AIUB-GRACE gravity field solutions for G3P: processing strategies and instrument parametrization

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Abstract. This paper discusses strategies to improve the GRACE monthly solutions computed at the Astronomical Institute of the University of Bern (AIUB) which are contributing to the Horizon 2020 project G3P - Global Gravity-based Groundwater Product. To improve the AIUB-GRACE gravity field solutions, we updated the use of the Level-1B observations and adapted the background models, and improved the processing strategies in terms of instrument screening and parametrization. We used the Release 3 K-Band product (KBR) and star camera data (L1B RL03), and adopted the Release 6 of the Atmospheric and Ocean De-aliasing (AOD1B RL06) product. For the accelerometer parametrization, we used arc-wise full scale factor matrix and arc-wise third-order polynomial biases. The new accelerometer parametrization is effective to reduce noise over the oceans in gravity field solutions especially for the late years of the GRACE mission when the thermal control was switched off. In this paper, we show that the outliers in KBR antenna offset correction (AOC) are projected into the range-rate residuals; therefore, we used the KBR AOC as the main source for outlier detection and eliminated the AOC above a threshold for all data before the gravity field processing.

1 Introduction

The Global Gravity-based Groundwater Product (G3P) is a collaborative Horizon 2020 project between twelve European institutions coordinated by the German Research Centre for Geosciences (GFZ, (Güntner et al., 2020)). One of the key objectives of the G3P project is to process Gravity Recovery And Climate Experiment (GRACE, Tapley et al. (2004)) and GRACE Follow-On (GRACE-FO, Tapley et al. (2019)) Level-1B instrument data. GRACE and GRACE-FO provide a unique type of Earth observation from space (Wahr et al., 1998), total water storage variations on the continents, which is essential to calculate the variations in groundwater storage by subtracting other compartments of water storage variations such as glaciers, snow, soil moisture and surface water bodies derived from other Earth observation data or models.

The Astronomical Institute of the University of Bern (AIUB) is one of the GRACE/GRACE-FO analysis centers contributing to the G3P project. AIUB has produced monthly GRACE gravity field solutions since 2011. The first monthly GRACE series was released in 2011, (Meyer et al., 2012) and the second series in 2016, AIUB-RL02, (Meyer et al., 2016). Beside the GRACE

gravity field solutions, GPS-based GRACE orbits are also processed at AIUB and are made publicly available (Arnold and Jäggi, 2020). The AIUB-RL02 of monthly gravity field models contributed to the combined monthly models in the frame of the European Gravity Service for Improved Emergency Management (EGSIEM) project (Meyer et al., 2019) coordinated by AIUB (Jäggi et al., 2019). AIUB-RL02 lacks the late years of GRACE gravity field solutions in 2016 and 2017. Therefore a new AIUB-G3P is prepared with the following objectives:

- contribute to the Global Gravity-based Groundwater Product (G3P).

- contribute to the International Association of Geodesy (IAG) service COST-G (International Combination Service for Time-variable Gravity Field Solutions) (Jäggi et al., 2020).

- update the input observations and background models for GRACE gravity field recovery to be consistent with the other contributors to the COST-G (see section 2).

- improve gravity field recovery processing.

- provide the complete time series of monthly GRACE gravity field solutions from 2002 to 2017.

2   GRACE orbit dynamic model

AIUB-G3P, like its two predecessors AIUB-RL01 (Meyer et al., 2012) and AIUB-RL02 (Meyer et al., 2016), is based on the Celestial Mechanics Approach (CMA) (Beutler et al., 2010), which treats gravity field estimation as a generalized orbit determination problem. The equations of motion for both GRACE satellites are:

$$\ddot{\boldsymbol{r}} = \boldsymbol{a}_g + \boldsymbol{a}_{ng} + \boldsymbol{a}_{emp} \tag{1}$$

where $\ddot{\boldsymbol{r}}$ is the acceleration of the satellite, second time derivative of the satellite position vector, $\boldsymbol{a}_g$ denotes accelerations due to all gravitational forces, $\boldsymbol{a}_{ng}$ denotes accelerations due to all non-gravitational forces and $\boldsymbol{a}_{emp}$ denotes empirical accelerations designed to overcome deficiencies remaining in the force models.

The CMA solves equation (1) as a linearized least-squares estimation where gravity field coefficients and all other orbit related parameters are estimated together. Kinematic positions and K-Band range-rate data are used as observables to estimate orbit and gravity field coefficients such that the orbit trajectories are solving equation (1).

The gravitational models ($\boldsymbol{a}_g$) in equation (1) are called the background gravity models. The details of the background gravity models for AIUB-G3P are provided in Table 1.

For $\boldsymbol{a}_{emp}$, constrained piecewise constant accelerations at 15 minutes intervals in all three directions of the local orbital frame were estimated (Jäggi et al., 2006).

For $\boldsymbol{a}_{ng}$, the GRACE accelerometer data is used. The accelerometer measurements given in the ACC1B data product, are affected by unknown scale factors, biases and random noise (Kim, 2000). Ideally, the scale factor matrix **S** (equation

Table 1. Background models for AIUB-G3P with maximum spherical harmonic degree (d/o) (if applicable).

Model	Description	Reference
A priori gravity	AIUB-GRACE03S (static part), d/o 160	
Solid Earth tides	IERS 2010 conventions	(Petit and Luzum, 2010)
Ocean tides	FES2014b, d/o 100	(Carrere et al., 2016)
Atmosphere and oceanic variability	AOD1BRL06, d/o 100	(Dobslaw et al., 2017)
Solid Earth pole tide	IERS 2010 conventions	(Petit and Luzum, 2010)
Ocean pole tide	IERS 2010 conventions, d/o 100	(Desai, 2002)
N-Body perturbations	DE421	(Folkner et al., 2009)

2) should be an identity matrix, but it contains diagonal elements and non-zero off-diagonal elements due to small instrument imperfections causing mutual influence of the accelerometer axes among each other. In order to account for these imperfections, a fully-populated scale factor matrix is used for AIUB-G3P:

$$\mathbf{S} = \begin{bmatrix} s_x & \alpha + \zeta & \beta - \epsilon \\ \alpha - \zeta & s_y & \gamma + \delta \\ \beta + \epsilon & \gamma - \delta & s_z \end{bmatrix} \tag{2}$$

5 The off-diagonal components are composed of a symmetric shear α, β and γ and a skew- symmetric rotation part ζ, ϵ and δ. For more details on interpretation of these elements we refer to (Klinger and Mayer Gürr, 2016). For previous AIUB releases, the off-diagonal elements have been neglected, i.e. the scale factor matrix was assumed to have main diagonal elements only. To account for instrument imperfections and misalignment, for AIUB-G3P both main diagonal and off-diagonal elements of the scale factor matrix (cf. Eq. 2) were estimated on a daily basis.

10 To account for bias changes due to temperature variations according to (Klinger and Mayer Gürr, 2016), a bias vector $\boldsymbol{b}$ is estimated daily using a third order polynomial. Four coefficients were estimated in each direction, therefore twelve accelerometer bias coefficients were estimated on a daily basis for each satellite.

The main observations are a combination of kinematic orbit positions for each satellite and inter-satellite K-Band range-rate measurements. The combination is realized through daily normal equations and is accumulated for one month to solve for 15 monthly spherical harmonics coefficients of the Earth's gravity field. The kinematic orbits of the GRACE satellites are determined in a precise point positioning from the undifferenced GPS phase observations (Jäggi et al., 2006). The kinematic orbits rely on reprocessed GPS orbits from the CODE analysis centre (Steigenberger et al., 2011). For kinematic orbit determination maps of the empirical phase center variation of the GRACE GPS antennas (Jäggi et al., 2009) were re-estimated. The kinematic orbits for the whole GRACE lifetime can be downloaded from http://ftp.aiub.unibe.ch/LEO_ORBITS/GRACE/RL01/. 20 The specifics of the GRACE data products are given in the Table 2.

Table 2. Data products for AIUB-G3P

Product ID	Release	Data Rate
KBR1B	RL03	5-second range-rate
KIN	AIUB in-house	30-second position
ACC1B	RL02	1 second linear acceleration
SCA1B	RL03	1 second quaternion

Although we can not see the star camera data in the equation (1) explicitly, they appear implicitly in two ways in GRACE gravity field recovery:

– transforming the linear ACC1B product to inertial frame (Darbeheshti et al., 2017),

– calculating KBR antenna offset correction in KBR1B product.

5   The SCA1B product is used to define the KBR antenna offset correction (AOC) in the KBR1B product. The KBR instrument measures the distance between the antenna phase centers, which are placed nominally on the satellite frame x-axis, almost 1.5 m away from the satellites' center of mass. Consequently, any pointing jitter (deviations of the satellites' attitudes from their nominal attitudes) causes a geometric error in the ranging measurement. In the absence of such misplacements and in the absence of pointing jitter, this effect would be constant and hence not effect the measured (biased) KBR range. The GRACE

10   KBR1B data product files contain a column, which is called antenna offset correction (AOC) term (Case et al., 2010). It has to be added to the KBR ranging measurement. A second and third column is also provided, computed by numerical differentiation, describing the correction for range-rate and range-acceleration.

Although the AOC is improved in GRACE KBR1B RL03, AOC outliers exist and need to be removed. AOC rate is in the range of $\pm 0.5 \mu m/s$ (Klinger, 2018), therefore the values beyond $\pm 1 \mu m/s$ are considered outliers. Figure 1 shows range-rate

15   AOC columns from GRACE KBR1B RL02 and GRACE KBR1B RL03 for two days in 2006. There are not any outliers in the day 264, but for both RL02 and RL03, day 290 contains outliers. The corresponding amplitude spectral density (ASD) plot of these two days show although the high frequency noise (greater than $10^{-2} \mu m/s/\sqrt{Hz}$) has been filtered out from the AOC, AOC RL03 still contains outliers that correspond to the satellite events like calibration maneuvers for different instruments.
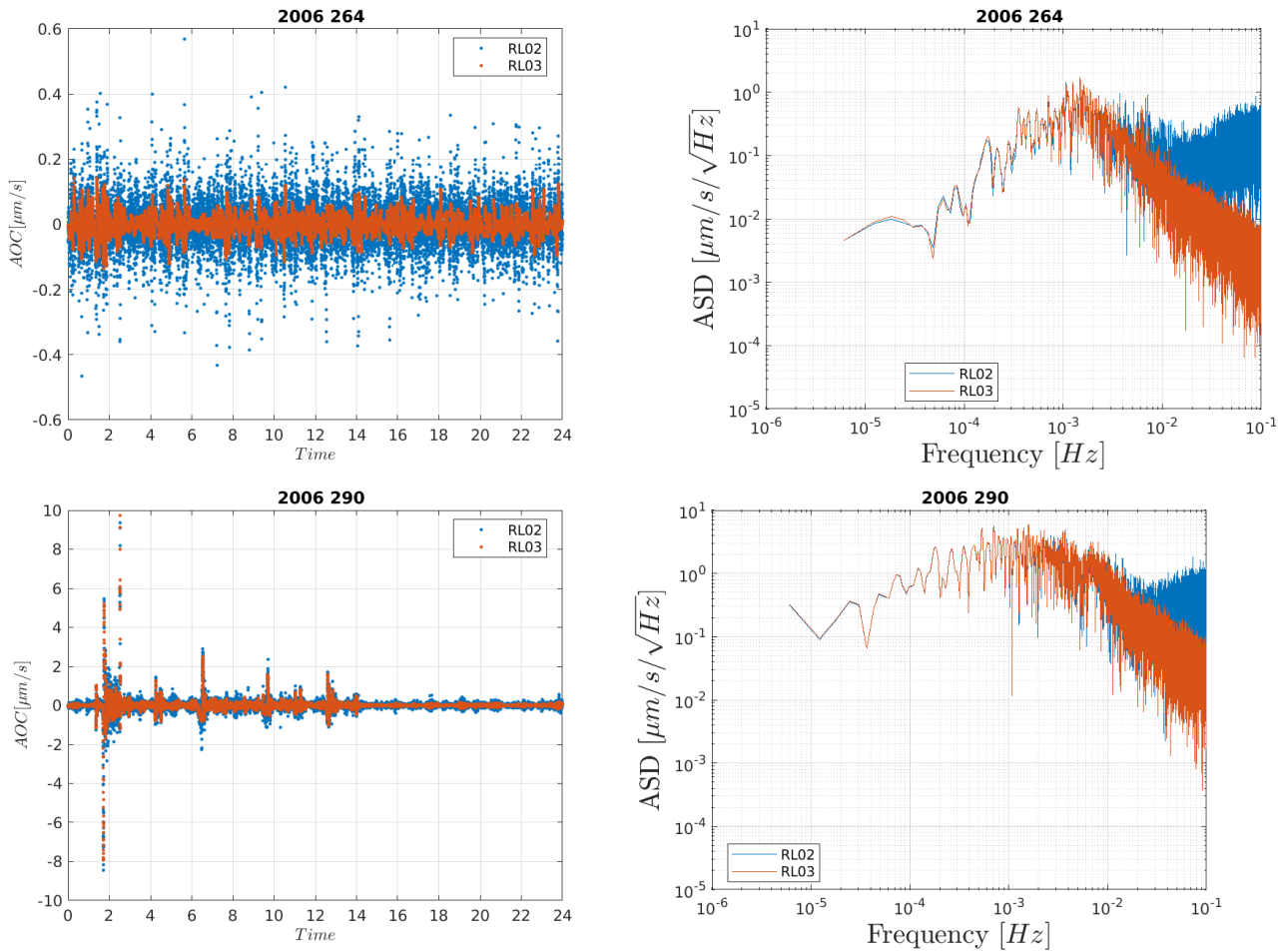
Figure 1. Range-rate AOC for days 264 (no outliers) and 290 (containing outliers) with the corresponding ASD.

3 Pre-processing: Level 1B data Screening

In theory, the GRACE L1B data products can be used directly for gravity field recovery, but there are outliers in the data that need to be removed before the gravity field recovery processing. Data screening for 15 years of GRACE data and for every instrument is a challenging task. The cause of systematic errors and outliers has been studied by (Goswami, 2018) and (Klinger, 2018). In this work we have only focused on finding an effective way to find outliers in GRACE data.

The overall error (including outliers) in the instrument data and background models are projected in range-rate residuals in case of GRACE gravity field recovery. Figure 2 shows how outliers in range-rate AOC are mapped into range-rate pre-fit residuals.
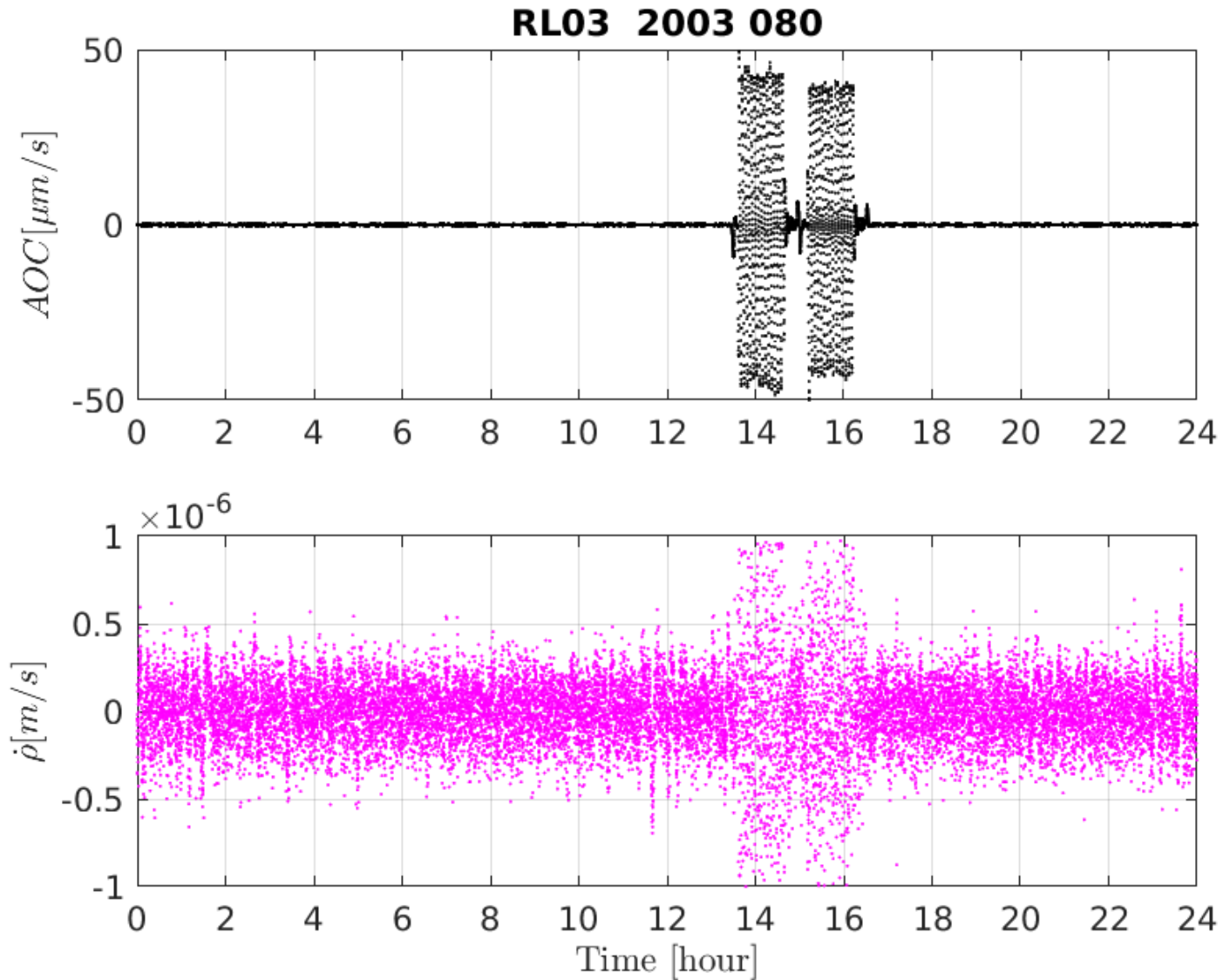
Figure 2. Outliers in AOC (day 80, 2003) are mapped into the KBR range-rate pre-fit residuals.

AOC and ACC Screening

AIUB-RL02 screening was based on inspection of the range-rate residuals and removing outliers by gap tables (Meyer et al., 2016). For AIUB-G3P, a novel screening strategy has been developed. This approach involves scrutinizing the GRACE L1B data product, specifically KBR1B and ACC1B. When an outlier is identified in the daily KBR1B and ACC1B, the correspond-
5   ing day is flagged. Subsequently, the epoch of the outlier is excluded using monthly session tables in the Bernese software.

The AIUB GRACE gravity field solutions are constructed by estimating orbital parameters for each 24-hour arc. The epochs of these daily arcs are recorded in the session tables. In the presence of an outlier, the affected epoch is removed, leading to the segmentation of the daily arc. New orbital parameters are then estimated for the revised arcs. As a result, while the general AIUB monthly gravity solution is typically based on daily arcs, months with outliers in the instrument exhibit shorter arcs in the monthly gravity solution.

We performed the data screening in three major steps: (1) threshold-based outlier detection of KBR1B AOC rate data product, (2) threshold-based outlier detection of ACC1B data product, and (3) empirical elimination of days that degraded final monthly gravity field solution. Table 3 summarizes the threshold values and margins used for threshold-based outlier detection for first and second steps. Margin means the time span before and after an outlier detected in the data. We used absolute value thresholds for the AOC rate data product, because the AOC rate is in the range of $\pm 0.5 \mu m/s$. For ACC1B data product, we used daily median based threshold, because we estimate ACC scale factors and biases on daily basis.

Table 3. Level-1B data screening: Threshold-based outlier detection.

Data product	Data type	Threshold		Margin
KBR1B	antenna offset correction (range-rate)	$\|AOC_{\dot{\rho}}^{i}\| < 1$	$\mu m/s$	10 minutes
ACC1B	linear acceleration	$\|a_x^i - \tilde{a}_x\| < 10$	$\mu m/s^2$	10 minutes
		$\|a_y^i - \tilde{a}_y\| < 10$	$\mu m/s^2$	10 minutes
		$\|a_z^i - \tilde{a}_z\| < 10$	$\mu m/s^2$	10 minutes
		$\tilde{a}$ is the median of a day		

Figure 3 shows the periods of outliers in the AOC rate and linear ACC data for GRACE A and GRACE B in all three axes. The years 2006 and 2007 are representative of high quality of GRACE data. There are complete twelve months of instrument data products from 2003 to 2010, therefor there is not any data gap in the AOC rate and linear ACC data for years 2006 and 2007. GRACE data products are only available until end of June 2017. Since April 2011, the onboard instruments are shut down for approximately 40-50 days during each 161 day to extend GRACE batteries's life time (Tapley et al., 2015), that's why there are AOC rate and linear ACC data gaps for 2016 and 2017, the last years of GRACE lifetime, where the quality of GRACE instrument data products is degraded.

The first column of figure 3 shows that the AOC outlier time length in 2007 is more than twice as 2006 (4 hours in 2006 versus 10 hours in 2007). In general, a satellite event like a calibration maneuver causes outliers in AOC. GRACE satellite events are published in the Sequence of Events file. For 2017, a much larger outlier threshold ($3 \mu m/s$) had to be used for AOC, because with a $1 \mu m/s$ AOC threshold, we would not have any data left to solve for the gravity field recovery.

Columns two and three of figure 3 show that there are much less outliers in ACC data than AOC. GRACE A ACC data for the years 2006 and 2007 is of high quality, but there are some outliers in the GRACE B ACC data. In October 2016, the accelerometer on-board GRACE B was permanently powered-off to reduce the stress on the remaining battery cells. Since

then, no GRACE B accelerometer data is available (except for May 2017). To allow for gravity field recovery, the GRACE B accelerometer transplant data (Bandikova et al., 2019) have been made available. Figure 3 shows that the bias along y axis in GRACE B in November 2016 suddenly changes and follows the bias in GRACE A, this pattern continues in 2017, except in May, when real GRACE B ACC data is again available. In June 2017 the bias in GRACE B y axis is again the same as for GRACE A.
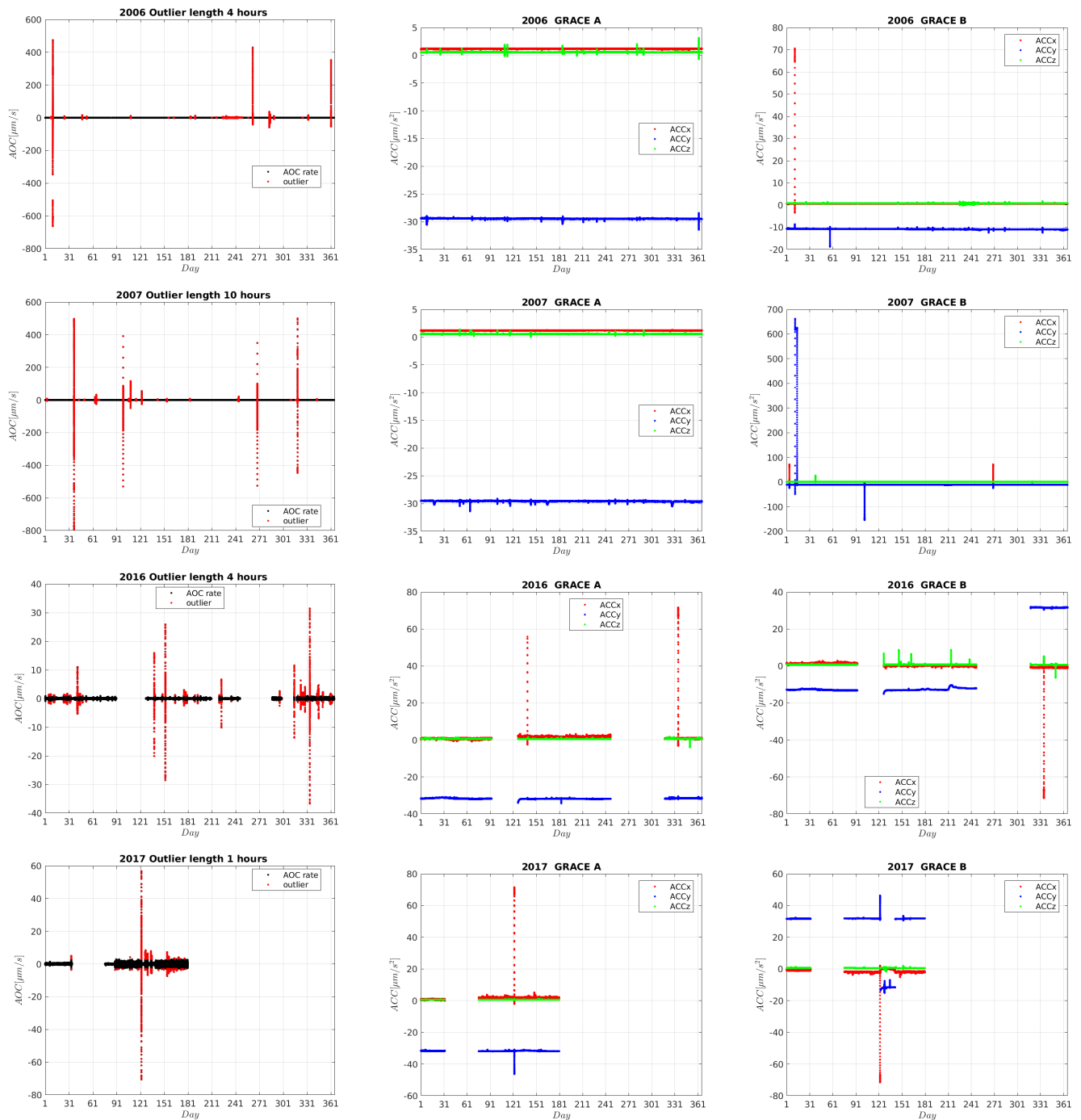
Figure 3. Annual plots of AOC rate (first column) and ACC1B accelerometer linear accelerations along three axes for 2006, 2007, 2016 and 2017. Red vertical lines in first column are outliers in AOC. For linear accelerations, vertical lines are outliers along three axes.

Empirical elimination of whole days

The empirical elimination of entire days has been incorporated as the final stage of data screening in generating the AIUB-RL01, AIUB-RL02, and AIUB-G3P solutions. For the empirical elimination procedure, n monthly gravity field solutions are produced for each month, where n is the number of days in each month. In each gravity field solution, one whole day of data

5   is eliminated. Then, by plotting and comparing the n gravity field solutions in terms of the difference degree amplitudes of geoid heights, days that corrupt the monthly gravity solution may be recognized. To compute the difference degree amplitudes, selecting a reference gravity field solution is crucial. In this context, our choice is the monthly gravity field solutions produced by the Institute of Geodesy at Graz University of Technology, ITSG-GRACE2018. This decision is motivated by the intention to benchmark our solution against a high-quality GRACE gravity solution. Furthermore, our solution closely aligns with ITSG-

10   GRACE2018 in terms of input observations, background models, and processing strategies. The deliberate use of a monthly model takes into account the varying quality of GRACE solutions from month to month, especially towards the end of the GRACE mission. Figure 4 demonstrates this procedure for July 2011. For this month, there is a dataset spanning 27 days. In the first iteration, 27 gravity solutions were generated, each excluding one day (resulting in the use of 26 days per solution). The legend denotes the day number that was omitted. For example, in July 2011, in the first iteration, day 1 in the legend

15   corresponds to day 186, day 2 to day 187, and so forth. Moving to the second iteration, day 186 is eliminated, resulting in 26 gravity solutions. In this iteration, day 1 corresponds to day 187. Subsequently, for the third iteration, day 187 is eliminated, and for the fourth iteration, day 188 is omitted. Remarkably, by the 4th iteration, after eliminating three entire days, all the gravity solutions converge closely. Their quality even surpasses that of the AIUB-RL02 monthly gravity field solution.
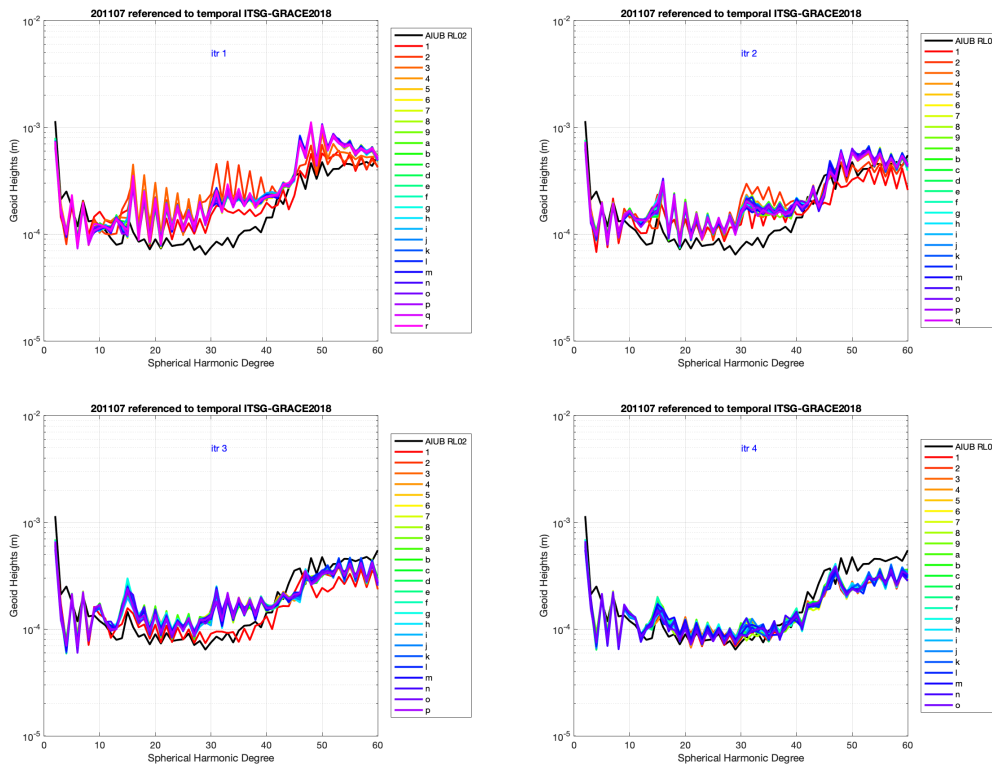
Figure 4. The empirical elimination procedure for July 2011 involves iteratively removing one day at a time. In the first iteration, day 186 (denoted as 1 in the legend) is eliminated, followed by day 187 in the second iteration, and day 188 in the third iteration. The consistently lower position of the red curves in these iterations suggests that days 186, 187, and 188 are corrupting the gravity solution. The legend indicates the corresponding day number eliminated in each gravity field solution.

To diagnose why these three days corrupt the gravity field solution, it is helpful to look at pre-fit residuals (Darbeheshti et al., 2018) of observations. Pre-fit residuals in context of gravity field recovery are observed value minus computed value, where the computed value is independent of gravity field estimation. Figure 5 shows daily root mean square (RMS) of pre-fit residuals for GRACE A and GRACE B orbits, ranges and range-rates in July 2011. Days 186, 187 and 188 show large RMS for all pre-fit residuals, which is in agreement with the empirical elimination procedure.
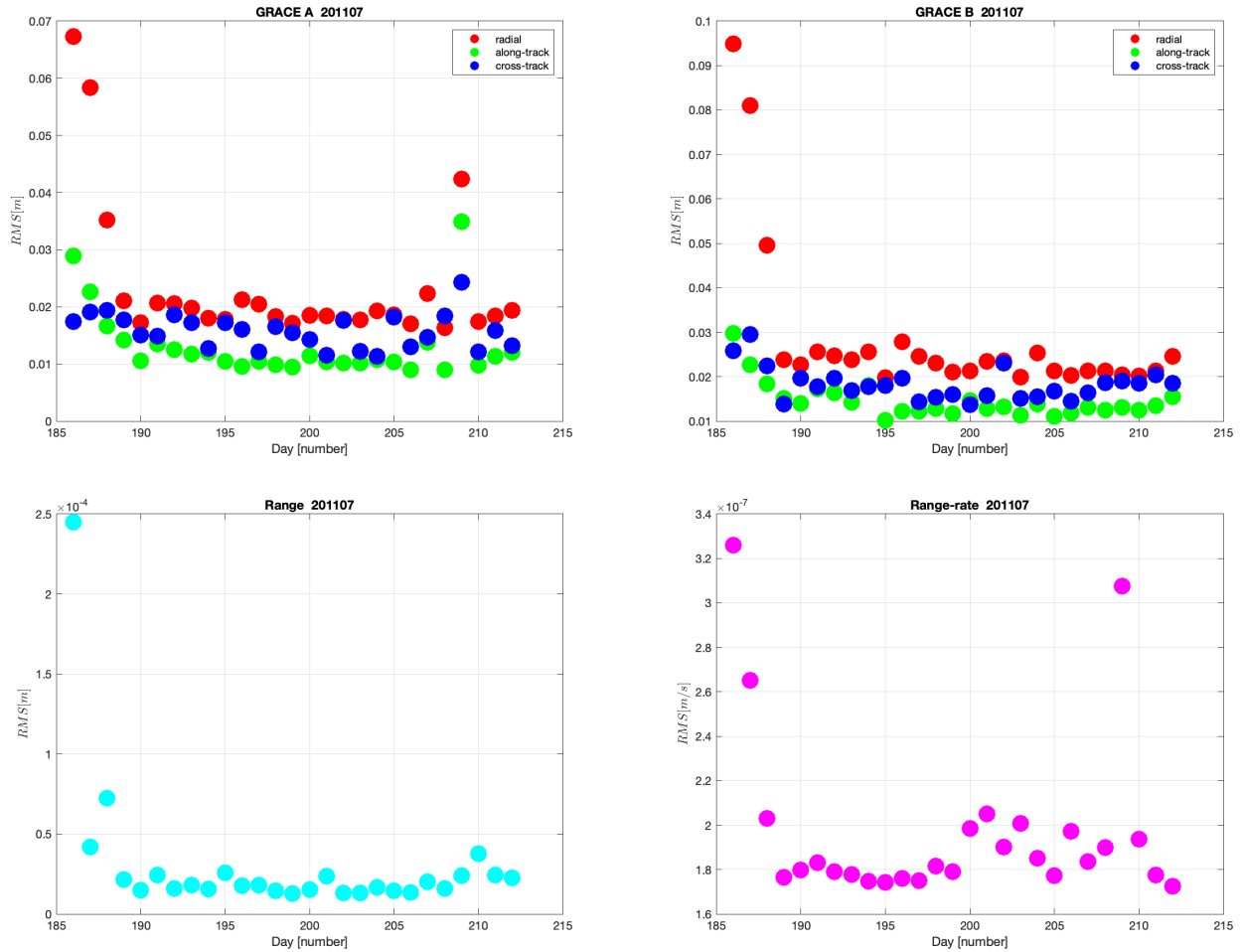
Figure 5. Daily pre-fit residual RMS for GRACE A orbit (radial (red), along- rack(green), cross-track(blue) directions, GRACE B orbit, range and range-rates for July 2011.

4 Evaluation of new AIUB-G3P GRACE

In this section, we compare new monthly GRACE solutions for G3P project, AIUB-G3P to AIUB-RL02. To maintain consistency, all comparisons in this section are referenced to a 'mean model'. The 'mean model' was computed by averaging monthly gravity field solutions from the Center for Space Research at the University of Texas, Austin (CSR Release 06), the German Research Centre for Geosciences (GFZ Release 06), the Centre National d'Etudes Spatiales/Groupe de Recherche de Geódeśie Spatiale (CNES_GRGS_RL04) and the Institute of Geodesy at Graz University of Technology (ITSG-Grace2018) for the time period 2004-2017.

An overall comparison of the AIUB-RL02 and AIUB-G3P is shown in Figure 6. For comparison, we only considered the months where AIUB-RL02 is available. The new AIUB-G3P shows the lower noise level, which is the result of the improvements in the processing chain.
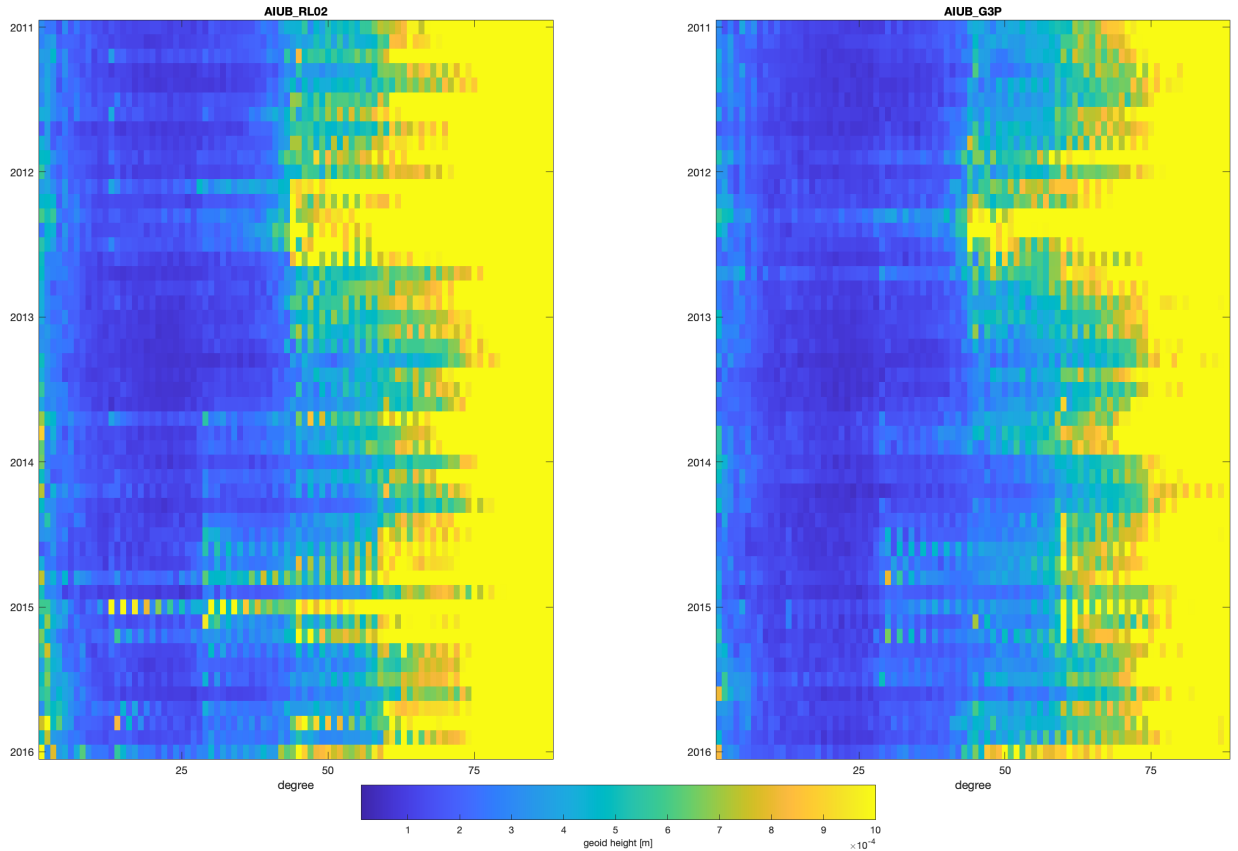
Figure 6. Difference degree amplitudes with respect to the 'mean model' for GRACE (February 2011 to August 2016) for AIUB-RL02 and AIUB-G3P.

One approach for evaluating GRACE gravity monthly solutions involves calculating the standard deviation (STD) of vari-
5 ability over the oceans, where hydrological signals are not expected. The discrepancies between the monthly solution and the 'mean model' are assessed on a grid with a cell size of 3 degrees, corresponding to a spherical harmonic expansion up to degree and order 60. Secular and seasonal variations are fitted to all grid cells and subtracted to eliminate long-periodic signals of oceanic origin. The grid cells are weighted by the cosine of the latitude to account for their different sizes, and the standard deviation over all ocean cells is computed. To prevent contamination from continental signals, the shoreline is shifted by three
10 grid cells (equivalent to 9 degrees) into the oceans (Meyer et al., 2016).

Figure 7 shows the standard deviations computed in this way for AIUB-RL02 and AIUB-G3P GRACE gravity field solutions. AIUB-G3P solution shows a significant improvement over AIUB-RL02 in the later years of GRACE lifetime, mainly after April 2011. There are few months in 2005 and 2009 for which the gravity field solutions are slightly worse in AIUB-G3P in terms of noise over the ocean. The reason for this degradation is still unknown to us.
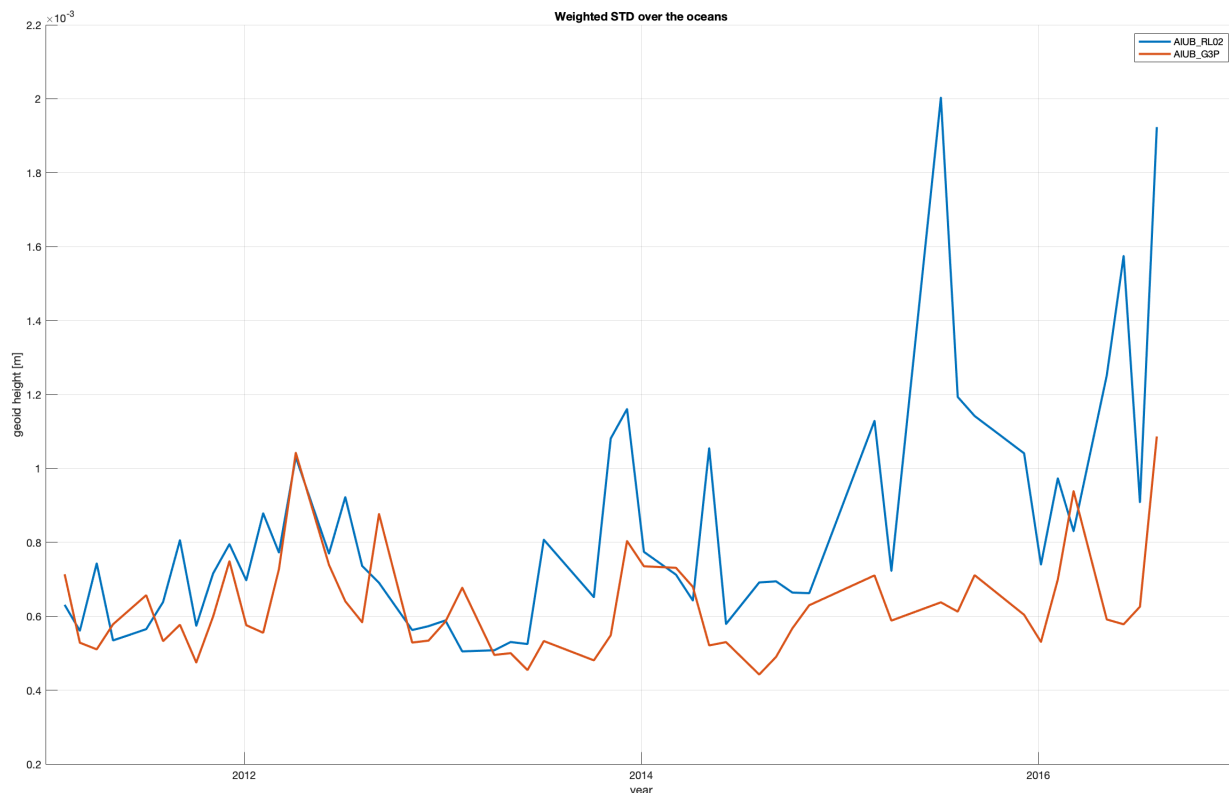
Figure 7. Weighted STD over the oceans for AIUB-RL02 and AIUB-G3P.

5 Major improvements in the processing chain for AIUB-G3P

As mentioned in Section 2, two significant changes in the processing chain have contributed to the improvement of AIUB-G3P:

- Accelerometer parameterization: In AIUB-RL02, only the diagonal elements of the scale factor matrix were calculated for each accelerometer in each arc. In AIUB-G3P, the full scale factor matrix was computed for each accelerometer in each arc, aligning with the recommendations by Klinger and Mayer Gürr (2016).

10 – Updating AOD release: The Atmospheric and Oceanic Dealiasing (AOD) release was updated from RL05 to RL06.

The impact of these two changes is assessed in Figure 8 for the years 2016-2017, a period during which the quality of GRACE observations was degraded. AIUB-RL02 solution is based on AOD-RL05 and diagonal scale factor accelerometer parametrization, while AIUB-G3P is based on AOD-RL06 and full scale factor accelerometer parametrization. In the legend 'AOD-RL05' indicates the same set up as AIUB-G3P, but using AOD-RL05 instead of AOD-RL06 and 'Diagonal' shows the same set up as AIUB-G3P, but diagonal scale factor accelerometer parametrization instead. Figure 8 shows the full scale factor matrix for accelerometer parametrization is important for late years of GRACE data. The effect of full scale factor accelerometer parametrization is even more important than updating to AOD-RL05, as it is clear from the noise over the ocean, the solution with AOD-RL05 is below the solution with diagonal scale factor accelerometer parametrization.
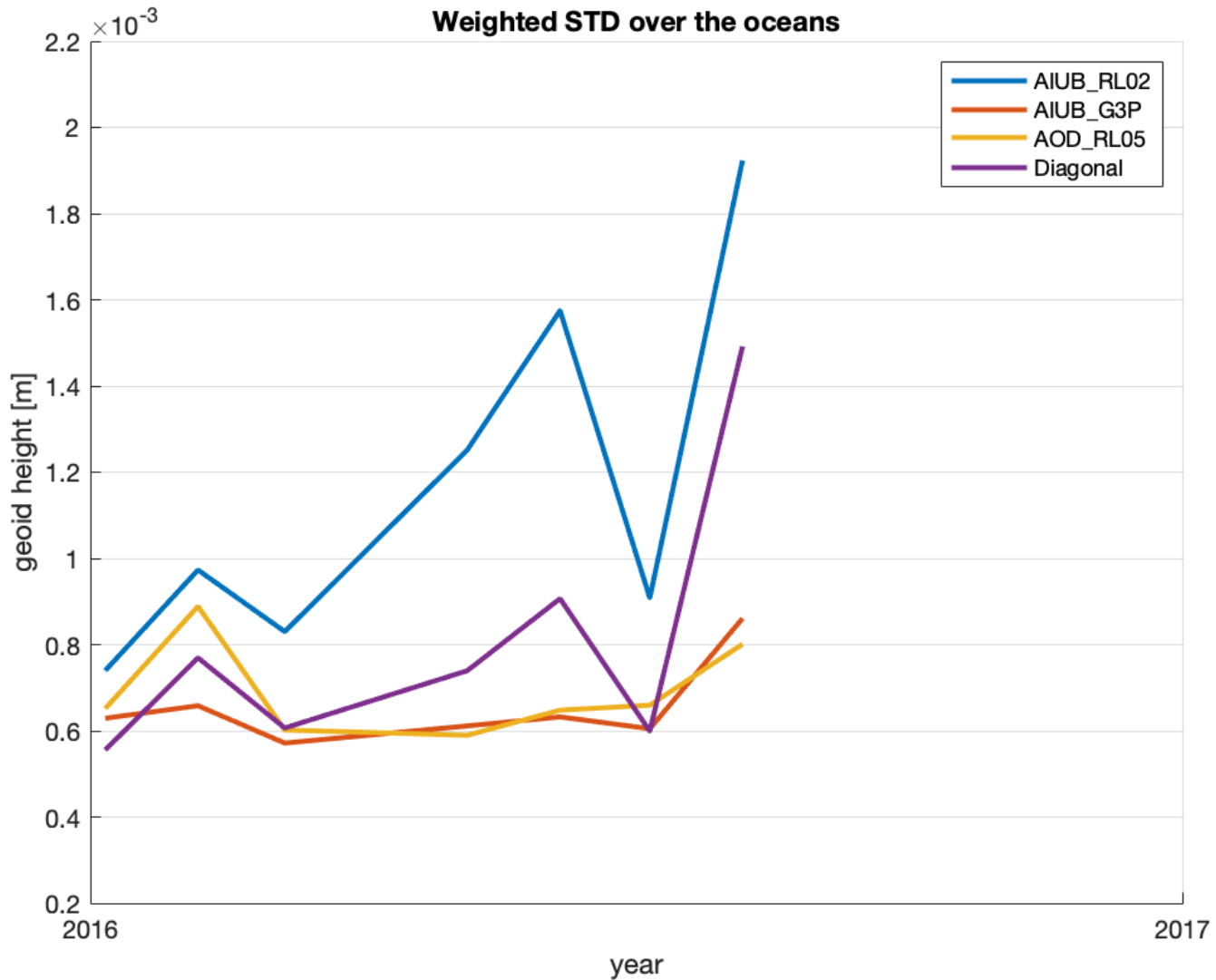
Figure 8. Weighted STD over the oceans for the years 2016 and 2017, where AIUB-RL02 data is available. 'Diagonal' shows AIUB-G3P set up with diagonal scale factor accelerometer parametrization and 'AOD-RL05' shows AIUB-G3P set up with AOD-RL05.

Figure 9 shows the elements of accelerometer full scale factor matrix for AIUB-G3P GRACE B. The main-diagonal elements of the accelerometer cross-track axis are more scattered than elements of the along-track and radial axes, which is related to the smaller sensitivity of the cross-track axis compared to other two axes. Additionally, the shear and rotational elements associated with the less-sensitive cross-track axis (δ and γ) are non-zero and are increasing for the late years of GRACE. The sheer and

rotational elements are absorbing accelerometer imperfections and misalignments, resulting in the better quality of AIUB-G3P than AIUB-RL02 in figure 7.
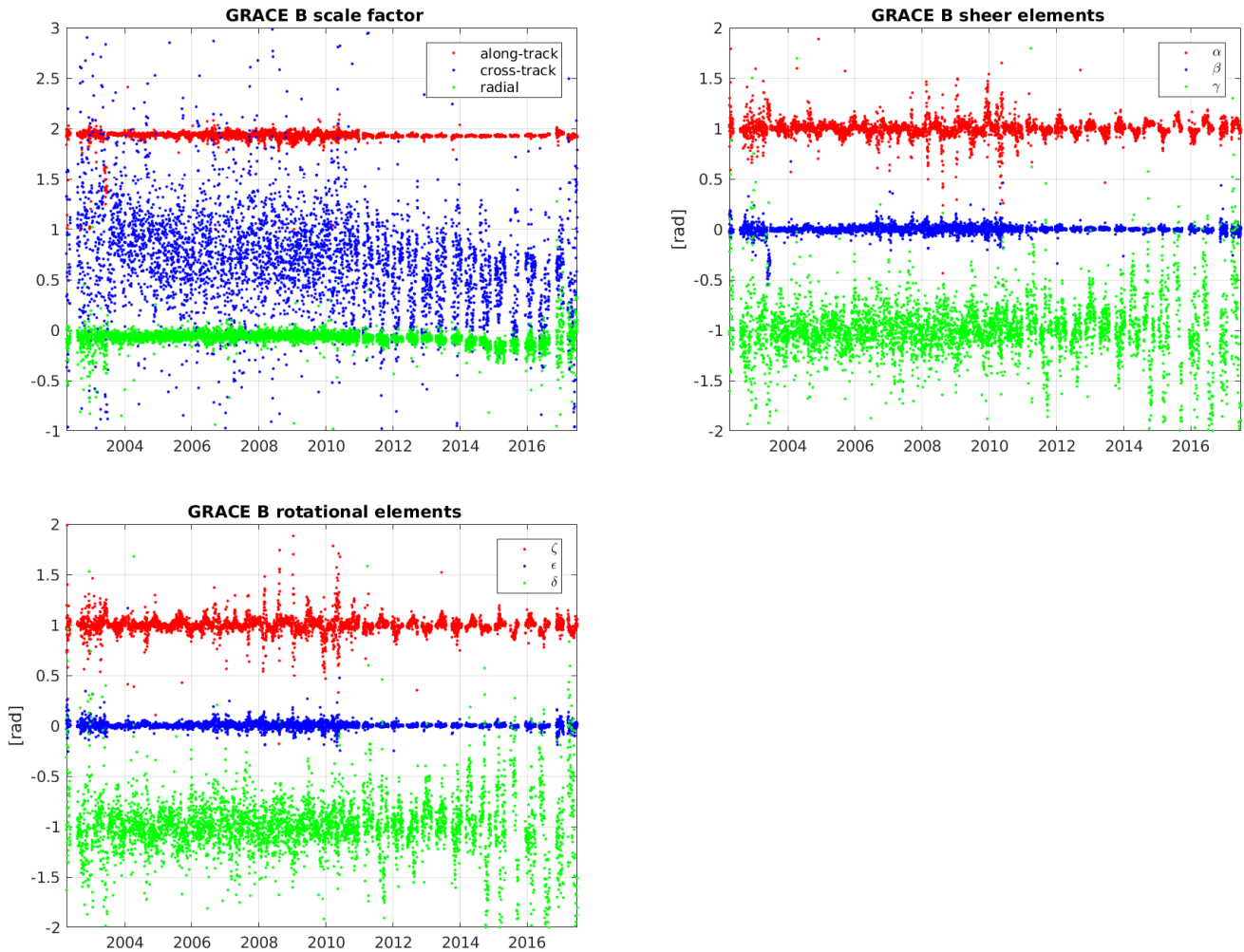
Figure 9. Elements of the scale factor matrix for GRACE B (up) Main diagonal elements in along-track, cross-track and radial direction; for a better illustration, a constant offset of ± 1 is added to the red and green graphs (middle) shear elements and (bottom) rotational elements.

5   Conclusions

In this paper, the importance of Level-1B data pre-processing methodologies to improve GRACE gravity field solutions were
5   demonstrated on the basis of AIUB processing chain and the transition from AIUB-RL02 (Meyer et al., 2016) to AIUB-G3P. Also the contribution of individual updates to the overall accuracy improvement of AIUB-G3P was highlighted. In particular, the effects and benefits of an automated AOC data screening, and a full scale factor accelerometer parametrization

were analyzed in detail. The full time series of GRACE AIUB-G3P gravity solutions can be accessed from the International Center for Global Earth Models website (ICGEM, (Ince et al., 2019)) at http://icgem.gfz-potsdam.de/series/03_other/AIUB/AIUB-G3P.

Data availability.

5   The full time series of GRACE AIUB-G3P gravity field solutions (Darbeheshti et al., 2023) is available at http://icgem.gfz-potsdam.de/series/03_other/AIUB/AIUB-G3P.

Author contributions. Ulrich Meyer and Adrian Jäggi have made contributions to the software heritage utilized in this project and reviewed the article. Martin Lasser developed accelerometer parametrization code. Daniel Arnold processed GRACE kinematic orbits. Neda Darbeheshti performed the GRACE AIUB-G3P gravity field processing and prepared the manuscript with contributions from all co-authors.

Competing interests. The authors declare that they have no conflict of interest.

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