

An introduction to the GRUAN processor

Satellite Applications Tech Memo 46

January 15, 2016

Fabien Carminati, William Bell, Stefano Migliorini, Stuart Newman,
and Andrew Smith



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Abstract

As part of the GAIA-CLIM project, reference quality radiosonde data from the GCOS reference upper-air network (GRUAN) will be used to characterize the uncertainties in numerical weather prediction (NWP) model fields, as well as simulated radiances derived from these fields. The comparison of collocated geophysical fields and simulated radiances between radiosondes and model fields is made possible through a new software developed at the Met Office and aimed to be part of the EUMETSAT-hosted 'Virtual Observatory' tool-set. The software, referred to as the GRUAN processor, has been designed and is in a preliminary state of development, and although data have been successfully processed, critical components are still to be developed. The present document introduces the top-level design of the GRUAN processor, details its key components, and gives an overview of the planned improvements. Preliminary outputs, although not scientifically robust in their current state of development, illustrate the possible range of future applications, including but not limited to, the assessment of uncertainties in NWP or reanalysis both in observation and radiance spaces.

1 Introduction

The European Union's Horizon 2020 research and innovation funded Copernicus programme has been established with the aim of maximizing the benefits from Earth Observing systems (EOS). The programme provides a framework for scientific and technological innovations aimed at delivering high-quality traceable information fit for the particular needs of multiple end users (<http://www.copernicus.eu/>).

Space-borne observational datasets are EOS key-components and therefore must be subject to high standards of calibration and validation to meet Copernicus stakeholders requirements. In most cases however, commonly used validation techniques involving satellite inter-comparisons, in-situ datasets, reanalysis, and or operational numerical weather prediction (NWP) do not yet provide essential data characteristics such as metrological traceability or robust uncertainty quantification.

The Gap Analysis for Integrated Atmospheric ECV CLimate Monitoring (GAIA-CLIM) project aims to address those challenges by improving the use of in-situ observations to better characterise a set of atmospheric Essential Climate Variables (ECVs) derived from satellite observations as well as the level 1 data from which these quantities are derived (<http://www.gaia-clim.eu/>). The project outcomes will be made available in an EUMETSAT hosted 'Virtual Observatory' where data, data characteristics, and tools will be available to end users for a broad range of applications.

As part of the Met Office led GAIA-CLIM work package (WP) 4, assessment of new satellite datasets, including FY-3C MWTS-2 and MWHS-2, GCOM-W AMSR-2, and F-19 SSMIS are being carried out using data assimilation systems employed in NWP and reanalysis. This WP also aims to demonstrate how reference quality radiosonde data, from the GCOS reference upper-air network (GRUAN), can be used to assess uncertainties in model background fields (http://www.dwd.de/EN/research/international_programme/gruan/home.html). The characterisation of uncertainties in NWP simulated radiances will in turn serve to establish uncertainties in satellite radiance measurements.

This document introduces the preliminary software design proposed to monitor GRUAN data with respect to global NWP fields (WP4 Task 4.3), hereafter referred to as GRUAN processor. Section 1 summarizes GRUAN specifics and pre-processing. In section 2, the GRUAN processor top design is detailed. Preliminary illustrative results and future improvements of the GRUAN processor are discussed in section 3. A summary finalizes this document in section 4.

2 Datasets

GRUAN is an international reference observing network, built on existing observational facilities, carrying out atmospheric observations of temperature, humidity, wind, and pressure with Vaisala RS92 radiosondes. The network is designed to provide long-term high-quality observations from the surface to the stratosphere for climate monitoring, and to provide direct in-situ observations for atmospheric studies. The principal goal of GRUAN is to serve as a baseline to diagnose long-term trends in more spatially complete datasets, including satellite observations, and recalibrate them when necessary.

To date, GRUAN relies on a dozen sites world wide, as illustrated in figure 1, although this number is expected to grow to 30-40 sites in the future. Certified sites must comply with strict requirements including the validation against complementary measurements and comprehensive uncertainty analyses. Observations and uncertainties must be documented, traceable to measurement standard, ideally SI, and include a complete meta-data description.

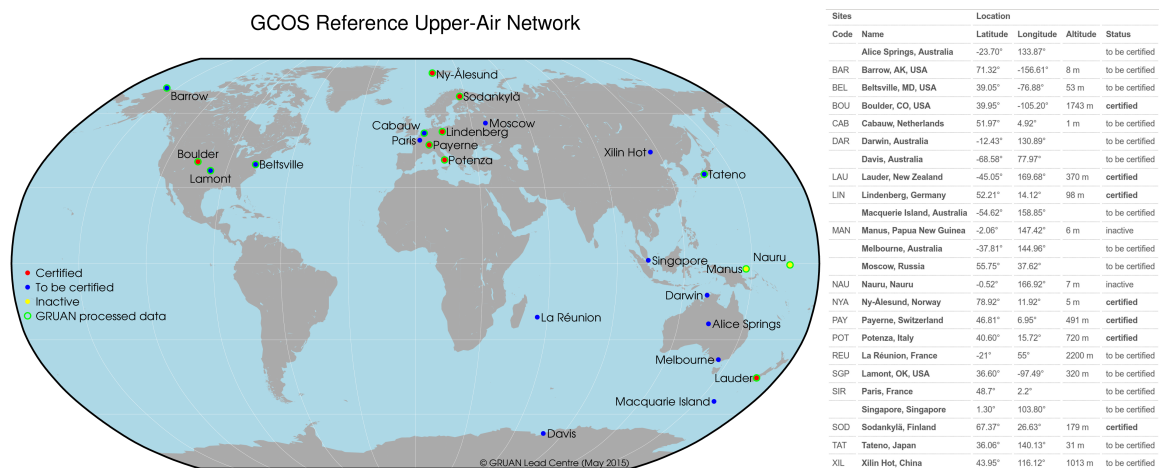


Figure 1: Overview of the GCOS Reference Upper-Air Network (GRUAN). Active sites are marked in green (from official GRUAN website http://www.dwd.de/EN/research/international_programme/gruan/home.html). Right hand-side table give the latitude, longitude, altitude, and operational status of each station.

Although GRUAN raw observations are available, the final data product is a calibrated bias-corrected measurement. The correction developed by the GRUAN lead centre accounts for known errors and biases to the extent of current knowledge, and is based on laboratory studies and field inter-comparisons (Dirksen et al., 2014). Vertically resolved uncertainty analysis (individually determined for each data point) follows the recommendations of the guide for expressing uncertainty in measurement (BIPM, 2008) and encompasses a correlated component of the uncertainty arising from calibration and corrections, and an uncorrelated component determined from statistical analyses (Immler et al., 2010).

For the needs of this study, GRUAN temperature, humidity, and pressure, as described in Immler and Sommer (2011) and Dirksen et al. (2014), are considered.

The dominant source of error in temperature profiles is a systematic bias caused by solar radiative heating. A correction model accounting for pressure, ascent speed, and actinic flux has been established from laboratory experimentations carried out in Lindenberg (lead centre) where measurements were performed in a vacuum chamber with sunlight as the light source. The implemented temperature correction is an average of that from the GRUAN model and the Vaisala model. Night-time long-wave radiative cooling bias, although small compared to day-time solar heating, is also accounted for using the Vaisala correction. The sensor response time (varying with temperature) was estimated to be small enough to be left uncorrected. Temperature spikes caused by balloon and/or payload motion are removed thanks to a low-pass filter based algorithm. The filter constrains the profile resolution to 10 seconds (50 m), although temperature profiles keep a 1 second sampling. The total temperature uncertainty after correction is the geometric sum of the squared individual correlated (calibration, albedo, and experimental fitting parameters) and uncorrelated (random, radiosonde rotation, and ventilation) uncertainties (for details see Dirksen et al., 2014, Table 2).

GRUAN relative humidity (RH) is measured by the Vaisala Humicaps humidity sensor, and given in percent RH over liquid water. Note that both GRUAN and Vaisala use the Hyland and Wexler (1983) formulation for their calculation of the saturation vapour pressure. The sensor is affected by a dry bias induced by solar heating, time-lag at low temperature, and temperature-dependent calibration errors. The latter effect causes a dry bias at low temperature that cannot result from solar heating (observed at night) and attributed by Miloshevich et al. (2006) to calibration inaccuracies. An empirical correction has been developed at GRUAN lead centre based on comparisons with cryogenic frost point hygrometers. This correction is applied ahead of radiative and time-lag related corrections. The radiative dry bias results from a decrease in RH inside the radiosonde because of the increase in temperature associated to the solar radiative heating. GRUAN correction is derived from the ratio of saturation vapour pressure in and outside of the sensor for temperatures estimated in a similar way to the temperature sensor correction (function of pressure, ventilation speed, and actinic flux). At low temperature, the sensor response time increases significantly (typically below -40°C), which results in a depreciated vertical resolution in the humidity profile. This principally affects the upper troposphere-lower stratosphere (UTLS) region. GRUAN time-lag correction algorithm is designed in the same vein as that introduced by Miloshevich et al. (2004) and relies on an exponential kernel complemented by a low-pass filter. As for the temperature, the filter constrains the humidity resolution to 10 seconds or more (for 1 s sampling) depending on the temperature-dependent time constant applied in the algorithm. The total humidity uncertainty is expressed as the square root of the geometric sum of the squared total correlated (accounting for calibration, temperature-dependence, radiative-induced dry bias, and time-lag) and uncorrelated (random) uncertainties (for details see Dirksen et al., 2014, Table 5).

The GRUAN vertical coordinate (geopotential height, geometric altitude, and pressure) is determined by the redundant measurements of a pressure sensor and a GPS receiver. Pressure measurements are used in the lower part of the profile where the noise in the geometric altitude, calculated from pressure data, is lower than the noise in GPS-based altitude. GPS data are used from the altitude where the pressure-based altitude noise becomes greater than that of GPS derived altitude. The geometric altitude is then converted back into a pressure profile from which is calculated the geopotential height. The geometric altitude uncertainty results from the cumulative uncertainties from below and above the pressure-to-GPS-based switch altitude. The pressure-based altitude uncertainty is the square root of the geometric sum of the squared uncorrelated uncertainty (station barometer for the launch altitude and random noise at launch), uncorrelated random error, and uncertainty of the geometric pressure altitude composed of a correlated component (pressure sensor calibration and bias with barometer) and an uncorrelated random component. The GPS-based uncertainty is the square root of the geometric sum of the squared uncorrelated random uncertainty and correlated recalibration and geometric pressure altitude at the switch altitude uncertainties. The uncertainty on the pressure profile is calculated from the the uncertainty on the geometric altitude with the barometric equation (see Dirksen et al., 2014, equation 26).

Along with GRUAN data, the GRUAN processor, further described in the next section, supports modelled atmospheric profiles from Met Office Unified Model fields files/PP files, GRIB files, NWP SAF 60-level ECMWF analysis, and NWP SAF 91-level ECMWF short-range forecasts. More generally, any model input file must contain multi-level pressure, temperature, and humidity fields, as well as the surface pressure, 2 m temperature, 2 m humidity, skin temperature, latitudinal and longitudinal wind speed, land-sea mask, orographic height, and sea-ice fraction fields. Further details can be found in Smith (2014a).

3 GRUAN Processor

The GRUAN processor has been developed from the EUMETSAT NWP SAF Radiance Simulator (Smith, 2014a, 2014b). This section presents the Radiance Simulator top-level design, summarised in figure 2, before introducing the changes to the system for the processing of GRUAN datasets, shown in figure 3.

RadSim

The Radiance Simulator (RadSim) can be seen as composed of three main parts: input, simulator, and output.

RadSim input consists of a namelist file containing the path to the location of the mandatory input data and variables (model datafile, file type, and RTTOV coefficients), the satellite characteristics to be simulated (platform, instrument, and satellite ID), and optional entries to be set up for specific simulation needs. The namelist file also contains general control variables, RTTOV-specific options, and output control variables that can be left in their default configuration or edited as required. The path to an optional text file containing meta-data related to where the radiances are to be simulated can be added to the namelist input file. If meta-data are provided (latitude, longitude, surface elevation, land-sea mask, and satellite zenith angle) the model profiles will be simulated at the location pointed to in the meta-data, otherwise the radiances will be simulated at the profile locations.

The simulator itself is composed by a reading section, a data pre-processing section, and a processing section.

The reading section reads the namelist input file, checks that all mandatory input are correctly set up, and checks the validity of data and configuration. Then, model fields are read in and variables are stored in the format used in RadSim. When provided, the simulator reads in and stores the meta-data.

The pre-processing consists in a rearrangement of the geolocation coordinates into RadSim format with coordinate rotation and gridding applied when necessary. When meta-data are provided, model fields are horizontally interpolated to the meta-data location(s) with a bi-linear approach weighting each point by the four adjacent points of a rectangular grid cell. This section also handles the model fields conversion to units supported by the radiative transfer model. Supported conversions are potential temperature to temperature, 2 m dew point temperature to 2 m specific humidity, and relative humidity to specific humidity. The latter makes use of the saturation vapour pressure as defined in the Magnus formulation (WMO, 2008) and approximates the relative humidity RH as the ratio of specific humidity q by the specific humidity at saturation q_s , so that $q = RH \times q_s$.

In the last section, model fields are transferred to the format used by the radiative transfer model. The model by default is RTTOV 11.2 (<https://nwpsaf.eu/deliverables/rtm/>), although RadSim

will support different versions. RTTOV is initialised (as a function of the options defined in input) and run for each profiles. RTTOV outputs are stored back to RadSim format before to be written out.

RadSim output are written to one netcdf file containing the simulation attributes (satellite ID, platform, instrument, channels, wave number, and validity time) and observation fields (latitude, longitude, satellite zenith and azimuth angles, land-sea mask, surface type, quality control information and flags, emissivity, and either brightness temperature or radiances depending of the chosen input option). Additionally, depending on the configuration of the input file, RTTOV variables (temperature, humidity, ozone Jacobians, and transmittances) and model fields (including, but not limited to temperature, pressure, and specific humidity) can also be saved in the output file.

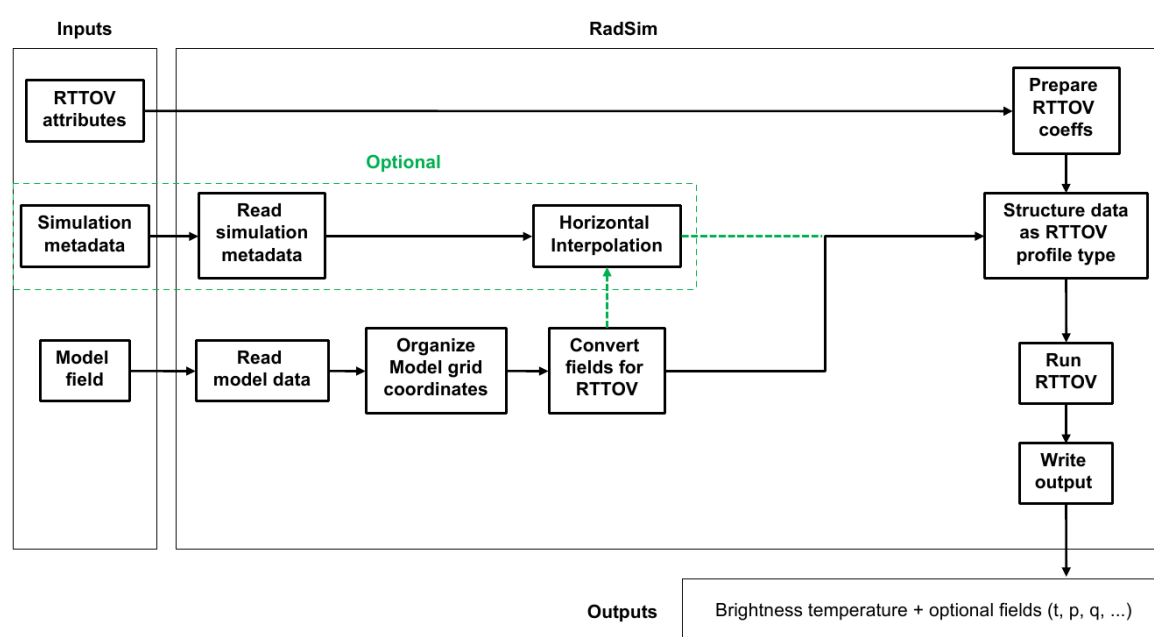


Figure 2: Schematic representation of the top-level design of the NWP SAF Radiance Simulator. Green lines represent the optional steps in the processing.

GRUAN processor

In order to process GRUAN data, the following modifications have been made for the RadSim-based GRUAN processor.

GRUAN delivers single radiosonde profile data files. Each file contains raw data, bias-corrected data, uncertainty estimates, and global attributes such as time, location, or conditions at launch site. A new optional entry has been added to the namelist input file recording the path to GRUAN data file. If no data file is provided, then the GRUAN processor will behave in a similar way to RadSim and process the model data file only. RTTOV default options remain unchanged, except the cloud liquid water option (used in microwave simulations), which is set to false as we assume

clear sky simulations. A meta-data text file becomes complementary when a GRUAN data file is provided. It indicates the location (of the launch site) where the model fields are to be interpolated. A library of meta-data text files has been created with information related to each GRUAN active launch site.

The simulator structure (a reading, pre-processing, and processing section) remains similar to that of RadSim, although major changes are introduced in order to process GRUAN data. The reading section now supports the netcdf format of GRUAN files. GRUAN pressure, temperature, and relative humidity profiles are transferred and stored in a format similar to that used in RadSim. GRUAN uncertainty profiles are also stored in a similar way.

The pre-processing section has been subject to two major updates. First, the conversion of relative humidity to specific humidity has been revised as follows:

The relative humidity is given by:

$$RH = \frac{e}{es} \quad (1)$$

with e the vapour pressure and es the saturation vapour pressure over liquid as defined by Hyland and Wexler (1983), and used by GRUAN and Vaisala, such as:

$$\ln(es) = \frac{C1}{T} + C2 + C3 \times T + C4 \times T^2 + C5 \times T^3 + C6 \times \ln(T) \quad (2)$$

with:

$$C1 = -5.8002206 \times 10^{3.0}$$

$$C2 = 1.3914993 \times 10^{0.0}$$

$$C3 = -4.8640239 \times 10^{-2.0}$$

$$C4 = 4.1764768 \times 10^{-5.0}$$

$$C5 = -1.4452093 \times 10^{-8.0}$$

$$C6 = 6.5459673 \times 10^{0.0}$$

The specific humidity is given by:

$$q = \frac{\epsilon e}{(p - (1 - \epsilon) e)} \quad (3)$$

with ϵ the ratio of the molecular weights of water vapour by the molecular weights of dry air.

Replacing 1 in 3 gives:

$$q = \frac{\epsilon RH es}{(p - (1 - \epsilon) RH es)} \quad (4)$$

4 Preliminary results, limitations and future improvements

At the time of writing of the present document, the GRUAN processor is in a preliminary functioning state ready for technical check-out. GRUAN profiles are being processed alongside Met Office NWP data for sanity check purposes. It is important to note that the GRUAN processor does not account yet for number of critical processes (e.g. clouds screening, radiosonde drift, or ascent time). At this stage, outputs are not yet suitable for scientific use.

Figure 4 shows GRUAN profiles compared to the Met Office model after being processed by the GRUAN processor. The radiosonde was launched in Boulder, CO, USA, on August 25, 2015, at 16:54 UTC, from an altitude of 1743 m. The balloon reached the altitude of 28012.4 m (16.85 hPa) with a payload of 1757 g (gross weight of 3257 g including the balloon). As model input, the temporally closest Met Office UM fieldsfile (20150825T1800Z) was selected. The GRUAN processor was set up to simulate brightness temperatures at ATMS channel frequencies.

The absolute and relative difference (radiosonde – model) in specific humidity are shown on Fig. 4 top-left and top-right plots, respectively. The absolute difference in temperature is shown on the bottom-left plot. Profiles are compared at model levels (70) with a simple match of the closest pressure level in the radiosonde profiles to each model level. Note that the lowermost and uppermost matches, both in humidity and temperature, have a difference of 0. This is because the GRUAN processor outputs the radiosonde merged profiles (with model data below and above GRUAN lowest and top levels) used for the calculation of the simulated brightness temperatures. Red lines represent the GRUAN total uncertainty interval. The absolute difference in brightness temperature in function of ATMS channels is shown on the bottom-right plot. The green box represents the temperature-sensitive channels peaking in the troposphere and lower-stratosphere where information from the radiosonde is available. The blue box is similar to the green box but for humidity-sensitive channels.

A detailed analysis of those differences would be meaningless as, again, the processor is not yet optimized or fully validated. Nevertheless, some interesting features can be observed.

The model, as expected, seems to reproduce tropospheric temperature better than humidity. This results in smaller ΔBT in temperature-sensitive channels than humidity-sensitive channels in the highlighted boxes.

Common features are found near the surface and in the UTLS, where both humidity and temperature large differences are evident. Surface biases may predominantly be caused by the temporal mismatch between model and radiosonde (about 1 hour). Biases in the UTLS may however result from the radiosonde horizontal drift (several kilometres) that is not accounted for since model fields are interpolated to the launch site location assuming vertical ascent of the sonde. Generally speaking, the radiosonde ascent time potentially introduces further temporal mismatch as the bal-

$RS_{GRUAN} - NWP_{MO}$ Boulder 2015082518

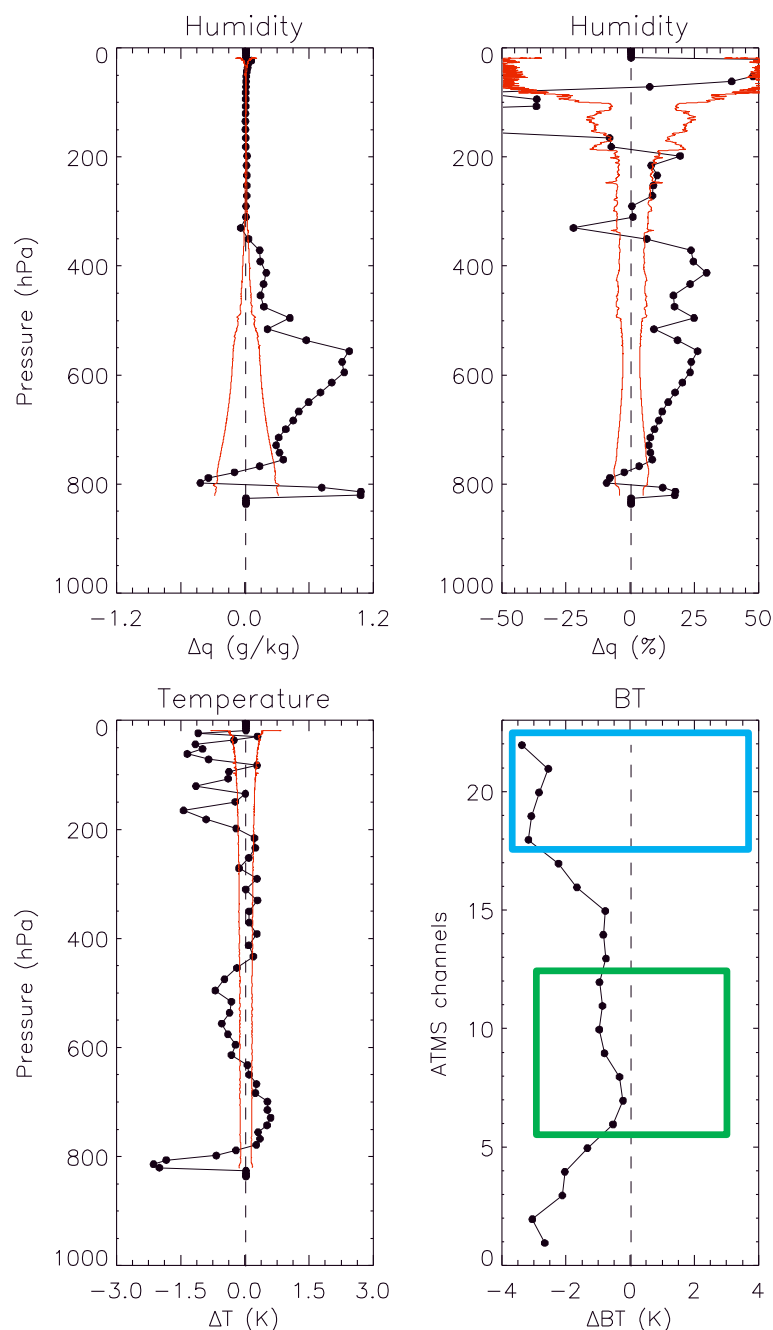


Figure 4: (Top) Absolute (left) and relative (right) difference in specific humidity between processed radiosonde observations and Met Office NWP fields ($RS_{GRUAN} - NWP_{MO}$) from the GRUAN processor for August 25, 2015, 18:00 UTC, Boulder, CO, USA. Comparison is made on model pressure levels. Red lines show GRUAN total uncertainty window. (Bottom left) Same as top left but for temperature. (Bottom right) Absolute difference in simulated brightness temperature ($RS_{GRUAN} - NWP_{MO}$) for ATMS channels. The green box shows tropospheric temperature-sensitive channels. The blue box shows the tropospheric humidity-sensitive channels.

loon rises into the UTLS, except that in the present case, this would tend to reduce the temporal difference between sonde and model as the balloon was launch roughly one hour before the model cycle.

Finally, large mid-tropospheric (700-400 hPa) discrepancies are present in the humidity profiles. This possibly reflects a cloud layer crossed by the radiosonde, absent in model fields due to temporal and spatial mismatches.

Necessary improvements to the GRUAN processor will gradually be implemented. On a short term perspective (with GAIA-CLIM annual meeting on Feb 9-12, 2016, as objective), efforts will be conducted towards the implementation of four upgrades:

1. GRUAN surface pressure at launch station will be read in and stored as a surface parameter.
2. A cloud screening will be carried out for both GRUAN and model profiles to avoid contamination in RTTOV cloud-free simulations. The filter will be implemented ahead of the merging step. It will consist in the determination of a critical relative humidity profile (RH_c), defined by Geleyn (1980) (and subsequently by Salonen and Uppala, 1991) as follows:

$$RH_c = 1 - \alpha \sigma (1 - \sigma) (1 + \beta (\sigma - 0.5)) \quad (5)$$

where the parameters $\alpha = 2$ and $\beta = \sqrt{3}$, and $\sigma = \frac{P(i)}{P(surf)}$ is the ratio of pressure at the i^{th} level and at surface.

Any level where $RH > RH_c$ will be considered as being within a cloud layer, and will be screened out. A critical specific humidity q_c , obtained by replacing RH_c in 4, will be used when RH is not available as follows:

$$q_c = \frac{\epsilon RH_c es}{(p - (1 - \epsilon) RH_c es)} \quad (6)$$

3. Uncertainty-based screening will be carried out after the cloud screening. The aim is to remove data with unreasonably large uncertainty (e.g. total uncertainty over 100
4. GRUAN uncertainties will be propagated in RTTOV in order to estimate the uncertainty window for the simulated radiances. This can be achieved by generating hybrid profiles where GRUAN data are incremented by the associated uncertainties, simulate the radiances, and repeat the operation with hybrid profiles decremented by uncertainties. This will result in simulated radiances relative to the incremented and decremented profiles marking the upper and lower bounds of the uncertainty window associated to GRUAN data. Total uncertainties will be considered in first instance, although the correlated and standard deviation part of the total uncertainty will be treated in a similar way in the longer term.

Other upgrade tasks will be implemented later in 2016.

The spatial interpolation will be revisited to account for the sonde drift. The latitude and longitude associated to each measure is provided in GRUAN data files. A subset of n pairs of lat–lon coordinates could be extracted from GRUAN data file (e.g. one for each model level) and replace the meta-data currently provided in input. Model fields would consequently be interpolated at the n locations, providing n profiles for each fields. A single profile (by field) will be reconstructed, level by level, using data at the model level matching the sonde level at n^{th} location.

Temporal interpolation will be implemented to account for the mismatch between the launch time of the sonde and model cycle times. The interpolation will also need to account for the balloon ascent time. This will require to use two model data files, one from the cycle before the sonde launch time, and one from the cycle after the sonde reaches its ceiling. The temporal interpolation should occur after the spatial interpolation but before single profiles are reconstructed. Hence, model fields can be interpolated at launch time + ascent time of the n^{th} location.

Finally, two possible but not mandatory upgrades could be: a) the vertical interpolation of the reconstructed model profiles (after spatial and temporal interpolation) on the GRUAN levels in order to process both GRUAN and model data the exact same way in RTTOV, and b) the use of radio occultation observations to fill the upper part of GRUAN profiles (rather than model data). Both upgrades are preliminary suggestions and will require further consultation with the various project members.

It is worth noting that the radiative transfer model RTTOV also introduces a degree of uncertainty when simulating radiances. The accuracy in RTTOV has been the subject of several studies (e.g. Matricardi, 2009). Nevertheless, independent studies will be conducted at the Met Office to determine to what extent this may impact the GRUAN processor results.

5 Summary

The characterisation of uncertainties in numerical weather prediction and reanalysis fields, and subsequently in simulated satellite observations, is a major challenge that will be addressed in the GAIA-CLIM project. In that regard, observations from the reference quality radiosonde GRUAN network are being used at the Met Office to assess, both in observation and radiance spaces, uncertainties associated with model data. Comparisons of geophysical fields and brightness temperatures between radiosonde observations and model fields have been made possible using the GRUAN processor, a NWP SAF Radiance Simulator-based collocation and (radiance) simulation tool, developed at the Met Office for the needs of this project. This document introduces the preliminary design and outputs of the GRUAN processor.

In its current version, the processor can process GRUAN and model data (in Met Office or ECMWF format) for a given location (defined in meta-data input). Model fields are interpolated at the location of the radiosonde launch site and the RTTOV radiative transfer model simulates radiances (or brightness temperatures) for both datasets at this location. The processor outputs allow direct assessment of model temperature, humidity, and brightness temperature against GRUAN given the known GRUAN uncertainties.

Nevertheless, the processor does not yet account for crucial processes such as the radiosonde horizontal drift or ascent time. Therefore, the preliminary results presented in this document are not, at the current time, exploitable for detailed scientific use, but at this stage represent a preliminary technical check of the functioning of the processor.

The necessary updates for a scientifically viable version of the processor are planned to be implemented during 2016. Main improvements will include, but not limited to, relative humidity-based cloud screenings, the simulation of radiances accounting for GRUAN uncertainties, refined spatial interpolations accounting for the sonde drift, and temporal interpolations accounting both for the exact launch time and balloon ascent time. The subsequent analysis of a statistically significant sample of GRUAN data is expected to provide the first estimation of uncertainties in NWP fields, and associated simulated radiances, by the end of the year.

Acknowledgements

We gratefully acknowledge European Unions Horizon-2020 program GAIA-CLIM project that supports the work of Fabien Carminati and William Bell.

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Met Office

FitzRoy Road, Exeter
Devon, EX1 3PB
UK

Tel: 0370 900 0100

Fax: 0370 900 5050

enquiries@metoffice.gov.uk

www.metoffice.gov.uk