields (GK-SAO), errors are consistently reduced for all degrees larger than 20, indicating that substantial medium-scale variability is taken up by the Kalman solution. This effect is also seen in the PSD of the k-band range-rates, that drops in particular at periods between 1 and 30 min, which corresponds to frequencies of 16 and 0.6 mHz, respectively. Note that in ITSG-Grace2016 constrained daily gravity field solutions are co-estimated with the monthly solution to mitigate temporal aliasing effects, but ocean tide model errors in the diurnal and semi-diurnal frequency band cannot be captured with daily sampling. Considering the magnitude of these errors, the error characteristics of ITSG-Grace2016 are closer to a G-SAOT scenario than to any of the GK scenarios. We conclude from those simulations that the Kalman Smoother analysis scheme is well suited to reduce aliasing artefacts in the science products of a GRACE-like mission.

3 EVALUATING THE ITSG-GRACE2016 DAILY KALMAN SMOOTHER SOLUTIONS

After demonstrating that estimating daily Kalman Smoother fields reduces the errors compared to the GRACE solutions that only use a dealiasing model, the real ITSG-Grace2016 daily Kalman Smoother solutions are analysed, to show that they indeed contain realistic oceanic signals in the submonthly frequency band. While the coefficients from the simulations are constrained towards and co-estimated with the monthly mean, the published daily Kalman smoother solutions are constrained towards a long-term mean field including trend and annual signal. This also implies that two different process dynamics were used, as the variability relative to a long-term mean field is quite large compared to variations relative to monthly averages. Nevertheless, even though the published ITSG-Grace2016 daily gravity field time-series and the co-estimated daily fields used for the GK simulations are independent data sets, they are produced in a similar manner and it is safe to assume they include similar signals.

In order to properly interpret the Kalman Smoother results in the spatial domain, we first reassess the expected geophysical signals at submonthly periods induced by non-tidal mass transport processes that potentially contribute to temporal aliasing. Over the continents, we use the Land Surface Discharge Model (LSDM; Dill 2008) in its

Table 2. Specification of gravitational forces and its associated errors applied for the numerical satellite gravity mission performance simulation experiments.

	Truth	S	SAO	SAOT
Static gravity	GOCO05s	EGM96	EGM96	EGM96
Non-tidal time-variable gravity	AOHIS	id.	DEAL + AOerr	DEAL + AOerr
Ocean tides	FES2014b	id.	id.	EOT11a
Direct tides	DE421 ^a	id.	id.	id.
Earth tides	IERS2010 ^b	id.	id.	id.

^aPlanetary and lunar ephemeris (Folkner *et al.* 2009).^bIERS 2010 Conventions (Petit & Luzum 2010). **Figure 1.** Power spectral densities of range-rate residuals (left-hand panel) and degree variances of true (solid lines) and estimated (dashed lines) errors (right-hand panel) for different simulation settings: GRACE-like mission with errors in the static gravity field (G-S), with additional errors in the non-tidal atmospheric and ocean dealiasing model (G-SAO), and with additional errors in the ocean tide model (G-SAOT). Signal and estimated errors for the ITSG-Grace2016 monthly solution for January 2006 are provided for comparison, as well as the baseline error estimate from Kim (2000). **Figure 2.** Power spectral densities of range-rate residuals (left-hand panel) and degree variances of true (solid lines) and estimated (dashed lines) errors (right-hand panel) for a GRACE-like mission with errors in the non-tidal atmosphere-ocean dealiasing model treated in the conventional way as error-free *a priori* background model (G-SAO); and with the additional estimation of daily Kalman Smoother fields in addition to the background model (GK-SAO). Signal and estimated errors for the ITSG-Grace2016 monthly solution for January 2006 are provided for comparison, as well as the baseline error estimate from Kim (2000).

latest configuration as applied for the prediction of Earth rotation excitations (Dill *et al.* 2018). Over the oceans, we utilize the Max-Planck Institute Ocean Model (MPIOM; Jungclaus *et al.* 2013) in its configuration for the latest release 06 of AOD1B (Dobslaw *et al.* 2017). Water storage variability is converted into equivalent surface pressure (i.e. 1 cm of water equals 1 hPa) before combining with ocean bottom pressure. All model data is available with daily sampling over the period 2003–2012. Mass variations are separated into four frequency bands by means of a series of 4th order Butterworth

filters, and standard deviations for every location on a global 1° grid are presented (Fig. 3). Note that GRACE satellites also measure the signals from the continental ice sheets, which is not represented in the numerical model data used here for comparison.

For periods shorter than 3 d we find almost no signals over the continents, whereas ocean areas have larger variability, in particular in coastal regions at higher latitudes. All Nordic Seas, Hudson Bay, East China Sea, Gulf of Thailand, Gulf of Carpentaria and the Patagonian Shelf encounter mass variability exceeding 2 hPa.

Figure 3. Standard deviation of daily mass anomalies expressed in surface pressure equivalent (hPa) due to water storage simulated by LSDM and ocean bottom pressure from MPIOM during 2003–2012 separated into periods (a) shorter than 3 d; (b) 3–10 d; (c) 10–30 d; and (d) longer than 30 d as obtained from a series of 4th order Butterworth filters.

Furthermore, signals related to fast changes in the Antarctic Circumpolar Current (ACC) reach 1 hPa. For the periods between 3 and 10 d the signals in similar coastal areas are still dominant, now exceeding 5 hPa, and the variability of the ACC is becoming even more important, with a very prominent maximum just south of the East Pacific Rise. Water storage variations over the continents remain much smaller than the oceanic signals also for this frequency band.

For the periods between 10 and 30 d, variability remains strongest on the continental shelves and along the path of the ACC, but there are now also relevant signals on the continents. Terrestrial water storage variations reach 1 hPa in regions with humid tropical climate as Brazil and Southeast Asia. Over the oceans, locations of strongest variability in the ACC shift somewhat in position in line with the eigenfrequencies of the most important resonant modes constituting the signal. For periods longer than 30 d, the oceanic variability continues to have similar magnitude and spatial distribution as for the 10–30 d band, but the seasonal variations in terrestrial water storage now clearly dominate, with standard deviations reaching 10 hPa almost everywhere over the continents—a notable exception being the deserts—and often exceeding 20 hPa in the regions with high precipitation rates, especially if the climate is characterized by monsoons, and along the large river systems, such as the Amazon, Kongo and Mekong.

It becomes obvious from Fig. 3 that the wind-driven ocean bottom pressure variability at high-frequencies is so strong that reasonable

ocean signals can only be deduced from monthly mean gravity fields if those signals are accounted for at each particular overflight of the satellites. Non-tidal ocean bottom pressure variability is thus part of the standard dealiasing model AOD1B. Submonthly variations of terrestrial water storage instead are much smaller than the corresponding oceanic signals at identical frequencies, and also much smaller than the monthly mean and seasonal variations, so that temporal aliasing errors would not dominate estimates over the continents. Model data of high-frequency water storage variations are thus deliberately not taken into account in standard GRACE processing.

We now turn to the global gravity field estimates from GRACE, specifically the ITSG-Grace2016 daily solutions (Mayer-Gürr *et al.* 2016) as obtained with the Kalman smoother approach discussed above. Available over the period 2003–2012 up to $d/o = 40$, the data is synthesized onto an 1° equiangular grid and subsequently separated into four frequency bands by means of a series of 4th order Butterworth filters (Fig. 4). Note that the oceanic and atmospheric variability reduced during the dealiasing process with AOD1B RL05 has not been restored here, meaning that only the so-called GSM products are used that reflect mass variability either not considered *a priori*, or introduced erroneously by means of imperfect background models. While a significant portion of the signal is removed during the dealiasing, if the dealiasing model is added back, we cannot be certain if the signal in the GRACE solutions is really captured by GRACE or it comes from the model. Since

Figure 4. Standard deviation of mass anomalies expressed in surface pressure equivalent (hPa) derived from daily ITSG-Grace2016 Kalman solutions during 2003–2012 as separated into periods (a) shorter than 3 d; (b) 3–10 d; (c) 10–30 d; and (d) longer than 30 d as obtained from a series of 4th order Butterworth filters.

GRACE is most commonly used to study seasonal and interannual signals, we would like to see whether it also captures submonthly oceanic signals in addition to the signals successfully simulated by the dealiasing model.

For the shortest periods below 3 d, the day-to-day variability in ITSG-Grace2016 over the continents is very small and never exceeds 0.3 hPa. Variations in the open ocean are also small in tropical regions but somewhat higher at moderate latitudes. The largest variability is seen in several semi-enclosed ocean basins like North Sea, Yellow Sea, Gulf of Thailand and Gulf of Carpentaria. All of these regions have very high variability also in MPIOM (see Fig. 3), and many of them are known today to be affected by errors in AOD1B RL05 (Dobslaw *et al.* 2013) as discussed in Dobslaw *et al.* (2016). Since ITSG-Grace2016 daily solutions use AOD1B RL05 for dealiasing, any errors in AOD1B RL05 are passed on to the ITSG-Grace2016 solutions. More recent GRACE solutions that use AOD1B RL06 and therefore MPIOM for dealiasing are consequently not affected by the same errors. For periods between 3 and 10 d, signals of more than 2 hPa are present everywhere in the Arctic Ocean and the Nordic Seas and particularly strong variability is visible along the Siberian Shelf and in Hudson Bay. Other semi-enclosed basins like North, Mediterranean and Black Sea, and some resonant basins in the Southern Ocean show enhanced variability as well. Increased variability in the regions of the ACC is also evident in this frequency band. Signals over the continents are still much smaller and hardly exceed 1 hPa.

Between 10 and 30 d, residual signals in the oceans are still dominating the ITSG-Grace2016 solutions. Most prominent areas are East Siberian, Baltic and Black Sea. The signal variability over the continents approaches 2 hPa in western Antarctica and at the southern tip of Greenland. Both regions are characterized by marine climate with strong snowfall events and the rapid passing of low pressure systems which might not be captured too well by the European Centre for Medium-Range Weather Forecasts (ECMWF) numerical weather model utilized for the atmospheric part of AOD1B. Residual signals at periods of 30 d and longer are dominated by the seasonal and interannual variations in terrestrial water storage and ice mass change, while the oceanic signals are much weaker. Signals over the continents contained in ITSG-Grace2016 are generally in line with model predictions in terms of both regions and magnitudes. Note that LSDM does not simulate ice dynamics and thus does not reflect the variability in Antarctica and Greenland, as well as in glaciated high-mountain regions like Alaska and Patagonia to full extent. To conclude, while the regions with highest variability are the same in the simulated and in ITSG-Grace2016 fields on all period bands, the oceanic variability is significantly reduced in the GRACE fields due to the subtraction of the AOD1B product.

As an external validation measure, we use a data set of approximately 150 *in situ* ocean bottom pressure time-series originally compiled by Macrandar *et al.* (2010) and processed as described by Poropat *et al.* (2018). Data segments with very strong drifts are removed from the time-series, trends are calculated and removed, as

well as jumps that are present in many time-series due to recovery and redeployment of sensors. Time-series are checked for outliers, hourly values are calculated via averaging for all instruments with higher temporal sampling, and tidal signals are estimated and subtracted. Finally, all data segments from the same location are stacked into one series. Since the AOD1B product has been removed during dealiasing, and has not been restored to the ITSG-Grace2016 fields, the daily means of the same AOD1B RL05 product have been removed from each *in situ* ocean bottom pressure time-series. To compare daily bottom pressure estimates of ITSG-Grace2016 with *in situ* ocean bottom pressure, a reduction in standard deviation is calculated (Fig. 5):

$$STDR = \frac{STD[p^{insitu}] - STD[p^{insitu} - p^{GRACE}]}{STD[p^{insitu}]}, \quad (1)$$

where p^{insitu} and p^{GRACE} are the time-series of *in situ* measured and GRACE-based ocean bottom pressure, respectively. The measure is negative in cases where GRACE increases the *in situ* variability and zero when subtracting GRACE does not alter the variability of the *in situ* data. Positive values indicate that some variability measured by *in situ* ocean bottom sensors is also contained in ITSG-Grace2016 daily Kalman solutions. Since *in situ* measurements are pointwise, while GRACE measures averages over larger areas, perfect correspondence between them is not expected. Furthermore, since the submonthly atmospheric and oceanic variability removed during dealiasing has not been restored, we only expect good agreement between GRACE and *in situ* time-series in regions where the AOD1B RL05 product is not performing well. In areas and for periods in which AOD1B RL05 performs very well, there is not much signal left in the GRACE and *in situ* data after AOD1B has been subtracted, resulting in time-series with very low signal to noise ratio that are difficult to compare and usually have negative standard deviation reductions.

For periods below 3 d, we see positive results at a few stations only, mostly in the Arctic Ocean and in the Sargasso Sea. Over the poles, GRACE observations are available every 90 min, and AOD1B RL05 is well known to be affected by errors due to the generally limited number of meteorologic and oceanographic observations at polar latitudes. On the other hand, the reasons for positive results in the Sargasso Sea are not as obvious because the dealiasing model performs quite well in that region (Dobslaw *et al.* 2017; Poropat *et al.* 2018). Similar results are also found at the Arctic polar stations in the period band between 3 and 10 d, with additional strong signals in two regions of the ACC. For the vast majority of stations away from the Arctic Ocean, however, ITSG-Grace2016 daily fields explain only a small portion or no signals seen by the *in situ* stations. We note, however, that most of the variability in the GSM fields is found in regions not covered by *in situ* stations available to us. This applies in particular to most of the semi-enclosed seas, the Siberian Shelf, and many of the resonant regions in the Southern Ocean.

For periods between 10 and 30 d on the other hand, 53 per cent of the *in situ* stations show reduced standard deviations when ITSG-Grace2016 is subtracted, the largest of them being in the ACC region, where for some stations around 40 per cent of variability is detected by GRACE, but obviously not captured by AOD1B RL05. This clearly indicates that some fraction of the ocean bottom pressure variability measured by the *in situ* gauges is indeed captured by the daily ITSG-Grace2016 Kalman Smoother solutions, meaning that the sampling characteristics of GRACE allow to reliably observe signals at weekly periods and longer. For the longest periods, ITSG-Grace2016 Kalman solutions have a similar number of locations with positive reductions of standard deviation, but their

spatial distribution is somewhat different. We thus conclude that the Kalman smoother scheme applied in ITSG-Grace2016 indeed captures submonthly variability not predicted by the non-tidal dealiasing model AOD1B and thus contributes to less temporal aliasing errors. The validation results from *in situ* ocean bottom pressure thereby fully confirm the simulations presented above.

4 ERROR BUDGET OF A FUTURE DOUBLE-PAIR MISSION

In view of the high reliability of our simulation environment as demonstrated by the consistency of the GRACE-like simulation with real data from ITSG-Grace2016, we now reconsider the potential benefit of a second pair of satellites in addition to a polar-flying GRACE mission (Fig. 6). In contrast to many other studies, we do not assume improved instrument accuracies, but only add two more satellites at an inclined orbit of 70° with an altitude of 429 km and a satellite separation of 120 km. In case that only errors in the static gravity field are assumed (B-S), we confirm the findings from the GRACE-like simulations that instrument noise and static gravity errors do not contribute substantially to the error budget. In the case of aliasing due to errors in both the non-tidal (B-SAO) and tidal models (B-SAOT), errors induced into the monthly gravity fields are much larger than the instrument noise but do not grow as rapidly with increasing degree as within the GRACE scenarios. This generally confirms that a doubled amount of available observations and the different orientation of the along-track distance measurements (89° versus 70° inclination) contribute substantially to stabilizing the solutions in particular at higher orders, thereby reducing the strength of the characteristic north–south stripes and thus leading to more isotropic spatial error correlations.

We also assess the impact of different analysis schemes under the presence of errors in static gravity, non-tidal atmosphere and ocean, and tidal mass variability. Compared to the standard case of conventional dealiasing (B-SAOT), we note that the implementation of the Kalman Smoother (BK-SAOT) does not improve the results. We relate this effect to a sufficiently dense coverage with observations of different heading angles that contribute to a better compensation for residual dealiasing errors already in the standard processing. We further note that pre-elimination of daily low-degree fields (BW-SAOT) has a negative effect on the accuracy of the monthly gravity fields: the spectral resolution restriction imposed by limiting the solution space of the daily solutions to degree and order 30 induces a sharp increase in the errors at degrees 31 and higher. It remains open if this is a general feature of pre-elimination schemes or rather related to our particular implementation, but we advise caution and further study before implementing a future gravity mission that critically relies on such an analysis scheme.

5 SUMMARY AND CONCLUSIONS

Based on contemporary estimates for GRACE sensor accuracies, global ocean tide model errors, and non-tidal atmosphere and ocean dealiasing model uncertainties, we demonstrated our ability to accurately confirm error degree variances of the January 2006 monthly solution of the ITSG-Grace2016 gravity field series within a closed-loop simulation setting. Degree variances of true errors obtained from the differences of the recovered gravity field and the synthetic time-variable gravity field used for the simulation are closely aligned to the corresponding error estimates obtained from the variance component estimation, thereby confirming both the plausibility

Figure 5. Standard deviation reduction of ocean bottom pressure (hPa) when subtracting daily ITSG-Grace2016 GRACE estimates from daily *in situ* observations separated into periods (a) shorter than 3 d; (b) 3–10 d; (c) 10–30 d; and (d) longer than 30 d as obtained from a series of 4th order Butterworth filters.

Figure 6. Degree variances of true (solid lines) and estimated (dashed lines) errors for different simulation settings of a double-pair mission with errors only in the static gravity field (B-S), with additional errors in the non-tidal atmosphere-ocean dealiasing model (B-SAO), and with additional errors in the tidal dealiasing model (B-SAOT) (left-hand panel); and for different analysis schemes for a double-pair mission with errors in the static gravity field and the non-tidal and tidal dealiasing models: standard dealiasing by means of *a priori* models (B-SAOT), co-estimation of daily fields by means of a Kalman Smoother (BK-SAOT), and the pre-elimination of daily low-degree fields (BW-SAOT) (right-hand panel). Signal and estimated errors for the ITSG-Grace2016 monthly solution for January 2006 are provided for comparison.

of the introduced uncertainties as well as the robustness of our *a posteriori* error quantification procedure.

As long as error-free *a priori* tidal and non-tidal models are assumed, the simulated errors in the monthly gravity field align exceptionally well to the predictions of Kim (2000) issued prior to the launch of the mission, thereby underlining that those early estimates about the GRACE baseline errors are indeed highly realistic and remain a valid target for current and future GRACE reprocessing efforts. The simulations further indicate that errors at low degrees reduce substantially for a GRACE-like mission when high-frequency non-tidal signals are co-estimated by a Kalman Smoother as applied within the ITSG-Grace2016 processing. Validation of the ITSG-Grace2016 daily gravity fields with *in situ* ocean bottom pressure indicates that they indeed contain signals of ocean mass variability not reflected in the applied dealiasing model, and thus provide geophysically relevant information not known *a priori*.

For a future double-pair configuration, we note that the relative impact of aliasing errors is substantially smaller even for present-day model and instrument error levels. Interestingly, the co-estimation of daily fields with a Kalman Smoother has a rather minor impact only. The pre-elimination of daily normal equations, instead, raises the overall error level in our simulations, in particular at degrees and orders in the vicinity of the selected cut-off degree. It is thus concluded that pre-elimination and its consequences on the overall gravity field accuracy should be studied further before implementing a future gravity mission tailored to deliver information of submonthly variability based on any pre-elimination analysis scheme.

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<https://www.tugraz.at/institute/ifg/downloads/gravity-field-models/>. The *in situ* OBP data is available from the PANGEA database. For this paper L. Poropat analysed the geophysical signals in the daily gravity fields, performed the *in situ* validation, and wrote the manuscript together with H. Dobsław. A. Kvas performed the satellite mission simulation experiments. T. Mayer-Gürr and H. Dobsław designed the study and contributed to the interpretation of results.

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