Algorithms for inverting radio occultation signals in the neutral atmosphere

This document describes briefly the algorithms, gives references to the papers with more detailed descriptions and to the subroutines used in the Fortran-77 code 'roam' which inverts radio occultation (RO) signals acquired by closed loop tracking. All inversion algorithms are based on the assumption of local spherical symmetry of refractivity in sufficiently large region (several hundred kilometers radius) around the occultation (ray tangent) point.

<u>Input data</u>: time (specified with constant increment), positions and velocities of the satellites (GPS and LEO) in inertial Cartesian reference frame, L1 and L2 excess phases and amplitudes.

<u>Output data</u>: L1, L2 and ionosphere free bending angles, impact parameter, neutral atmospheric refractivity and "dry" pressure and temperature, height over MSL, latitude and longitude of the estimated ray tangent point (in the Earth fixed reference frame) and azimuth of the occultation plane.

Inversion of radio occultation signals in the neutral atmosphere consists of the following steps.

1) Filtering (smoothing) of L1 and L2 excess phases and calculation of excess Doppler frequency shifts.

2) Truncation of RO signals based on Doppler climatology test.

3) Calculation of L1 bending angle from Doppler (geometric optics).

4) Estimation of the occultation (ray tangent) point and azimuth of the occultation plane.

5) Transfer of the reference frame to the local center of sphericity estimated under the occultation point.

6) Calculation of L1 and L2 bending angles from Doppler frequency shift (geometric optics).

7) Calculation of L1 bending angle by radio holographic methods from raw complex signal.

8) Combining (sewing) (6) and (7) L1 bending angles.

9) Ionosphere calibration of the bending angle.

10) Optimal estimation of the bending angle by use of climatology.

11) Retrieval of refractivity (Abel inversion).

12) Retrieval of "dry" pressure and temperature (by integration of hydrostatic equation).

1) Filtering (smoothing) of L1 and L2 excess phases and calculation of excess Doppler frequency shifts.

Noise in acquired L1 and L2 RO signals results in that the phase of RO signal is out of the space restricted by the assumption of spherical symmetry used in the inversion algorithms. This, in turn, results in that the bending angle calculated from Doppler (in geometric optics approximation) is a multi-valued function of the impact parameter. The multi-valued function may not be inverted by the Abel inversion. The noise is filtered from the excess phase prior to calculation of the bending angles and impact parameters in geometric optics. Two filters are used in the code. Both filters allow analytical calculation of derivative of the phase (Doppler). The choice of the filter is controlled by input parameter.

Fourier filter. The phase is subjected to Fourier transform. First, the spectrum is multiplied by windowing function of Gaussian shape. The width of the windowing function is the input parameter. The inverse transformed spectrum returns the smoothed phase. The smoothing window is inversely related to the width of the spectral windowing function. Second, the spectrum is multiplied by the windowing function and by imaginary frequency. Then the inverse transformed spectrum returns the smoothed derivative of the phase (Doppler). The discontinuities of the raw phase at the ends of time interval result in corruption of the returned (smoothed) function near the ends due to spectral aliasing. To suppress this effect, prior to the Fourier transform, the raw phase is extrapolated beyond the ends of the initial RO time interval with smooth transition to constant (zero).

Spline regression + Fourier filter. This method does not require extrapolation of the raw phase function beyond the ends of the initial RO time interval. The main trend from the phase is removed by cubic spline regression (least squares fit of the phase by cubic spline specified on a sparse grid). Then the residual phase (which varies around zero and does not have large discontinuities at the ends) is subjected to Fourier filtering and calculation of the residual Doppler. The derivative of the spline regression is calculated analytically, by differentiating cubic polynomial. Then the Doppler is equal to the sum of the Dopplers obtained from the spline regression and from the filtered residual.

The size of the smoothing window is controlled by input parameter.

Subroutines:

filter0.f – Fourier filtering of a function.

filter1.f – Fourier filtering of the derivative of a function.

filter.f – Spline regression + Fourier filtering of a function and of the derivative of the function.

2) Truncation of RO signals based on Doppler climatology test.

Truncation of RO signal is based on the magnitude of deviation of the observed (smoothed) L1 excess (atmospheric) Doppler from the Doppler calculated based on orbits (positions and velocities) and refractivity climatology (based on CIRA+Q model, Kirchengast et al., 1999). For large enough distance from limb to receiver, like ~3300km for COSMIC satellites, the fractional variability of the excess Doppler frequency shift of RO signal is much smaller than the fractional variability of the bending angle for a given height in the atmosphere. For COSMIC satellites the L1 excess Doppler variability must be ~ ± 10 Hz. When the difference of the observed and modeled Dopplers is larger, this indicates that most likely the acquired RO signal was subjected to receiver tracking errors. In this case the signal is truncated at earlier time, when the difference exceeds 5 Hz (the threshold for the truncation depends on LEO height). Calculation of the Doppler frequency shift from GPS and LEO orbits and bending angle model based on refractivity climatology is described by Sokolovskiy, 2001b.

Subroutines:

ray.f – calculates zenith angles of the ray connecting GPS and LEO for their given positions and for a given bending angle as function of impact parameter.

dop.f – calculates excess Doppler frequency shift for given positions and velocities of GPS and LEO and given zenith angles of the ray.

3) Calculation of L1 bending angle from Doppler (geometric optics).

Calculation of bending angle and impact parameter from Doppler frequency shift is described in step (6). At first, this is done in the original, Earth centered, reference frame for the purpose of estimation of the occultation (ray tangent) point.

Subroutines:

eps.f – calculates bending angle, impact parameter and zenith angle of the ray for given positions and velocities of GPS and LEO and given excess Doppler frequency.

correct.f – approximation of a multi-valued function by close single-valued function.

4) Estimation of the occultation (ray tangent) point and azimuth of the occultation plane.

The occultation plane is defined by vectors k_1' and k_2' from the center of reference frame to GPS and to LEO. The occultation point, i.e. the point on Earth's surface to which the retrieved refractivity profile is assigned, is estimated under the tangent point of the ray connecting GPS and LEO for which L1 excess phase is equal 500 m. This, on average, corresponds to 3-4 km height. The direction vector k_{p}' from the center of the reference frame to the occultation point is calculated by rotation of the vector k_2' toward k_1' in the occultation plane by the angle $\pi/2 + \alpha/2 - \phi_2$ where ϕ_2 is the zenith angle of ray at k_2' . The occultation point is defined by latitude and longitude in the Earth fixed reference frame. The geocentric latitude is converted to geodetic latitude. The azimuth angle of the occultation plane is the angle between the occultation plane and the meridian plane at the occultation point.

Subroutines:

perigee.f – calculates latitude and longitude of ray perigee (tangent) point for given positions of GPS and LEO and given bending angle of the ray.

azimuth.f – calculates azimuth of the occultation plane for given positions of GPS and LEO and given latitude and longitude of the ray tangent point.

gast.f – calculates rotation angle between the inertial and the Earth fixed reference frames for a given date and time (for conversion of longitude).

5) Transfer of the reference frame to the local center of sphericity estimated under the occultation point.

Oblateness of the Earth can introduce significant retrieval errors (depending on the latitude) when solving inverse problem under the assumption of spherical symmetry in the Earth centered reference frame (Syndergaard, 1998). In order to minimize these errors the reference frame is transferred from the Earth's center to the effective center of curvature of the Earth's reference ellipsoid. The curvature of the reference ellipsoid is different in latitudinal and longitudinal directions. The local center of sphericity is defined as the local curvature center at the estimated occultation point in the direction of the occultation plane (defined by azimuth at step (4)).

Subroutines:

curvcent.f – calculates local curvature radius of the Earth's reference ellipsoid for given latitude, longitude and azimuth.

6) Calculation of L1 and L2 bending angles from Doppler frequency shift (geometric optics).

Calculation of the bending angles and impact parameters from Doppler frequency shift is performed under the assumption of single-ray propagation between transmitter (GPS) and receiver (LEO). This is assumption is feasible above the moist troposphere, where the multipath propagation is not common. The equation which relates the Doppler frequency shift to zenith angles of ray at transmitter and receiver:

$$\frac{f + f_{dop}}{f} = \frac{1 - \frac{\rho}{h_2} \frac{\rho}{v_2} / c}{1 - \frac{\rho}{h_1} \frac{\rho}{v_1} / c} = \frac{c - v_2 \cos(\gamma_2 - \phi_2)}{c - v_1 \cos(\gamma_1 - \phi_1)}$$

where $h_{1,2}$ are ray direction vectors at transmitter and receiver (multiplied by refractive indices (set to 1)), $v_{1,2}$ are modulo of projections of the velocity vectors in the occultation plane, $\gamma_{1,2}$ are zenith angles of velocity vectors, $\phi_{1,2}$ are ray zenith angles, is solved concurrently with the Snell's equation:

$$r_1 n_1 \sin \phi_1 = r_2 n_2 \sin \phi_2 = a$$

by iterative method. This allows for solving for two zenith angles $\phi_{1,2}$. Then the impact parameter *a* and the bending angle α of ray are calculated:

$$\alpha = \phi_1 + \phi_2 + \theta - \pi$$

where θ is the central angle between the satellites. <u>Subroutines</u>:

eps.f - see above

correct.f - see above

lintp.f – linear interpolation of the bending angle on a given impact parameter grid.

7) Calculation of L1 bending angle by radio holographic methods from raw complex signal.

Under conditions of multipath propagation, common in moist troposphere, calculation of bending angle and impact parameter from Doppler is not applicable (its application results in bending angle being a multi-valued function of impact parameter). Under multipath propagation, the bending angle as function of impact parameter is derived from raw complex RO signal (from both the phase and the amplitude) by radio holographic (RH) methods that allow solving for (disentangling) multiple rays. The current version of 'roam' code includes four radio holographic methods: (1) back propagation (BP); (2) sliding spectral (radio optics) (SS); (3) canonical transform (CT); and (4) full spectrum inversion (FSI). The choice of a method is controlled by input parameter.

All RH methods are 2-D, i.e. applied for electromagnetic (EM) field in the occultation plane. All RH methods have to be applied for stationary EM field (from immovable transmitter) received on a given trajectory. Under the assumption of

spherical symmetry, this is equivalent to constant radius of transmitter. The CT method requires specification of the received EM field on a straight line trajectory. The FSI method requires specification of the EM field on a circular trajectory. To apply RH methods, at first, new (virtual) positions of transmitter and receiver and the total phase path between them are calculated by use of the Snell's law (equivalent to straight line continuation of geometric optical rays) so that the new virtual position of transmitter has constant radius. For the FSI method, the new virtual position of receiver, also, has constant radius. For CT method the EM field is back propagated (BP) from the new virtual receiver trajectory to straight line.

(1) BP method consists of propagation of complex EM field in a vacuum back to limb by use of the EM field on the virtual observation trajectory as the boundary condition and by numerical calculation of Kirchhoff integrals (in vicinities of stationary points) (Gorbunov and Gurvich, 2000). The BP is equivalent to straight line continuation of rays in GO. Although the BP EM field is different from true EM field inside the atmosphere, it preserves impact parameters of the rays. Closer to atmosphere, where it is assumed no multipath, the BP EM field is calculated on auxiliary trajectory (normal to initial direction of propagation, located 200 km from limb toward receiver) and its phase used for calculation of arrival angles (bending angles and impact parameters) of the rays.

(2) SS method consists in Fourier analysis of the complex received EM field in sliding window (aperture). Different harmonics are associated with different plane waves (rays) arriving at the aperture. The frequency of a harmonic defines the arrival angle (the bending angle with account for position of the GPS and the Snell's law) and the position of the center of the aperture and the arrival angle define the impact parameter. Each ray, also, is associated with spectral power. All rays from all apertures are combined and sorted according to their impact parameter. Then the arrays of the impact parameters and the bending angles are subjected to sliding averaging by weighting with their spectral powers (Sokolovskiy, 2001a). Thus the smoothed bending angle as a single-valued function of the impact parameter is obtained.

(3) CT method transforms the complex wave function, specified on straight line trajectory, from coordinate to impact parameter representation, by an integral transform (Gorbunov, 2002). The integral transform is reduced to two (forward and inverse) Fourier transforms and transformation of the spectrum (that corresponds to substitution of variable) between them and is computationally efficient. The derivative of the phase of the transformed wave function is related to ray arrival angle (bending angle with account for position of the GPS and the Snell's law). The most CPU time consuming part of the CT method is the BP from the observation trajectory to the auxiliary straight line trajectory normal to initial propagation direction located 1000 km from limb toward receiver.

(4) FSI method, also, is a type of the canonical transform, which in case of circular transmitter and receiver orbits is reduced to simply one Fourier transform. The

frequency is directly related to impact parameter and the derivative of the phase of the Fourier spectrum is linearly yields the bending angle (Jensen et al., 2003).

The SS, CT and FSI methods, by definition, provide the bending angle as a singlevalued function of the impact parameter. The BP method may result in multi-valued function (in particular, in case of super refraction). For GPS and close to circular LEO orbit, the FSI method is an optimal method (most accurate and fast) for calculation of bending angles and impact parameters under multipath propagation (in moist troposphere).

Subroutines:

gpstat.f – for given positions of GPS and LEO and excess phase between them, calculation of the new virtual positions (2-D in occultation plain, by Snell's law, by assuming straight line propagation, by setting GPS radius to constant) and the new excess phase.

bp.f – calculation of the array of positions on a straight line auxiliary trajectory in radial direction, specified by central angle, and back propagation of complex EM field (phase and amplitude) from an arbitrary trajectory to the auxiliary trajectory.

bend.f – calculation of bending angles and impact parameters from the phase on a 2-D trajectory given position of the receiver.

spectr.f – calculation of bending angles and impact parameters from complex EM field (phase and amplitude) specified on arbitrary 2-D trajectory given position of the receiver and the size of sliding window (aperture).

spectr1.f – calculates the sliding spectrogram of RO signal specified on 2-D trajectory (not used in inversion process, for visualization purpose only, contains stop statement).

gpstat1.f – rotation of the 2-D reference frame so that X axis becomes parallel to the line GPS-limb, and calculation of the new positions of GPS and LEO (for application of the CT method).

bp1.f – calculation of array of positions on a straight line auxiliary trajectory in the direction normal to X axis, specified by distance, and back propagation of complex EM field (phase and amplitude) from an arbitrary trajectory to the auxiliary trajectory (for application of the CT method).

ct.f – canonical transform of the complex EM signal (phase and amplitude) specified on the straight line trajectory for a constant radius of transmitter and calculation of impact parameters, bending angles and amplitudes.

gpsleofix1.f – geometric optical propagation of the phase from arbitrary transmitter and receiver trajectories to close circular trajectories (with radii corresponding to the end of occultation) by use of given ray zenith angles at transmitter and receiver (for application of the FSI method).

gpsleofix0.f - the same as gpsleofix1.f, but bending is not taken into account (propagation along straight lines transmitter-receiver).

fsi1.f – full spectrum inversion of the complex EM signal (phase and amplitude) specified on circular trajectory for a constant radius of transmitter and calculation of impact parameters, bending angles and amplitudes. Upsampling of raw signal is performed by linear interpolation of amplitude and phase.

fsi0.f – the same as fsi1.f, but up-sampling is performed by Fourier interpolation of complex raw signal.

pha2dop.f – calculation of Doppler from phase by connecting raw phase (defined between $-\pi$ and π).

dop2pha.f – calculation of the continuous (accumulated) phase from Doppler.

runav.f – running averaging of an array.

medav.f – running median averaging of an array.

revers.f – inverts the order of a 1-D array.

filter0.f – see above.

filter.f - see above.

lintp.f – see above.

correct.f – see above.

8) Combining (sewing) (6) and (7) L1 bending angles.

Multipath propagation in moist troposphere result in strong fluctuation and large tracking errors on L2 RO signal, which makes the L2 signal unusable. Large and abrupt noise increase on L2 Doppler or large mean deviation between L1 and L2 Dopplers (whichever occurs at higher altitude) are used as indicator of multipath propagation and define altitude below which L1 bending angle derived from Doppler (step 6) is replaced by the bending angle derived by RH methods (step 7). Also, below this height L2 Doppler is not used (step 9).

Subroutines:

append.f – appends one array to another.

9) Ionospheric calibration.

Ionospheric calibration of RO observables in 'roam' uses linear combination of L1 and L2 bending angles at a given impact parameter (Vorob'ev and Krasil'nikova, 1994). To reduce the effect of larger noise on L2 due to semi-codeless tracking under AS, the modified linear combination is used (Rocken et al, 1997):

$$\alpha(a) = \alpha_1(a) + \frac{f_2^2}{f_1^2 - f_2^2} [\tilde{\alpha}_1(a) - \tilde{\alpha}_2(a)]$$

where $\tilde{\alpha}_1(a)$ and $\tilde{\alpha}_2(a)$ are obtained from L1 and L2 excess phases subjected to filtering with larger smoothing window than that used for $\alpha_1(a)$. This results in overall error reduction by reduction of the effect of L2 noise however, at the expense of a certain increase of uncalibrated ionospheric effects.

10) Optimal estimation of the bending angle by use of climatology.

While magnitude of the neutral-atmospheric bending angle and its weather-related variations (signal) decrease exponentially with height, the magnitude of the noise (after the filtering and the ionospheric calibration) remains about constant and overshadows the signal above a certain height (which can be significantly different between different occultations due to different magnitude of the residual ionospheric noise). To reduce the effect of noise propagation from high to low altitudes, after the Abel inversion, the observation bending angle is subjected to optimal estimation (under certain assumptions) by use of the bending angle for a climate model as the 1st guess. This results in that the optimized bending angle is a linear combination of the observation and the first guess with weighting coefficients varying with height

$$\alpha_{opt}(a) = w_{obs}(a)\alpha_{obs}(a) + w_{guess}(a)\alpha_{guess}(a)$$

The weighting functions w(a) depend on the method of estimation of the observation errors and of the errors of the 1st guess (based on high altitude refractivity climatology). The standard observation is estimated from rms deviation of the observation bending angle from the 1st guess between 60 and 80 km. The fractional standard error of the first guess (climatology) is assumed to be constant (Kuo et al., 2004). In another option, the standard error of the 1st guess is estimated from rms deviation of the observation bending angle from the 1st guess is estimated from rms deviation of the observation bending angle from the 1st guess between 20 and 60 km (Lohmann, 2004). In the latter approach, additionally, the correlation distances of the observation and the 1st guess errors are estimated and used for calculation of damping factors in the optimized bending angle (with account for the frequency response of the Abel inversion). The choice of option for the optimization and the choice of the climate model for the 1st guess are controlled by input parameter.

Subroutines:

standref.f, standref1.f, standref2.f, standref3.f – calculation of standard refractivity profiles for given day of year and latitude and different climatology models: (1) CIRA; (2) CIRA+Q; (3,4) NCAR.

direct.f - calculation of the bending angle as the function of impact parameter from refractivity as the function of refractional radius (the transform inverse to the Abel inversion).

noiserr.f – calculation of the mean and standard deviation of the observation and the 1^{st} guess bending angles between 60 and 80 km.

estimk.f – calculation of the mean and standard deviation of the observation and the 1^{st} guess bending angles between 20 and 60 km.

correl.f – calculation of the correlation functions for the observation and the 1^{st} guess errors.

correllengths.f – calculation of the correlation lengths for the observation and the 1^{st} guess errors.

obsvarprof.f – calculation of the observation error variance profile.

11) Retrieval of refractivity (Abel inversion).

The optimized bending angle $\alpha_{opt}(a)$ (step 10) is obtained in the height range defined by RO observations. If RO starts below 150 km, the optimized bending angle is extended up to 150 km height by setting $\alpha_{opt}(a) = \alpha_{guess}(a)$ by using exponential extrapolation of the $\alpha_{guess}(a)$ above the top height. Thus optimized and extended bending angle profile is subjected to Abel inversion (the large top height allows setting zero boundary condition at the top):

$$n(x) = \frac{1}{\pi} \int_{x}^{x_{top}} \frac{\alpha_{opt}(a)}{\sqrt{a^2 - x^2}} da$$

where x = rn(r) and $N = 10^6(n-1)$ and $z = r - r_{curv} + \Delta z_{geoid}$, where r_{curv} is the local curvature radius at the occultation point (step 5) and Δz_{geoid} is geoid correction.

Subroutines:

invert.f – calculation of refractivity as the function of radius from bending angle as the function of impact parameter (Abel inversion).

zoversea.f - geoid correction of altitude over the MSL.

12) Retrieval of "dry" pressure and temperature (by integration of hydrostatic equation).

Under the assumption of dry air, the retrieved refractivity is directly proportional to density $N = c\rho$. Then pressure is retrived by integration of the hydrostatic equation: $p(z) = c^{-1} \int_{z}^{z_{top}} g(z')\rho(z')dz'$ and temperature is derived from the equation of state: $T = mp / R\rho$.

Subroutines:

tempres.f – calculation of "dry" pressure and temperature profiles from refractivity profile. Pressure and temperature are initialized to zero at the top.

tempres 1.f – the same as tempres.f, but temperature is initialized by a given value at a given height (data number).

References.

Gorbunov., M.E., and A.S. Gurvich, Comparative analysis of radioholographic methods of processing radio occultation data. Radio Sci., 35(4), 1025-1034, 2000.

Gorbunov, M.E., Canonical transform method for processing radio occultation data in lower troposphere. Radio Sci., 37, 1076, doi:10.1029/2000RS002592, 2002.

Jensen, A.S., M.S. Lohmann, H.-H. Benzon, and A.S. Nielsen, Full spectrum inversion of radio occultation signals. Radio Sci., 38, 1040, 10.1029/2002RS002763, 2003.

Kirchengast, G., J. Hafner, and W. Poetzi, The CIRA-86&Q_UoG model: An extension of the CIRA-86 monthly tables including humidity tablesand a Fortran 95 global moist air climatology model. Eur. Space Agency, IMG/UoG Techn. Rep. 8., 1999.

Kuo, Y.-H., T.K. Wee, S. Sokolovskiy, C. Rocken, W. Schreiner, D. Hunt and R.A. Anthes, Inversion and error estimation of GPS radio occultation data. J. Met. Soc. Japan, 82(1B), 507-531, 2004.

Kursinski et al., Observing Earth's atmosphere with radio occultation measurements using the Global Positioning System. J. Geophys. Res., 102(D19), 23,429-23,465, 1997.

Lohmann, M. S., Application of dynamic error estimation for statistical optimization of radio occultation bending angles. Radio Sci., 40 (RS3011), doi:10.1029/2004RS003117, 2005.

Lohmann, M. S., Dynamic error estimation for Radio Occultation bending angles retrieved by the FSI technique. Radio Sci., submitted, 2005.

Rocken et al., Analysis and validation of GPS/MET data in the neutral atmosphere. J. Geophys. Res., 102(D25), 29,849-29,866.

Sokolovskiy, S.V., Modeling and inverting radio occultation signals in the moist troposphere. Radio Sci., 36(3), 441-458, 2001a.

Sokolovskiy, S.V., Tracking tropospheric radio occultation signals from low Earth orbit. Radio Sci., 36(3), 483-498, 2001b.

SPARC Intercomparison of Middle Atmosphere Climatologies. WCRP-116. WMO/TD-No.1142. SPARC Report No.3. Edited by: W.Randell, M.-L.Chanin and C.Michaut. 88pp. 2002.

Syndergaard, S., Modeling of the effect of the Earth's oblateness on the retrieval of temperature and pressure profiles from limb sounding. J. Atmos. Solar-Terr. Phys., 60, 171-180, 1998.

Syndergaard, S., Retrieval Analysis and Methodologies in Atmospheric Limb Sounding Using the GNSS Occultation Technique, DMI Scientic Report 99-6, Copenhagen, 1999.

Vorob'ev, V.V. and T.G. Krasil'nikova, Estimation of accuracy of the atmospheric refractive index recovery from Doppler shift measurements at frequencies used in the NAVSTAR system, Izv. Russ. Acad. Sci., Atmos. Ocean. Phys., Engl. Transl., 29, 602-609, 1994.

Addendum 1: Processing of radio occultation signals recorded in open-loop mode

Alternatively to the phase-locked loop (PLL) tracking, L1 RO signal may be recorded in open-loop (OL) mode below a certain height of ray TP (L2 signal, currently, may not be recorded in the OL mode). Above that height both L1 and L2 RO signals are recorded in the PLL mode. The OL tracking is raw sampling of complex signal (I and Q) after down-conversion with the frequency model precalculated in RO receiver without a feedback from received signal. In the OL mode, both the rising and the setting RO signals may be recorded. The OL signal is considered as a sequence of un-connected complex samples that have to be connected, i.e. the phase extracted and the cycle ambiguities resolved between the samples, in the post-processing. The C/A code modulation is removed from RO signal in receiver while the 50 bps navigation data modulation (NDM) remains on the OL RO signal and has to be removed in the post-processing.

With account for the OL RO signals, the format of the atmPhs files has been modified. In particular, these files now contain the receiver Doppler model which is set to -999 for the PLL tracking. If other than -999 is found the L1 signal is processed as the OL, otherwise as the PLL. Rising occultations are reversed, so all ooccultations are processed as the setting occultations.

Because of the un-removed NDM, the OL data in atmPhs files are not interpolated on a standard time grid, but supplied with individual GPS time tags. The sampling frequency in 'roam' code is changed from integer to real*8 and it is calculated by dividing the difference between the last and the first time tags by the number of samples. The OL complex signal is down-converted by use of the excess Doppler model calculated from orbits and the bending angle model obtained from CIRA+Q refractivity (the same model is used for the detection of tracking errors in PLL mode). The down-converted signal is subject to removal of the NDM. (i) If the gpsBit file is present in the argument line (after the parms file) then the NDM is removed by synchronizing the data bit sequence contained in the gpsBit file with the RO signal in the GPS time. (ii) If the gpsBit file is not present in the argument line, the NDM is removed by inverting the phasor when the phasor rotation between adjacent samples exceeds $\pi/2$. After the NDM is removed, the phase is connected between the adjacent samples by recursively adding $0,\pm 2\pi$ whichever minimizes the difference of the phase from the previous sample. After the phase is connected between the samples, the OL signal is further processed as the PLL signal. The RO signal is truncated for the inversion purpose when the SNR smoothed with 1 s window drops below (and never emerges) 150% of the mean SNR estimated during the last 3 s.

The Doppler model for the down-conversion of the OL RO signal can be corrected (refined) by using of the residual frequency as the function of time obtained from the sliding spectrogram of the down-converted signal thus minimizing the frequency miss-modeling. Currently this is intended for research purposes and not recommended for mass processing. The corresponding section of the code (ends at 777) is bypassed by setting iolss=0.

Addendum 2: Error estimation

Roam provides errors estimates for the retrieved bending angle and refractivity profiles. Errors are first estimated for the bending angle profiles and then propagated to refractivity errors following the procedures described in (Syndergaard, 1999). Different error estimation techniques are applied for the

Geometrical Optical (GO) processing and for the Radio Holographic (RH) processing.

For the GO processing bending angle observation errors are estimated from differences between 1st guess and observation bending angles between 60 – 80 km as described in Section 10. These errors are adjusted with height according to the variations in the *SNR* by assuming that bending angle errors are proportional to the inverse *SNR*, which is a good approximation for high *SNR*. Furthermore, the bending errors are also adjusted in order to account for errors in impact parameters stemming from Doppler errors as suggested by (Syndergaard, 1999). In this case the height varying bending angle standard deviation σ_{obs} may be expressed as:

$$\sigma_{obs}(a) = \sigma_{obs}^{u} \left(\frac{SNR^{u}}{SNR(a)}\right)^{3/2}$$

where *SNR* is the *SNR* of L1 (which is assumed to be proportional to the *SNR* for L2) and Superscript *u* refers to the average value in the height interval 60-80 km. The bending angle errors computed from the expression above corresponds to the GO bending angle errors supplied by roam. The refractivity computed by roam is based on the statistical optimized bending angle profile as described in Section 10. Hence, in order to estimate refractivity errors, the errors in the 1^{st} guess bending angle profile must be estimated as well in order to estimate the total errors in the optimized bending angle profile. This is done from differences between 1^{st} guess bending angles and observed bending angles in the height range from 20-60 km (Lohmann, 2004).

For the RH processing statistical optimization is not applied and the estimated bending angle errors are directly propagated to refractivity errors. Bending angle errors are estimated by mapping fluctuations in the RH log-amplitude to bending angle errors (Lohmann, 2005). This is done by exploiting that the variances, of the RH log-amplitude, χ , and the RH phase, φ , are related through:

$$\sigma_{\varphi}^2 \approx \sigma_{\chi}^2$$

which allows for estimation of the RH phase errors from the χ fluctuation. The estimated RH phase errors can readily be propagated to bending angle errors and subsequently to refractivity errors.