Response to Referee #2

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Manuscript:

Innerkofler, J., Kirchengast, G., Schwärz, M., Marquardt, C., and Andres, Y.: *GNSS radio occultation excess phase processing for climate applications including uncertainty estimation*, Atmos. Meas. Tech. Discuss. [preprint], https://doi.org/10.5194/amt-2023-28, in review, 2023.

The authors thank the reviewer very much for the constructive and detailed feedback to the manuscript. We thoroughly considered all comments and carefully revised the manuscript accounting for them. Below are our point-by-point responses.

Comments by the reviewer are cited black upright, our responses are red. Line numbers used in our responses refer to the original AMT Discussions paper and text updates in the revised manuscript are quoted below in blue)

All citations referenced are provided in the bibliography of the revised manuscript.

Summary

This paper "GNSS radio occultation excess phase processing for climate applications including uncertainty estimation" by Innerkofler et al. describes a new RO excess phase processing system including excess phase uncertainty estimation for Metop series satellites. The excess phase profiles derived with such system are compared against those from different processing centers with different POD and excess phase algorithms. The uncertainty estimation of excess phase thus can be helpful to trace the excess phase errors back to SI standard. The main purpose of such "reprocessing" of operational missions is to provide climate quality data records. First there indeed exist the needs in RO community for reprocessing of Metop A/B/C excess phase datasets for inter-center comparison so that the structural uncertainties in the dry temperature can be traced back to excess phase or observational level. There are CDR products from EUMETSAT ROM SAF, but their RO products are based on existing excess phase profiles from other processing centers. UCAR CDAAC also has different versions of RO datasets for the same missions. Second, determining the uncertainty of RO bending angle retrievals are often limited to local spectral width (LSW), which is hard to connect with the excess phase uncertainty. Thus this study, the excess phase processing with uncertainty estimation, is scientifically important and a significant contribution to GNSS RO community, not only because it can be used for quality control for excess phase profiles, but also because the excess phase uncertainties can be further possibly quantified to derive the bending angle uncertainties. Technically, the processing system uses improved GNSS/Leo POD solutions, follows the standard excess phase processing procedure adopted by other missions/centers but with rigorous quality control. It uses the zero-differencing clock bias removal algorithm which depends on the ultra-stable clock onboard the Metop-

Satellites. The RO excess phase processing algorithm description is solid and covers all the related aspects. The quality control relies on the excess phase modeling, including geometric and atmospheric modeling, which is a significant step in excess phase algorithm. Overall, the excess phase processing of three three-months periods for Metop A/B/C shows successful reprocessing of Metop RO excess phase profiles, with uncertainty estimation, and within expected differences compared with datasets from other centers. The system can be used to generate a long time series for climate applications. Overall, this paper is well written and organized, with technical description in details, and presents the results clearly. The logic of the study is scientifically sound. The excess phase uncertainty estimation can be applied to other missions. I recommended this paper to be published at AMT after some minor revision.

Thank you for the valuable feedback, and your further specific suggestions below that helped to improve our manuscript.

One thing we want to point out here is that EUMETSAT ROM SAF, as application facility of the satellite data, has their own excess phase retrieval for the Metop satellites.

I am little bit concerned the large difference in excess phase in lower atmosphere (Figure 15) from UCAR. What's the main reason caused the large difference in standard deviation/biases? Is this related to how the excess phase model and/or the filtering/smoothing algorithm used for excess phase processing? The author should explain that in depth. Is this a proof that the actual uncertainties maybe larger than proposed (e.g: the STD compared with UCAR at 3.5 km MSL is more than 40cm, but the uncertainty in excess phase is less than 4cm.)?

In this study we aim for an uncertainty estimation of the observational data; the inter-comparison of excess phase data from different processing centers might include additional structural uncertainties due to the different processing schemes not captured in the uncertainty budget. In particular, the larger deviation of UCAR data in the lower troposphere indicates representation uncertainties from until yet unknown sources. The authors believe that the characteristics of the differences indicate an issue in the processing in the transition of closed loop and open loop measurements. To reassure this assumption. further research will be needed which could be a valuable future task within a broader inter-center comparison (similar to what, e.g., Steiner et al. (2020) did along the retrieval step from bending angle to atmospheric profiles retrieval). We included the following text in the summary & conclusion section of the manuscript:

"We note that the results from the inter-comparison between excess phase data processed by EUMETSAT, WEGC, and UCAR experience larger differences in the lower troposphere than we quantified in the uncertainty budget. This indicates additional structural uncertainties arising from different processing schemes not captured in the estimated uncertainties of the observational data. In order to address this substantial differences a broader inter-center comparison study is advised."

Though the excess phase uncertainty estimation is important, how this uncertainty can be translated into the Doppler shift and then into bending angle is not clearly mentioned. Some discussion on how the excess phase uncertainty propagates further into bending angle should be given for the cases given. After all, the bending angle or derived temperature products are the Essential Climate Variable.

In the revised manuscript we now provide a paragraph discussing the propagation of the estimated uncertainties at excess phase through the subsequent retrieval chain. A detailed discussion of the uncertainty propagation from excess phase to bending angle is provided by Schwarz et al. (2018), which is one of the references in the manuscript. The added paragraph is as follows:

"The random and systematic uncertainty estimates at excess phase level are then propagated through the entire ODP retrieval chain in order to provide the final ECVs with their associated uncertainties. Additionally, the uncertainties quantified are employed in part of the retrieval operators of rOPS to improve the derivation of variables (e.g., ionosphere correction, statistical optimization, moist air retrieval). For details on the uncertainty propagation along this chain, starting from the estimates at excess phase level, see Schwarz et al. (2017, 2018); Schwarz (2018); Li et al. (2019)."

Technically, the excess phase processing in this study seem ignored both the GNSS and LEO satellite attitude information, please explain in detail how this can affect the error budget in excess phase.

Thank you for this relevant point; for the LEO attitude we considered nominal attitude with the assumption that for a satellite with a stable orientation like Metop the deviation compared to the application of measured or modeled attitude is small. However, within the ROM SAF validation activities it was found that this causes some residual biases at bending angle level (Alemany et al. 2022). However, with the scheduled implementation including quaternions in rOPS in a next update of the system this remaining weakness will be resolved. The impact of disregarding GNSS attitude is considered insignificant. Hunt et al. (2018) found that the effect of omitting GNSS attitude and phase center offsets amount for approximately 0.001 mm/s deviation in the Doppler shift, which is a negligibly small effect.

Figure 15, please explain why the STD profiles in figure 15 (e.g. left dotted line and right dotted line in any subfigure) are not symmetric even systematic bias approaches zero?

The STD shown in Figure 15 represents the 16 % and 84 % percentiles, indicating asymmetric distributions of the difference profile ensembles. We now note in the figure caption that percentiles are depicted.

Minor Comments:

Line 63, Is excess phase measurement accuracy/uncertainty really SI traceable given the excess phase model used, the GPS bit time series used, and the cycle slip correction uncertainty in the lower atmosphere?

In principle RO measurements are SI-traceable to the universal time standard. However, the use of auxiliary data in the processing and limitations in the tracking system, such as cycle slips, to some degree impede SI-traceability and the quality of the measurements. With rigorous handling of the auxiliary data, the modeled excess phase, and uncertainty budget, we aim to keep these influences as limited as possible.

Figure 2, Are the attitude data belong to the auxiliary datasets from IERS? Aren't they provided by the mission operation?

Yes, the LEO attitude information is usually provided by the mission operator in form of either measured or simulated Euler angles or quaternions. In case of Metop, EUMETSAT provides a yaw-steering model (EUMETSAT2005) and UCAR corresponding daily attitude files. We updated Figure 2 accordingly.

Line 106, In table I, I believe the LEO attitude is important and should be labeled. It looks the usage of the LEO attitude is optional. But how could you convert the antenna offsets from space body frame to ECI without attitude/quaternion information?

As stated in line 394 of the manuscript, the attitude correction using quaternion information is not yet implemented for Metop in rOPS. The conversion of the antenna offsets is based on nominal attitude of the satellite with the assumption that for a satellite with a stable orientation like Metop this correction is small. However, within the ROM SAF validation activities it was found that this causes some residual biases at bending angle level (Alemany et al. 2022). The team is currently working on the implementation of the attitude correction in rOPS. Also, more detailed information is now included in the manuscript but we do not include LEO attitude information in Table 1, since it could not yet be used for the calculations in this study. The added information reads:

"Corrections for the changing orientation of the satellite in space and the deviation from nominal attitude during orbital revolution are not yet implemented in rOPS. However, although for missions with stable orientation like Metop this correction is small, it was found that not applying the correction introduces a small residual bias in bending angle data (Alemany et al., 2022). Therefore, it is treated as a priority to include this correction in a next version of rOPS. On the GNSS transmitter side, neither GNSS antenna offsets nor attitude are modeled, since they have a far smaller effect on RO processing than the LEO antenna offsets (Hunt et al., 2018)."

Line 130, does this reconstruction include the POD phase/pseudo-range also (RINEX files)?

No, the reconstruction does not include raw navigation tracking data from the RINEX files, but the receiver and transmitter clock biases as well as position and velocity determined in the precise orbit determination. These data are needed to reconstruct the raw occultation measurement time stamps and for un-differencing of the NCO phase from the EUMETSAT L1a data files.

Line 138, I believe UCAR have a more specific data address (url) to point to the exact location of the datasets used.

Right, thank you for the comment. The new CDAAC data interface contains DOIs of the respective datasets. This information has now been added to the manuscript. We also seized the opportunity to as well add more specific information on the EUMETSAT data. It now reads:

"In this study publicly available excess phase profiles from EUMETSAT (https://eoportal.eumetsat.int; 2008/2013-JAS: DOI: 10.15770/EUM_SEC_CLM_0015, processor: YAROS-1.4; 2020_DJF: processor: GRAS-4.6.2) and CDAAC (Metop-A: DOI: 10.5065/789w-m137, version: 2016.0120; Metop-B: DOI: 10.5065/1k0w-2272, version: 2016.0120; Metop-C: DOI: 10.5065/p8es-mc74; version: 2019.2580) have been used for such intercomparison (Sect. 4.2)."

Line 205, this has puzzled me. I think this is different from that used by UCAR. At the mean event time, the straight line may not be tangent to the WGS-84 ellipsoid surface. Unless the tangent point can be defined first and then the time difference (really small though) can be neglected. Please explain. How sensible the different profile location definition can affect the excess phase quality control (atmospheric modeling), especially at lower atmosphere?

Yes, we are using a slightly different definition for the occultation's reference point that is only depending on geometry and not on the atmospheric state or the specific duration of the actually tracked occultation event (and yes, this is why these mean tangent point locations can be computed beforehand and are independent of the occultation profiles retrieval process). Specifically, the mean event time is the time when the straight-line connection between GNSS and LEO is tangent to (i.e., just touches) the Earth's Ellipsoid, i.e., it is the time when the mean tangent point location is visited. We updated the description in the manuscript for better understanding as follows:

"The selected reference location of an event is defined on the Earth's ellipsoidal surface at the time when the straight-line connection between receiver and transmitter satellite is tangent to the Earth's surface (WGS-84/EGM2008, cf. Figure 3 for measurement geometry)."

Line 240, 'is used T and ln(p)', should be 'is used for T and ln(p)'? It would be better to give a reference for this interpolation scheme or a reason why these schemes are the best (e.g. ROPP manual compares different interpolation schemes). Different interpolation scheme can certainly affect how the bending angle bias look alike in different altitude.

Thank you, this is correct; the sentence was adapted in the manuscript. The horizontal 4-point polynomial (cubic) interpolation was adapted from a scheme originally implemented by M. E. Gorbunov (a detailed description was included in the PhD thesis of Lackner, 2010; Appendix A.3 therein). For vertical interpolation, several interpolation methods were compared and the most suitable selected. We included improved information on this as follows:

"Horizontal interpolation is performed by using a 4-point cubic-polynomial interpolation technique (for a detailed description see Lackner, 2010). For vertical interpolation of *T* and ln(*p*) several interpolation methods were compared (linear, cubic-spline, Savitzky-Golay filter) and the most robust fit through the nodes of the ECMWF altitude levels was selected. As a result, the vertical interpolation to the fixed-altitude grid z is performed for T and $\ln(p)$ using a natural cubic-spline interpolation, while the q profiles are interpolated linearly."

Line 260, the angle ζ should be between the velocity vector and the leo position vector, please label correctly in Figure. 3.

Thank you for noting, the angle ζ is now labeled correctly in the updated version of the manuscript.

Line 285, Carries phase can't be called phase pseudo-range, since the time measurements and phase measurements use different mechanisms in GNSS positioning techniques. It would be more appropriate to use its name 'carrier phase' than 'phase pseudo range.'

In line 285, the term "phase pseudorange" is just used in brackets, for introductory purposes, in order to also point to the terminology in the widely used book by Hofmann-Wellenhof et al. (2008). In line 287 we do clarify that more commonly the term "carrier phase" measurements is used. We don't use the term "pseudorange" in the remainder of the paper.

Line 337, Rewrite Eq. 5 to be consistent with Eq. 4, such as the ionosphere correction has opposite sign with atmospheric delay term, missed C in the third item in Eq. 5, inconsistent sign (+/-) between receiver/transmitter clock bias correction, etc.

Thank you for the detailed review of the equations. We corrected the formulae as proposed.

Line 346-349, some terms are misleading. You do not need to correct the clock bias, but to remove it. the antenna offset needs to be calculated in the proper coordinate system and added to the mass center of the satellites. The distance is not between satellites, but between receiver and transmitter antennas (pcvs/or offset since pcvs may not be used here). Please rewrite accurately.

Thank you, the text passage was re-written accordingly, as follows:

"This process includes the removal of receiver and transmitter clock biases, relativistic corrections, the calculation of the signal travel time, proper coordinate transformation of the antenna offsets and addition to the satellite's COM, and the calculation of the geometric distance between receiver and transmitter satellite antennas (see Figure 6)."

Figure 6 and from other context, why the LEO/GNSS satellites attitude input is optional? Are all the antennas offsets/pcvs defined in such a way that the attitude is not needed? How does this affect the error budget and excess phase itself? If attitude are not needed, you may also need to explicitly explain how the antenna offsets are applied.

Please also see the answer regarding the LEO attitude above.

Line 395-397, I do not understand the sentence ' common coordinate transformation from satellite body frame to ECI', isn't this the satellite attitude information (usually given as quaternions).

This is referring to the coordinate transformations of the LEO RO antenna offsets, which are defined in the satellite body frame assuming nominal attitude, to ECI. This step is needed to successfully and properly apply the offsets to the satellite's position and velocity (also given in ECI). As stated in Line 394-295, and discussed in other comments in this response to the reviewer, the attitude information is not yet taken into account, but will (in a next update of the system) be inserted exactly at this step of the processing.

Line 410: Here the time delay correction does not consider the GNSS antenna offset. There is neglected time bias of about 2/C (assume GNSS antenna offset length of 2m) about 7 ns. Please justify how this affects the excess phase calculation with zero-differencing methods. For single differencing, this may be absorbed by differencing itself.

This is considered to be a small effect, since the pointing of the GNSS antenna is very stable over the short duration of an occultation, and the non-time dependent part of this effect will cancel out in the derivation of the excess phase to Doppler. Hunt et al. (2018) found that the effect of omitting GNSS attitude and antenna offsets only amount to approximately 0.001 mm/s deviation in the Doppler shift, which is a negligibly small effect.

Line 436-437, down sampling of RS data to 50HZ, the authors used the 20 samples arithmetic mean. Please explain how the 20 samples arithmetic mean affect the cycle slips (if not corrected yet) especially for lower atmosphere.

The cycle slip correction is performed right before the down-sampling based on the 1000 Hz RS (I/Q) data. Cycle slips remaining undetected by this step will increase the arithmetic mean of the respective sample and can only be accounted for in the uncertainty budget.

Line 453, the Metop POD antenna are not designed to track high rate GNSS signals thus the single differencing may not be effectively used (as COSMIC does) with low rate POD antenna observations.

Exactly, for the application of the single differencing method for the Metop mission, the reference link data measured at the zenith antenna with 1 Hz would need to be up-sampled to match the 50 Hz high-rate occultation link data. This introduces additional noise and reduces the quality of the calculated excess phase data. Therefore, for RO missions with ultra-stable onboard oscillators (USOs, like on Metop), the preferred method is to eliminate the LEO clock errors using the clock biases estimated in POD (i.e., to apply zero differencing).

Line 505, Aren't the sampling rate defined at the receiver time with a constant interval? Please explain what caused the drift.

The raw measurement time stamps of GRAS exhibit a frequency offset and irregularities due to external temperature changes (Montenbruck et al., 2008). The frequency offset is corrected for and resulting time stamps are (very) slightly deviating from nominal sampling rate. From Table 4 we can see that for Metop data this obviously is not an issue, however, since for no Metop profile considered in this study the sampling check failed (i.e., we observe a rejection rate of 0 %).

Line 549, what's the criteria to use 7.5 m/s.

The value was empirically derived by detailed sensitivity examinations from analyses of event ensemble from multiple RO missions (done within the work of Seidl 2018).

Line 614, DLL already defined at line 310.

Thank you, now the acronym is introduced only at line 310.

Line 619, please define the t_{bot}^{DLL} and t_{top}^{DLL}. This looks quite small. Given one minute of travel time in the lower atmosphere, the cycle slip error is only 0.001m=1mm? If this is true, how do you explain large excess phase difference in lower troposphere between different processing centers?

Regarding the larger excess phase differences in the lower troposphere, please see the "main comments" section of this review above. However, we re-checked technical Metop documentation for a more reliable quantitative estimate. We did not come over a clear quantitative estimate but agree that the current setting was clearly too small. We now try to better reflect the effect by adopting a more plausible change of 1 mm/s, i.e., reflecting a 1% slip fraction per second relative to the half-cycle length (about 10 cm), more consistent with the documentation.

Therefore, to account for these undetected cycle slips as an estimated basic uncertainty, we include a change-rate factor c = 1 mm/s, reflecting a 1% slip fraction per second relative to the half-cycle length. This leads to a gradual excess phase decrease (cumulative negative bias) with decreasing altitude from the time of highest altitude t_{top}^{DLL} to lowest t_{bot}^{DLL} in DLL measurement mode:

Line 655, Why does the Metop-C have less daily RO profiles than Metop-A/B?

In the 2020-DJF period Metop-B/C feature a similar number RO profiles. In the earlier measurement periods 2008-JAS and 2013-JAS we can observe larger numbers of RO profiles per satellite. The decrease in the number of profile counts in the later 2020-JAS period is due to missing closed loop observations in the input data. We added the following declaration to the revised manuscript:

"Overall, on average, the daily number of profiles amounts to 647 profiles (Metop-A), 610 profiles (Metop-B), and 559 profiles (Metop-C). In the later 2020-JAS period EUMETSAT input data contains files with missing closed loop (either L2 or both frequencies), which reduces the number of processed event in this later study period."

Line 731-732, it is hard to follow what the authors talk about. Are they trying to compare the setting and rising differences in total profile numbers or to compare inter-center difference?

Here we refer to Figure 13 and the total number of difference profiles depicted as function of altitude therein. As described it can be observed that differences between the number of setting and rising occultations exist in dependence of the altitude.