Variability and Dynamics of the Earth's Atmosphere from GPS Radio Occultation

Kumulative Habilitationsschrift

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Barbara Scherllin-Pirscher

Karl-Franzens-Universität Graz
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Synopsis

Abstract

This habilitation thesis reveals the high potential of Radio Occultation (RO) observations to study atmospheric processes in the Upper Troposphere and Lower Stratosphere (UTLS) region. The quality of individual RO profiles and of climatological fields based on single and multiple satellites is discussed. It is shown that both the high accuracy and precision of the data set (best data quality from approximately 8 km to 25 km) as well as its high vertical resolution and long-term stability are outstanding characteristics and unique in this combination. This allows gaining detailed insights and better understanding of atmospheric processes in the UTLS.

We exploited the full potential of the RO record by investigating atmospheric variability and dynamics. It is shown that tropical temperature variability in the UTLS occurs on very different time scales. In the tropical tropopause region, quasi-stationary waves associated with interannual variability and the annual cycle account for about one third of total resolved variance. The remaining two thirds are associated with atmospheric equatorial waves.

El Niño–Southern Oscillation (ENSO)-related interannual temperature anomalies occur as a zonal-mean and an eddy component, which feature different spatial characteristics and temporal evolutions. Applying Empirical Orthogonal Function (EOF) analysis separately at each vertical level allows deriving vertically-resolved ENSO and Quasi-Biennial Oscillation (QBO) indices that can be used, e.g., in climate trend analyses. Interannual variability of tropical tropopauses is also dominated by ENSO and QBO. At mid- and high latitudes, tropopause characteristics are also modulated by the strength of the polar vortex and Sudden Stratospheric Warming (SSW) events.

A further pillar of research within the habilitation framework embraces the investigation of atmospheric dynamics outside the tropics. It is shown that gridded fields of RO data can be used to infer high-quality climatological wind fields. Since 2006, RO sampling is even dense enough to resolve synoptic atmospheric variability and to investigate atmospheric blocking at mid-latitudes.

All these findings are introduced and summarized in the first part of this habilitation thesis. More detailed information is given in the 13 peer-reviewed journal papers that can be found in the second part of this thesis.

1. Variability and Dynamics of the Earth's Atmosphere from GPS Radio Occultation

1.1. Introduction and context

1.1.1. RO measurement principle and data characteristics

Information about the thermodynamical characteristics of the neutral atmosphere can be derived from Global Positioning System (GPS) signals that are modified on their way through the atmosphere: GPS satellites at orbit altitudes of approximately 20 200 km transmit electromagnetic waves at two carrier frequencies in the L-band at $f_1 = 1575.42$ MHz and $f_2 = 1227.60$ MHz (Hofmann-Wellenhof et al. 1997; Hofmann-Wellenhof et al. 2008). A GPS receiver on a different device is able to replicate the signal and to compare it to the received one. The difference between the two signals is caused by the relative motion of the transmitter and the receiver (kinematic Doppler shift), by the Earth's refractive field (ionosphere- and neutral atmosphere-induced Doppler shifts), transmitter and receiver clock errors, as well as measuring inaccuracies such as orbital errors or delays in electronic hardware (Hofmann-Wellenhof et al. 2008).

All GPS measurements are affected by these contributions. However, depending on specific needs, the user aims at maximizing the information of one of these components while minimizing the contributions of the others. The GPS receiver, e.g., that is used in everyday life for information about time, position, and velocity, uses information from the kinematic Doppler shift. In atmospheric sciences, however, the state of the ionosphere or neutral atmosphere are retrieved by extracting information of the ionosphere- or the neutral atmosphere-induced Doppler shift and calculating further derived atmospheric parameters (see Section 1.1.2 for more information about the neutral atmosphere retrieval).

The GPS receiver used for RO measurements is mounted on a Low Earth Orbit (LEO) satellite. The relative motion of the two satellites yields a near-vertical scan through the atmosphere. It takes about one to three minutes to scan a large part of the atmosphere from top downwards or from bottom upwards.

The capability of the RO technique is mature. Beneficial characteristics comprise (Melbourne et al. 1994; Kursinski et al. 1997; Sherwood et al. 2006; Anthes 2011; Scherllin-Pirscher et al. 2017a; Schwarz 2018):

1. unprecedented accuracy and precision, which originate from precise time measurements due to highly stable clocks onboard the satellites,
2. all-weather capability and availability of atmospheric profiles during day and night due to the use of GPS signals at microwave frequencies, which are able to penetrate through clouds and are independent of sunlight,
3. global coverage of the measurements, if the LEO satellite is in a near-polar orbit (which is the case for most RO missions so far),
4. self-calibration and long-term stability, which originate from the retrieval principle, which is based on phase change profiles rather than on absolute phases,
5. a high vertical (but relatively low horizontal) resolution due to the limb sounding geometry of this active remote sensing technique,
6. virtually independent information of height and derived atmospheric variables such as pressure or temperature because the vertical height grid is established and adopted as the independent vertical coordinate early in the retrieval, and
7. integrated uncertainty propagation that can be implemented in the RO processing scheme and quantifies and traces systematic and random uncertainties including vertical error correlations and gives resolution estimates.

1.1.2. Retrieval of atmospheric parameters

The quantities of interest for the scientific RO community are the ionosphere-induced and the neutral atmosphere-induced Doppler shifts. The former is used to retrieve profiles of electron density and total electron content of the ionosphere. The latter quantity is used to derive profiles of thermodynamic atmospheric parameters mainly from the troposphere up to the stratosphere. From now on, I will focus on the neutral atmosphere retrieval.

To retrieve high quality profiles of atmospheric parameters, it is crucial to monitor errors and (if possible) remove all contributions to the measurement besides the quantity of interest. Relativistic effects can be corrected by modeling. Synchronization and drift errors of GPS clocks are monitored by the GPS control segment.

Receiver clock errors that arise from non-ultra-stable clocks on the LEO satellite can be removed by single or double differencing methods (Schreiner et al. 2009).

If all these components are accounted for, the remaining signal, also called "excess phase" or "excess phase delay" or "phase delay" (Syndergaard 1999), still contains contributions of the kinematic Doppler shift, the ionosphere-induced Doppler shift, the neutral atmosphere-induced Doppler shift, and potential multipath errors. The latter means that the receiver detects multiple signals, that propagated along different paths (Gorbunov 2002). While local multipath effects can be reduced using directional antennas and modeling (Kursinski et al. 1997), atmospheric multipath effects, which can be caused by sharp vertical variations in atmospheric refractivity structures, have to be removed later in the retrieval process (e.g., Gorbunov 2002; Jensen et al. 2006).

Excess phases and amplitudes of both GPS signals are derived as a function of time. Precise orbit information (i.e., positions and velocities of the transmitter and the receiver satellites), determined with an appropriate Precise Orbit Determination (POD) software, is interpolated to the same time-grid.

Knowledge of the occultation geometry and excess Doppler (i.e., differentiated excess phase) allows the calculation of the atmospheric bending angle, usually done for GPS signals at both frequencies, separately. These bending angles still contain the contributions of the ionosphere and neutral atmosphere and are available as a function of their respective impact parameters (e.g., Melbourne et al. 1994). The ionosphere-induced part of the bending angle can be removed by linearly combining these two bending angle profiles as a function of a common impact parameter (Vorob'ev and Krasil'nikova 1994).

The refractive index is calculated by inversion of an Abel integral equation (Steiner 1998). This step requires accurate knowledge of the bending angle at high altitudes (in the mesosphere and above). Since the quality of RO measurements decreases with height (i.e., worse signal-to-noise ratio at high altitudes due to very small bending angles), a priori information is usually used as an extrapolation (e.g., Scherllin-Pirscher et al. 2015). The quality of these data and details of merging RO with a priori data are crucial as they can induce noticeable errors in stratospheric retrieval products and therefore affect the quality of derived atmospheric profiles (Gobiet et al. 2007).

Atmospheric parameters such as density, pressure, and temperature can be derived from refractivity profiles by applying the state law of an ideal gas and the hydrostatic integral. Since atmospheric moisture also contributes to the bending angle, these parameters (also called "dry atmospheric parameters") are of best quality in regions where humidity is negligible. In the (lower) troposphere, however, where moisture becomes significant, these parameters also contain a humidity-induced contribution which causes large biases relative to true physical atmospheric quantities (Scherllin-Pirscher et al. 2011b; Danzer et al. 2014). True physical atmospheric parameters (and also humidity) can only be retrieved using additional background information (e.g., Kursinski and Hajj 2001; Poli et al. 2002; Rieckh et al. 2017).

Several studies investigated the quality of retrieved atmospheric products from RO by comparing them to independent measurements or analysis/reanalysis data from Numerical Weather Prediction (NWP) systems (e.g., Gobiet et al. 2007; He et al. 2009; Ladstädter et al. 2015). All these studies confirmed high quality of RO products in the UTLS.

1.1.3. Added value of RO data in atmospheric sciences

A deeper understanding of the Earth's atmosphere can be obtained from observations, analysis/reanalysis products, and atmospheric models. All these different sources of information have their limitations but complement each other if used together.

Since global or regional circulation models provide physically consistent information about the state of the atmosphere, they can be used to improve understanding of underlying physical processes. Experimental model setups allow to explicitly study processes, e.g., by switching them on or off or by modifying sub-processes or their parameterizations. Model assumptions or simplified representation of physical processes, however, can limit the validity of model results.

Mostly independent information about the state of the atmosphere that is usually limited to only a few atmospheric parameters, can be obtained from observations. However, availability of observations is limited in space and time, affecting their representativeness for a larger spatial domain or longer time scale. Furthermore, each measurement is also affected by its uncertainty.

Since analysis and reanalysis products rely on both model and observation information, these data give insights of the atmosphere that comes closest to the real state when looking at the entire four-dimensional spatio-temporal scale. While processes cannot be studied in an experimental design, these data give (almost) physically consistent information about the state of the atmosphere that can be used to investigate relationships between different atmospheric variables at different spatial and temporal scales.

Atmospheric measurements and analysis/reanalysis products are only independent from each other if (i) the observation is not assimilated into the model and if (ii) the retrieval of the measurement is not based on any information from an analysis or reanalysis. In 2006, NWP centers started assimilating RO measurements into their models operationally (Healy 2007; Aparicio and Deblonde 2008; Cucurull

and Derber 2008), yielding improved forecast skills, in particular in the southern hemisphere (e.g., Healy 2008; Rennie 2010) and in remote regions such as over tropical oceans (e.g., Liu et al. 2012). This means, however, that RO observations and NWP analyses/reanalyses are not independent anymore and one might raise the following question: What is the added value of RO data compared to analysis or reanalysis products when studying atmospheric processes?
Revisiting the characteristics of RO measurements (see Sect. 1.1.1), we get the following answer:

Accuracy and precision: Due to their high accuracy and precision, RO data can be used to validate atmospheric models, analysis and reanalysis products, and measurements from observing systems other than RO. In the UTLS, most analyses/reanalyses that assimilate RO observations have similar quality as RO data themselves. However, in particular at high altitudes (above approximately 40 km), where impact of RO on NWP analyses/reanalyses is limited, RO data (primarily early retrieval products such as bending angle and refractivity) have an added value due to their high accuracy and precision (Scherllin-Pirscher et al. 2015).

Vertical resolution: In the UTLS, the vertical resolution of RO measurements is better than the vertical resolution of analysis and reanalysis products. This is also true for most retrieved RO profiles, even if the retrieval algorithm degrades their vertical resolution due to vertical integrations and smoothing (Noersomadi and Tsuda 2017; Noersomadi et al. 2018). High vertical resolution is important when investigating, e.g., thin vertical layers such as the tropopause or atmospheric waves with short vertical wavelengths.

Long-term stability and consistency: The difference between analyses and reanalyses is that the latter are always based on the exactly same model version while the model system of an analysis can change (usually improve) with time. However, the performance of both NWP systems change with available measurements that are assimilated (e.g., Poli et al. 2010). Since self-calibrating RO measurements do neither exhibit an instrument drift nor a satellite-to-satellite bias, they have a major advantage compared to analysis/reanalysis products. Despite of the use of a priori information in the RO inversion process, long-term stability and consistency of retrieved RO products is still superior in the RO core region between about 8 km and 25 km.

Estimation of errors and uncertainties: While errors and uncertainties from retrieved RO profiles can be derived empirically (Scherllin-Pirscher et al. 2011a) or with integrated uncertainty propagation (Schwarz et al. 2017; Schwarz et al.

> 2018), they are not fully understood from analysis and reanalysis products RO (Parker 2016). However, detailed knowledge of errors and uncertainties is important to understand strengths and limitations of a data set. This information is therefore crucial for drawing appropriate conclusions about the system under investigation (Parker 2016).

Producing new scientific results from GPS RO is therefore a matter of exploiting these properties with sufficient density (Sherwood et al. 2006).

While first RO measurements of the Earth's atmosphere were performed by the Global Positioning System/Meteorology (GPS/MET) mission in 1995 (Rocken et al. 1997), a continuous RO record is available since the early 2000s (Wickert et al. 2001; Hajj et al. 2004). A vast increase of RO measurements occurred in 2006 after the launch of the Formosa Satellite Mission #3 (FORMOSAT-3)/Constellation Observing System for Meteorology (COSMIC) (F3C) constellation, which consists of six individual satellites (Anthes et al. 2008). Since 2006, important modes of atmospheric variability that operate over a wide range of spatial and temporal scales can be resolved (see Section 1.4.1).

In the next sections, I will discuss the quality of RO data from different processing centers and different satellites and give detailed information about error characteristics of individual RO profiles as well as of RO climatological fields. Then, I will exploit the full potential of the RO record and investigate atmospheric variability and dynamics by means of selected examples.

1.2. The reproducibility and consistency of the RO record

1.2.1. Reproducibility and structural uncertainty of CHAMP data

Due to the measurement principle, RO observations are characterized by very high quality (see Section 1.1.1). In the retrieval process, however, several assumptions limit the accuracy and precision of derived results that can again affect the reproducibility and consistency of the RO record.

Major limitations of the GPS RO technique occur below approximately 5 km and above approximately 35 km. Specific height limits[1] depend on the retrieval

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[1] The standard coordinate for Global Navigation Satellite System (GNSS)-related data processing and therefore measurement height of RO observations is height above the Earth's ellipsoid. Altitude (or Mean Sea Level (MSL) altitude) is height above the Earth's geoid. The geoid undulation is the height difference between the Earth's geoid and ellipsoid. In general, it is smaller than ±100 m. Geopotential height refers to height above the Earth's geoid but also accounts for the geographic and vertical effects of local gravity anomalies. Differences between geopotential height and MSL altitude are smaller than 300 m up to 35 km (Scherllin-Pirscher et al. 2017a).

product. The CHAllenging Minisatellite Payload (CHAMP) RO record (2002 to 2008) served as an excellent data source for a better understanding of the sensitivity of retrieved atmospheric profiles from different RO processing chains.

The first research question raised in this thesis therefore is:

Research question 1

How large is the structural uncertainty of retrieved CHAMP profiles as well as of CHAMP climatological fields?

Several institutions process RO measurements: the Radio Occultation Meteorology (ROM) Satellite Application Facility (SAF) at the Danish Meteorological Institute (DMI) in Copenhagen, Denmark, the European Organization for the Exploitation of Meteorological Satellites (EUMETSAT) in Darmstadt, Germany, the German Research Center for Geosciences (GFZ) in Potsdam, Germany, the Jet Propulsion Laboratory (JPL) in Pasadena, CA, USA, the University Corporation for Atmospheric Research (UCAR) in Boulder, CO, USA, and the Wegener Center for Climate and Global Change (WEGC) in Graz, Austria. All these centers have a different scientific focus that ranges from operationally providing RO data of a specific satellite in near-real-time for data assimilation to providing derived RO products of several satellites to the general scientific user community.

Depending on the aim and focus, some centers start their processing with raw measurement data and the retrieval of excess phase, others use excess phase and orbit information derived by other processing centers and start with the inversion process (i.e., the retrieval of bending angles). Some processing results are therefore not entirely independent from each other.

In a very first study, Ao et al. (2003) performed an intercomparison study of CHAMP RO data using processing results of three centers (GFZ, JPL, and UCAR). The authors found generally good agreement between retrieved RO data sets with monthly mean fractional refractivity differences being smaller than 0.3 % from 10 km to 25 km and monthly mean temperature differences smaller than 1 K from 10 km to 20 km.

Using only matching pairs of CHAMP measurements from GFZ and UCAR, von Engeln (2006) performed an intercomparison study for bending angle, refractivity, and dry temperature. Similar to Ao et al. (2003), the author also found good agreement between the data sets between 10 km and 25 km with best agreement for early retrieval products (i.e., bending angle). Due to large biases at high altitudes (up to 5 K in temperature at an altitude of 35 km) and varying biases in different latitude bands, von Engeln (2006) concluded that the agreement of these retrieval products was not sufficient for climate monitoring and suggested further coordination among the processing centers.

This was realized by the RO Trends Intercomparison Working Group, which was established in 2007. The aim of this group was to examine the suitability of the RO record as a climate benchmark data set. First results were published by Ho et al. (2009b). The authors investigated monthly-mean zonal-mean fields of CHAMP refractivity processed by four retrieval centers (GFZ, JPL, UCAR, and WEGC) and found fractional refractivity differences among the centers smaller than 0.2 % between an altitude of 8 km and 25 km. Errors in fractional refractivity trends were about 0.03 % per 5 years if differences in spatial-temporal sampling were accounted for.

To further investigate the reproducibility of RO data, Ho et al. (2012) used the CHAMP record from 2002 to 2008 from six processing centers (DMI, EUMETSAT, GFZ, JPL, UCAR, and WEGC) to quantify differences and standard deviations of retrieved profiles of individual centers relative to the all-center mean. Statistics was obtained only from those profiles, that were classified as "high quality profiles" by all centers. It is interesting to note that only 30 % of all CHAMP profiles entered this statistics due to different quality aspects of individual centers.

In the global layer from 8 km to 30 km, Ho et al. (2012) found mean differences of bending angle, refractivity, and dry temperature between −0.08 % and +0.12 %, −0.03 % and +0.02 %, −0.27 K and +0.15 K, respectively. The corresponding standard deviations were within 0.02 % for bending angle, 0.01 % for refractivity, and 0.06 K for dry temperature. Best agreement was found close to the tropopause (12 km to 20 km).

In a complementary study, Steiner et al. (2013) used all retrieved high-quality profiles from each center and calculated sampling error-corrected monthly-mean zonal-mean fields. This study revealed lowest structural uncertainty in the tropics and at mid-latitudes (50°S to 50°N) from 8 km to 25 km, where trends over 7 years were <0.03 % for bending angle and refractivity and <0.06 K for dry temperature. GPS RO therefore meets Global Climate Observing System (GCOS) climate requirements for air temperature, which are 0.05 K/decade for the troposphere and 0.1 K/decade for the lower stratosphere. Larger structural uncertainty above 25 km was attributed to different bending angle initialization; limited agreement at high latitudes was explained by higher atmospheric variability that caused a larger residual sampling error. Results of Ho et al. (2012) and Steiner et al. (2013) confirmed the high quality of RO retrieval products from all processing centers and demonstrated that trends in gridded RO fields are essentially independent of the processing center.

Research answer 1: Reproducibility and structural uncertainty

In the global layer from 8 km to 30 km individual atmospheric profiles of the CHAMP satellite retrieved by six processing centers (DMI, EUMETSAT, GFZ, JPL, UCAR, and WEGC) agree within −0.08 % and +0.12 % in bending angle, −0.03 % and +0.02 % in refractivity, and −0.27 K and +0.15 K in temperature. Corresponding standard deviations are smaller than 0.02 % for bending angle, 0.01 % for refractivity, and 0.06 K for dry temperature. Best agreement is found close to the tropopause (12 km to 20 km) (Ho et al. 2012).

Sampling error-corrected monthly-mean zonal-mean fields have lowest structural uncertainty in the tropics and at mid-latitudes (50°S to 50°N) from 8 km to 25 km, where trends over 7 years are <0.03 % for bending angle and refractivity and <0.06 K for dry temperature (Steiner et al. 2013).

GPS RO therefore meets GCOS climate requirements for air temperature (0.05 K/decade for the troposphere and 0.1 K/decade for the lower stratosphere).

1.2.2. Consistency of the multi-satellite RO climate record

The CHAMP RO record ended in 2008. In order to use a longer RO time series, e.g., for climate applications, the CHAMP record has to be merged with data from other RO missions. The overlap of different RO satellite systems allows to determine potential inter-satellite biases.

Therefore, the second research question raised in this thesis is:

Research question 2

What is the quality and concistency of the RO multi-satellite record?

The consistency of different RO satellites was first investigated by Hajj et al. (2004) examining differences between co-located soundings of the CHAMP and the Satelite de Aplicaciones Cientificas-C (SAC-C) satellites. This study revealed mid- to upper-tropospheric (5 km and 15 km) differences of dry temperature of 0.1 K (mean) with a standard deviation of 0.86 K. Smaller separation of the occultation pairs of F3C satellites as well as their parallel occultation planes revealed even better precision of these measurements as investigated by Schreiner et al. (2007) and Anthes et al. (2008). These studies showed Root Mean Square (RMS) differences of fractional refractivity smaller than 0.2 % between 10 km and 20 km. Larger differences were found by Ho et al. (2009a), who compared retrieved profiles from

CHAMP and F3C. Mean differences were within −0.35 K and 0.25 K and standard deviations increased from 2 K in the mid-troposphere to 4 K at 10 hPa. In the lower troposphere (below 500 hPa), even larger differences (−2 K) and standard deviations (6 K) were found due to different signal tracking algorithms of CHAMP and F3C.

While Hajj et al. (2004), Schreiner et al. (2007), Anthes et al. (2008), and Ho et al. (2009a) used co-located profiles of different satellites, Foelsche et al. (2009a) examined the agreement of zonal-mean seasonal-mean fields of different F3C satellites. This study showed that atmospheric climatologies from these satellites agree well up to an altitude of approximately 35 km. After subtraction of the estimated respective sampling errors, differences between RO climatologies from different F3C satellites were smaller than 0.1 K almost everywhere between 8 km and 35 km altitude. Systematic differences between F3C and CHAMP were slightly larger above 30 km (≈0.5 K), mainly due to the higher amount of background information used in the retrieval of CHAMP profiles. Similar results were obtained by Foelsche et al. (2011) and Steiner et al. (2011).

Using both, individual profiles of different RO satellites as well as gridded climatological fields, Angerer et al. (2017) investigated the WEGC Occultation Processing System version 5.6 (OPSv5.6) record consisting of retrieved profiles of CHAMP, Gravity Recovery and Climate Experiment (GRACE), SAC-C, Communications/Navigation Outage Forecasting System (C/NOFS), Meteorological Operational (Metop), and F3C. Level 1 input data of all these satellites were based on the UCAR processing.

Improvements of the receiver quality from 2001 to 2017 were clearly evident in bending angle noise at high altitudes with best data quality found for the Metop satellites. Bending angle bias, which is a measure for the consistency of the level 1 processing, was in good agreement for all satellites. This is important because erroneous bending angles cause non-negligible errors in refractivity, which are then further propagating to thermodynamic atmospheric variables. Global temperature fields were found highly consistent between 8 km and 25 km, where differences from the multi-satellite mean were smaller than 0.1 K for all satellites.

Above 25 km, retrieved atmospheric profiles were increasingly influenced by a priori information with the least amount of a priori information found for the Metop satellites due to superior bending angle quality. This can, however, seriously degrade the suitability of the RO record for climate applications: If a priori information is biased relative to RO, the bias propagates into retrieved thermodynamic atmospheric variables. Since this bias is largest for measurements with a high amount of a priori information and since RO receiver and data quality improved over time, the amount of a priori information decreases over time leading to a spurious trend in retrieved atmospheric parameters of the multi-satellite RO record. There would also be a spurious trend if the quality of a priori information changed with time, which was the case for European Centre for Medium-Range Weather Forecasts (ECMWF) data (e.g., Foelsche et al. 2009b). It is important to avoid this effect for climate applications and to use the OPSv5.6 multi-satellite record only below about 30 km for refractivity and below 25 km for temperature.

Research answer 2: Quality and consistency

The WEGC RO multi-satellite record OPSv5.6 is of very high quality and consistency. Global temperature fields are highly consistent between 8 km and 25 km, where differences from the multi-satellite mean are smaller than 0.1 K for all satellites. Above 25 km, retrieved atmospheric profiles are increasingly influenced by a priori information with the least amount of a priori information found for the Metop satellites due to superior bending angle quality. To avoid a spurious trend in retrieved atmospheric parameters, the OPSv5.6 multi-satellite record should only be used below about 30 km for refractivity and below 25 km for temperature (Angerer et al. 2017).

To further investigate the suitability of GPS RO as climate benchmark record, the uncertainty of different satellites from different retrieval centers will be evaluated. This study is currently performed by colleagues at WEGC (preliminary results of Mochart (2018) and A. K. Steiner, personal communication, 2018).

1.3. Error characterization of RO retrieval products

Detailed knowledge of the errors of RO retrieval products is essential when using these data in atmospheric research. This habilitation thesis includes error characterization of both, individual RO profiles and RO-based climatological fields.

1.3.1. Error characterization of individual RO profiles

The third research question raised in this thesis is:

Research question 3

How large are the errors of individual atmospheric profiles from GPS RO?

A first theoretical analysis of the propagation of random, Gaussian-distributed errors from excess phase to bending angle, refractivity, and dry atmospheric parameters was performed by Syndergaard (1999). This study discussed error propagation from each step to the next one in detail. Rieder and Kirchengast (2001) complemented and extended this work by applying a Bayesian error analysis and characterization formalism.

Observational error estimates based on real RO measurements from CHAMP and SAC-C were first provided by Kuo et al. (2004). This study confirmed highest accuracy between 5 km and 25 km with refractivity observational errors smaller than 0.5 %. Errors increased towards the surface and above 25 km.

Similar results were obtained by Steiner and Kirchengast (2005) using an ensemble of simulated RO profiles and by Steiner et al. (2006) who investigated the quality of retrieved atmospheric profiles from the CHAMP satellite. Steiner et al. (2006) also provided a simple analytical error model for CHAMP refractivity, that can be used, e.g., in data assimilation systems.

Scherllin-Pirscher et al. (2011a) followed Steiner and Kirchengast (2005) and Steiner et al. (2006) and investigated the error characteristics of CHAMP, GRACE, and F3C in terms of bending angle, refractivity, dry pressure, dry geopotential height, and dry temperature. Scherllin-Pirscher et al. (2017a) extended this study and investigated error characteristics of retrieved physical atmosphere parameters. Retrieved atmospheric profiles were referenced to "true" co-located profiles of ECMWF analysis fields. The standard deviation of the difference profiles and the estimated ECMWF model error were both used to quantify the observational error. Between 4 km and 35 km global mean observational errors of CHAMP, GRACE, and F3C agreed within 0.3 % in bending angle, 0.1 % in refractivity, and 0.2 K in dry temperature. Retrieval products of UCAR and WEGC were also in good agreement.

Based on the empirically-derived error estimates of different latitude regions and different months, Scherllin-Pirscher et al. (2011a) provided a simple analytical model of the observational error. The model represents the observational error's vertical structure (introduced by Steiner and Kirchengast 2005; Steiner et al. 2006), its latitudinal and seasonal dependence.

For bending angle, refractivity, and dry atmosphere parameters, the model assumes smallest, constant observational errors in the tropopause region (0.8 % for bending angle, 0.35 % for refractivity, 0.15 % for dry pressure, 10 m for dry geopotential height, and 0.7 K for dry temperature). While an exponentially increasing error was adopted in the stratosphere, the increase in the troposphere closely followed an inverse height power-law. Larger stratospheric observational errors in hemispheric winter at high latitudes were modeled by varying the stratospheric error scale height.

In the troposphere, Scherllin-Pirscher et al. (2017a) found decreasing observational errors for physical temperature and potential temperature due to increasing influence of background information. However, the same observational error model as introduced by Scherllin-Pirscher et al. (2011a) was used with adapted model parameters to properly describe the linearly decreasing errors below 15 km.

In order to be able to model full error covariance matrices for bending angle and refractivity, Scherllin-Pirscher et al. (2011a) also provided information about the vertical error correlation structure of these two variables up to 50 km. Results revealed that the error correlation structure of bending angle can be described by a Mexican Hat function and refractivity error correlations follow a simple exponential form. These results were consistent with Steiner and Kirchengast (2005) and Steiner et al. (2006).

Note that the new Reference Occultation Processing System (ROPS) developed at the WEGC provides integrated uncertainty propagation of retrieved profiles as introduced by Schwarz et al. (2017) and Schwarz et al. (2018).

Research answer 3: Errors of individual RO profiles

Individual atmospheric profiles from RO measurements have smallest (constant) observational errors in the tropopause region, where errors are within 0.8 % in bending angle, 0.35 % in refractivity, 0.15 % in dry pressure, 10 m in dry geopotential height, and 0.7 K in dry temperature. Observational errors exponentially increase in the stratosphere. Largest stratospheric observational errors are found in hemispheric winter at high latitudes. In the troposphere, the errors of bending angle, refractivity, and dry atmospheric parameters increase following an inverse height power-law (Scherllin-Pirscher et al. 2011a). Decreasing tropospheric observational errors are found for physical temperature and potential temperature due to increasing influence of background information (Scherllin-Pirscher et al. 2017a).

1.3.2. Error characterization of RO gridded fields

Individual RO profiles can be used to calculate gridded atmospheric fields. This can be performed by binning and averaging as described, e.g., by Foelsche et al. (2008) and Pirscher (2010) or by optimally interpolating data, e.g., with a Bayesian interpolation technique (Leroy et al. 2012). Independent of the details of their generation, RO gridded fields are affected by several errors, including (i) systematic errors, (ii) sampling errors, and (iii) statistical (random) errors.

The fourth research question raised in this thesis is:

Research question 4

How large are the errors of RO gridded atmospheric fields?

Systematic errors of RO gridded fields are caused by the measurements themselves and by assumptions made in the data processing (Scherllin-Pirscher et al. 2011b). A dedicated study by Danzer et al. (2013) investigated the ionospheric influence on retrieved neutral-atmosphere profiles. The authors found that the ionospheric residual daytime bias of observed RO data increases from low to high solar activity. This ionospheric error propagated down and left a temperature bias larger than 2 K at 35 km.

Other sources for the systematic error include, e.g., errors in excess phase measurements and orbit determination, errors due to local multipath and due to background information-dependent initialization of bending angle profiles, the spherical symmetry assumption in the retrieval, strong horizontal gradients, tracking errors, super-refraction, and the degradation of the quality of the L2 signal (Scherllin-Pirscher et al. 2011b). Between about 10 km and 20 km (specific height limits slightly depend on the atmospheric parameter), the systematic error was estimated to about 0.1 % in bending angle, 0.05 % in refractivity, 0.1 % in dry pressure, 7 m in dry geopotential height, and 0.1 K in dry temperature (Scherllin-Pirscher et al. 2011b), and 0.15 K in potential temperature (Scherllin-Pirscher et al. 2017a). In general, the total climatological error was dominated by the systematic error.

The sampling error in gridded atmospheric fields is caused by undersampling true atmospheric variability in the four-dimensional space. It can be estimated from a reference atmosphere, which adequately represents atmospheric variability (e.g., Pirscher 2010). Pirscher et al. (2007), Foelsche et al. (2008), and Scherllin-Pirscher et al. (2011b) found that the sampling error is largest in regions with high atmospheric variability such as observed at winter high latitudes, where it can reach several Kelvin. Systematic undersampling of the true diurnal cycle yields a local time component error, which is much smaller as it rarely exceeds 0.15 K (Pirscher et al. 2007; Foelsche et al. 2009a).

Subtracting the estimated sampling error from an RO gridded field leaves a residual sampling error. It is caused by limitations of the reference atmosphere, which does not fully represent true atmospheric variability. Scherllin-Pirscher et al. (2011b) estimated the residual sampling error and found that it amounts to approximately 30 % of the original sampling error. Between 10 km and 20 km, the residual sampling error is about 0.045 % in bending angle, refractivity, and dry pressure, 3 m in dry geopotential height, 0.09 K in dry temperature (Scherllin-Pirscher et al. 2011b), and 0.15 K in potential temperature (Scherllin-Pirscher et al. 2017a).

The statistical (random) error strongly depends on the number of measurements going into the statistics. It can be estimated from the observational error of individual profiles (Scherllin-Pirscher et al. 2011a) divided by the square-root of the number of profiles. (Scherllin-Pirscher et al. 2011b) and (Scherllin-Pirscher et al. 2017a) showed that this error component is significantly smaller than the others if sampling size is large. For typical monthly mean 10°-zonal mean climatologies of CHAMP (200 measurements per bin) and F3C (3600 measurements per bin), the statistical error between approximately 10 km and 20 km (specific height limits again slightly depend on the atmospheric parameter) is approximately 0.06 %/0.015 % in bending angle, 0.025 %/0.006 % in refractivity, 0.01 %/0.0025 % in dry pressure, 0.7 m/0.17 m in dry geopotential height, 0.05 K/0.012 K in dry temperature (Scherllin-Pirscher et al. 2011b), and 0.01 K/0.06 K in potential temperature (Scherllin-Pirscher et al. 2017a).

Scherllin-Pirscher et al. (2011b) created an error model that can be used to model all three individual error components as well as the total climatological error. The model can be applied to all relevant RO variables from bending angle, refractivity, to dry and physical atmosphere parameters (Scherllin-Pirscher et al. 2017a) and accounts for vertical, latitudinal, and seasonal variations. The total climatological error is smallest at low latitudes between about 10 km and 20 km, where it is about 0.12 % in bending angle, 0.07 % in refractivity, 0.12 % in dry pressure, 8 m in dry geopotential height, and 0.15 K in dry temperature for single-satellite climatologies. Towards higher latitudes, the error increases to 0.4 % in bending angle, 0.3 % in refractivity, 0.5 % in dry pressure, 30 m in dry geopotential height, and 0.6 K in dry temperature in winter time.

Note, that these errors are still small compared to other UTLS observing systems of thermodynamic atmospheric variables and that the claim, that “RO data are of high accuracy and precision” is still valid. Therefore, the data are well suited for investigating atmospheric variability in the UTLS.

Research answer 4: Errors of RO gridded fields

RO gridded fields are affected by systematic errors, (residual) sampling errors, and statistical (random) errors. In general, the resulting total climatological error is dominated by the systematic error, which can contain a non-negligible residual ionospheric contribution (Danzer et al. 2013). The statistical error strongly depends on the number of measurements per bin.

The total climatological error is smallest at low latitudes between about 10 km and 20 km, where it is about 0.12 % in bending angle, 0.07 % in refractivity, 0.12 % in dry pressure, 8 m in dry geopotential height, and 0.15 K in dry temperature. Towards higher latitudes, the error increases to 0.4 % in bending angle, 0.3 % in refractivity, 0.5 % in dry pressure, 30 m in dry geopotential height, and 0.6 K in dry temperature in winter time (Scherllin-Pirscher et al. 2011b). These errors are small compared to those of other UTLS observing systems.

1.4. Atmospheric variability observed with GPS RO

1.4.1. Tropical temperature variability associated with quasi-stationary and transient sub-seasonal waves

The atmospheric thermal structure and its variability are coupled with dynamical and physical processes and play a fundamental role for many aspects of the Earth's climate system. At low latitudes, interannual variability, the annual cycle, and sub-seasonal variability are all strongly pronounced. Their interactions, however, are complex but important to understand the entire system.

The fifth research question raised in this thesis therefore is:

Research question 5

What type of tropical atmospheric variability can be observed with GPS RO?

Atmospheric climate change draws a lot of attention because of its global environmental and social impact. The relatively short RO record (continuous observations are only available since 2001) requires sufficiently small errors for detecting temperature trends in the global UTLS. Leroy et al. (2006) suggested that temperature trends should be detectable within 10 to 20 years and first studies were performed in 2008 and 2009 (Schmidt et al. 2008b; Steiner et al. 2009).

Including very first RO measurements from the GPS/MET mission from 1995 and 1997, Steiner et al. (2009) found a significant cooling trend in the tropical lower stratosphere for the month of February from 1997 to 2008. In the upper tropical troposphere, no significant trend was detected because of obscuring ENSO variability. Using RO data from 2001 to 2010, Lackner et al. (2011) found an increase of tropical geopotential height of approximately 15 m/decade, a warming of about 0.3 K/decade in the tropical upper troposphere and a cooling of about

0.6 K/decade in the tropical lower stratosphere. Ao and Hajj (2013) used RO data from 2002 to 2011 and found a widening of the tropical belt of about 1° latitude/decade in the northern hemisphere. In the southern hemisphere, however, they did not find a statistically significant trend signal.

It is not straightforward to use RO data to investigate tropical temperature variability associated with the solar cycle because of the obscuring ionospheric residual in retrieved neutral-atmosphere RO profiles. Remember, e.g., that Danzer et al. (2013) found an ionospheric residual daytime temperature bias that was larger than 2 K at 35 km during high solar activity (see also Section 1.3.2).

Randel and Wu (2015) and Scherllin-Pirscher et al. (2017b) used RO measurements and investigated tropical temperature variability associated with natural variability modes. While Randel and Wu (2015) focused on zonal-mean temperature variability, Scherllin-Pirscher et al. (2017b) closely investigated longitudinally-resolved tropical temperature variability.

Both studies and also Wilhelmsen et al. (2018) confirmed that the dominant stratospheric variability mode is associated with the QBO, which manifests itself as alternating easterly and westerly zonal winds. It has a period of approximately 28 months and large impacts on the entire global stratosphere (Baldwin et al. 2001). Randel et al. (2003) showed first the QBO pattern in tropical RO temperature using data from the GPS/Met satellite. Schmidt et al. (2004) and Schmidt et al. (2005) used longer time series of CHAMP measurements and showed that maximum QBO-related anomalies were within ±4.5 K between 22 km and 31 km. Randel and Wu (2015) found a peak of QBO-related variability (>3 K^2) at approximately 26 km.

Interannual tropical tropospheric variability is dominated by the ENSO phenomenon, which emerges from the atmosphere-ocean interaction in the tropical Pacific. First studies of ENSO using RO data were performed in the framework of climate change detection studies (Lackner et al. 2011; Steiner et al. 2011). In a dedicated study, Scherllin-Pirscher et al. (2012) investigated the vertical and spatial structure of ENSO using RO data and showed that anomalies are mostly within ±2 K. The study of Randel and Wu (2015) revealed a peak of zonal-mean temperature variability of approximately 0.4 K^2 at 19 km. More details about the atmospheric response from ENSO can be found in Section 1.4.2.

A clear tropical annual cycle of zonal-mean temperatures (variance up to 10 K^2) is evident only close to the tropopause between 16 km and 22 km (Randel and Wu 2015). Resolving longitudinal variability reveals also some seasonal variability in the tropical troposphere below 14 km (Scherllin-Pirscher et al. 2017b). Largest temperature anomalies (±2 K) related to the annual cycle were found close to the tropopause at 18 km from November to May with strong negative anomalies east of the convective regions of the Maritime Continent (including Malaysia, New Guinea, Indonesia, and the surrounding seas) and over the western Pacific (Scherllin-Pirscher et al. 2017b).

On average, tropical quasi-stationary waves associated with the annual cycle and interannual variability account for one third (1 K^2) of total resolved variance (3 K^2) in the tropical tropopause region.

Equatorial sub-seasonal variability (here defined as variations with periods shorter than 100 days) essentially contains signals of the Madden Julian Oscillation (MJO) and equatorial waves. The MJO (also called equatorial intraseasonal oscillation) mainly occurs in the equatorial Indian ocean and western Pacific ocean, where organized deep convection and precipitation propagate eastward at an average speed of 5 $\mathrm{m\,s^{-1}}$. It is a dominant atmospheric oscillation pattern in the tropics with a local intraseasonal period of 30 days to 90 days (Zhang 2005). Zeng et al. (2012) investigated the MJO with RO data and found an MJO-related warm RO temperature anomaly smaller than 1 K in the middle and upper troposphere over the Indian and western Pacific oceans. At the cold point tropopause, associated temperature anomalies were distinctively larger (up to 2 K) (Kim and Son 2012; Zeng et al. 2012).

Alexander et al. (2008) performed space-time spectral analysis of gridded F3C data in the equatorial lower stratosphere. The authors found that equatorially trapped Kelvin waves and Mixed Rossby gravity waves (MRGW) with zonal wave numbers larger than -5 dominated the wave spectra. Westward propagating equatorial Rossby waves with meridional mode number $n = 1$ and eastward propagating equatorial inertia-gravity waves with $n = 0$ were only weakly resolved. Therefore, I focus here on eastward propagating Kelvin waves and westward propagating MRGW that were both already predicted by Matsuno (1966) and observed by Yanai and Maruyama (1966) and Wallace and Kousky (1968).

Atmospheric Kelvin waves are eastward propagating oscillations that are observed in the equatorial troposphere and stratosphere (within 15°N and 15°S). Typically, these waves are characterized by periods from 4 to 30 days, wave numbers 1 to 6, and an eastward phase speed between 15 $\mathrm{m\,s^{-1}}$ and 30 $\mathrm{m\,s^{-1}}$ (Randel and Wu 2005). Temperature variations associated with atmospheric Kelvin waves can be larger than 3 K (Scherllin-Pirscher et al. 2017b) and explain about two thirds (2 K^2) of total resolved variance in the tropical tropopause region.

Scherllin-Pirscher et al. (2017b) also showed that Kelvin waves are highly transient in time. In the lower and middle stratosphere (above 20 km), these waves are strongly modulated by the QBO with enhanced wave activity during the westerly shear phase of the QBO. In the tropical tropopause region, however, peaks of enhanced Kelvin-wave activity were irregularly distributed in time without any distinct periodicity. While several peaks in Kelvin wave activity coincided with peaks of zonal variance of sub-seasonal waves of convection, other maxima were not evidently related. The nature of these modulations in Kelvin waves near the tropopause remains poorly understood and requires further investigation.

MRGW travel westwards with periods smaller than 5 days. Typically, these waves have zonal wave numbers larger than -5 and a westward phase speed between 20 $\mathrm{m\,s^{-1}}$ and 30 $\mathrm{m\,s^{-1}}$ (Alexander et al. 2008). Amplitudes of MRGW were found to be smaller than 1.2 K at 22 km and smaller than 0.6 K at 16 km (Alexander et al. 2008).

Due to their high vertical resolution, RO data were also used to investigate characteristics of atmospheric gravity waves (e.g., Tsuda et al. 2000; de la Torre et al. 2004; Ratnam et al. 2004; Schmidt et al. 2008a; Wang and Alexander 2010; McDonald 2012; Nath et al. 2015). Several studies found large temperature perturbations associated with gravity waves in the tropical lower stratosphere (e.g., Tsuda et al. 2000; Ratnam et al. 2004; Schmidt et al. 2008a). In the altitude range from 17.5 km to 22.5 km, Wang and Alexander (2010) found temperature amplitudes of atmospheric gravity waves between 0.8 K and 1 K with largest amplitudes found over land. While vertical wavelengths were only about 5 km, horizontal wavelengths were found to be between 3000 km and 4000 km. Wang and Alexander (2010) identified low-intrinsic frequency inertio gravity waves to dominate gravity wave activity.

Tropical temperature variability with relatively short periods is associated with migrating diurnal tides. Alexander and Tsuda (2008), Zeng et al. (2008), Pirscher et al. (2010), and Xie et al. (2010) studied atmospheric tides with RO observations and consistently found increasing amplitudes with decreasing density (i.e., increasing height) due to the wave energy conservation (Chapman and Lindzen 1970). In the tropics, migrating diurnal tides reach an amplitude of approximately 1 K at an altitude of 30 km (Pirscher et al. 2010).

Besides these interannual, annual, and intra-annual modes, tropical temperature variability can also be modulated by events that happen on an irregular basis such as tropical cyclones, volcanic eruptions, or SSW events. Using RO data from 2001 to 2012, Biondi et al. (2015) found negative temperature anomalies near the cloud top of tropical cyclones. Looking into detail revealed different characteristics of temperature profiles in (or close to) tropical cyclones for northern and southern hemisphere ocean basins.

Mehta et al. (2015) investigated the UTLS temperature time series from 2001 to 2010 and found a warming signal associated with two volcanic eruptions in 2006. Between 16 km and 18.5 km, temperature increased from 0.5 K to 0.8 K. Biondi et al. (2017) investigated the thermal structure before and after two volcanic eruptions in June 2011 and found an upper troposphere cooling signal after the eruption of the Puyehue volcano, which mainly released volcanic ash into the atmosphere. In contrast, a significant stratospheric warming signal was found after the eruption of the Nabro volcano, which mainly released water and sulfur dioxide into the atmosphere.

The impact of SSW events on tropical temperature variability was confirmed by Randel and Wu (2015), who found two distinct peaks in tropical temperature time series that were associated with two well-known large SSW events in 2002 and 2009.

Research answer 5: Tropical atmospheric variability

Tropical temperature variability in the UTLS occurs on very different time scales. In the tropical tropopause region, quasi-stationary waves associated with interannual variability and the annual cycle account for about one third of total resolved variance. The remaining two thirds are associated with atmospheric equatorial waves (Scherllin-Pirscher et al. 2017b). Several studies exploited the high potential of RO data and investigated (i) atmospheric climate change, (ii) interannual variability associated with the QBO and ENSO, (iii) the annual cycle, (iv) the MJO, (v) equatorial planetary-scale waves such as Kelvin waves and MRGW, (vi) gravity waves, (vii) migrating diurnal tides, and irregular events such as tropical cyclones, volcanic eruptions, and SSW events.

1.4.2. Three-dimensional atmospheric response of ENSO

Global weather and climate are influenced by the interannual ENSO phenomenon. During the warm ENSO phase, Sea Surface Temperature (SST) anomalies over the equatorial eastern Pacific enhance convection and rainfall over the tropical eastern and central Pacific. Large-scale atmospheric waves that are generated by convection, influence weather outside the tropics from high northern latitudes (e.g., Song and Son 2018) to high southern latitudes (e.g., Turner 2004). Domeisen et al. (2019) gave a comprehensive review about observational and modeling studies that contributed to our current knowledge of ENSO teleconnections. The research question is:

Research question 6

What is the three-dimensional atmospheric response of ENSO in the UTLS?

In recent decades, numerous studies investigated the influence of ENSO on atmospheric temperature. These studies consistently showed that the warm phase of ENSO (El Niño) is associated with tropospheric warming and stratospheric cooling at tropical latitudes. Relative to the forcing mechanism in the eastern Pacific, the atmospheric zonal-mean temperature signal is lagged by one or two seasons (e.g., Angell 1981; Su et al. 2005; Chou and Lo 2007).

Using observations from the Microwave Sounding Unit (MSU) instrument, Yulaeva and Wallace (1994) and Calvo Fernández et al. (2004) found different atmospheric ENSO signatures for the zonal-mean and for deviations from the zonal-mean ("eddy") temperature components, whose evolutions were not simultaneous. Similar results were found by Trenberth and Smith (2006), Trenberth and Smith (2009), and Zhou and Zhang (2011), who identified two distinct modes of ENSO-related variability, which were in general agreement with zonal-mean and eddy ENSO signals.

Motivated by these studies, Scherllin-Pirscher et al. (2012) investigated the vertical and spatial structure of ENSO in more detail by exploiting the unprecedented vertical resolution and global coverage of RO. Data were used for the period August 2006 to December 2010 and gridded into 5° latitude by 5° longitude boxes with a 100 m vertical spacing. Monthly mean anomalies were calculated from subtracting the mean annual cycle. The ENSO signal was identified by Principal Component Analysis (PCA) and multiple linear regression analysis.

This study confirmed that ENSO-related interannual temperature anomalies naturally decompose into zonal-mean and eddy components. Since these components are caused by different underlying physical processes, they feature different spatial characteristics and temporal evolutions.

Zonal-mean tropospheric warming was found during the warm ENSO phase. It was most pronounced between 8 km and 15 km (approximately 2 K), which was in good agreement with previous studies. It can be explained by the anomalous heat flux from the tropical Pacific ocean to the atmosphere (Seager et al. 2003). The transition from tropospheric warming to stratospheric cooling, linked to enhanced tropical upwelling (Randel et al. 2009; Calvo et al. 2010) during El Niño, occurred close to the tropopause at approximately 17 km. Correlation to the monthly Niño 3.4 SST index revealed a lag between the SST forcing and the atmospheric zonal-mean response of 3 months.

The atmospheric eddy component, in contrast, responded rapidly (within 1 month) to ENSO forcing. The signal was symmetric about the equator and showed a low-latitude dipole between the Indian Ocean and the Pacific Ocean centered slightly west of the date line (180°). Off-equatorial maxima were centered around 20°N to 30°N latitude in both hemispheres. This pattern was consistent with

Rossby and Kelvin wave circulations induced by equatorial heating anomalies (Gill 1980; Highwood and Hoskins 1998). Maximum amplitude was attained in the upper troposphere near 11 km and (with opposite polarity) in a shallow layer near the tropopause at approximately 17 km. This shallow response near the tropopause results from hydrostatic horizontal pressure gradients associated with deep convective heating (Holloway and Neelin 2007). At mid latitudes, eddy ENSO signals were out-of-phase with those at low latitudes.

Research answer 6: Three-dimensional atmospheric response of ENSO

ENSO-related interannual temperature anomalies occur as a zonal-mean and an eddy component, which feature different spatial characteristics and temporal evolutions.

The warm ENSO phase is characterized by zonal-mean tropospheric warming (most pronounced between 8 km and 15 km) and zonal-mean stratospheric cooling. The warming to cooling transition occurs close to the tropopause at approximately 17 km. Strongest atmospheric zonal-mean response is observed about 3 months after maximum ENSO SST. The eddy ENSO signal features a low-latitude dipole between the Pacific Ocean and the Indian Ocean and is symmetric about the equator. During the warm ENSO phase, tropospheric warming/cooling is strongest over the Pacific/Indian Ocean near 11 km. The node to a spatial signal with opposite polarity occurs at approximately 14 km and the reversed signal is strongest in a shallow layer near the tropopause. This atmospheric eddy component responds rapidly (within 1 month) to ENSO forcing (Scherllin-Pirscher et al. 2012).

Scherllin-Pirscher et al. (2012) clearly showed that the three-dimensional atmospheric response of ENSO is complex and cannot be described by a simple one-dimensional time series. It is therefore important to closely investigate the temporal evolution of the full three-dimensional field. This was done by Wilhelmsen et al. (2018) and is summarized in the next section.

1.4.3. Vertically-resolved indices of ENSO and the QBO

The temporal evolution of atmospheric variability modes can be described by specific indices. These indices characterize the nature of the mode and quantify the phenomenon. Underlying data are usually some kind of anomalies calculated from measurements at selected meteorological stations or gridded fields of climate variables. In order to describe the target pattern, indices are derived from variables closely associated with the phenomenon. ENSO, for example, is usually quantified by either SST anomalies averaged over specific regions and/or mean sea level pressure measured at specific locations (Kaplan 2010). Similarly, the phase of the QBO is described by equatorial winds at pre-defined pressure levels (Baldwin et al. 2001). Conventional QBO indices are provided at 30 hPa and 50 hPa.

Since ENSO and the QBO exhibit different signatures at different heights, these indices do not describe their full three-dimensional atmospheric responses. It is important, however, to fully account for natural atmospheric variability including its vertical characteristics in climate trend analyses. The seventh research question therefore is:

Research question 7

Is it possible to calculate meaningful vertically-resolved ENSO and QBO indices from RO data? If so, what is their added value?

To answer this question, Wilhelmsen et al. (2018) used tropical temperature measurements from RO and applied an EOF analysis to identify major modes of natural variability following two independent approaches. First, they decomposed atmospheric variability from the entire vertical and horizontal temperature field from 30°S to 30°N (5° × 5° horizontal resolution) and from 2 km to 35 km (200 m vertical spacing). Second, they used the two-dimensional horizontal temperature fields and applied an EOF analysis separately at each vertical level. This second approach exploits the high vertical resolution of RO.

Decomposing atmospheric variability from the entire vertical and horizontal RO temperature field revealed QBO- and ENSO-related variability from EOF1 to EOF4. Together, they explained about 65 % of total variability. While EOF1 and EOF2 were closely associated with the QBO (correlation coefficients between Principal Component (PC) time series and 30 hPa and 50 hPa QBO winds were larger than 0.8), EOF3 and EOF4 were obviously linked to ENSO (correlation between PC3+PC4 and the Niño 3.4 SST index was larger than 0.8 at a lag of 3 months).

Decomposing atmospheric variability from two-dimensional horizontal temperature fields provided more detailed information about the vertical structure of temperature variability. Patterns of the first and second EOF were clearly associated with ENSO and the QBO in the troposphere and stratosphere, respectively. Corresponding PC time series were highly correlated with conventional ENSO and QBO indices. Explained variance of the sum of EOF1 and EOF2 peaked at 14 km (70 % of total variance) and at 25 km (85 % of total variance). Less variance was explained close to the tropical tropopause region at 17 km, where irregular events such as volcanic eruptions or SSW events as well as sub-seasonal variability

associated with the MJO, e.g., contribute to tropical temperature variability (see Section 1.4.1 for more details).
PC time series from this approach can be used as indices as they describe natural atmospheric variability mainly associated with ENSO and the QBO. Since these indices cover the vertical details of atmospheric variability, they can easily be used in climate trend analyses because there is no need to account for response time lags at different altitude levels. This is of great benefit for climate trend analyses with data that have high vertical resolution.

Research answer 7: ENSO and QBO indices

Major modes of natural variability can be identified by EOF analysis. The high vertical resolution of RO can be exploited by applying an EOF analysis separately at each vertical level. This allows deriving vertically-resolved ENSO and QBO indices.
In the troposphere and stratosphere, the first and second EOFs are clearly associated with ENSO- and QBO-related variability (Wilhelmsen et al. 2018). PC time series from this EOF analysis can be used as indices. Since these indices cover the vertical details of atmospheric variability, they can easily be used in climate trend analyses because there is no need to account for response time lags at different altitude levels. This is of great benefit for climate trend analyses with data that have high vertical resolution.

1.4.4. Global variability of the thermal tropopause

The tropopause marks the transition layer between the convectively well-mixed troposphere and the stably stratified stratosphere. The variability of physical tropopause properties is complex because it reacts to both tropospheric and stratospheric changes. Since tropopause characteristics are also known to provide valuable information about climate change (e.g., Sausen and Santer 2003), detailed understanding of its natural variability is crucial. The eighth research question raised in this thesis therefore is:

Research question 8

What are the spatio-temporal characteristics of the tropopause observed with GPS RO?

Already in the very early years of RO, these data were used to better understand thermodynamical characteristics of the tropopause region. Nishida et al. (2000) used RO data from the GPS/Met satellite to investigate the tropopauses' seasonal and longitudinal variability. The authors showed that RO data are suitable to resolve rapid temperature variations near the tropical tropopause. Randel et al. (2003) extended their analysis and found that sub-seasonal variability of cold-point tropopause temperature and height were caused by wave-like fluctuations originating from inertia-gravity waves and other tropical oscillations such as Kelvin waves.

Two years of RO measurements of the CHAMP satellite were used by Schmidt et al. (2004), who investigated the spatio-temporal variability of the lapse-rate and cold-point tropopause mainly in the tropics but also on the global scale and gave further insights into their annual cycles, horizontal variability, and inter-annual variability associated with the QBO.

The combined set of CHAMP and SAC-C data were used by Schmidt et al. (2005) and Kishore et al. (2006), who analyzed tropopause characteristics in terms of altitude, temperature, pressure, potential temperature, and sharpness. Randel et al. (2007b), Grise et al. (2010), and Noersomadi et al. (2018) calculated and analyzed static stability from RO to better characterize the temperature inversion layer right above the tropopause.

Detailed investigations of the lapse-rate tropopause and cold-point tropopause spatio-temporal characteristics were performed by Son et al. (2011) and Kim and Son (2012), who exploited the F3C record.

Rieckh et al. (2014) used the RO record of more than 12 years and investigated characteristics of lapse-rate tropopause altitude and temperature. This study confirmed the well-known latitudinal structure of high and cold tropical tropopauses (tropopause height between 16 km and 17 km and tropopause temperature between 190 K and 195 K) and low (warm) extra-tropical tropopauses (tropopause height between 8 km and 12 km and tropopause temperature mainly between 210 K and 220 K). While little variability was found at low latitudes and in the summer polar region (standard deviations about 1.5 km to 2 km and 5 K to 10 K, for tropopause height and temperature, respectively), large variability was detected close to the subtropical break and at mid- and high latitudes in hemispheric winter (standard deviations larger than 4 km and 20 K, respectively).

Longitudinal variability was found to be much smaller than latitudinal variations. Noticeable latitudinal asymmetries were identified in the tropics above South Asia, where tropopause height was up to 1 km higher than the zonal mean in boreal summer. This pattern was linked to deep convective activity, which increased tropopause height. Zonal asymmetries were also found in the northern hemisphere mid-latitudes above eastern Canada and eastern Russia, where tropopause height was up to 3 km lower than the zonal mean in boreal winter. These zonal asymmetries were attributed to tropospheric processes associated with Rossby wave activity.

Rieckh et al. (2014) also investigated temporal tropopause variations in terms of the mean annual cycle and interannual variability. At low latitudes, amplitudes of seasonal variations were within 0.5 km for tropopause height and 3.5 K for tropopause temperature. Annual cycles of northern and southern hemisphere low latitudes were in phase with maxima found in southern hemisphere summer and minima found in southern hemisphere winter. While incoming radiation was found to drive seasonal variations in the tropical southern hemisphere, the Brewer–Dobson Circulation (BDC) with strong tropical upwelling in northern hemisphere winter was found responsible for the seasonal cycle of tropical tropopause characteristics in the northern hemisphere.

At mid- and high latitudes the annual cycle was significantly stronger (amplitudes up to 2 km and 5 K, even larger at southern hemisphere high latitudes) and in phase with incoming radiation or atmospheric dynamics (strengths of the polar vortex).

Interannual variability was dominated by ENSO and the QBO at low latitudes and by the strength of the polar vortex and SSW events at high latitudes. The strongest ENSO signal was found above the tropical central Pacific, where tropopause height increased and tropopause temperature decreased during the warm ENSO phase. A more longitudinally uniform signal was found for the QBO response with a lower (warmer) tropopause during westerly QBO winds at 50 hPa and higher (colder) tropopause during easterly QBO winds. During SSW events, when stratospheric temperatures can increase by up to 50 K within a couple of days, tropopause was found lower and warmer compared to normal conditions.

It is interesting to note that Rieckh et al. (2014) also revealed some distinct features of multiple tropopauses, which were mainly found close to the equator, in the extra-tropics between 20° and 40° N/S, and at high latitudes in the winter hemisphere. In the extra-tropics between 20° and 40° N/S multiple tropopauses are of most interest for this thesis because they are linked to the characteristic break in the thermal tropopause near the subtropical jet (Randel et al. 2007a). Climatological wind fields from RO are discussed in the next section.

Research answer 8: Tropopause characteristics

Rieckh et al. (2014) used the RO record of more than 12 years and investigated characteristics of lapse-rate tropopause altitude and temperature. In agreement with many other studies, Rieckh et al. (2014) also found high and cold tropical tropopauses, which featured only little variability. Annual cycles at northern and southern hemisphere low latitudes were in phase with amplitudes within 0.5 km and 3.5 K for height and temperature, respectively. Tropical interannual variability was dominated by ENSO and the QBO.

In the extra-tropics (apart from the polar region), tropopauses were low and warm. Large variability occurred close to the subtropical break and at mid latitudes in hemispheric winter. The amplitude of the annual cycle was up to 2 km in tropopause altitude and 5 K in tropopause temperature.

While only little tropopause variability was found in the summer polar region, large variability occurred in hemispheric winter (partly because lapse-rate tropopauses are ill-defined in polar winter). The annual cycle was in phase with incoming radiation or atmospheric dynamics (strengths of the polar vortex). Interannual variability was dominated by the strength of the polar vortex and SSW events.

1.5. Atmospheric dynamics derived from GPS RO

The retrieval and error characteristics of thermodynamic atmospheric variables from GPS RO measurements were explained in detail in Sections 1.2 and 1.3 of this thesis. Since the RO processing is independent of the dynamical state of the atmosphere, dynamical properties cannot be derived from individual RO measurements. However, according to the theory, atmospheric dynamics can be derived from RO gridded fields. This section gives more detailed information about that and shows how accurate dynamical atmospheric features can be derived from GPS RO.

1.5.1. Climatological wind fields from GPS RO

There are currently very limited measurements of vertically-resolved profiles of tropospheric and stratospheric winds that are globally available. Radiosonde measurements can be used to infer wind by tracking their position with time but these measurements are mainly available in the northern hemisphere over land. The same is true for radar wind observations.

Geostationary satellites such as the European Meteosat satellites or the U.S. Geostationary Operational Environmental Satellite (GEOS) satellites carry instruments (Spinning Enhanced Visible Infra-Red Imager (SEVIRI) and Advanced Baseline Imager (ABI), respectively) that track clouds or water vapor features and allow the computation of cloud motion winds. These measurements, however, are only available over limited areas. Polar orbiting satellites (such as Metop, Aqua, and

Terra) perform similar measurements on a global scale but these measurements are only available for cloud-covered height layers.

In this regard, the launch of the ADM-Aeolus satellite on 22 August 2018 was a milestone because its Atmospheric Laser Doppler Instrument (ALADIN) provides vertically-resolved wind measurements that will be needed for a better understanding of the Earth's atmospheric dynamics. However, it will take a while until these data can be used to study variability of wind on an annual- and interannual time scale. Therefore, it is worth investigating if RO data can be used to provide information about vertically-resolved climatological wind fields.

Leroy (1997) was the first who suggested deriving climatological wind fields from RO data. Since RO provides virtually independent information of the vertical height grid and retrieved thermodynamic atmospheric profiles, geopotential height of pressure levels and the Montgomery potential of potential temperature levels can be computed. If these physical quantities are of high quality, it should be possible to derive reliable and high quality information of horizontal wind fields in terms of geostrophic and gradient winds.

The ninth research question raised in this thesis therefore is:

Research question 9

Is it possible to obtain high-quality climatological wind fields from GPS RO? If so, what can we learn from these data?

Almost 20 years after Leroy (1997) suggested deriving climatological wind fields from RO, Scherllin-Pirscher et al. (2014) and Verkhoglyadova et al. (2014) confirmed that high-quality climatological wind fields outside the tropics can indeed be inferred from horizontal RO geopotential height gradients on pressure levels. Both studies showed that RO-derived geostrophic and gradient winds clearly capture all of the main wind features. Dominating error sources are the sampling error and ageostrophy. Accounting for the sampling error (i.e., subtracting the estimated sampling error from geopotential height fields), Scherllin-Pirscher et al. (2014) found that biases are, in general, smaller than 2 $\mathrm{m\,s^{-1}}$. Larger biases (up to 10 $\mathrm{m\,s^{-1}}$) were caused by the geostrophic/gradient wind approximation, which is violated close to the subtropical jet and at high latitudes. Residual sampling errors and systematic errors from RO were found to be very small.

Scherllin-Pirscher et al. (2017a) calculated geostrophic wind of sampling error-corrected climatological fields of both geopotential on isobaric surfaces and the Montgomery potential on isentropic surfaces. Maximum column wind speeds were then calculated to investigate vertical characteristics of climatological wind in the upper troposphere from 500 hPa to 50 hPa above the tropopause.

Scherllin-Pirscher et al. (2017a) found maximum monthly-mean geostrophic wind speeds in the winter hemisphere at mid-latitudes. At the location of maximum column wind speed, geopotential height, pressure, and potential temperature varied widely between about 9 km and 13 km, 180 hPa and 250 hPa, and 330 K and 360 K, respectively.

The absolute maximum of maximum column wind speed between 20° S/N and 50° S/N was then used to identify the jet stream core, which was most frequently found above the western Pacific close to China in the northern hemisphere. In the southern hemisphere, however, it was distributed in different longitudinal regions during one year. In both hemispheres, the jet stream wind speed revealed a distinct seasonal cycle with highest speeds in hemispheric winter (about 70 $\mathrm{m\,s^{-1}}$ in the northern hemisphere in January and about 60 $\mathrm{m\,s^{-1}}$ in the southern hemisphere in July). Geopotential height, pressure, and potential temperature showed hardly any seasonal cycle at jet stream core location in the northern hemisphere. In the southern hemisphere, a distinct annual cycle was found for all parameters, with potential temperature and geopotential height being in phase with wind speed (maximum in austral winter) and pressure being out of phase with wind speed (maximum in boreal winter).

Climatological wind fields from GPS RO were already used to study the generation and specific characteristics of internal gravity waves. Pišoft et al. (2018) calculated the vertical rotation of the RO wind direction and found that in the northern hemisphere, wind rotation exceeds 180° mainly over the northern Pacific. Comparison to the maximum growth rate of disturbances arising from the Rayleigh–Taylor convective instability, which is a measure for the probability of internal gravity wave breaking, revealed high correspondence between the spatial distribution of the critical rotation of background wind and the maximum growth rate of the disturbances. This study also confirmed the importance of the region close to east Asia and the north Pacific as a unique source of gravity wave drag in the lower stratosphere.

Research answer 9: Climatological wind fields

Outside the tropics, high-quality climatological wind fields can be inferred from horizontal RO geopotential height gradients on pressure levels or from horizontal gradients of the RO Montgomery potential on potential temperature levels. Accounting for the sampling error, biases are, in general, smaller than 2 $\mathrm{m\,s^{-1}}$. Larger biases (up to 10 $\mathrm{m\,s^{-1}}$) are caused by the geostrophic/gradient wind approximation, which is violated close to the

subtropical jet and at high latitudes. Residual sampling errors and systematic errors from RO are very small (Scherllin-Pirscher et al. 2014).
RO geostrophic wind fields can be used, e.g., to investigate spatial and temporal characteristics of climatological winds. Scherllin-Pirscher et al. (2017a) showed that the wind speed in the jet stream core (i.e., the location of the absolute maximum of maximum column wind speed between 20° S/N and 50° S/N) has a distinct seasonal cycle with highest speeds in hemispheric winter.

1.5.2. Atmospheric blocking from GPS RO

Atmospheric blocking occurs when a persistent and stationary high-pressure system blocks the climatological westerly flow at mid-latitudes for several days to weeks. Blocking episodes are often associated with anomalous weather patterns and extreme events (e.g., Cattiaux et al. 2010; Matsueda 2011; Mattingly et al. 2015; Brunner et al. 2019) but key mechanisms still are not entirely clear and occurrence is underestimated in current weather and climate models (e.g., Pfahl et al. 2015). Accuracy, precision, and high vertical resolution of GPS RO might help to better understand the three-dimensional state of the atmosphere before, during, and after blocking events. The tenth research question raised in this thesis therefore is:

Research question 10

Is it possible to detect atmospheric blocking with GPS RO and what are its limitations?

Blocking occurs on synoptic spatial and temporal scales. To detect this atmospheric phenomenon, it is therefore mandatory to compute atmospheric fields with high spatial and temporal resolution. Brunner et al. (2016) calculated daily atmospheric fields from GPS RO on a 2.5° × 2.5° longitude–latitude grid by applying a weighted average. This study showed that RO data are dense enough to resolve synoptic atmospheric variability reasonably well and associated errors (mainly the sampling error) are small enough to further investigate atmospheric blocking.
Two well-known blocking events from summer 2010 (blocking over Russia) and late winter/early spring 2013 (blocking over Greenland) were analyzed in detail. A standard blocking detection algorithm, which is based on latitudinal geopotential height gradients at the 500 hPa pressure level was applied. These latitudinal geopotential height gradients are linked to the geostrophic flow described in Section 1.5.1. One of the blocking criteria requires an easterly geostrophic flow equatorwards of

the selected grid point and a strong westerly geostrophic flow polewards of the selected grid point.

Brunner et al. (2016) showed that this distinct anomalous blocking feature did not only occur at the 500 hPa level, but it reached from the atmospheric boundary layer at least up to 300 hPa, sometimes even up to the tropopause. Apart from that, geopotential height increased up to 300 m in the upper troposphere and temperatures increased up to 10 K in the middle and lower troposphere.

Using RO data from 2006 to 2016, Brunner and Steiner (2017) investigated the representation of main blocking regions in the northern and southern hemisphere for different seasons and found that blocking regions are correctly resolved in both hemispheres and also capture seasonal blocking variability. Insufficient sampling, however, led to a slight underestimation of blocking frequencies compared to three reanalysis products. To overcome this problem, more RO measurements with denser sampling at mid and high latitudes are required but this will only be achieved with a sufficient number of RO satellites in polar orbit. It might take a while to have these measurements because the second cluster of Formosa Satellite Mission #7 (FORMOSAT-7)/COSMIC #2 (COSMIC-2) (F7C2), which was supposed to be in polar orbit, was canceled due to a lack of funding in October 2017.

Research answer 10: Atmospheric blocking

From 2006 onwards, RO data sampling is dense enough to resolve synoptic atmospheric variability reasonably well and to investigate atmospheric blocking at mid-latitudes (Brunner et al. 2016). Compared to different reanalyses, however, a slight underestimation of blocking frequencies was found by Brunner and Steiner (2017), who attributed this bias to too sparse measurement density.

Acknowledgments

Working as a PostDoc and project leader is probably one of the most challenging and stimulating, but also valuable and outstanding experiences. I spent most of this time working in the field of RO and this time was awesome. I started with an ASP program, funded by NCAR, Boulder, CO, USA, returned to the University of Graz, Austria, worked as a visiting scientist at EUMETSAT, Darmstadt, Germany and at DMI, Copenhagen, Denmark. Then I had a position within the Hertha-Firnberg program funded by the Austrian Science Fund (FWF), where I was head of my own project and could realize my own project ideas. Thereby, I had the chance to collaborate with well-known and highly experienced researchers, visiting them at their home institutes and inhaling their stimulating working atmosphere. I had the freedom to study scientific questions that were not only important for the scientific community but also attractive for me.

The Wegener Center, University of Graz, Austria, was my scientific home base. My research was embedded in the ARSCliSys research group, led by Gottfried Kirchengast, Andrea Steiner, and Ulrich Foelsche. I would like to thank Gottfried for all his support during my time at WEGC, for sharing his knowledge, work inspiration, helpful discussions, and valuable criticisms. His diligent and accurate working style strongly influenced my work attitude. Without Andrea, who was not only co-applicant of my Hertha-Firnberg proposal and mentor during the project phase, but is also a close friend, I would probably not have finished this habilitation thesis. She supported my scientific work with a great amount of perseverance and gave invaluable feedback and motivation whenever needed. Uli also supported me whenever possible. As co-supervisor of my PhD work, he not only introduced me to the RO community back in 2006, but also brought me in touch with Bill Kuo, one of the most impressive and amiable people I've ever met.

Bill was the one who encouraged me to apply for an ASP fellowship to spend some dedicated research time in the U.S. This was probably the best I could do at that time. I very much enjoyed working in Boulder and benefited from extensive discussions and helpful comments from colleagues of the awesome COSMIC group. Having the opportunity to give a short talk to the NFS director was something very special during my time as an ASP PostDoc in Boulder. Thank you, Rick Anthes, for giving me this chance. Rick is not only a top-ranking and well-known scientist

with altruistic behavior, he was also very helpful with problems in everyday life. Rick was the one who offered and made available his wife's bike for a month during one of my research visits in Boulder. I very much appreciated his help.

In Boulder, I also met Clara Deser, another amazing person. I'm very grateful for her constructive ideas and tireless support during our collaboration. Clara and also Stig Syndergaard from DMI, Copenhagen, strongly stimulated my research career and work attitude. They have the talent to write the most encouraging e-mails and spread their enthusiastic research spirit while—at the same time—pass on constructive criticism. I'm very grateful that I had the opportunity to meet and collaborate with these wonderful people. I would also like to thank Kent Lauritsen from DMI for his continuous support and responsiveness during our successful collaboration.

During my Hertha-Firnberg project, I had the opportunity to spend some research time at Harvard University, Cambridge, MA, USA, collaborating with Stephen Leroy from the Anderson group. Furthermore, I had the chance to visit Bill Randel at NCAR and to collaborate with Joowan Kim, who was at NCAR at that time. I extremely benefited from their hospitality and criticism. I'm very grateful to these three people for sharing their expertise and giving professional guidance.

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I very much enjoyed working in the field of RO and using these wonderful data to study certain aspects of the atmosphere. About three years ago, I moved on to work in a completely different scientific field namely air quality modeling and data assimilation. I again met a few amazing people but I still often miss my former RO colleagues. However, I'm always happy to see them again in very different situations: having a coffee or joint dinner in Graz with colleagues from WEGC, doing a ROM-SAF review and getting together with colleagues from DMI in Copenhagen, or meeting COSMIC people in the hallway of FL4 and going out for lunch or an after-work beer in Boulder. Thank you all.

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Most of all, I would like to thank my family, especially Marko and my parents for their understanding and support, which enabled me to complete this work.

Part II.

Selected papers

1. Research questions and selected papers

1.1. The reproducibility and consistency of the RO record

The following papers answered the research questions

Research questions

1. How large is the structural uncertainty of retrieved CHAllenging Minisatellite Payload (CHAMP) profiles as well as of CHAMP climatological fields?
2. What is the quality and consistency of the Radio Occultation (RO) multi-satellite record?

and significantly enhanced the knowledge about the reproducibility and consistency of the RO record.

Ho et al. (2012): S.-P. Ho, D. Hunt, A. K. Steiner, A. J. Mannucci, G. Kirchengast, H. Gleisner, S. Heise, A. von Engeln, C. Marquardt, S. Sokolovskiy, W. Schreiner, **B. Scherllin-Pirscher**, C. Ao, J. Wickert, S. Syndergaard, K. Lauritsen, S. Leroy, E. R. Kursinski, Y.-H. Kuo, U. Foelsche, T. Schmidt, and M. Gorbunov (2012), Reproducibility of GPS radio occultation data for climate monitoring: Profile-to-profile inter-comparison of CHAMP climate records 2002 to 2008 from six data centers. *J. Geophys. Res.*, 117, D18111, doi:10.1029/2012JD017665.

Steiner et al. (2013): A. K. Steiner, D. Hunt, S.-P. Ho, G. Kirchengast, A. J. Mannucci, **B. Scherllin-Pirscher**, H. Gleisner, A. von Engeln, T. Schmidt, C. Ao, S. S. Leroy, E. R. Kursinski, U. Foelsche, M. Gorbunov, S. Heise, Y.-H. Kuo, K. B. Lauritsen, C. Marquardt, C. Rocken, W. Schreiner, S. Sokolovskiy, S. Syndergaard, and J. Wickert (2013), Quantification of structural uncertainty in climate data records from GPS radio occultation, *Atmos. Chem. Phys.*, 13, 1469–1484 doi:10.5194/acp-13-1469-2013.

Angerer et al. (2017): B. Angerer, F. Ladstädter, **B. Scherllin-Pirscher**, M. Schwärz, A. K. Steiner, U. Foelsche, and G. Kirchengast (2017), Quality aspects of the Wegener Center multi-satellite GPS radio occultation record OPSv5.6. *Atmos. Meas. Tech.*, 10, 4845–4863, doi:10.5194/amt-10-4845-2017.

1.2. Error characterization of RO retrieval products

The following papers answered the research questions

Research questions

3. How large are the errors of individual atmospheric profiles from Global Positioning System (GPS) RO?
4. How large are the errors of RO gridded atmospheric fields?

and provided error estimates of individual atmospheric profiles as well as of gridded climatological fields from GPS RO. An empirical error model, which accounts for the errors' vertical, latitudinal, and seasonal variations, was established.

Scherllin-Pirscher et al. (2011a): **B. Scherllin-Pirscher**, A. K. Steiner, G. Kirchengast, Y.-H. Kuo, and U. Foelsche (2011), Empirical analysis and modeling of errors of atmospheric profiles from GPS radio occultation, *Atmos. Meas. Tech.*, 4, 1875–1890, doi:10.5194/amt-4-1875-2011.

Scherllin-Pirscher et al. (2011b): **B. Scherllin-Pirscher**, G. Kirchengast, A. K. Steiner, Y.-H. Kuo, and U. Foelsche (2011), Quantifying uncertainty in climatological fields from GPS radio occultation: an empirical-analytical error model, *Atmos. Meas. Tech.*, 4, 2019–2034, doi:10.5194/amt-4-2019-2011.

Danzer et al. (2013): J. Danzer, **B. Scherllin-Pirscher**, and U. Foelsche (2013), Systematic residual ionospheric errors in radio occultation data and a potential way to minimize them. *Atmos. Meas. Tech.*, 6, 2169–2179, doi:10.5194/amt-6-2169-2013.

Scherllin-Pirscher et al. (2017a): **B. Scherllin-Pirscher**, A. K. Steiner, G. Kirchengast, M. Schwärz, and S. S. Leroy (2017), The power of vertical geolocation of atmospheric profiles from GNSS radio occultation, *J. Geophys. Res. Atmos.*, 122, 1595–1616, doi:10.1002/2016JD025902.

1.3. Atmospheric variability observed with GPS RO

The following papers answered the research questions

Research questions

5. What type of tropical atmospheric variability can be observed with GPS RO?
6. What is the three-dimensional atmospheric response of El Niño–Southern Oscillation (ENSO) in the Upper Troposphere and Lower Stratosphere (UTLS)?
7. Is it possible to calculate meaningful vertically-resolved ENSO and Quasi-Biennial Oscillation (QBO) indices from RO data? If so, what is their added value?
8. What are the spatio-temporal characteristics of the tropopause observed with GPS RO?

and significantly contributed to the current knowledge of natural atmospheric variability in the tropics associated with quasi-stationary and transient sub-seasonal waves, provided QBO and ENSO indices that can be used for climate trend analyses, and gave deeper insight into natural variability of tropopause altitude and temperature.

Scherllin-Pirscher et al. (2017b): **B. Scherllin-Pirscher**, W. Randel, and J. Kim (2017), Tropical temperature variability and Kelvin-wave activity in the UTLS from GPS RO measurements, *Atmos. Chem. Phys.*, 17, 793–806, doi:10.5194/acp-17-793-2017.

Scherllin-Pirscher et al. (2012): **B. Scherllin-Pirscher**, C. Deser, S.-P. Ho, C. Chou, W. Randel, and Y.-H. Kuo (2012), The vertical and spatial structure of ENSO in the upper troposphere and lower stratosphere from GPS radio occultation measurements, *Geophys. Res. Lett.*, 39, L20801, doi:10.1029/2012GL053071.

Wilhelmsen et al. (2018): H. Wilhelmsen, F. Ladstädter, **B. Scherllin-Pirscher**, and A. K. Steiner (2018), Atmospheric QBO and ENSO indices with high vertical resolution from GNSS radio occultation temperature measurements, *Atmos. Meas. Tech.*, 11, 1333–1346, doi:10.5194/amt-11-1333-2018.

Rieckh et al. (2014): T. Rieckh, **B. Scherllin-Pirscher**, F. Ladstädter, and U. Foelsche (2014), Characteristics of tropopause parameters as observed with

GPS radio occultation. *Atmos. Meas. Tech.*, 7, 3947–3958, doi:10.5194/amt-7-3947-2014.

1.4. Atmospheric dynamics derived from GPS RO

The following papers answered the research questions

Research questions

9. Is it possible to obtain high-quality climatological wind fields from GPS RO? If so, what can we learn from these data?
10. Is it possible to detect atmospheric blocking with GPS RO and what are its limitations?

and showed that high-quality climatological wind fields can indeed be inferred from RO outside the tropics, which also allows studing jet stream variability including the location of the jet stream core. Furthermore, since 2006 RO sampling density is dense enough to detect atmospheric blocking.

Scherllin-Pirscher et al. (2014): **B. Scherllin-Pirscher**, A. K. Steiner, and G. Kirchengast (2014), Deriving dynamics from GPS radio occultation: Three-dimensional wind fields for monitoring the climate, *Geophys. Res. Lett.*, 41(20): 7367–7374, doi:10.1002/2014GL061524.

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2. Contributions to selected papers

Ho et al. (2012): I performed the computational work and post-processing necessary to make available individual GPS RO profiles of the Wegener Center for Climate and Global Change (WEGC) Occultation Processing System (OPS) retrieval. Furthermore, I contributed with extensive discussions during the analysis work and contributed to the paper text.

Steiner et al. (2013): I performed the computational work and post-processing necessary to provide individual GPS RO profiles of the WEGC OPS retrieval. Furthermore, I provided advice during data analysis and feedback during manuscript preparation. I also contributed to the paper text.

Angerer et al. (2017): I significantly contributed to the study design, provided advice and feedback on the method and the interpretation of the results. I also contributed significantly to the paper text.

Scherllin-Pirscher et al. (2011a): Together with Andrea K. Steiner and Gottfried Kirchengast, I formulated the initial idea and developed the design of this work. Furthermore, I collected the data, performed the analysis, created all figures, and wrote the manuscript. Co-authors provided advice and contributed to the paper text.

Scherllin-Pirscher et al. (2011b): Together with Andrea K. Steiner and Gottfried Kirchengast, I formulated the initial idea and developed the design of this work. Furthermore, I collected the data, performed the analysis, created all figures, and wrote the manuscript. Co-authors provided advice and contributed to the paper text.

Danzer et al. (2013): Together with Ulrich Foelsche and Julia Danzer, I developed the design of this work. I collected University Corporation for Atmospheric Research (UCAR) data, provided advice and feedback on the method and interpretation of the results. I also contributed significantly to the paper text.

Scherllin-Pirscher et al. (2017b): Together with Andrea K. Steiner and Gottfried Kirchengast, I formulated the initial idea and developed the design of this work. Furthermore, I collected the data, performed the analysis, created all figures, and wrote the manuscript. Work was supported by advice and contributions of the co-authors.

Scherllin-Pirscher et al. (2017a): I formulated the initial idea of the project and developed the design of this work. Furthermore, I performed the analysis, created all figures, and wrote the paper. Co-authors provided advice and contributed to the paper text.

Scherllin-Pirscher et al. (2012): I formulated the initial idea of the project and developed the design of this work. Furthermore, I performed the analysis, created all figures, and wrote the paper. Co-authors provided advice and contributed to the paper text.

Wilhelmsen et al. (2018): Together with Andrea K. Steiner, I formulated the initial idea of the work. Furthermore, I significantly contributed to the study design, provided advice on the method and interpretation of the results. I also contributed to the paper text.

Rieckh et al. (2014): Together with Ulrich Foelsche, I formulated the initial idea of this work, which mainly is the outcome of Therese Rieckh's diploma thesis, supervised by U. Foelsche and me. We also developed the study design. Furthermore, I provided advice and feedback on the method, on the interpretation of the results, and contributed to the paper text.

Scherllin-Pirscher et al. (2014): I formulated the initial idea of the project and developed the design of this work. Furthermore, I collected the data, performed the analysis, created all figures, and wrote the paper. Work was supported by advice and contributions of the co-authors.

Brunner et al. (2016): Together with Andrea K. Steiner, I provided guidance on all aspects of the study with a focus on the study design, method, and interpretation of the results. Furthermore, I contributed to the paper text.

Acronyms

ABI Advanced Baseline Imager

ALADIN Atmospheric Laser Doppler Instrument

BDC Brewer–Dobson Circulation

CHAMP CHAllenging Minisatellite Payload

C/NOFS Communications/Navigation Outage Forecasting System

COSMIC Constellation Observing System for Meteorology

COSMIC-2 Constellation Observing System for Meteorology (COSMIC) #2

DMI Danish Meteorological Institute

ECMWF European Centre for Medium-Range Weather Forecasts

ENSO El Niño–Southern Oscillation

EOF Empirical Orthogonal Function

EUMETSAT European Organization for the Exploitation of Meteorological Satellites

F3C Formosa Satellite Mission #3 (FORMOSAT-3)/COSMIC

F7C2 Formosa Satellite Mission #7 (FORMOSAT-7)/COSMIC #2 (COSMIC-2)

FORMOSAT-3 Formosa Satellite Mission #3

FORMOSAT-7 Formosa Satellite Mission #7

GCOS Global Climate Observing System

GEOS Geostationary Operational Environmental Satellite

GFZ German Research Center for Geosciences

GNSS Global Navigation Satellite System

GPS Global Positioning System

GPS/MET Global Positioning System/Meteorology

GRACE Gravity Recovery and Climate Experiment

JPL Jet Propulsion Laboratory

LEO Low Earth Orbit

Metop Meteorological Operational

MJO Madden Julian Oscillation

MRGW Mixed Rossby gravity waves

MSL Mean Sea Level

MSU Microwave Sounding Unit

NWP Numerical Weather Prediction

OPS Occultation Processing System

OPSv5.6 Occultation Processing System version 5.6

PC Principal Component

PCA Principal Component Analysis

POD Precise Orbit Determination

QBO Quasi-Biennial Oscillation

RMS Root Mean Square

RO Radio Occultation

ROM Radio Occultation Meteorology

ROPS Reference Occultation Processing System

SAC-C Satelite de Aplicaciones Cientificas-C

SAF Satellite Application Facility

SEVIRI Spinning Enhanced Visible Infra-Red Imager

SST Sea Surface Temperature

SSW Sudden Stratospheric Warming

UCAR University Corporation for Atmospheric Research

UTLS Upper Troposphere and Lower Stratosphere

WEGC Wegener Center for Climate and Global Change

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