

Standard RO Inversions in the Neutral Atmosphere 2013 - 2020 (Processing Steps and Explanation of Data)

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Hereafter: TX is transmitter (GNSS); RX is RO receiver (in LEO).

Input data

'atmPhs' files contain times, positions and velocities of the TX and RX, excess phases and SNRs (multiplied by 10) sampled at 50 Hz rate. The excess phases are corrected for the TX and RX clock drifts. The positions and velocities are specified in the inertial reference frame with z-axis pointed to the North Pole. The time tags correspond to the reception times. Additionally, atmPhs files contain receiver phase and range models used in the open loop (OL) mode. In the closed loop (CL) mode, these models are set to -999.

'gpsBit' files contain time sequences of the navigation data modulation (NDM) bit flips (0,1) collected by ground receivers from occulted TX during the time intervals that cover the time intervals of the occultations. Each sample has the quality flag (0,1). The time tags correspond to the transmission times. The 'gpsBit' files are created for all occultations, but they may be empty if NDM data was not available.

The file containing bending angle model calculated from CIRA+Q refractivity climatology for different latitudes (step = 10 deg) and months (step = 1 month) [Kirchengast et al., 1999]. Used as the reference model for processing OL data in the troposphere.

The file containing refractivity profiles calculated from NCAR climatology [Randel et al., 2002] for different latitudes (step = 10 deg) and months (step = 1 month). Used as the background model for optimizing bending angles in the stratosphere to minimize the error propagation before the Abel inversion.

Retrieval of the profiles (processing steps)

- 1) Calculation of the array of heights of straight-line TX-RX over the reference-ellipsoid using positions of the TX and RX.
- 2) Reversing of the data order for rising occultations (by converting all occultations to setting).

3) Calculation of the number of samples corresponding to Fresnel's scale in a vacuum for the distance from RX to limb and the time derivative of the height of straight line.

4) Calculation of L1 Doppler model (for each data sample) based on TX and RX orbits [Sokolovskiy, 2001] and refractivity climatology [Kirchengast et al., 1999]. This is the post-processing model, different from the model used in RX.

4.1) Calculation of the zenith angles of rays for the CIRA+Q bending angle model and positions of the TX and RX. Bending angles and impact heights over the reference ellipsoid are also calculated.

4.2) Calculation of the Doppler frequency shifts from positions, velocities and ray zenith angles at the TX and RX.

5) Detection of the presence of raw open loop (OL) data.

6) Processing of the raw OL data (if detected) [Sokolovskiy et al., 2009A].

6.1) Calculation of the phase model by integration of the L1 Doppler model.

6.2) Down-conversion of the raw RO signal (un-connected phase, which includes the receiver phase model) by use of the L1 phase model. Operations described in the steps (6.4-6.8) are performed on the down-converted RO signal.

6.3) If gpsBit file is not empty, then alignment of the NDM replica with RO signal using time tags and propagation time between TX and RX. If gpsBit file is empty, then go to the step (6.7).

6.4) Check the NDM bit quality in the OL section of RO signal. If at least one sample has quality flag '0', then go to the step (6.7).

6.5) Removal of the NDM from the RO signal by applying replica (adding pi to the phase when the phase flip is detected from the replica).

6.6) Check for miss-alignment of the NDM replica with RO signal (this happens rarely, likely due to shifting of the time tags by receiver). Calculate the rms of the phasor rotations between the adjacent samples for the top 1 sec of the OL data (where the troposphere-induced modulation is minimal). Repeat this calculation by shifting NDM replica within a limited time interval. For most of the occultations, the minimum of the rms is at the shift = 0. If the minimum is found at a shift other than zero (typically,

several samples), then that shift is used to align the NDM replica. In this case, the occultation is processed, but the output parameter alerting about NDM replica misalignment using time tags, is generated.

6.7) Removal of NDM from RO signal without a replica. When the modulo of the phasor rotation angle between the adjacent RO samples exceeds $\pi/2$, the phasor is inverted (π is added to raw phase).

6.8) Connection of the phase. Adding $2*\pi$, 0 or $-2*\pi$ (whichever minimizes the modulo of the phasor rotation angle between adjacent RO samples) to the phase.

Comment: steps 6.7 and 6.8 are similar to signal processing in RX operating in PLL mode and extracting phase in 2 quadrants, except there is no feedback (dependency of the model on previously extracted phase).

6.9) Up-conversion of the NDM-removed, phase-connected RO signal with the post-processing phase model.

6.10) Output of the auxiliary (diagnostic) data: the differences between the receiver and the post-processing Doppler and range (integrated Doppler) models; phasor rotation angle between adjacent samples; the sliding spectrogram of the NDM-removed RO signal.

7) Correction of the L2 phase: replacement of the -999 (in OL mode) by the model (to reduce the edge effect after filtering) and correction of the full cycle slips (in CL mode).

8) Estimation of the optimal window win-opt for the filtering of L4 bending angle used to correct L1 bending angle. This is based on the minimization of the fluctuation of LC Doppler at 60-80 km [Sokolovskiy et al., 2009B]. The optimal window win-opt is searched in the interval between the window defined for L1 win-1 (step 3) and 3 times larger window win-2.

9) Filtering of the excess phases and calculation of the Doppler frequency shifts. The filter: sliding polynomial regression (Savitzky-Golay filter, [Press et al., 1992]) of the 3rd order applied 3 times (to suppress high frequencies). Both L1 and L2 phases are filtered with three windows: win-1, win-2 and win-opt (see step 8).

10) Truncation of the RO signal at the bottom of an occultation.

10.1) For the CL data, the truncation is based on the difference between the L1 Doppler filtered with the window win-1 and the L1 Doppler model. The RO signal is checked

from the top toward the bottom. When the difference for the first time increases above the threshold value (10 Hz), the RO signal is checked from that point backward and truncated at the point where the difference first time decreases below the threshold value (5 Hz).

10.2) For the OL data, the truncation currently is based on the SNR [Sokolovskiy et al., 2010].

10.2.1) The L1CA SNR is boxcar-filtered with the window set to 1.5 sec. The minimum of the filtered SNR is determined and used as the reference snr-min.

10.2.2) The filtered SNR is checked from bottom to top. When it increases first time above threshold value ($3 * \text{snr-min}$) then:
the filtered SNR is checked backward (from top to bottom); when it decreases first time below threshold value ($1.5 * \text{snr-min}$), then:
the filtered SNR is continued to be checked from top to bottom until it stops to decrease; this is the truncation point.

10.2.3) The minimum of the RMS-averaged SNR in the sliding window 1.5 sec also is calculated and provided on output as the scalar parameter.

11) Calculation of latitude and longitude of ray tangent point from the position vectors of the TX and RX, the standard bending angle (calculated in step 4.1) and the Snell's equation.

12) Calculation of the azimuth of the occultation plane (counted from the direction to North) at the ray tangent point from the position vectors of the TX and RX and latitude and longitude of ray tangent point (calculated in step 11).

13) Calculation of latitude and longitude of the conventional "occultation point" (a scalar parameters assigned to retrieved profiles). This point corresponds to the excess phase equal to 500 m.

14) Calculation of the center and radius of local curvature of the reference ellipsoid at the "occultation point" (calculated in step 13) in the direction of the azimuth (calculated in step 12) [Syndergaard, 1998].

15) Calculation of the positions of the TX and RX in the inertial reference frame with the center shifted to the center of local curvature of the reference ellipsoid (calculated in step 14). These positions are used in step (17).

16) Conversion of the longitudes from the inertial to the Earth-fixed reference frame by accounting for the rotation angle for a given observation time.

17) Calculation of L1 and L2 bending angles and impact parameters from L1 and L2 Doppler frequency shifts, positions (calculated in step 15) and velocities of the TX and RX [Kursinski et al., 1997]. Bending angles are calculated from the Doppler shifts obtained by smoothing the excess phases with three filtering windows defined in step (9).

18) Correction of ambiguities: approximation of the multi-valued bending angle as function of impact parameter by single-valued function (does not change the single-valued bending angle).

19) Quality check of L2 signal.

19.1) Calculation of the maximal differences between the raw L1 and L2 excess Dopplers in the impact height intervals 40-60 km and 60-80 km.

19.2) Calculation of the height below which L2 signal is considered low quality based on the criteria: (i) high-pass filtered L2 excess Doppler exceeds threshold-1 or (ii) the difference between low-pass filtered L1 and L2 excess Dopplers exceeds threshold-2. This height may be used (optionally) for dynamic transition between the standard ionospheric correction and extrapolation.

20) Wave optics processing (phase matching) [Jensen et al., 2004].

20.1) Calculation of the impact height (impact parameter minus local curvature radius) grid with the step 1 m. Bottom height = 0 km. Top height = settable parameter (currently 20 km) + 1 km (to eliminate filtering edge-effect).

20.2) Calculation of the bending angle on the impact height grid defined in step (20.1) by phase matching. Step (20.2.1) is performed for L1 RO signal for all occultations. Step (20.2.2) is performed for L2 RO signal only if OL L2C is scheduled for wave optics processing. This is controlled by input parameter (currently not applied for standard processing).

20.2.1) For each impact height, the complex integral (Re,Im), which transforms RO signal from coordinate to impact parameter representation, is calculated analytically, by using linear interpolation of the connected phase and mean constant amplitude (SNR) between high rate samples. For each impact height, the location of the main stationary point (absolute local minimum of the phase) is calculated. When the stationary point is

closer to the end of truncated RO signal than pre-defined threshold, the flag is set (this flag can be used for optional conservative truncation of the retrieved bending angle profile). The raw phase of the calculated complex signal (integral), $\text{atan2}(\text{Im}, \text{Re})$, is connected in the same way as in step (6.7). The frequency, calculated from the raw connected phase, is low-pass filtered and the smoothed (reference) phase is subtracted from the raw phase. The residual phase is re-connected and appended back to the reference phase. Alternatively, the residual complex signal is low-pass filtered, the phase is extracted, connected and appended back to the reference phase; this is the radio holographic filtering introduced by [Gorbunov et al., 2006]. The bending angle is calculated from the frequency of the transformed RO signal with or without the radio-holographic filtering (the use of the filtering is controlled by settable parameter). This step is done for L1 RO signal for all occultations.

20.2.2) If OL L2C data were detected and scheduled for wave optics processing, then the step (20.2.1) is applied for the L2 RO signal.

20.3) Low-pass filtering of the L1 and L2 bending angles. This is done with three windows (currently 100 m, 225 m, and 500 m). The three low-pass filtered bending angle profiles are merged at the two impact heights (currently, 7 km and 10 km). Transition is performed by applying smooth transition functions in the intervals 1 km.

20.4) Truncation of the retrieved bending angle profile. Calculation of the averaged value of the PM-transformed amplitude between 10 and 20 km, A_{max} . Three options: (i) the impact height where amplitude first time increases above $A_{\text{max}}/2$ (least conservative); (ii) the impact height where amplitude first time decreases below $A_{\text{max}}/2$ (most conservative); the transition height of the step-function least squares fitted to the raw transformed amplitude.

21) The low-pass filtered wave optics bending angle profiles are sampled on the output impact height grid. The output grid is defined above the lowest point based on the wave optics truncation by using 20 m step. The output grid extends to the top of an occultation or 150 km (whichever is higher). Sampling of the wave optics bending angle profile does not require interpolation. The geometric optics L1 and L2 bending angle profiles are linearly interpolated on the output grid.

22) The wave optics and the geometric optics L1 and L2 bending angle profiles are merged at the settable height (currently 20 km), by applying smooth transition function in the interval 1 km.

23) Above the settable transition height for extrapolation of the ionospheric correction (by default, 20 km), the function defined in [Zeng et al., 2016] is fitted to L1 - L2 geometric optics bending angle profile.

24) Above the transition height for extrapolation of the ionospheric correction, the L3 (ionosphere-free) bending angle is calculated by correcting L1 bending angle (win-1, see steps 8, 9) with the optimally smoothed L4 = L1 - L2 (win-opt, see steps 8, 9) bending angle [Sokolovskiy et al., 2009B]. Below, the transition height, the L1 bending angle is corrected by extrapolation of the function calculated in step (23) [Zeng et al., 2016]. The transition interval is 1 km.

25) Interpolation of latitude, longitude and azimuth profiles (defined in steps 11, 12 with the use of the step 4.1) on the standard output impact height grid (defined in step 21).

26) Optimization of the bending angle profile.

26.1) Calculation of the standard refractivity profile for the day of an occultation and the latitude and longitude (defined in step 13), for the NCAR climatology model [Randel et al., 2002]. Interpolation in height is log-spline. Interpolations in latitude and day are linear.

26.2) Calculation of the standard bending angle profile as function of impact height on the standard output impact height grid (defined in step 21), from the standard refractivity profile (calculated in step 26.1). Hereafter this profile is called 1st guess.

26.3) Mixing the observational L3 bending angle profile with the background profile.

26.3.1) Merging (mixing) the optimally smoothed observational L3 bending angle profile (L1 is smoothed with the win-1 and L4 is smoothed with the win-opt, see steps 8, 9) with the more heavily smoothed observational L3 bending angle (both L1 and L2 are smoothed with the win-2, see steps 8, 9). The transition interval is settable (currently, 30-40 km).

26.3.2) Fitting the $c \cdot (\text{1st guess})^b$ bending angle profile (26.2) to the observational bending angle profile, thus solving for coefficients c and b . This is done by direct fitting (as opposed to linear fitting in the logarithm space). Hereafter, this profile is called the fitted 1st guess. The fitting interval is settable (currently is set to 35-60 km).

26.3.3) Merging (mixing) the bending angle profile calculated in step (26.3.1) with the fitted 1st guess calculated in step (26.3.2). The transition interval is settable (currently is set to 35-60 km).

26.3.4) Merging (mixing) the bending angle profile calculated in step (26.3.3) with the 1st guess profile (26.2). The transition interval is settable (currently is set to 55-65 km). Hereafter, this profile is called the optimized bending angle profile.

27) Abel inversion of the optimized bending angle profile [Kursinski et al., 1997]. The integration starts at 150 km (this does not require explicit specification of the upper boundary condition).

28) Correction of the heights and impact heights for the geoid undulation calculated for the latitude and longitude of the occultation point (defined in step 13) and the JGM-2 geoid model.

29) Calculation of the pressure and temperature profiles using the equation for refractivity, the hydrostatic equation and the equation of state for dry air. Optionally, the temperature can be initialized at a settable height (currently this initialization is not used, i.e. both pressure and temperature are implicitly initialized by the climatology-based 1st guess).

Output scalar parameters

There is a set of 80 output scalar parameters briefly explained in the atmPrf files. The parameters, related to the boundary layer, the tropopause and the sporadic E-layer, are explained below in more details.

1) The height of the strongest inversion layer. This height is commonly used as a proxy for the depth of the boundary layer over the regions where the top of the boundary layer is well pronounced (such as the sub-tropical ocean west of continents). There are several proxies for this height explained below.

1.1) The height of the maximum bending angle lapse. This height is calculated by maximizing the cost function, calculated on the bending angle as the function of impact height [Sokolovskiy et al., 2007]. The impact height is converted to TP height after the Abel inversion.

1.2) The height of maximum refractivity lapse. This height is calculated by finding maximum of the refractivity (retrieved as function of height by Abel inversion) lapse in the running window of fixed length (currently, the length is set to 300 m).

1.3) The height of most pronounced break point of the refractivity profile (the refractivity is the function of height, as in 1.2). This height is calculated by finding maximum angle between linear regressions in two adjacent running windows of fixed lengths (currently, the lengths are set to 300 m).

2) The height and temperature of the tropopause. The two definitions are used: (i) the cold point and (ii) the WMO definition of the 1st and 2nd tropopause.

3) Detection of the sporadic E-layers (structures), the corresponding TP heights and vertical thicknesses of the structures [Zeng and Sokolovskiy, 2010].

Output data

'atmPrf' file contains 13 main and 2 additional vectors (profiles), and 80 scalar parameters. There are two reference vectors (arguments). 1) The impact height over the geoid sampled with constant 20 m step above the truncation point (20.4) which is the argument for bending angle. 2) The corresponding height of tangent point which also is the argument for bending angle and simultaneously the argument (as the height over the MSL) for the retrieved local atmospheric parameters, refractivity, pressure, temperature. The vectors (functions) are : L1 and L2 bending angles; L3 (ionosphere-free) bending angle, proxy for L1 bending angle error; L1 bending angle confidence parameter; latitude; longitude; azimuth; refractivity; pressure; temperature.

The 2 additional vectors (profiles) are explained below (in retrieval changes).

Error estimation

Error estimation is applied below the height used for extrapolation of the ionospheric correction (currently set to 20 km). A proxy for the BA error is calculated from the local spectral width (LSW) of L1 RO signal transformed to impact parameter representation by the phase matching. The LSW is estimated in the sliding window after down-conversion of the transformed signal by the reference model - the low-pass filtered phase. The LSW is estimated by least squares fitting of the simple analytical model to the power spectrum [Liu et al., 2018]. The LSW is assigned to the center of sliding window. The LSW estimated as the function of impact height is subject to low-pass filtering. The LSW represents the uncertainty of BA related to the effect of non-spherically symmetric

irregularities in the lower troposphere. The LSW is not an absolute rms error, but a proxy, i.e., should be subject to empirical scaling to convert to absolute error.

Quality control

Preprocessing check

Occultations are not inverted unless the top tangent point altitude is above 60 km and the bottom tangent point altitude is below 10 km.

Quality control tests in retrieved profiles

Inverted occultations are tagged 'BAD' when any of the following applies (current settings of QC parameters are used):

- 1) Maximum relative difference between bending angle and climate model between 25 and 40 km exceeds 0.25.
- 2) Standard deviation of the relative difference between bending angle and climate model between 25 and 40 km exceeds $3E-5$.
- 3) Maximum relative difference between refractivity and climate model between 10 and 60 km exceeds 0.5.
- 4) L1 SNR averaged between 60 and 80 km is less than 200 V/V
- 5) Maximum absolute difference of L1 and L2 excess phase finite differences between 20 and 40 km exceeds 0.1 m/sample
- 6) Standard deviation of the difference between bending angle and climate model between 60 and 80 km exceeds $1.5E-4$ rad.
- 7) Mean difference between bending angle and climate model between 60 and 80 km exceeds $1E-4$ rad.

Updates applied in 2020

New input files

'conPhs' files contain same information as atmPhs files, but additionally NDM is removed and phase is connected. This is done in the separate code which is based on steps 4-7 of the inversion code (2013-2020) with some modifications.

The inversion code can use conPhs and atmPhs + gpsBit files. The way of handling of the input file is determined automatically.

Retrieval updates

- 1) When conPhs file is detected on input, steps 5-7 in the inversion code are bypassed.
- 2) Phase matching is revised.
 - 2.1) The hard-coded parameters which control the radio holographic filtering are replaced by input parameters.
 - 2.2) BA error estimation based on LSW is revised and included in the phase matching code. Updated calculation of the LSW includes three different options (definitions). Selection of the option for output is controlled by input parameter.
 - (i) Least squares fitting of the model to local spectral power as function of the frequency [Hui et al., 2018].
 - (ii) Weighting of the local spectral power with the square of the frequency [Gorbunov et al., 2006].
 - (iii) Weighting of the local spectral power with the modulo of the frequency.Option (i) does not depend on the reference model, but has precision limited by spectral resolution. Options (ii) and (iii) depend on the reference model, but precision is not limited. Option (ii) more heavily weights spectral components with large deviations from the model than option (iii). Based on testing, currently option (iii) is selected and provided on output (included in atmPrf files).
- 3) Pre-processor which includes: additional down-conversion based on the spectrogram of RO signal in time representation, low-pass filtering and truncation based on the LSW, is added as an option (currently not enabled).
- 4) Down-sampling is added as an option (currently not enabled).

- 5) Truncation of retrieved bending angles based on the least squares fitting of step-function to transformed amplitude will be applied for all processing modes: real-time, post-processing and re-processing. Additionally, an optional conservative truncation height (based on the stationary point in the phase matching) is included as output parameter.
- 6) Parallel processing of L1 without L2 (using climatology above 20 km) for all occultations is included. The "L1 only" bending angle and tangent point height vectors and the scalar parameters (BA lapse, N break point) are calculated separately for each occultation and included in the atmPrf files.
- 7) A flexible option to use static or dynamic transition height for extrapolation of the ionospheric correction when L2 is "bad" is included. Options: (i) static always; (ii) dynamic always; (iii) dynamic when L2 is bad below the static height; (iv) dynamic when L2 is bad above static height.
- 8) For calculation of lat, lon profiles based on orbits and climatology, the following option is added: linear extrapolation below the point of maximum gradient. This may reduce the effect of negative bias of refractivity gradient in CIRA+Q climatology in the bottom 1 km on determination of lat, lon (needs further testing, currently not enabled).
- 9) Effect of topography on retrieved profiles is calculated. The following parameters are provided on output. (i) Flag (Yes/No) whether terrain affects the ray with the lowest retrieved height of tangent point obtained after standard truncation and Abel inversion. If Yes, then: (ii) the lowest height of tangent point of the ray not affected by terrain; (iii) the highest terrain point along the ray paths and its height, lat, lon.
- 10) Detection of the tropopause is modified by changing the bottom height used to start tropopause search and by applying additional constraint on temperature. The former is needed to capture very low tropopause in high latitudes; the latter is needed to eliminate the effect of strong dry temperature variations not related to the tropopause.
- 11) Tops of all output vectors (profiles) are increased from 60 km to 80 km (needed for only the ionosphere-free BA, other vectors are filled by -999 between 60 and 80 km).
- 12) The list of output scalar parameters which characterize the retrieved profiles and can be used for QC is increased. All output scalar parameters are explained in the atmPrf files.

Comments

1) Processing of L1 without L2 (update 6) is aimed at obtaining useful information about ABL depth from significant number of COSMIC-1 rising occultations where L2 was either not acquired or acquired with low SNR and large tracking errors.

2) Dynamic transition height (update 7) currently is applied for COSMIC-2 L2P rising occultations only (all other occultations are processed with fixed transition height 20 km). This is because current L2P acquisition has a problem. Once the problem is resolved, this option will be disabled.

3) This document outlines basic standard processing. There may be some differences for different missions (for example, see comment 2 above) and processing modes (real-time, post-processing, re-processing). Available CDAAC datasets and other documentation may be viewed at <https://cosmic.ucar.edu/what-we-do/data-processing-center/data/>.

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