NPROVS Manual (ATBD)

(Preliminary Draft)

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1. Introduction

This document primarily serves as a user manual concerning NPROVS data collection and graphical analysis applications. NPROVS compiles daily collocation datasets of global radiosonde (and dropsonde), satellite and nwp observations and facilitates "retrospective" satellite product assessment. These include special radiosondes from the GRUAN and JPSS dedicated radiosonde program. Over 20 international satellite sounding product systems (and NWP) are collocated with each radiosonde and an extensive database of collocations since 2008 is archived (stewardship at STAR). Collocations are the single closest from each product suite to each radiosonde, providing an efficient and informative collection of observations. Graphical applications allow users to analyze the collocation samples ranging from overall global monitoring to deep-dive case studies and includes access to the original satellite orbital data; anywhere, anytime. NPROVS supports assessments not only for the satellite data but also for the radiosondes, dropsondes including subsampling of radiosonde instrument types. NPROVS features enterprise assessments, namely the comparisons of multiple satellite product suites against identical radiosonde observations. Enterprise assessment (as feasible) is considered optimal for product comparison.

The document covers four basic areas covering data sources, pre-Processing, collocation processing and assessment. An introductory discussion of enterprise validation, a unique core objective of NPROVS, is also provided.

2. Enterprise Assessment

The NPROVS objective is rooted in enterprise validation, defined as the use of identical groundtruth (radiosondes ...) to assess multiple satellite product suites. The original idea was to create a centralized program at NOAA which would collocate all the (operational, legacy ...) sounding product suites (international) to each 'conventional" radiosonde. This includes the generation of global statistics vs radiosondes for each product suite for use in routine monitoring. NPROVS also access internal "Test (R&D)" products made available by Providers to quantify differences relative to operational counterparts, supporting RTO. The NPROVS program was initiated at STAR (OPDB) in 2006 and during the (2-year) development phase it was recognized that flexibility to identify collocations for any specified combination of radiosonde and product (suite) combinations for analysis (vertical statistics) was pivotal to success; the trick was in selecting them. This is manifested in the Profile Display (PDISP) graphical analysis application, a centerpiece of NPROVS.

Prior to 2006 (ATOVS, TOVS, DMSP), separate systems to collocate radiosondes for each product (10+ separate systems) were operated (at ORA later to become STAR) and the primary basis of (individual) operational assessments (back in the days when satellite soundings were assimilated in nwp) ... systematic differences among these separate "collocation" systems (approaches) was evident.

The NPROVS collocation data processing at STAR began in April 2008. Upon the emergence (circa 2015?) of the phrase "enterprise algorithms", the use of the same "science" to derive products across different sensors, "enterprise assessment" was coined as use of the same "ground truth (radiosondes)" to assess products across different product suites (science). Enterprise assessment lends confidence that statistical differences observed across the given set of products are real. Interpreting the differences in the context of respective performance is secondary (but unavoidable), smaller differences are better. As discussed, a constraint looms in that the product suites compared have 'similar" local overpass times. NPROVS provides a centralized capability to provide collocation datasets and assessment that facilitates both traditional (one suite, one radiosonde) and enterprise (multiple suites, same radiosondes) strategies; one-stop shopping.

NPROVS integration of routine satellite product suite collocation with JPSS dedicated radiosonde program observations began in 2013, and soon after GCOS Reference Upper Air Network (GRUAN) were included; also corresponds to the onset of operational NUCAPS hyper-spectral sounding products from NPP. The addition of GRUAN introduced fully characterized reference radiosondes, and agreement by GRUAN to process JPSS dedicated radiosondes from GRUAN/ARM sites provided reference baselines for use in cal/val (and R&D). Expansion to special radiosondes from research experiments (AEROSE, ARM Mobile, CIRA, CALWATER ...) followed; GRUAN (LC) processed 2013 AEROSE radiosondes into reference with recent observations pending.

NPROVS Special nicely compliments the more routine monitoring nature of NPROVS Conventional. However with NPROVS Special, the assessment baseline includes fully characterized reference radiosonde targeted at satellite overpass, a most delicious validation fruit particularly in an enterprise context.

3. Data Access

Schematic of the NPROVS is shown in Figure 1. Two separate Radiosonde datasets, Conventional (left) and Special (right) are compiled each day. Each serves as a baseline for collocation with each of the satellite product suites (and satellites) indicated in the blue boxes, over twenty satellite product suites; Test (R+D) suites are included as available. This is done daily creating daily collocation files and ultimately the NPROVS Conventional and Special Collocation Archives. The NPROVS Special collocation archive links directly to VALAR, which provides satellite SDR for subsets of "timely" collocations key for R&D.



Figure 1: NPROVS Processing and Data Management Schematic operated daily

3.1 Radiosondes (Red)

3.1.1 NPROVS Conventional

NPROVS Conventional collocates all satellite product systems and ECMWF Analysis with conventional radiosondes managed by the World Meteorological Observation (WMO). These are accessed via NOAA Global Forecast System (GFS) 6-hour PREPBUFR files and include available dropsonde (NOAA, etc) observations. Radiosonde and dropsonde are (normally) reported at mandatory (standard) and significant levels and include the GFS 6-hour forecast (initialization) interpolated (by NWS) to each report level along with QC markers assigned during assimilation.

3.1.2 NPROVS Special

NPROVS Special collocates all satellite product systems and ECMWF with special radiosondes which are accessed in their original high density format (1-sec, 6-sec ...) from the following sources:

Global Climate Observing System (GCOS) Reference Upper Air Network (GRUAN) currently provides radiosondes at 21 sites. GRUAN was established to build a climate data record using reference geophysical observations of the Troposphere and Stratosphere. GRUAN processing includes fully characterized uncertainties for Temperature and RH profiles.

Satellite synchronized observations from the joint NOAA Joint Polar Satellite System (JPSS) and the US Department of Energy's (DOE) Atmospheric Radiation Measurement (ARM) dedicated radiosonde program managed at STAR and the University of Wisconsin at Madison. The program objective is to assist in the cal/val of NUCAPS temperature and moisture sounding (EDR) JPSS satellites (currently NOAA-20). Radiosondes are launched at three ARM sites, Southern Great Plains in Oklahoma, US; North Slope Alaska in Alaska, US; and Eastern North Atlantic on Graciosa Island. Radiosondes are launched thirty to forty minutes before satellite (currently NOAA-20) overpass and in select cases is followed by a second launch about 10 minutes before overpass. Radiosondes are typically processed by GRUAN (LC) into reference observations.

Radiosonde Intercomparison and Validation (RIVAL) partnership between GRUAN / ARM / JPSS and managed by STAR / Univ Madison (Wisconsin). Dual (Vaisala RS41/RS92) radiosonde (on one balloon) are launched similar to JPSS dedicated program (above) including select cases of a second launch typically RS41). RIVAL covered the 3 ARM sites from February 2018 through February 2020 with RS92 radiosondes processed by GRUAN (LC) into reference; RS41 reference processing is pending.

JPSS funded dedicated radiosondes in coordination with Aerosol and Ocean Science Expedition (AROSE) campaigns onboard the NOAA Science Vessel Ronald H Brown (RHB) since 2013. These are typically annual experiments in the Atlantic Basin intended to study Saharan Air Layer (SAL) dust events; six 30-day campaigns since 2013. GRUAN processing is available for the 2013 campaigns and pending for others.

JPSS funded dedicated radiosondes (NPP) in coordination with CALWATER (Jan-Feb, 2015) and El-Nino Rapid Response (Feb-March 2016) campaigns to study (NUCAPS) during Atmospheric Rivers impacting the US West Coast. Radiosondes targeted both NPP and MetOp polar satellites.

CIRA (Ft Collins) dedicated radiosondes collocated with NPP, May 2016; no GRUAN Processing

ARM Mobile facility radiosondes including at Darwin, Ascension Island (Atlantic Basin), Alaska and Antarctica.

3.2 Satellites (Blue)

The satellites, associated sounding product suites with links (w/ sensors) are:

S-NPP and NOAA-20

NOAA Unique Combined Atmospheric Processing System (NUCAPS) Microwave Integrated Retrieval System (MIRS)

MetOp A, B and C

NUCAPS

Infrared Atmospheric Sounding Interferometer (IASI) from EUMETSAT GPS Receiver for Atmospheric Sounding (GRAS) from EUMETSAT MIRS Advanced TIROS Observational Vertical Sounder (ATOVS)

NOAA-18, 19

<u>MIRS</u> ATOVS

NASA-Earth Observing System (EOS) - Aqua

Advanced InfraRed Sounder (AIRS v6; begin 2013)

Constellation Observing System for Meteorology lonosphere and Climate (COSMIC); C-1 (4/2008 to 3/2020) and C-2 (3/2020 ...)

University Corporation for Atmospheric Research (UCAR)

KOMPSAT; begin December, 2019 (Korea Multi Purpose Satellite-5)

Satellite product suites include the temperature and water vapor profiles and additional ancillary information available per product suite.

The polar satellite profiles infra-red and microwave based profiles are the native 100 vertical pressure level (layer) profiles; ATOVS are at native 40 vertical pressure levels.

COSMIC, GRAS and KOMPSAT are Global Navigation Satellite System (GNSS) profiles are the original high density with partial vertical subsampling as described in Section 4.2.

3.3 Numerical Weather Prediction (NWP) (Red and Blue)

- a. NOAA GFS 6-hour forecast (appended during assimilation) and Analysis
- b. ECMWF 6-hour Analysis
- c. NOAA CFSR (Climate) appended retrospectively via 90-day re-processing

The NOAA GFS 6-hour forecast are those originally interpolated (during nwp assimilation) to the conventional radiosonde (and dropsonde) mandatory (standard) and significant levels. The GFS Analysis are received in gridded format from NCEP

ECMWF 6-hour Analyses are received in gridded format through a previous agreement (MOU) between NOAA/JPSS and ECMWF.

NOAA CFSR (interpolated to conventional radiosonde) is retrospectively appended to the NPROVS collocation data record upon availability from the NWS; typically 90-days.

Further details for each of the NWP datasets is given in Section 4.2

4. Data Processing

Conventional observations are the operational WMO radiosondes and dropsonde reported at the mandatory and significant pressure levels and accessed from the GFS PREPBUFR files. The GFS 6-hour forecast interpolated (by NCEP) to the reported mandatory and significant levels is also available.

Special observations are the original high-density (1-sec) radiosonde data from a given site or campaign. If GRUAN processed reference observations are available they are stored, otherwise the original "vender processed" (non-reference) observations are retained.

Conventional and Special reports are each processed into a "Unified" radiosonde format.

4.1 Unified Radiosonde Format

4.1.1 Conventional

The original NCEP PREPBUFR contains the conventional WMO radiosonde report data (mandatory and significant levels) for pressure, temperature, depoint temperature and wind. These are accessed from the numerical weather prediction (NWP) assimilation data stream and also include 1) QC marks and 2) the GFS 6-hour forecast at each Raob (Section 4.3)) level determined during assimilation. These are retained on the Unified file.

The incoming radiosonde data are initially tested for completeness, including data gaps, which include use of the QC marks and GFS 6-hour data. Only data with valid QC markers (defined below ?) and for which the temperature was within 10K of the GFS 6-hour forecast are considered. Remaining data then undergo profile completeness and gap checks (*Ryan document ?*) to insure a minimum 5km vertical extent in the troposphere (below 200 hPa) with no gaps. Gap limits are variable ranging from about 1km in the lower troposphere to 3km at 100 hPa and 5km above 10 hpa. If a gap is observed the radiosonde is capped at the highest level below the gap. Report data above the gap are retained on the unified file but not used for assessment.

Associated software:

- Radiosonde Profile Completeness
 - Function: Rb2rtv.f
 - o Reject profile if vertical extent of merged array is less than 5 km
- Gaps
 - Function: Gapchk2.f
 - Checks for gaps in the merged array of mandatory and significant pressure levels. If a gap is detected, the number of pressures in the merged array is adjusted to reflect the index of the pressure where the gap begins, and the remainder of the merged pressures above that point are set to missing values
 - o If profile after the gap adjustment is not 5km vertical extent the Raob is rejected

Radiosonde which pass the minimum 5km continuity test are considered for collocation with satellites. Radiosonde data records include ancillary information and tests to characterize the radiosonde profile including:

- WMO Radiosonde site identification code
- Radiosonde Instrument type
- Terrain Type (land, Sea (including Ship), Coast
- Day, Night, Dusk
- Surface Pressure and Temperature
- Superadiabatic
 - Function: Chksu2.f
 - Checks for superadiabatic layers; determines the potential temperature at a given level (up to tropopause) and sets flag to "1" if not monotonically decreasing and "2" if increase exceeds 1K.
- Supersaturation
 - Function: mergechk.f
 - Checks to see if dew point temperature is greater than reported atmosphere temperature at any level and reports RH
- Inversions (Surface, aloft)
 - Function: Invers.f
 - Checks on interpolated temperature profile for inversions and returns a value that reflects the presence of an inversion. If an inversion starts within 1km (flexible) of the reported surface pressure, it is labeled a surface inversion.
- Vertical pressure range
- Moisture Profile Shape (Index)
 - Function: Tier2ts1.f
 - Water vapor mixing ratio profiles are characterized from 0, monotonically decreasing to 3, numerous increases and decreases
- TPW and LPW
- Tropopause Pressure
 - o Extracted in uraobs6500.f
- Profile Stability Indices (10+ including CAPE, Lifted Index...)
- Radiosonde Drift (latitude, longitude, time)
- Global Network
 - Global Climate Observing System (GCOS)
 - GCOS reference Upper Air Network (GRUAN)
 - o Satellite Upper Air network (SUAN; NPROVS internal)

Characterizations and test results are stored on the Unified file and useful for sub-sampling collocation samples for analysis using NPROVS graphical applications (Section 6.2) For example, using the Inversion flag, one can sub-sample collocations by radiosonde profiles which have surface temperature inversions useful in boundary layer assessments.

4.1.2 Special

Contrary to conventional radiosondes, the original high-density observations (1-sec) of altitude, pressure, temperature, dewpoint temperature and wind are the initial baseline for NPROVS Special processing. These data come from a variety of data sources contingent on a given site. Each site typically processes their data differently, some are delayed and as a result the NPROVS team must accommodate multiple formats and file types which can also change over time. This requires extensive "bookkeeping" to insure that the data is read correctly and does not introduce error, for example, unit conversions (e.g. Celsius to Kelvin, Relative Humidity to Water Vapor Mixing Ratio, etc).

Although a large portion of the Special radiosonde observations originate from the GRUAN Lead Center (LC), the format of these observations may vary over time or include new reference instruments and formats. Each requires unique consideration when accessing data from specific periods. If observations from a given site are not available, the original vendor data is queried from the launch site and specific site protocols (which can also change over time) must be adhered. For example, GRUAN observations from Lauder (New Zealand) and Beltsville (USA) were not available from the LC for an extended period and during this time the original vendor data directly accessed from the site was stored in NPROVS Special. Eventually, GRUAN versions became available at the LC and replaced the vendor versions. Such replacement occurs during periodic NPROVS "reprocessing" (maintenance) which is discussed in Section 5.4

Whatever the source, the hi-density parameters are read from the radiosonde record and converted to a predefined set of atmospheric layers identical to the polar satellite products. This is done using the "convert_layers" subroutine initially developed by the Atmospheric InfRared Sounder (AIRS) Science Team (**Reference**) to create a standard set of 101 Boundaries (and 100 layers at effective pressure) layers suitable for Radiative Transfer Algorithm (RTA) processes. The "convert_layers" subroutine embodies the original AIRS Science Team Approach (ASTA) (reference Nalli JGR 2016) and provided to NPROVS by the STAR/JPSS NUCAPS Algorithm Development Team (web site).

The conversion for hi-density to 101 boundary levels begins with interpolation to the 101 boundary pressures followed by averaging (boundary pairs) to create layer means at effective pressure. The report surface pressure (lowest level) must be equal or greater than the lowest boundary (or bottom level) pressure ... actually .ge. the bottom layer effective pressure.

However, H20 Vapor includes additional steps:

- 1) calculate total column abundance for water vapor mixing ratio (WVMR),
- 2) determine WVMR for each layer (at effective pressure) down to surface pressure

Notice that the moisture is defined at effective pressure whereas the temperature is initially defined at a given boundary then converted to effective pressure. Table 1 lists the 101 boundary and 100 effective layer pressures for Temperature and H20 vapor profiles.

QC checks are done on 100 layer profiles after "conv_layers" and are similar to the quality control checks performed on the conventional raobs from the PREPBUFR files (Section 4.1.1); for example, a profile must extend 5km in the troposphere without a gap. The main difference is that checks against NWS QC flags are not available since Special radiosondes are (typically) not assimilated into the NOAA GFS (nor ECMWF).

Similarly, all reports meeting the 5km continuity requirement undergo profile characterization tests similar to those for conventional radiosondes (Section 4.1.1)

In summary, the goal of radiosonde preprocessing is to efficiently compress data from a given high-density radiosonde within one 8500-byte unified report file. Efficiency is also defined in the context of assessing satellite sounding profiles which are retrieved using Radiative Transfer Models (ASTA). The 100 layer effective pressure profiles stored on the unified (SpeciaL) file serves as an optimal baseline for such assessments. The original hi -density Radiosonde observations are preserved and available off-line.

Unified reports for NPROVS Special are produced daily but delayed fourteen days to account for different latency periods of observations across the various radiosonde sources.

4.2 Satellites

Each of the 20+ satellite product suites integrated into NPROVS have geophysical and data format differences which must be understood, reconciled and restructured into a unified structure that facilitates a consistent representation of respective product suite information. This includes parameters needed for collocation and (meaningful) assessment (using graphical applications).

Describe the process for re-format and attachment of each product suite to the radiosonde collocation data record for each radiosonde (Blue and Red in Fig 1)..

All satellite product suite data are stored as received by each provider (NOAA,EUMETSAT, NASA, UCAR, SAF). These include the temperature (K) and water vapor mixing ratio (g/kg) profiles plus ancillary data unique to each profile suite. All product suites are collocated with a given radiosonde, each the single closest observation from a given suite.

Polar satellite product suites include respective/combined hyperspectral infra-red and advanced microwave product soundings (T and H20 vapor). The EUMETSAT GRAS, COSMIC and KOMPSAT Global Navigation Satellite System (GNSS) product suites are based on Radio

Occultation (RO) measurements and include additional Tdry profiles representing a candidate reference temperature in the stratosphere. Associated first guess profiles are included for all product suites except MiRS. Each product suite includes QC and other ancillary information as available from the respective providers and used (as recommended by a given provider) in the context of sampling options for assessments. The respective polar orbiting and GNSS satellite product suites are listed below (as of March 2021):

Polar Orbiting Satellites:

NOAA NUCAPS (NOAA-20, NPP; MetOp-A,B) ... plus Test suites for NOAA-20 and NPP NOAA MiRS (NOAA-20, NPP, MetOp-A,B,C, NOAA-18,19) EUMETSAT IASI (MetOp-A,B,C) NASA Aqua-AIRS (v6.1) NOAA ATOVS Metop-B

GNSS Constellations:

UCAR COSMIC 1,2 EUMETSAT GRAS (MetOp-A,B,C) KOMPSAT-5

Polar orbiting satellite and GNSS COSMIC (C1, C2) are accessed directly from the respective provider agencies, namely NOAA, EUMETSAT, NASA and University Corporation for Atmospheric Research (UCAR) for COSMIC (<u>http://www.cosmic.ucar.edu/cdaac</u>). EUMETSAT GNSS Receiver for Atmospheric Sounding data (GRAS) and KOMPSAT are available from the Radio Occultation Meteorology (ROM) Satellite Application Facility (SAF; www.romsaf.org).

The polar satellite profiles infra-red and microwave based profiles are stored at the native 100 vertical pressure level (layer) profiles; ATOVS are at native 40 vertical pressure levels.

COSMIC, GRAS and KOMPSAT are Global Navigation Satellite System (GNSS) profiles are accessed at the native high density but stored after partial vertical subsampling as described in Section 4.2.

4.3 Numerical Weather Prediction

- i. ECMWF analysis
- ii. GFS 6-hour forecast
- iii. GFS Analysis
- iv. GFS Climate Forecast System Re-analysis (CFSR)

ECMWF Analysis for Temperature and H20 vapor are gridded fields at 0000, 0600, 1200, and 1800 Z. Ninety-one (91) vertical pressure levels thinned from the 137 model sigma levels and horizontal resolution of 0.258 degree (Eresmaa and McNally 2014) are available.

The GFS 6-hour forecast is only available for conventional radiosondes and interpolated to the mandatory and significant report levels as described in Section 3.3

The NOAA Global Forecast System (GFS) Analysis for Temperature and H2O vapor are gridded fields at 0000, 0600, 1200, and 1800 Z. Forty-seven (47) vertical pressure levels (original) at 0.25 degree (**Reference ...**) are available.

The GFS CFSR is accessed similar to GFS 6-hour forecast but retrospectively (90-day delay).

The GFS 6-hour forecast and CFSR data are those included in the PREPBUFR files generated in the NCEP data assimilation (Section 4.1.1). CFSR (and GFS ?) atmospheric profiles, at 64 vertical levels and 0.38-km horizontal resolution, are 4D interpolated to radiosonde profiles (J. Wollen 2018, personal communication; Saha et al. 2010), meaning that radiosonde balloon drift in space and time is taken into account. The balloon drift information is retained on the Unified Radiosonde File (Section 4.1).

5. Collocation Processing

The conventional and special radiosondes serve as baseline for collocation with each satellite product suite and the collocation strategy is the same for all. Conventional collocations are typically available within 12-36 hours of a given observation. Special observations are processed on a 14-day delay.

5.1 Collocation Strategy

The collocation strategy identifies the "single closest" satellite profile (any retrieval type) from each suite among all candidates that are within 150 km and 6-hours a given radiosonde. This essentially assures at least one collocation per polar satellite. Distance is measured at the surface and thirty (30) minutes is added to the Raob launch time effectively synchronizing the collocation to the vicinity of 300 hPa; 30 minutes is not added for GNSS. This also favors collocations with radiosondes prior to overpass particularly for cases with larger time difference.

Collocations are compiled daily, the data-day is 0 to 2359Z as defined by the radiosonde, and include post processing (next day) to assure selection of the single closest satellite sounding across the 0Z date change. Typically, satellite profiles from a single satellite overpass are candidates for collocation and the closest in distance is the default selection. However, in mid-latitude and polar regions, multiple candidate orbits can occur and the respective time and distance differences are weighted (70km per hour) to determine the single closest profile; in most cases these are the closest in time..

Most Conventional (and a few Special) radiosondes are typically available twice daily at 0Z and 12Z. There are cases (< 5%) when radiosondes at a given site are 6-hourly (or less) and a few regions (Europe) with sites within 50 to 100 km. In these cases the same satellite sounding can be collocated with different radiosondes. Although overall undesirable, they are retained and can be of interest.

Radiosonde candidates for collocation and assessment must have at least a 5km vertical extent of qualified observations in the troposphere with no gaps; there are no vertical extent limits for dropsondes. Radiosondes also undergo a series of QC tests which includes looking at the NCEP "qc" flags tests assigned for each mandatory and significant level during NWS assimilation. A description of all QC tests can be found in Appendix B. All raobs which pass QC are candidate for collocations with sounding product suites

5.2 Collocation Steps

- a. Raob must pass QC,
- b. Identify "single, closest" observation per polar satellite product suite that is within -6 to +7 hours of Raob launch time "plus 30 minutes" and 150 km of launch site
- c. Identify "single closest" observation per GNSS constellation that is within +/- 6 hours and 250km at 100 hPa.
- d. In cases multiple candidate observations use the the closeness parameter (C) to determine the single closest observation:
 - C = [Delta (Time) x F] + Distance, where F is factor 72 (km/h)
- e. Single closest observation is selected regardless of any ancillary information, such as terrain, QC flag, cloudiness, etc (ancillary data are stored and available for use later)
- f. Apply 0Z filtering approach to latest 2-days of collocations to assure the selection of the single closest observation across the 00Z date change

In cases of multiple candidate collocations, a generic approach is employed for selecting a single closest collocation from respective satellite systems. A closeness parameter C, where $C = [Del(t) \times F] + Distance$, where F is a penalty factor (km/h). For example, setting F to zero would result in the closest observation in distance being selected regardless of time, and making F large would result in the closest observation in time being selected regardless of distance. The goal is to set a pragmatic value of F for consistent collocation selection among all satellites at any time and location.

Data records for each radiosonde containing all the collocated satellite product suites are stored for each day, referred to as the dailly collocation file.

5.3 Collocation Datasets

The NPROVS system produces an output file that contains every individual collocation for a single day. The file is a binary format used internally by NPROVS. The binary file is then converted to netCDF format for use outside of NPROVS.

The netCDF files are initially single day files, after 0Z filtering, that correspond to the initial binary format. The program CombineNetCDF performs the binary to netCDF conversion. This program was designed to also combine single day files into a file that contains multiple days. The CombineNetCDF program also has the ability to customize the data platforms that are written to the netCDF file as well as the parameters for each data platform that are copied. Together, these capabilities allow for the creation of netCDF files that can be customized for particular purposes.

Although the specific contents of the NPROVS netCDF file canl vary based on the selected data platforms and the number of days (or period) of data, the general format of the file is:

```
NPROVS netCDF
Global attributes
Date group 1
      Collocation_info
             Dates
             Times
             Latitudes
             Longitudes
       Data platform 1
             Parameter 1
             Parameter 2
             ...
             Parameter n
       Data platform 2
       ...
       Data platform n
Date group 2
•••
Date group n
```

The "Date_group" data groups typically contain data for one day. If a file contains data for multiple days, there will usually be one "Date_group" for each day.

Within each "Date_group" are several subgroups. There will always be a "Collocation_Info" subgroup that contains the dates, times, latitudes and longitudes for every collocation. There will also be one or more "Data_platform" groups which contain the parameter data for each data platform (radiosondes, satellite data, forecast data).

5.4 Reprocessing the Collocation Dataset

5.4.1 Conventional

- a) As needed to append extended period of missing data
- b) Routinely to append CFSR (approximate 90-day delay)

5.4.2 Special

Automatic re-processing of 60-day old data is routinely done to append "tardy" observations onto the NPROVS Special record.

Re-processing of the entire Special Dataset is also done to append "new" observations, for example a new site, new observations from a given site and/or new satellites. In these cases the radiosondes/satellites may be months/years old and therefore cannot be automatically included in the system. At the discretion of NPROVS staff, a reprocessing initiates with the high density radiosonde reformatting to the unified reports across the entire NPROVS Special dataset to append new profiles. These new unified reports are then collocated with existing/new satellites and/or NWP products. Done in this manner, special circumstances of appending and collocating observations are integrated at once across the Radiosonde and Satellite product landscapes. Subsequently, new GRUAN sites/products via the Lead Centre and/or new satellites (ie GPSRO ...) are able to be retrospectively inserted into the NPROVS Special record.

6. Assessment

A core assessment provided by NPROVS are the ensemble vertical statistics comparing the collocated radiosonde and satellite observations .

NPROVS provides a complete vertical profile assessment capability using the graphical applications (NARCS, PDISP, ODS described in Section 6.2). These applications span from global time series to regional, seasonal, weekly, daily and individual collocation analysis and deep dive case-studies.

Assessments are rooted in the vertical statistics package contained in PDISP. Vertical statistics are calculated consistent with Nalli, 2015 originally developed by the AIRS Science Team.

6.1 Vertical Statistics

Vertical statistics within NPROVS are calculated and displayed within ProfileDisplay. The radiosonde observations are those described for Conventional (Section 4.1.1) and Special (Section 4.1.2). Since the conventional radiosonde are received at mandatory and significant levels, these are interpolated to the 101 boundary and ultimately the 100 effective pressure levels (Appendix B). The hi-density Special radiosondes have already been converted to the 100 effective pressures (approximate 500m resolution in troposphere) so no interpolation is needed.

The 100 effective pressure levels match the derived retrieval levels provided in most of the satellite product suites. The exception is GNSS profiles which are originally derived (received) at much higher vertical density and ultimately "subsampled" down to the 100 level effective pressures for assessment..

Subsequently, all the radiosonde and satellite profiles are available and typically assessed at the 100 effective pressures. However, there are user options (within PDISP) to further downgrade the vertical density, including to 30 effective pressure levels (approximate 1km resolution; Appendix B) more consistent with typical polar satellite sensor sensitivity.

PDISP also provides user options to use specific, "customized" sets of collocations for assessment. These contain options for inter-comparing multiple satellite suites using collocations which contain the desired satellite product suites. For example, a user can compare NUCAPS and AIRS soundings (which pass QC or not ...) that are each within 2 hours of a given radiosonde over a desired region. Furthermore, users can select based on radiosonde attributes including instrument type, day / night, surface inversion, etc and or satellite sounding attributes including QC flag, terrain etc. These features are further outlined in Section 6.2

Users also have options to display the statistics in a variety of ways, for example as vertical statistics covering desired atmospheric pressure levels (y-axis) and dynamic range (x-axis), scatter plots including associated slopes and intercept at a given level or to simply browse the individual collocations (case studies).

The vertical statistic (or scatter plot) generation begins once the user has sub-selected the desired collocations and attributes. Only collocations that are within the chosen sample are used during the generation of statistics; enterprise assessment. Once selected, users are provided with additional options prior to the statistics calculation. These include selecting the baseline profile and a variety of weighting options, for example, in the context of global distribution and moisture statistics.

There are four primary options available with respect to global distribution representation: The **first, default option**, simply treats each collocation individually.

The **second**, **bin option**, sorts the collocations according to the 27 (18) geographic bins used in legacy TOVS and ATOVS systems to compute the first guess and retrieval operators (Reale, 2012)

The **third**, **grid option**, sorts collocations into 10 degree by 10 degree latitude/longitude grid boxes (extended in polar regions) and then computes statistics which integrate each grid box The **fourth**, **weighting option**, initially sorts collocations by land and sea, respectively considering the terrain type of the radiosonde and selected product suite(s), and then applies a weighting of 0.7 to sea collocations and 0.3 to land. This method most closely matches the JPSS sounding product requirements.

Weighting (W) options for computing H20 vapor fraction statistics include three (3) choices: No weight,

Weight by H20 vapor magnitude or

Weight by H20 vapor magnitude squared.

The method (Nalli, 2016) originally sanctioned by the AIRS Science Team is to weight the bias by H20 vapor magnitude and to weight the Standard Deviation and RMS by the water vapor magnitude squared.

Once the options are selected, the program (PDISP) then begins calculating the statistics using every chosen profile. The program calculates running sums of the differences between the profile and the baseline while looping through all of the available collocations. The running sums are computed at every pressure. During the step the time differences, distance differences, maximum negative differences and maximum positive differences are also calculated. Running sums are maintained for temperature, water vapor mixing ratio, relative humidity and total precipitable water.

A particular issue is determining the lowest pressure boundary (101) and ultimately the surface air temperature for product suites that do not include this information. Most product suites provide surface pressure but only AIRS and the NWP models provide a surface air temperature. Assuming surface pressure is reported, the estimation of the lowest boundary and surface air temperature is done consistent with Berndt, 2020. The lowest boundary level ultimately used for statistics must exceed the reported surface pressure for each selected product suite. Surface air temperature is not routinely included in statistics *at this time*. Once the common lowest boundary is determined, the corresponding effective pressures are used for statistical comparison. Similarly, the topmost common boundary is used to determine the uppermost effective pressure for statistics. The topmost boundary is primarily defined by the Raob and rarely exceeds 5 hPa (4.92 hPa); satellite product suites extend above 0.1 hPa.

Once the sample and product suites are selected, the running sums are computed for each collocation and the calculation of the statistics for each of the platforms is performed. Statistics are computed for Temperature, H20 Vapor Mixing Ratio fraction (%) *and TPW* respectively; H2O vapor fraction (%) is defined as the H20 vapor difference / Baseline H20 vapor (g/kg). The calculated statistics are:

- Baseline mean
- · Profile mean
- Bias
- · Standard deviation
- · Root mean square
- · R-squared
 - Maximum difference (+ and -)
- Average distance
- Average time difference
- Average absolute time difference

After the statistics are calculated, the values are grouped and returned to the part of ProfileDisplay that displays the statistics. At this point the user has many options for displaying the statistics including choices to show temperature, water vapor fraction and/or, relative humidity in various formats including P**2/7, logarithmic and linear. Options for vertical statistics include pressure range, dynamique variable range, sample size constraints and plot color for a given product suite. One can also display as a scatter plots or within a table. Finally, the user can easily browse/display the individual profiles for a given set of statistics including easy identification of profiles with the maximum (+ or -) difference, see Section 6.2.2

STOP (6-5)

6.2 Graphical Applications

There are 3 applications, all written in Java language which allows platform independence so they run on any Java supported computer, such as Windows, Mac OS and Linux servers.

- 1. Orbital Display System (ODS) can show horizontal cross-section images of the Earth's atmosphere using data from a variety of sources including weather satellites and forecast models. Additionally, ODS can display vertical cross-sections of the atmosphere. Any location on a horizontal image can be selected to obtain additional data associated with the location or a Profile graph showing a Skew-T plot of all the level data. The User's Guide can be viewed on the NPROVS web site: ODS User's Guide.pdf
- 2. Profile Display (PDISP) displays collocated radiosonde and satellite profiles in Skew-T profile plots and can perform the calculation and display of vertical accuracy statistics and scatter plots. Additionally one can view where all the available collocations are mapped in color and user can sub-select collocations. This utility has improved over the years and we are getting ready for version 7 which will be able to import NetCDF files. The User's Guide can be viewed on the NPROVS web site: ProfileDisplay User's Guide

3. NPROVS Archive Statistics (NARCS) can display statistical plots archived over the span of all collocations since 2008 (2013 for the Special system). This includes mean bias, standard deviation and RMS. A new feature was added to display a color vertical cross-section of the statistics whereby each system can be picked from a list. Currently only have a <u>Quick Start guide</u> but some of the features are described.

6.3 Strategies

- a Horizontal Fields (ODS); see ODS User guide
- b Global Time Series (NARCS); see NARCS User Guide
- c Regional/Seasonal Performance Statistics (PDISP); see PDISP User Guide and PDISP Quick Start
- d Deep Dive (PDISP, ODS)

7. Summary / Path Forward

Summarize the system and its monitoring capability)...to be done.

In addition to the capability in satellite products monitoring as demonstrated in section xx, NPROVS (via analysis of collocation data accumulated since 2008) has also been utilized in other research and applications listed below.

a) Quantify the uncertainty of time and distance mismatches on the bias and standard deviation of the product being validated (Sun et al. 2010; Sun et al. 2017a).

b) Assess satellite products mission requirement by taking advantage of the large radiosonde sample from conventional network and high quality dedicated/GRUAN data (Sun et al. 2017a, b).

c) Correct radiation-induced temperature biases in conventional radiosonde types by using GPS RO Tdry as the reference (Sun et al. 2013). This provides the potential of updating the RADCOR which has been obselete in the NCEP NWP assimilation.

d) Quantify the measurement improvement of newly emerging Vaisala RS41 over Vaisala RS92 in support of their transition in GRUAN (Sun et al. 2019a; Sun et al. 2020).

e) Understand the consistency of GRUAN observations with satellite measurements in GSICS context (Sun et al. 2019b).

f) Detect long-term data continuity introduced by new radiosonde types (Tony?)

8. Appendices

A NPROVS Special Sites

| Station | Station ID | Data Record | Instrument Types | GRUAN |
|---|------------|---------------------------|---------------------|-------|
| Ascension Island | ASCENS | 29 Apr 2017 - Present | RS92 | |
| AEROSE 2013 | WTEC | 9 Jan 2013 - 7 Dec 2013 | RS92 | x |
| AEROSE 2015 | WTEC | 13 Feb 2015 -17 Nov 2015 | RS92 | |
| AEROSE 2017 | WTEC | 13 Feb 2017 - 7 Mar 2017 | RS41/RS92 | |
| McMurdo Station, Antarctica | 89664 | 30 Nov 2015 - 3 Jan 2017 | RS92 | |
| Western Antarctic Ice Sheet | WAIS | 4 Dec 2015 - 18 Jan 2016 | RS92 | |
| Barrow, North Slope Alaska | 70027 | 01 Jan 2011 - Present | RS41/RS92 | x |
| Howard University Beltsville, Maryland | BELTSV | 07 Mar 2012 - Present | RS92/RS41 | x |
| Hamburg, Germany | 10141 | 09 Jun 2016 - 06 Jan 2017 | RS41 | |
| Boulder, Colorado | BOULDE | 24 Aug 2011 - 31 Aug 2016 | RS92/RS41 | x |

| Cabauw, Netherlands | 06260 | 01 Jan 2011 - 16 Jan 2017 | RS92/RS41 | Х |
|---|--------|---------------------------|-----------|---|
| CalWater Campaign | ACAPEX | 12 Jan 2015 - 10 Feb 2015 | RS92 | |
| CIRA Colorado State University | CIRA | 6 May 2016 - 22 Sep 2016 | RS41/RS92 | |
| ENNR Campaign | WTEC | 16 Feb 2016 - 16 Mar 2016 | RS92 | |
| Christmas Island, ENRR | CXENRR | 26 Jan 2016 - 13 Mar 2016 | RS92 | |
| Darwin, Australia | 94120 | 01 Apr 2014 - 14 Jan 2015 | RS92 | |
| Eastern North Atlantic, Azores, Portugal | GRACIO | 28 Sep 2013 - Present | RS92/RS41 | х |
| Eureka, Canada | 71917 | 24 Oct 2012 - 18 Mar 2013 | RS92 | х |
| Gan, Maldives Islands | 43599 | 22 Sep 2011 - 09 Feb 2012 | RS92 | x |
| Lauder, New Zealand | LAUDER | 11 Dec 2012 - Present | RS41/RS92 | х |
| Lindenberg, Germany | 10393 | 01 Jan 2011- Present | RS92/RS41 | х |
| Manus, Papua New Guinea | 92036 | 01 Jul 2013 - 06 Jul 2014 | RS92 | х |
| Nauru Island | 91532 | 01 Jan 2011 - 26 Aug 2013 | RS92 | x |
| Ny Alesund, Svalbard, Norway | 01004 | 19 Oct 2012 - Present | RS92/RS92 | x |
| Oliktok Point, Alaska | OLIKTO | 10 Sept 2013 - Present | RS92 | |
| Ougadougou, Burkina Faso | 65503 | 17 Jul 2012 - 01 Aug 2012 | RS92 | х |
| Payerne, Switzerland | 06610 | 23 Sep 2011 - 19 Dec 2016 | RS92/RS41 | х |
| Potenza, Italy | 16300 | 23 Feb 2011 - 05 May 2016 | RS92/RS41 | Х |

| Reunion (La Reunion Island), France | REUNIO | 08 April 2013 - Present | RS92/RS41 | Х |
|--|--------|--------------------------------|-----------|---|
| San Cristobol, Galapagos, Ecuador | 84008 | 03 Aug 2012 - 26 Jan 2015 | RS92 | x |
| San Jose, Costa Rica | 78762 | 04/10/2012 - 02/21/2014 | RS92 | x |
| Singapore, Singapore | 48698 | 13 April 2016 - Present | RS41 | X |
| Southern Great Plains, Oklahoma | 74646 | 01 Jan 2011 - Present | RS92/RS41 | x |
| Sodankyla, Finland | 02836 | 05 Jan 2011 - 24 March 2017 | RS92/RS41 | X |
| Neumayer, Antarctica (DE) | 89002 | 18 Feb 2020 - Present | RS41 | |
| Tateno, Japan | 47646 | 06 June 2011 - Present | RS92/RS41 | X |
| Tenerife, Spain | 60018 | 01 Oct 2014 - 12 Dec 2017 | RS92/RS41 | x |
| Table Mountain Facility, California | TMFJPL | 22 Jul 2011 - 01 Jul 2016 | RS92/RS41 | x |

B Levels (100 layers, 30 layers ...)

9 References

Need NCEP Hydrocheck reference ... Need berndt, 2020 ...

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