Validation of Atmospheric Profile Retrievals from the SNPP NOAA-Unique Combined Atmospheric Processing System 1. Temperature and Moisture

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***Abstract*—This paper overviews the validation of the operational atmospheric vertical temperature and moisture profile (AVTP and AVMP) environmental data record (EDR) products retrieved from Cross-track Infrared Sounder (CrIS) and the Advanced Technology Microwave Sounder (ATMS), two passive sounding systems onboard the Suomi National Polar-orbiting Partnership (SNPP) satellite. The SNPP CrIS/ATMS sounder suite serves as the U.S. low earth orbit (LEO) satellite sounding system and will span the future Joint Polar Satellite System LEO satellites. The operational sounding algorithm is the NOAA-Unique Combined Atmospheric Processing System (NUCAPS), a legacy sounder science team algorithm capable of retrieving atmospheric profile EDR products with optimal vertical resolution under non-precipitating (clear to partly cloudy) conditions. The SNPP NUCAPS AVTP and AVMP EDR products are validated using extensive global *in situ* baseline datasets, namely radiosonde observations launched from ground-based networks and from ocean-based intensive field campaigns, along with numerical weather prediction model output. Based upon statistical analyses using these datasets, the SNPP AVTP and AVMP EDRs are determined to meet the JPSS Level 1 global performance requirements.**

***Index Terms*—NUCAPS, SNPP, JPSS, environmental satellite, atmospheric profiles, soundings, retrieval, validation, cal/val**

I. INTRODUCTION

The U.S. Suomi National Polar-orbiting Partnership (SNPP) satellite was launched in 2011 and is the first operational U.S. satellite to feature the high spectral-resolution ("hyperspectral") Cross-track Infrared Sounder (CrIS) and Advanced Technology Microwave Sounder (ATMS) sounding system (previously referred to collectively as the Cross-track Infrared Microwave Sounder Suite, CrIMSS [1]). The follow-on Joint Polar Satellite System (JPSS) is a U.S. National Oceanic and Atmospheric Administration (NOAA) operational satellite mission, in collaboration with joint international partnerships and the U.S. National Aeronautics and Space Administration (NASA) [2], that will support NOAA's weather, climate and environmental monitoring missions by providing operational timely global data to users. JPSS-series will feature CrIS/ATMS sounders onboard four satellites launched in the same orbit over the next two decades beginning in 2017. The CrIS/ATMS sounding system is designed to measure well-calibrated infrared (IR) and microwave (MW) radiances or sensor data records (SDRs) for synergistically retrieving atmospheric vertical profile environmental data records (EDRs) under non-precipitating conditions (clear, partly cloudy and cloudy) with relatively high vertical resolution ($\approx$2–5 km) in much the same manner as predecessor sounding systems, namely the MetOp-A and -B Infrared Atmospheric Sounding Interferometer (IASI) [3], [4] and the EOS-Aqua Atmospheric Infrared Sounder (AIRS) [5], [6]. The CrIS instrument is an advanced Fourier transform spectrometer (FTS) that measures high-resolution IR spectra in 1305 channels over three bands spanning $\nu = [650, 2550]$ cm^{-1} (high spectral resolution is hereafter simply referred to as "hyperspectral"). The ATMS is a MW sounder with 22 channels ranging from 23 to 183 GHz [7]. These two instruments operate in an overlapping field-of-view (FOV) formation analogous to AIRS, with ATMS FOVs resampled to match the location and size of the 3×3 CrIS FOVs for retrievals under clear to partly cloudy conditions.

While hyperspectral sounder SDRs (radiances) have generally come to be directly assimilated into global numerical weather prediction (NWP) models via variational analysis schemes, they also continue to be directly inverted operationally to retrieve orbital atmospheric profile EDRs in near-realtime as originally envisioned by satellite sounding pioneers [8]–[10] and [11]–[13]. The operational EDR retrieval algorithm for CrIS/ATMS is currently the NOAA-Unique Combined Atmospheric Processing System (NUCAPS) developed at NOAA/NESDIS/STAR [14], [15], which superseded the original Interface Data Processing Segment (IDPS) CrIMSS algorithm in September 2013. The NUCAPS algorithm processes CrIS/ATMS data based upon the heritage methodology developed for the EOS-Aqua AIRS and MetOp IASI systems, with the retrieval algorithm being a modular implementation of the multi-step AIRS Science Team retrieval algorithm Version 5 [16], [17]. For more details on the NUCAPS algorithm, the reader is referred to [15], [16] or the Algorithm Theoretical Basis Document [18] available online. The primary EDR parameters retrieved by NUCAPS are the atmospheric vertical temperature and moisture profiles (AVTP and AVMP), which are output on the University of Maryland Baltimore County (UMBC) radiative transfer algorithm (RTA) [19] 100 levels

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(i.e., layer boundaries) and layers, respectively. In addition to AVTP and AVMP, NUCAPS retrieves ozone (O_3) and carbon trace gases, including carbon monoxide (CO), carbon dioxide (CO_2) and methane (CH_4) profile EDRs on 100 RTA layers. Current users of the NUCAPS EDRs include NOAA National Weather Service (NWS) weather forecast offices (WFOs) via the Advanced Weather Interactive Processing System (AWIPS). Sounder EDRs are also invaluable for numerous global environmental research studies [20], [21].

The NUCAPS algorithm operates under clear to partially cloudy conditions by first cloud-clearing [16] the 3×3 CrIS FOV arrays, these being referred to as the "field-of-regard" (FOR). Figure 1 shows a schematic of the CrIS/ATMS FOV sampling for an example NUCAPS FOR. The current method selects a 3 × 3 array of ATMS footprints[1] based on a center footprint matched with CrIS, then simply averages the antenna temperature data records (TDRs) for each channel to obtain the value for a single MW footprint (thereby emulating the earlier AIRS/AMSU configuration illustrated in [5]). Although there are more sophisticated ways of doing this (e.g., matching individual footprints instead of simply the center), they have been found to have very small impact and may even lead to scene dependent biases. Then assuming radiance differences in the FOV are due only to clouds, a "clear-column" IR radiance spectrum is extrapolated for each FOR. More details and discussion on the cloud-clearing methodology and cloud-cleared radiance product can be found in numerous previously published papers [14], [16], [22]. The multi-step NUCAPS physical retrieval module then retrieves individual parameters sequentially (as opposed to simultaneously), using only channels rigorously determined to be sensitive to that parameter [23], beginning with temperature, then water vapor, followed by the ozone profile retrieval and trace gases. Figure 2 shows the selected CrIS IR channels in the longwave, midwave and shortwave IR bands, used for the AVTP, AVMP and ozone profile retrievals. The current operational NUCAPS algorithm (Version 1.5) runs on nominal CrIS resolution spectra at $\Delta\nu \approx 0.625$ cm^{-1}, 1.25 cm^{-1} and 2.5 cm^{-1} for the longwave, midwave and shortwave IR bands, respectively [1], [2].

To ensure that the SNPP NUCAPS retrieved EDR products meet their mission specification objectives, in this work we have conducted a formal validation of the AVTP and AVMP EDRs (v1.5 nominal CrIS resolution) using radiosonde collocations from land-based networks and ocean-based dedicated launches. Section II overviews the JPSS EDR calibration/validation (Cal/Val) program, Section III characterizes the operational algorithm performance (v1.5) based on rigorous statistical analyses, and finally Section V presents preliminary results (i.e., based on numerical model comparisons) of the NUCAPS algorithm for CrIS full-resolution data scheduled for operational delivery in July 2017 (v2.0.5) in preparation for the launch of the JPSS-1 satellite. Validation of the operational NUCAPS IR ozone profile product will be the subject of the Part 2 companion paper.

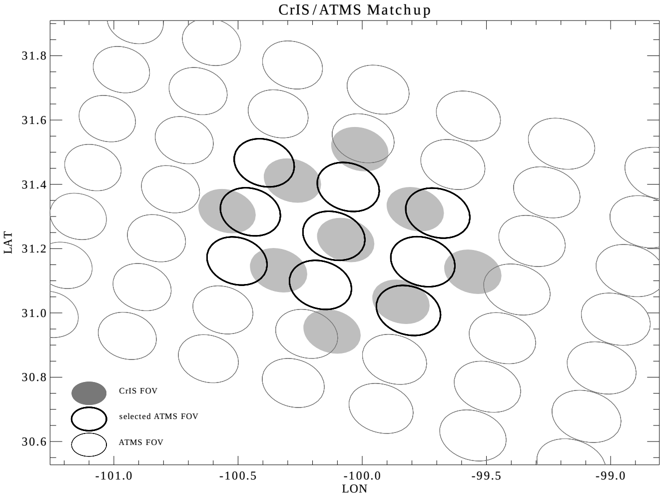

Fig. 1. Example CrIS/ATMS FOV configuration for a single NUCAPS FOR used for cloud-clearing. The cross-track scanning direction is roughly upper-left/lower-right and the grey unfilled ellipses show approximate ATMS FOV footprints for beam width 1.1° (channels 17–22) [7]. The grey ellipses show the 3×3 CrIS FOV footprints comprising a NUCAPS FOR, and the black unfilled ellipses show the selected ATMS footprints (based on the center footprint matched to a CrIS footprint) comprising an effective MW FOV analogous to the AIRS/AMSU configuration [5]. The ellipses depicted are approximations for illustration purposes only and do not represent the exact spatial footprints of those instruments.

II. JPSS Sounder EDR Cal/Val Overview

The direct goal of validating EDRs is to provide a general assessment and error characterization of the retrieved parameters relative to an assumed "truth" (or baseline) dataset. Continued assessments in this manner in turn enables ongoing development and/or improvement of algorithms. Validation of EDRs can also facilitate the routine monitoring of SDRs from which they are derived (e.g., sea surface temperature EDRs [24]).

To support cal/val and long-term monitoring of the SNPP satellite SDRs and retrieved EDRs, the JPSS Cal/Val Program defines four phases for cal/val of sensors and algorithms throughout the satellite mission lifetime [25]: Pre-Launch, Early Orbit Checkout (EOC), Intensive Cal/Val (ICV), and Long-Term Monitoring (LTM). In accordance with the JPSS phased schedule, the SNPP CrIS/ATMS EDR Cal/Val Plan was devised to ensure the EDR would meet the mission Level 1 requirements [26]. The CrIS/ATMS EDR Cal/Val Plan for the successor JPSS-1 satellite (or "J-1") was drafted during Jul–Aug 2015 and submitted on 31 December 2015.

The JPSS Level 1 Performance Requirements[2] for AVTP and AVMP are reproduced in Tables I and II, respectively. These serve as the metrics by which the system is considered to have reached Validated Maturity and has met mission requirements. It is noted that the requirements are defined for global, non-precipitating cases on 3–5 atmospheric "broad-

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[1] The term "footprint" refers to the sensor FOV projected onto the earth surface.

[2] In satellite product parlance, "Level 1" typically refers to the lowest level of the product chain (e.g., raw data records or SDRs) whereas "Level 2" refers to higher level EDRs or retrievals. However in the current context of JPSS requirements, "Level 1" is a programmatic term that refers to the "highest level" program requirement (L. Zhou, Personal Communication, 2017).

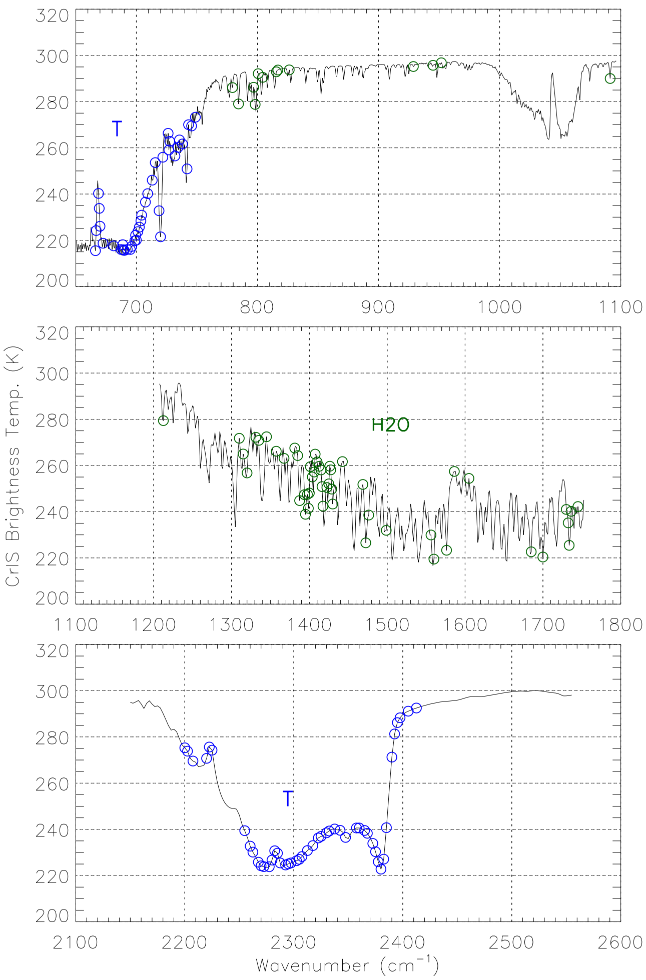

Fig. 2. Hamming apodized CrIS IR brightness temperature spectra for a marine nighttime case (10:22 UTC 9 June 2015, 6.5°N, 130.0°W) showing temperature and water vapor channels (blue and green circles, respectively) used in the NUCAPS multi-step physical retrieval: (top) longwave IR (unapodized nominal resolution 0.625 cm^{-1}), (middle) midwave IR (unapodized nominal resolution 1.25 cm^{-1}), and (bottom) shortwave IR (unapodized nominal resolution 2.5 cm^{-1}).

layers" that are computed as an average of "coarse-layers" ranging from 1–5 km in thickness for AVTP and 2 km for AVMP. "Partly Cloudy" conditions are defined by a successful cloud-clearing and IR retrieval converging to a solution. Conversely, "Cloudy" conditions are defined by cases where cloud-clearing is not successful and the IR algorithm is not able to converge to a solution, thereby resulting in a MW-only algorithm solution as the final product. It is in this manner that the NUCAPS system is capable of providing AVTP/AVMP retrievals for global, non-precipitating conditions. The original IDPS CrIMSS operational algorithm was validated through Beta and Provisional Maturities [27], and the successor SNPP NUCAPS algorithm formally attained Validated Maturity in September 2014 [25] based upon the analyses detailed below.

TABLE I
JPSS LEVEL 1 REQUIREMENTS[a] FOR CRIS/ATMS ATMOSPHERIC VERTICAL TEMPERATURE PROFILE MEASUREMENT UNCERTAINTY

Global AVTP Measurement Uncertainty Requirement[b]		
Atmospheric Broad-Layer	Threshold	Objective
Cloud-Free to Partly Cloudy (IR+MW)[c]		
Surface to 300 hPa[d] (1 km layers)	1.6 K	0.5 K
300 hPa to 30 hPa (3 km layers)	1.5 K	0.5 K
30 hPa to 1 hPa (5 km layers)	1.5 K	0.5 K
1 hPa to 0.5 hPa (5 km layers)	3.5 K	0.5 K
Cloudy (MW-only)[e]		
Surface to 700 hPa (1 km layers)	2.5 K	0.5 K
700 hPa to 300 hPa (1 km layers)	1.5 K	0.5 K
300 hPa to 30 hPa (3 km layers)	1.5 K	0.5 K
30 hPa to 1 hPa (5 km layers)	1.5 K	0.5 K
1 hPa to 0.5 hPa (5 km layers)	3.5 K	0.5 K

[a] Source: Joint Polar Satellite System (JPSS) Program Level 1 Requirements Supplement – Final, Version 2.10, 25 June 2014, NOAA/NESDIS.
[b] Expressed as an error in layer average temperature.
[c] Partly cloudy conditions are those where both the IR and MW retrievals are used and are typically scenes with $\leq 50\%$ cloudiness.
[d] The IR+MW surface to 300 hPa requirement is for over global ocean. Over land and ice mass, the Uncertainty is relaxed slightly to 1.7 K due to the state of the science of the land emissivity knowledge within the temperature sounding algorithm.
[e] Cloud conditions are those where only the MW retrievals are used and are typically scenes with $> 50\%$ cloudiness.

TABLE II
JPSS LEVEL 1 REQUIREMENTS[a] FOR CRIS/ATMS ATMOSPHERIC VERTICAL MOISTURE PROFILE MEASUREMENT UNCERTAINTY

Global AVMP Measurement Uncertainty Requirement[b]		
Atmospheric Broad-Layer	Threshold	Objective
Cloud-Free to Partly Cloudy (IR+MW)[c]		
Surface to 600 hPa	greater of 20% or 0.2 g kg^{-1}	10%
600 hPa to 300 hPa	greater of 35% or 0.1 g kg^{-1}	10%
300 hPa to 100 hPa	greater of 35% or 0.1 g kg^{-1}	10%
Cloudy (MW-only)[d]		
Surface to 600 hPa	greater of 20% or 0.2 g kg^{-1}	10%
600 hPa to 300 hPa	greater of 40% or 0.1 g kg^{-1}	10%
300 hPa to 100 hPa	greater of 40% or 0.1 g kg^{-1}	NS

[a] Source: Joint Polar Satellite System (JPSS) Program Level 1 Requirements Supplement – Final, Version 2.10, 25 June 2014, NOAA/NESDIS.
[b] Expressed as a percent of average in 2 km layers.
[c] Partly cloudy conditions are those where both the IR and MW retrievals are used and are typically scenes with $\leq 50\%$ cloudiness.
[d] Cloud conditions are those where only the MW retrievals are used and are typically scenes with $> 50\%$ cloudiness.

III. TEMPERATURE AND MOISTURE PROFILE ASSEMENT

Satellite sounder EDR validation methodology has been well-established in previous validation work (i.e., with AIRS and IASI), with the various approaches being roughly classified as part of a hierarchy that includes [28] (1) global numerical model comparisons, (2) satellite EDR intercomparisons, (3) conventional radiosonde assessments, (4) dedicated/reference radiosonde assessments, and (5) intensive campaign dissections. Those at the beginning of the hierarchy are typically employed in the early cal/val stages of a satellite's lifetime, whereas those near the top are employed during later stages.

A. Data

To allow for adequate validation of the SNPP operational sounder EDRs, JPSS has directly and indirectly funded a dedicated radiosonde program leveraging several collaborating institutions. Dedicated radiosondes are optimally collocated and synchronous with SNPP overpasses at various selected sites. In addition, we have leveraged GCOS Reference Upper Air Network (GRUAN) RAOB sites (discussed more below). Collocations of NUCAPS CrIS/ATMS FORs with RAOBs are facilitated via the NOAA Products Validation System (NPROVS) [29]. NPROVS routinely collocates single-closest EDR profile retrievals from multiple platforms (including SNPP) with RAOB launch "anchor points." Using this base RAOB-satellite collocation system, an EDR validation archive (VALAR) has been created whereby CrIS SDR and ATMS temperature data record (TDR) granules in the vicinity of RAOB "anchor points" are acquired for running offline retrievals, thus allowing validation flexibility (e.g., enables ozone and trace gas validation) and ongoing algorithm optimization and development.

Figure 3 shows JPSS-funded dedicated RAOB sites for the SNPP sounder validation effort as of this writing through 2016. These include U.S. DOE Atmospheric Radiation Measurement (ARM) sites [30], [31], namely Southern Great Plains (SGP), North Slope of Alaska (NSA), Tropical Western Pacific (TWP) (Manus Island), and Eastern North Atlantic (ENA) sites (the TWP site was discontinued in August 2014 and funded dedicated launches were subsequently transferred to the ENA site). JPSS has also supported ship-based dedicated radiosondes during intensive campaigns-of-opportunity over open-ocean during the 2013a,b/2015 NOAA Aerosols and Ocean Science Expeditions (AEROSE) [32], [33] and the Jan–Feb 2015 CalWater ARM Cloud Aerosol Precipitation Experiment (ACAPEX) [21], [34]. In addition to these, two collaborative land-based sites-of-opportunity (with data acquisition objectives spanning satellite sounder validation) include the Howard University Beltsville Center for Climate System Observation (BCCSO) site in Beltsville, Maryland, and combined RAOB and lidar data collected by The Aerospace Corporation from the Pacific Missile Range Facility (PMRF) site on Kauai, Hawaii [35]. Lastly, there are three GRUAN sites that fortuitously happen to collocate well with SNPP overpasses, these being Lindenberg, Germany (LIN), Cabauw, The Netherlands (CAB), and Sodankyla, Finland (SOD) [36]. The reason these sites "automatically" collocate is because of the local time zone, which is approximately UTC +1 hour. Given that synoptic launch times are at 00 and 12 UTC, the local times of launches from these sites are ≈01:00 and 13:00 LT. The sun-synchronous SNPP orbit has local equator crossing times of 01:30 and 13:30 LT, thus the satellite happens to overpass these locales just following the launches, thereby fortuitously "mimicking" dedicated launches.

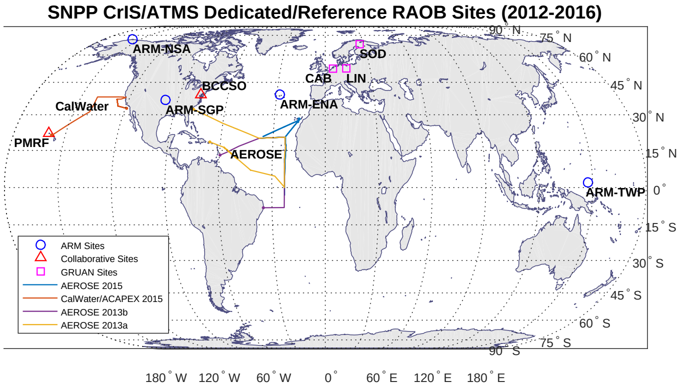
SNPP CrIS/ATMS Dedicated/Reference RAOB Sites (2012-2016)

Fig. 3. SNPP-dedicated and GRUAN reference RAOB truth sites used for JPSS CrIS/ATMS EDR cal/val over the period 2012–2016. Blue circles denote ARM sites (NSA, SGP, TWP and ENA), red triangles denote collaborative partner sites (BCCSO and PMRF), magenta squares denote collocated GRUAN reference sites (LIN, CAB and SOD), and different colored lines denote ocean-based intensive campaign ship tracks (AEROSE and CalWater/ACAPEX). Map projection is equal-area.

B. Error Analysis

Using these *in situ* data as the baseline, we compute coarse-layer and broad-layer uncertainties (defined in §II) for AVTP and AVMP EDRs derived from an offline emulation[3] of the operational NUCAPS algorithm running on nominal CrIS resolution data (Version 1.5). Details on the methodology for calculating coarse-layer statistics, namely bias, standard deviation (σ) and root-mean-square uncertainty (RMSE) are described in [28]; for AVMP, we consistently apply W^2 moisture weighting to both the bias and RMSE calculations [28]. To minimize mismatch error in our statistical analyses, stringent space-time collocation criteria are applied, namely quality-accepted retrievals within $\delta x \leq 75$ km radius and $-60 < \delta t < 0$ minutes of launches (the time criterion ensures the radiosonde is airborne coincident with the satellite overpass). These criteria strike a good balance between sample size and mismatch error [37]. For the MW-only retrievals, it is noted again here that the JPSS requirements are specified for "cloudy" cases (i.e., >50% cloudiness, defined by failure of the IR algorithm to obtain an accepted solution; cf. §II); thus, the MW-only samples are given by cases accepted by the MW-only quality flag but rejected by the IR+MW quality flag. Figure 4 shows a geographic histogram (on an equal-area map projection) of the distribution of the RAOB collocation sample, where it can be seen that the combination of the RAOB sites described above provide adequate coverage of global climate zones (tropics, midlatitudes and polar) along with land and ocean surfaces. However, it is also noted that midlatitude, land-based sites tend on dominating the sample, whereas the JPSS Level 1 Requirements are derived based on global model calculations that cover the earth's ocean/land/zonal

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[3] The offline code is an exact emulation of the operational code. However, the offline version generates additional diagnostic output files in Level 2 binary format which facilitate validation on large samples. The offline code also enables algorithm development.

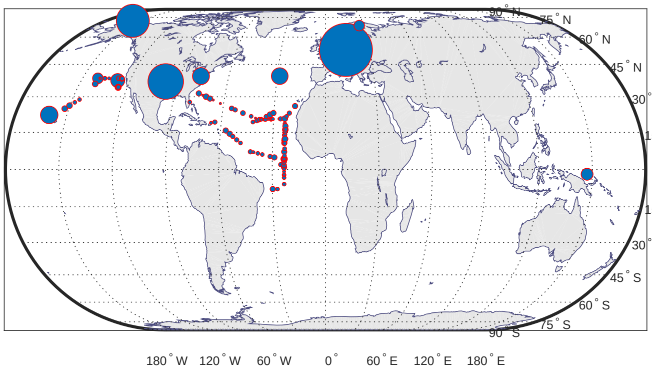

Fig. 4. Geographic histogram of SNPP CrIS/ATMS FOR-RAOB showing zonal representation of collocation data used in the global land/sea statistical error analysis. Circle areas depict the relative SNPP-RAOB collocation sample sizes for each RAOB launch location (prior to zonal and land/sea area weighting described in the text). Map projection is equal area.

surface areas. Therefore, we subsequently apply a geographic zonal area weighting scheme over 15° latitude zones and land/sea surface areas in our statistical calculations. This scheme gives proportionately greater weight to tropical ocean RAOB collocations and lesser weight to high-latitude land-based collocations, which is in accordance with the JPSS Requirements implicitly having such weighting built in.

The resulting global profile error statistics for AVTP and AVMP are given in Figures 5 and 6, respectively. The righthand plots show the bias statistics given by the coarse-layer means with $\pm 1\sigma$ given by the error bars. The JPSS Level 1 specification requirements are defined in terms of RMS statistics shown with dashed lines in the lefthand plots. The corresponding broad-layer results for AVTP and AVMP retrievals are shown with asterisks and summarized in Tables III and II, respectively. We find that both EDRs meet the JPSS requirements for both IR+MW and MW-only cases, with the only exception being MW-only AVTP for the upper tropospheric layer (30–1 hPa), which falls somewhat outside of the 1.5 K requirement for this layer. However, we see in Figure 5 that the collocation samples roughly fall off dramatically starting at about 14 hPa as radiosonde balloons tend on bursting somewhere below this level. In fact, it should be noted that the available 15 data points in top two layers above 5 hPa are due to merged lidar-RAOB data provided by the PMRF site [35]. In the right-hand plot an elevated random error (magenta $\pm 1\sigma$ bars) occurs in the coarse-layer between 10 and 5 hPa, and a significant negative bias (magenta line) occurs above 2 hPa, although this cannot be considered statistically significant. It should be noted that the MW-only samples correspond to cases rejected by the IR+MW quality flag, thus sample sizes are ≈30% the IR+MW sizes and generally correspond to more difficult geophysical cases. A more detailed examination of the AVTP performance from 110–10 hPa versus radio occultation measurements showing comparable results can be found in [38].

The reader may have also noticed that in Figure 6 the AVMP results for the 300–100 hPa broad-layer fall outside the requirements lines for both the IR+MW (blue asterisk) and MW-only retrievals, with an oscillation between significant positive and negative bias in the two coarse layers comprising the broad-layer. Some of these discrepancies are believed to be associated with biases and precision limitations in the RAOBs. For RAOB temperature it is due to radiation-induced biases [39], and for moisture it is associated with extremely low water vapor conditions, a known problem at higher levels of the troposphere [40]. For moisture this explanation is supported by a completely consistent pattern of discrepancies in bias with profiles from the European Centre for Medium-Range Weather Forecasts (ECMWF) model as seen in Figure 7. Nevertheless, the JPSS threshold requirements for AVMP (Table II) allow for the greater of a fractional error (%) or an absolute error ($\mathrm{g\,kg^{-1}}$). The AVMP results summarized in Table IV show in the last column absolute errors of 0.02 $\mathrm{g\,kg^{-1}}$, which are well below the 0.1 $\mathrm{g\,kg^{-1}}$ threshold, and thus in spite of the fractional differences the moisture product nevertheless meets requirements in upper layer. Based on the above results, we have concluded that the operational SNPP NUCAPS AVTP and AVMP EDRs meet the JPSS Level 1 requirements; similar statistical results versus RAOBs have been observed by [41].

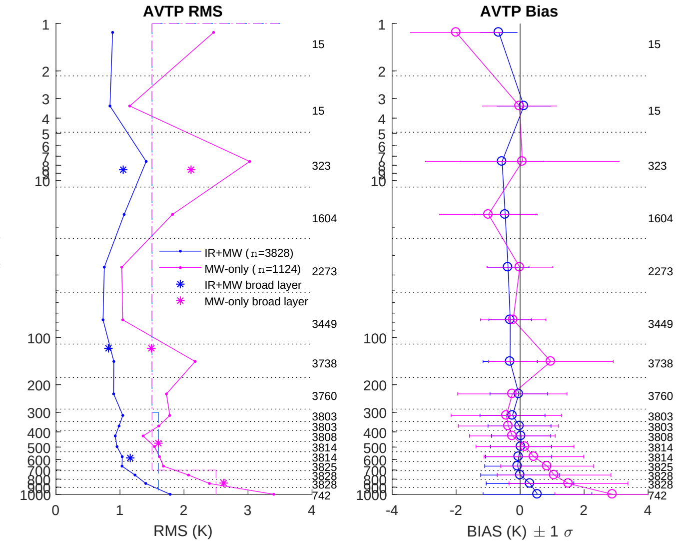

Fig. 5. Coarse-layer statistical uncertainty assessment of the NUCAPS atmospheric vertical temperature profile (AVTP) EDR retrievals (offline v1.5 operational emulation) versus collocated dedicated/reference RAOBs for retrievals accepted by the quality flag within space-time collocation criteria of $\delta x \leq 75$ km radius and $-60 \leq \delta t \leq 0$ minutes of launches over a sampling period of 9 January 2013 to 13 December 2015. The left and right plots show the RMSE and bias $\pm 1\sigma$ results, respectfully. NUCAPS IR+MW (clear to partly cloudy, defined by IR+MW accepted cases) and MW-only (cloudy, defined by the intersection of MW-only accepted cases and IR+MW rejected cases) performances are given in blue and magenta respectively, with IR+MW collocation sample size for each coarse layer given in the right margins. The light blue dashed line in the RMS plots (left) designate the JPSS Level 1 global performance requirements for "broad-layers," and the asterisks show the calculated broad-layer RMSE.

IV. LONG-TERM MONITORING

The long-term monitoring (LTM) of sounder profile EDRs is facilitated using conventional RAOB launches from synoptic WMO sites due to their ongoing regular launch schedule. Conventional RAOB collocations are routinely obtained via

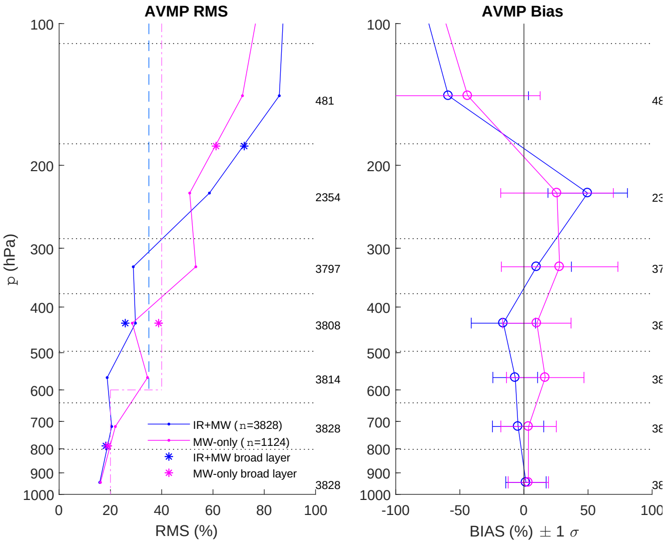

Fig. 6. As Figure 5 except for AVMP.

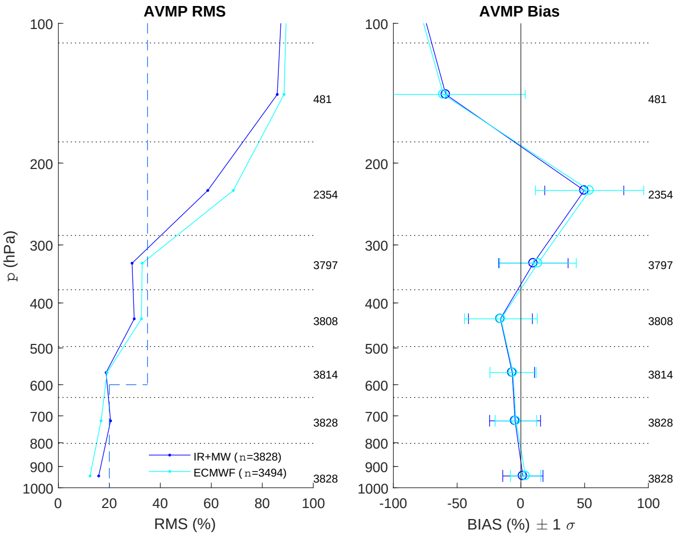

Fig. 7. As Figure 6 but showing statistical uncertainty assessments versus RAOBs of NUCAPS IR+MW moisture profile retrievals (blue lines) alongside collocated ECMWF output (analysis or forecast nearest in time) for reference (cyan lines).

TABLE III
VALIDATED GLOBAL AVTP EDR MEASUREMENT UNCERTAINTY

Atmospheric Broad-Layer	Land/Ocean	Ocean Only
Cloud-Free to Partly Cloudy (IR+MW)		
1014 to 300 hPa	1.16 K	1.08 K
300 hPa to 30 hPa	0.82 K	0.81 K
30 hPa to 1 hPa	1.05 K	1.08 K
Cloudy (MW-only)		
1014 to 700 hPa	2.62 K	2.46 K
700 hPa to 300 hPa	1.60 K	1.58 K
300 hPa to 30 hPa	1.49 K	1.42 K
30 hPa to 1 hPa	2.11 K	1.78 K

TABLE IV
VALIDATED GLOBAL AVMP EDR MEASUREMENT UNCERTAINTY

Atmospheric Broad-Layer	Fractional	Absolute
Cloud-Free to Partly Cloudy (IR+MW)		
1014 to 600 hPa	18.2%	1.23 $\mathrm{g\,kg^{-1}}$
600 hPa to 300 hPa	25.8%	0.30 $\mathrm{g\,kg^{-1}}$
300 hPa to 100 hPa	72.2%	0.02 $\mathrm{g\,kg^{-1}}$
Cloudy (MW-only)		
1014 to 600 hPa	19.0%	1.36 $\mathrm{g\,kg^{-1}}$
600 hPa to 300 hPa	38.8%	0.51 $\mathrm{g\,kg^{-1}}$
300 hPa to 100 hPa	61.2%	0.02 $\mathrm{g\,kg^{-1}}$

NPROVS, which collocates single-closest EDR profile retrievals from multiple platforms (including SNPP) with RAOB launch "anchor points" [29], and provides graphical user interface Java applet tools to assist EDR algorithm developers, users and validation scientists in the routine monitoring and diagnostic troubleshooting of sounding products. Profile statistics based on conventional RAOBs have been found to be similar to those obtained dedicated/reference RAOBs as reported by [41].

While NPROVS will always provide a low Earth orbit (LEO) satellite collocation with a RAOB using an inclusive ±6 h time window with launch times (scanning instruments onboard sun-synchronous LEO satellites provide twice-daily near global coverage), in this work we attempt to minimize mismatch error by employing tight space-time collocation criteria. For NPROVS-collocated conventional RAOBs we keep only single-closest FORs within $\delta x \leq 25$ km radius and $-30 < \delta t < 0$ minutes of launches ($\delta t \equiv t_{\mathrm{raob}} - t_{\mathrm{sat}}$). A typical distribution of conventional RAOB collocations with SNPP acquired over a month time period is shown in Figure 8. NPROVS archive statistics (NARCS) for monthly mid-troposphere temperature and moisture versus conventional RAOB collocations over the course of the SNPP mission life are shown in Figures 9 and 10 respectively. Blue lines show the results of the NUCAPS IR+MW retrievals (clear to partly cloudy) and cyan lines show the collocated AIRS retrievals for comparison. The solid lines show the bias statistics given by the coarse-layer means and the dotted lines show the RMS statistics. These results show reasonable interannual stability in the NUCAPS EDRs, with comparable performance against those obtained from the AIRS sounder relative to RAOBs, AIRS representing a mature, validated system [30], [42]–[45], with the primary exception being somewhat superior performance of AIRS AVTP relative to RAOBs. The AIRS improvement in accuracy is believed to be at least in part due to the non-linear neural-network first guess employed in the AIRS v6 algorithm. NUCAPS continues to use a linear regression for its first guess (similar to AIRS v5), which simply cannot capture the same degree of variability in fine

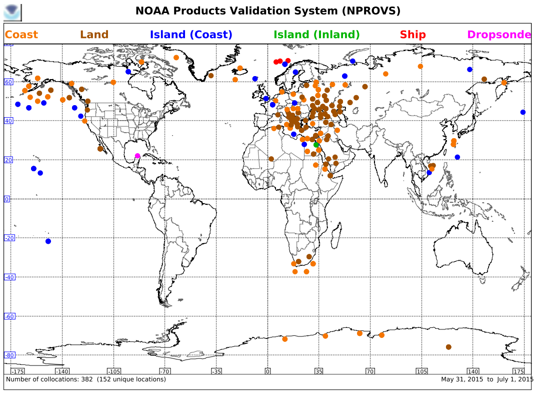

Fig. 8. NPROVS conventional synoptic RAOBs collocated with SNPP NUCAPS retrievals for June 2015 (single-closest FOR within 50 km radius of radiosonde launch sites and 0–30 minutes following launches).

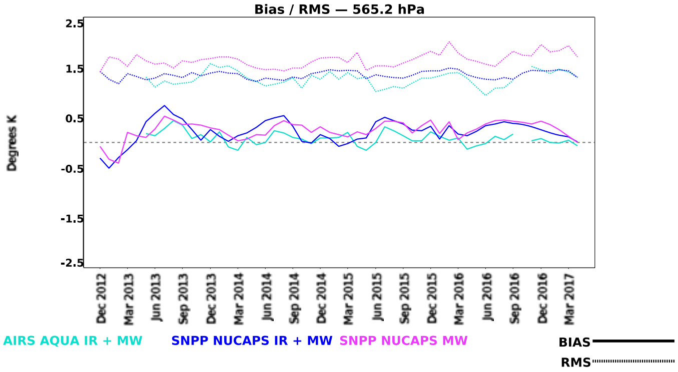

Fig. 9. NPROVS NARCS monthly statistical time-series for NUCAPS (operational v1.5) and AIRS (v6) temperature EDR retrievals versus collocated conventional RAOBs at a nominal mid-tropospheric RTA level (565.2 hPa). The solid and dotted lines show the bias and RMSE results, with blue, magenta and cyan lines indicating the NUCAPS IR+MW (clear to partly-cloudy), MW-only (cloud) and AIRS retrievals, respectively.

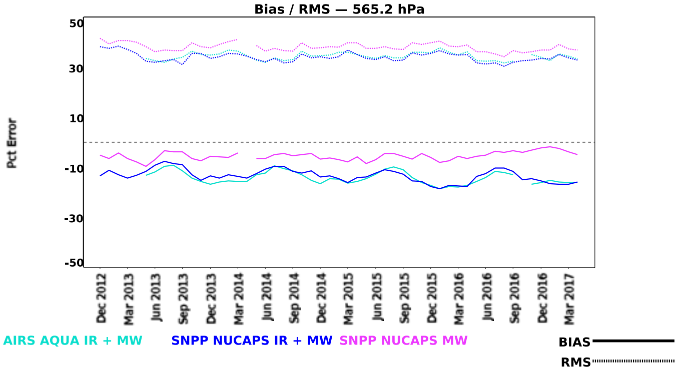

Fig. 10. As Figure 9 except for AVMP.

vertical structure for the physical retrieval to "pivot" off of, thereby yielding greater null-space errors with respect to high-resolution RAOBs.

V. PREPARATION FOR JPSS-1: CRIS FULL RESOLUTION

As mentioned in Section I, the operational SNPP NUCAPS v1.5 runs on CrIS spectra at the original nominal spectral resolution spectra of $\Delta\nu \approx$0.625 cm^{-1}, 1.25 cm^{-1} and 2.5 cm^{-1} for the longwave, midwave and shortwave IR bands, respectively. The reduced resolution in the midwave and shortwave bands is the result of the interferograms being truncated in those bands during operational processing of the SDRs. The reduction in spectral resolution in these bands was not anticipated to have a negative impact upon the primary temperature and moisture profile EDRs, but it was known that there would be adverse impact upon trace gases, especially carbon monoxide, and this was later empirically demonstrated by [46]. Requests for access to full-resolution CrIS ($\Delta\nu \approx$0.625 cm^{-1} in all three bands) from EDR science teams eventually led to offline production of full-spectral resolution (full-res) CrIS SDRs beginning in December 2014 [47]. In preparation for the ingest of operational full-res SDRs (including both SNPP as well as JPSS-1, to be launched tentatively in late 2017), a preliminary experimental offline NUCAPS version (v1.8.x) was developed to run on CrIS full-res data for demonstration studies [46]. The finalized version representing the operational delivery of the NUCAPS system in full-res mode (scheduled for July 2017) using the UMBC full-res RTA, has since been developed (v2.0.5) and is undergoing testing. CrIS full-res SDRs were not operationally available during the dedicated/reference RAOB acquisition period discussed in Section III, but the full-resolution SDRs were processed for a global Focus Day, 17 February 2015, for which global numerical ECMWF model comparisons have been performed (per the first method in the "validation hierarchy" referred to in Section III). Figures 11 and 12 correspondingly show the statistical profile errors for AVTP and AVMP, respectively. The results show the retrievals are comparable to the operational v1.5 (nominal-resolution CrIS) and generally meet JPSS Level 1 requirements.

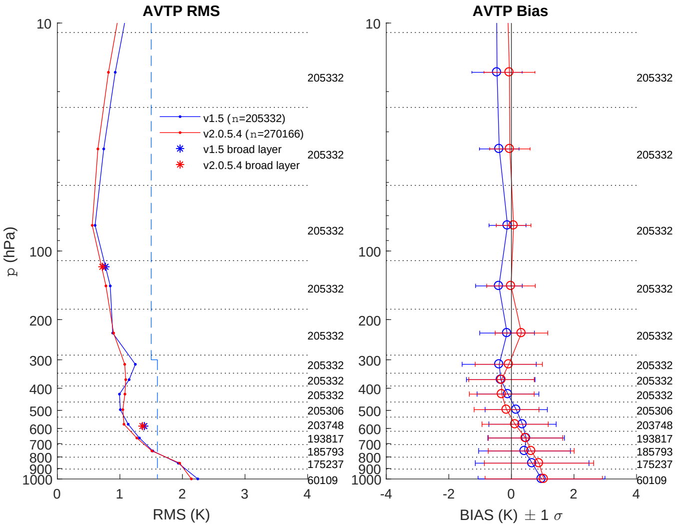

Fig. 11. As Figure 5 except statistical assessment of offline NUCAPS AVTP v2.0.5 (CrIS full-resolution, red lines) and v1.5 (CrIS nominal-resolution, blue lines) versus collocated ECMWF model output (analysis or forecast nearest in time) for retrievals accepted by the quality flag for a global Focus Day, 17 February 2015. Global yields for v2.0.5 and v1.5 accepted cases are 83.4% and 63.5%, respectively, indicating a marked improvement in the v2.0.5 acceptance rate.

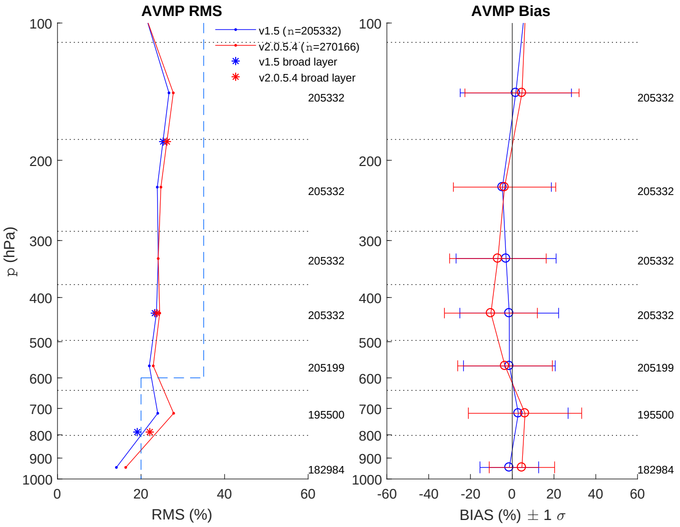

Fig. 12. As Figure 11 except for AVMP.

VI. Summary and Future Work

This work documents the formal validation of the SNPP NUCAPS temperature and moisture profile (AVTP and AVMP) EDRs based upon a globally representative sample of dedicated/reference RAOBs, where it has been shown that the NUCAPS EDRs meet JPSS Level 1 global performance requirements and have thus reached Validated Maturity. We note that the RAOB sites used in the analyses include those from three global zones (tropical, midlatitude and polar), as well as marine-based datasets obtained from ship over both the Pacific and Atlantic Oceans (i.e., AEROSE and CalWater/ACAPEX campaigns) under a range of very different thermodynamic meteorological conditions germane to users of sounder EDR (and SDR) products. The NUCAPS mid-tropospheric temperature and moisture show reasonable stability (seasonal variability of AVTP and AVMP biases roughly within 0.5 K and 10%, respectively, with no discernible interannual trends) over the SNPP lifetime, and the algorithm has been successfully implemented for future operational full-resolution CrIS data. The NUCAPS version for CrIS full-res data (v2.0.5) has undergone preliminary testing and is scheduled for operational delivery in July 2017. Validation of the operational SNPP NUCAPS IR ozone profile product will be the subject of a forthcoming companion paper.

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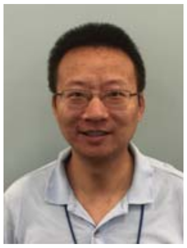
Dr. Barnet joined Science and Technology Corporation, Columbia, MD, USA in 2013 to support new applications for these advanced algorithms and now serves as the Joint Polar Satellite System (JPSS) Program Science subject matter expert for hyperspectral IR soundings. In 2014 he was also selected at the NASA Suomi National Polar-orbiting Partnership (SNPP) science team discipline lead for development of long-term datasets from the SNPP sounding instruments.



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