Validation of NOAA-Unique Operational Sounder Environmental Data Records (EDR)

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Intro: JPSS EDR Validation

- **Validation** is "the process of ascribing uncertainties to these radiances and retrieved quantities through comparison with correlative observations" (*Fetzer et al.,* 2003).
  - EDR validation provides implicit validation of SDRs
  - Includes validation of the cloud-cleared radiances (a Level 2 product shown to have positive impact on NWP; e.g., *Le Marshall et al.,* 2008)
  - EDR validation enables development/ improvement of algorithms
- **Users of sounder EDR observations** (AVTP, AVMP and trace gas) include
  - Weather Forecast Offices (AWIPS)
    - Nowcasting / severe weather
  - NOAA Data Centers (e.g., NGDC, CLASS)
  - Basic and applied science research/ investigation (e.g., *Pagano et al.,* 2013)

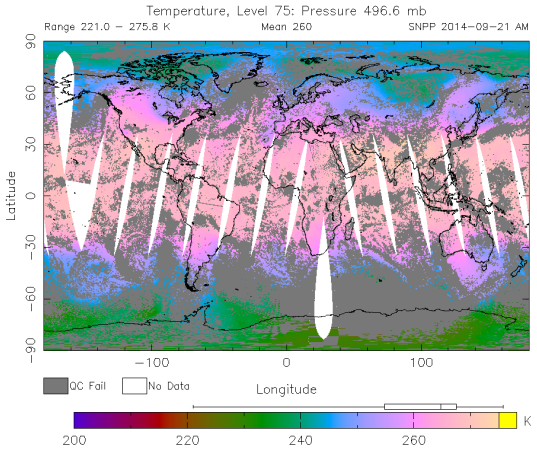
- **JPSS Cal/Val Phases**
  - Pre-Launch / Early Orbit Checkout (EOC)
  - **Intensive Cal/Val (ICV)**
    - Validation of EDRs against multiple correlative datasets
  - **Long-Term Monitoring (LTM)**
    - Characterization of all EDR products and long-term demonstration of performance
- In accordance with the JPSS phased schedule, the **SNPP CrIMSS EDR cal/val plan** was devised to ensure the EDR would meet the mission **Level 1 requirements** (*Barnet,* 2009)
- The **EDR validation methodology** draws upon previous work with AIRS and IASI (*Nalli et al.,* 2013, *JGR Special Section on SNPP Cal/ Val*)
  - Classification of various approaches into a "Validation Methodology Hierarchy"

CrIS/ATMS (CrIMSS) Sounder Operational EDR

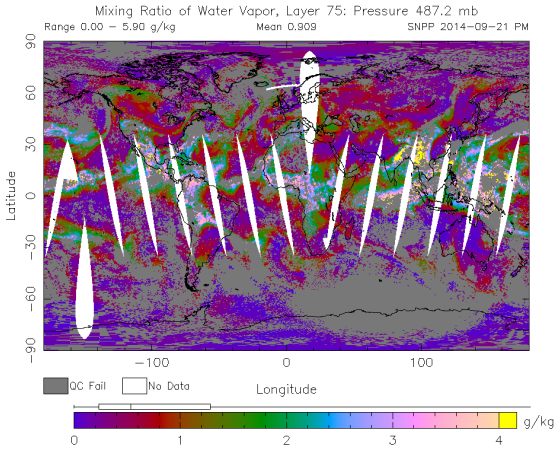
- **Original IDPS Algorithm**
  - Optimal Estimation (OE) algorithm originally developed by AER and NGAS
  - CrIMSS operational product (MX7.1) validated through Beta and Provisional Maturities (*Divakarla et al.,* 2014)

- **NOAA Unique CrIS/ATMS Processing System (NUCAPS) Algorithm** *(Gambacorta et al., Liu et al. talks)*
  - **Operational algorithm beginning Sep 2013**
    - Transition to NUCAPS validation ongoing over past year
    - **Stage-1 Validated Maturity achieved in Sep 2014**
  - Line-for-line modular implementation of the iterative, multistep AIRS Science Team retrieval algorithm
  - Non-precipitating conditions (cloudy, partly cloudy, clear)
  - AVTP, AVMP and trace gas profiles (O_3, CO, CO_2, CH_4)

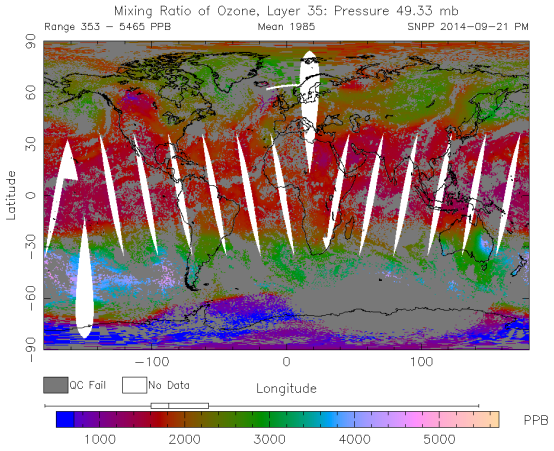
NUCAPS AVTP



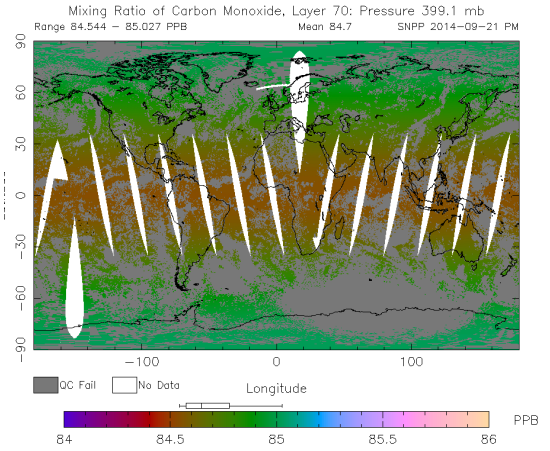
NUCAPS AVMP



NUCAPS O_3



NUCAPS CO



http://www.ospo.noaa.gov/Products/atmosphere/soundings/nucaps/index.html

CrIS/ATMS Sounder EDR L1 Requirements

AVTP and AVMP EDR

CrIS/ATMS Atmospheric Vertical Temperature Profile (AVTP) Measurement Uncertainty – Layer Average Temperature Error	
PARAMETER	**THRESHOLD**
AVTP, Cloud fraction < 50%, surface to 300 hPa	1.6 K / 1-km layer
AVTP, Cloud fraction < 50%, 300–30 hPa	1.5 K / 3-km layer
AVTP, Cloud fraction < 50%, 30–1 hPa	1.5 K / 5-km layer
AVTP, Cloud fraction < 50%, 1–0.5 hPa	3.5 K / 5-km layer
AVTP, Cloud fraction ≥ 50%, surface to 700 hPa	2.5 K / 1-km layer
AVTP, Cloud fraction ≥ 50%, 700–300 hPa	1.5 K / 1-km layer
AVTP, Cloud fraction ≥ 50%, 300–30 hPa	1.5 K / 3-km layer
AVTP, Cloud fraction ≥ 50%, 30–1 hPa	1.5 K / 5-km layer
AVTP, Cloud fraction ≥ 50%, 1–0.5 hPa	3.5 K/ 5-km layer

CrIS/ATMS Atmospheric Vertical Moisture Profile (AVMP) Measurement Uncertainty – 2-km Layer Average Mixing Ratio % Error	
PARAMETER	**THRESHOLD**
AVMP, Cloud fraction < 50%, surface to 600 hPa	Greater of 20% or 0.2 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction < 50%, 600–300 hPa	Greater of 35% or 0.1 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction < 50%, 300–100 hPa	Greater of 35% or 0.1 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction ≥ 50%, surface to 600 hPa	Greater of 20% of 0.2 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction ≥ 50%, 600–400 hPa	Greater of 40% or 0.1 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction ≥ 50%, 400–100 hPa	Greater of 40% or 0.1 $g \cdot kg^{-1}$ / 2-km layer

Source: L1RD (2014), pp. 41, 43

Trace Gas EDR

CrIS Infrared Trace Gases Specification Performance Requirements	
PARAMETER	**THRESHOLD**
CO (Carbon Monoxide) Total Column Precision	35%, or full res mode 15%
CO (Carbon Monoxide) Total Column Accuracy	±25%, or full res mode ±5%
CO_2 (Carbon Dioxide Total Column Precision	0.5% (2 ppmv)
CO_2 (Carbon Dioxide) Total Column Accuracy	±1% (4 ppmv)
CH_4 (Methane) Total Column Precision	1% (≈20 ppbv)
CH_4 (Methane) Total Column Accuracy	±4% (≈80 ppmv)
O_3 (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)	20%
O_3 (Ozone) Profile Precision, 260 hPa to sfc (1 statistic layer)	20%
O_3 (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)	±10%
O_3 (Ozone) Profile Accuracy, 260 hPa to sfc (1 statistic layer)	±10%
O_3 (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)	25%
O_3 (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)	25%

Source: L1RD (2014), pp. 45-49

Global requirements defined for lower and upper atmosphere subdivided into 1-km and 2-km layers for AVTP and AVMP, respectively.

Validation of NOAA-Unique Operational Sounder EDR

VALIDATION METHODOLOGY

Validation Methodology Hierarchy

(e.g., *Nalli et al.,* 2013)

1. Numerical Model (e.g., ECMWF, NCEP/GFS) Global *Comparisons*

- Large, truly global samples acquired from Focus Days
- Useful for early sanity checks, bias tuning and regression
- However, not independent truth data

2. Satellite EDR (e.g., AIRS, ATOVS, COSMIC) *Intercomparisons*

- Global samples acquired from Focus Days (e.g., AIRS)
- Consistency checks; merits of different retrieval algorithms
- However, IR sounders have similar error characteristics; must take rigorous account of averaging kernels of both systems (e.g., *Rodgers and Connor,* 2003)

3. Conventional RAOB Matchup *Assessments*

- WMO/GTS operational sondes launched ~2/day for NWP
- Useful for representation of global zones and long-term monitoring
- Large statistical samples acquired after a couple months' accumulation (e.g., *Divakarla et al.,* 2006)
- NOAA Products Validation System (NPROVS) (*Reale et al.,* 2012)
- Limitations:
  - Skewed distribution toward NH-continental sites
  - Mismatch errors, potentially systematic at individual sites
  - Non-uniform, less-accurate and poorly characterized radiosondes
  - RAOBs assimilated , by definition, into numerical models

4. Dedicated/Reference RAOB Matchup *Assessments*

- *Dedicated* for the purpose of satellite validation
  - Well-specified error characteristics and optimal accuracy
  - Minimal mismatch errors
  - Include atmospheric state "best estimates" or "merged soundings"
- Reference sondes: CFH, corrected RS92
  - Traceable measurement
- Detailed performance specification and regional characterization
- Limitation: Small sample sizes and geographic coverage
- E.g., **ARM sites** (e.g., *Tobin et al.,* 2006), AEROSE, ideally GRUAN

5. Intensive Field Campaign *Dissections*

- Include dedicated RAOBs, especially those *not* assimilated into NWP models
- Include ancillary datasets (e.g., ozonesondes, lidar, M-AERI, MWR, sunphotometer, etc.)
- Ideally include funded aircraft campaign using IR sounder (e.g., NAST-I, S-HIS)
- Detailed performance specification; state specification; SDR cal/val; EDR "dissections"
- E.g., **AEROSE**, **CalWater2**, JAIVEX, WAVES, AWEX-G, EAQUATE

Assessment Methodology: Reducing Truth to Correlative Layers

- The **measurement equation** (e.g., *Taylor and Kuyatt,* 1994) for retrieval includes forward and inverse operators (*Rodgers*, 1990) to estimate the measurand, $\mathbf{x}$, on forward model layers:

$$\hat{\mathbf{x}} = I[F(\mathbf{x},\mathbf{b}),\mathbf{b},\mathbf{c}]$$

- **Rigorous validation** therefore requires high-resolution truth measurements (e.g., dedicated RAOB) be **reduced to correlative RTA layers** (*Nalli et al.,* 2013, *JGR Special Section on SNPP Cal/Val*)
- **Radiative transfer approach** is to integrate quantities over the atmospheric path (e.g., number densities → column abundances), interpolate to RTA (arbitrary) levels, then compute RTA layer quantities, e.g.,

$$\sum_x(z) = \int_{z_t}^{z} N_x(z')\,dz'$$

Assessment Methodology: Statistical Metrics

- Level 1 AVTP and AVMP accuracy requirements are defined over **coarse layers**, roughly 1–5 km for tropospheric AVTP and 2 km for AVMP (Table, Slide 5).

AVTP

$$\mathrm{RMS}(\Delta T_{\mathfrak{L}}) = \sqrt{\frac{1}{n_j}\sum_{j=1}^{n_j}(\Delta T_{\mathfrak{L},j})^2} \qquad \mathrm{BIAS}(\Delta T_{\mathfrak{L}}) \equiv \overline{\Delta T}_{\mathfrak{L}} = \frac{1}{n_j}\sum_{j=1}^{n_j}\Delta T_{\mathfrak{L},j}$$

$$\mathrm{STD}(\Delta T_{\mathfrak{L}}) \equiv \sigma(\Delta T_{\mathfrak{L}}) = \sqrt{[\mathrm{RMS}(\Delta T_{\mathfrak{L}})]^2 - [\mathrm{BIAS}(\Delta T_{\mathfrak{L}})]^2}$$

AVMP and O_3

- W2 weighting was used in determining Level 1 Requirements
- To allow compatible STD calculation, W2 weighting should be consistently used for both RMS and BIAS

$$\Delta q_{\mathfrak{L},j} \equiv \frac{\hat{q}_{\mathfrak{L},j} - q_{\mathfrak{L},j}}{q_{\mathfrak{L},j}} \qquad \mathrm{RMS}(\Delta q_{\mathfrak{L}}) = \sqrt{\frac{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}(\Delta q_{\mathfrak{L},j})^2}{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}}},$$

water vapor weighting factor, $W_{\mathfrak{L},j}$,

$$\mathrm{BIAS}(\Delta q_{\mathfrak{L}}) = \frac{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}\,\Delta q_{\mathfrak{L},j}}{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}}, \qquad W_{\mathfrak{L},j} = \begin{cases} 1 & , \mathrm{W}^0 \\ q_{\mathfrak{L},j} & , \mathrm{W}^1 \\ (q_{\mathfrak{L},j})^2 & , \mathrm{W}^2 \end{cases}$$

$$\mathrm{STD}(\Delta q_{\mathfrak{L}}) = \sqrt{[\mathrm{RMS}(\Delta q_{\mathfrak{L}})]^2 - [\mathrm{BIAS}(\Delta q_{\mathfrak{L}})]^2}$$

Assessment Methodology: Use of Averaging Kernels (AKs)

- **AKs** define the **vertical sensitivity** of the sounder measurement system

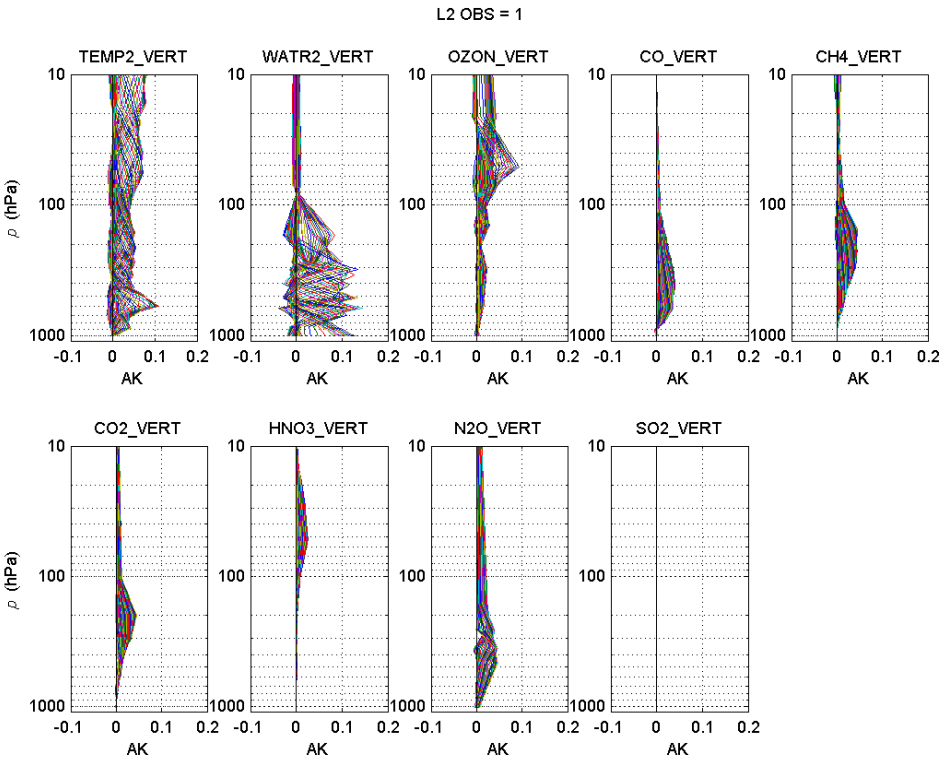
$$\mathbf{A} \equiv \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}}$$

- Facilitates intercomparisons of profiles obtained by two different observing systems

- Retrieval AKs can be used to "smooth" correlative truth (RAOBs reduced to RTA layers), thereby **removing null-space errors** otherwise present

$$\mathbf{x}_s = \mathbf{A}(\mathbf{x} - \mathbf{x}_0) + \mathbf{x}_0$$

NOAA-Unique IASI Averaging Kernels

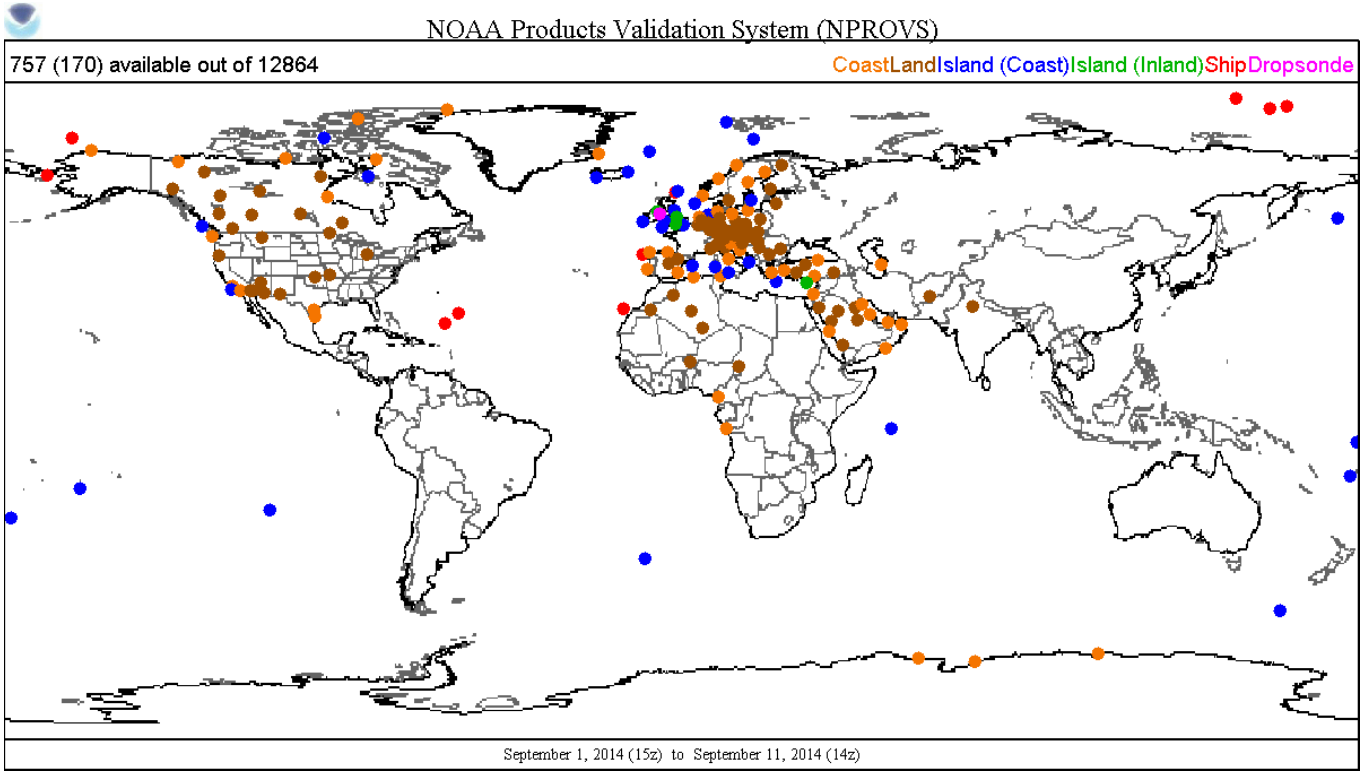


Validation of NOAA-Unique Operational Sounder EDR

NUCAPS VALIDATION STATUS

NPROVS Conventional RAOB Collocations

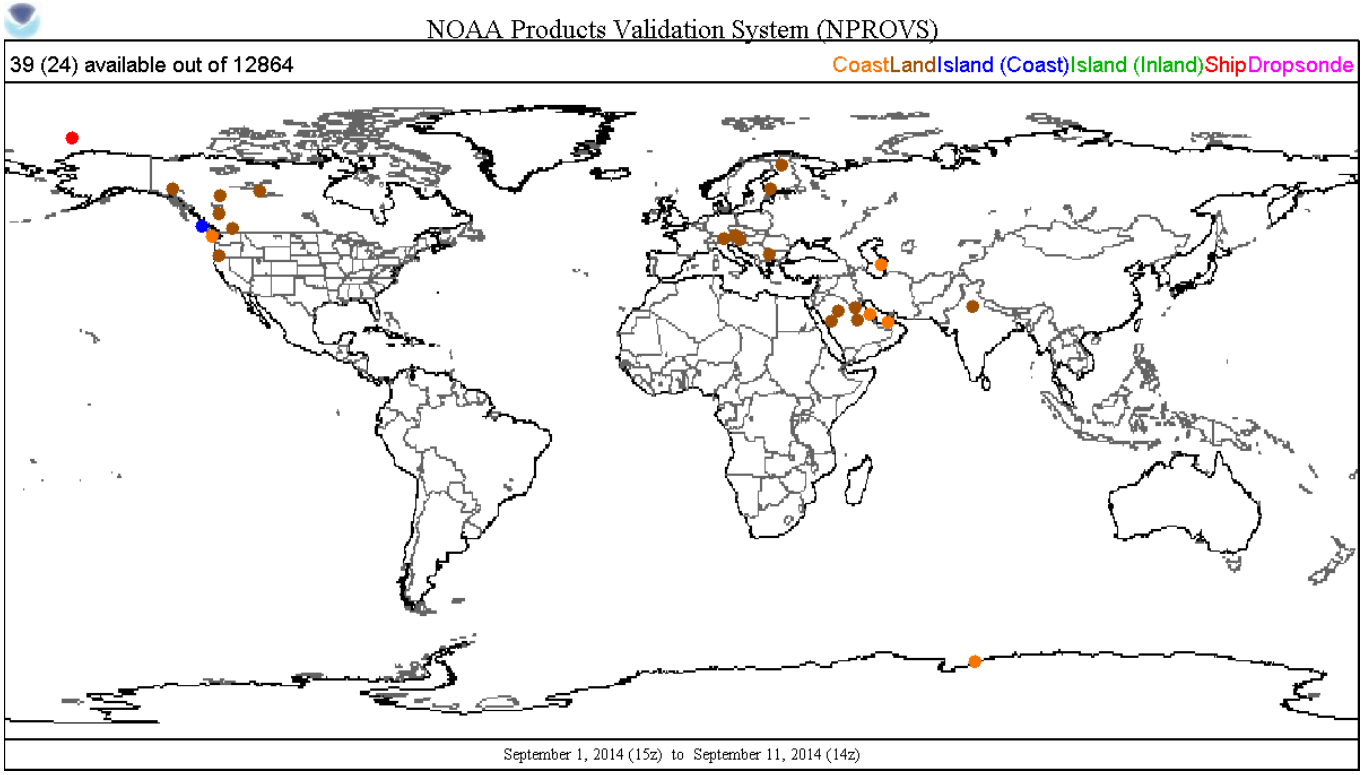
Single Closest FOR (*Reale et al.*, 2012)



- 1–11 Sep 2014
- **RS92 and RS41 sondes**
- Single-closest FOR
- **Space-time window 1**
  - **±3 h before/ after overpass**
  - **75 km**
- **Sample size 1**
  ***N* = 757**

NPROVS Conventional RAOB Collocations

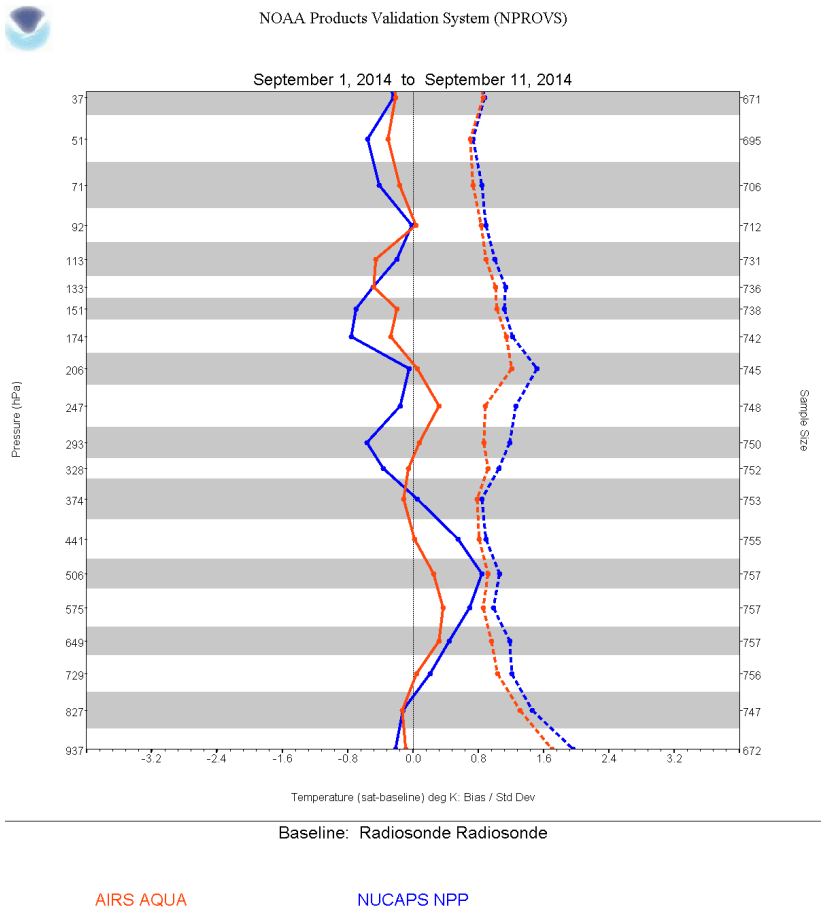
Single Closest FOR (*Reale et al.*, 2012)



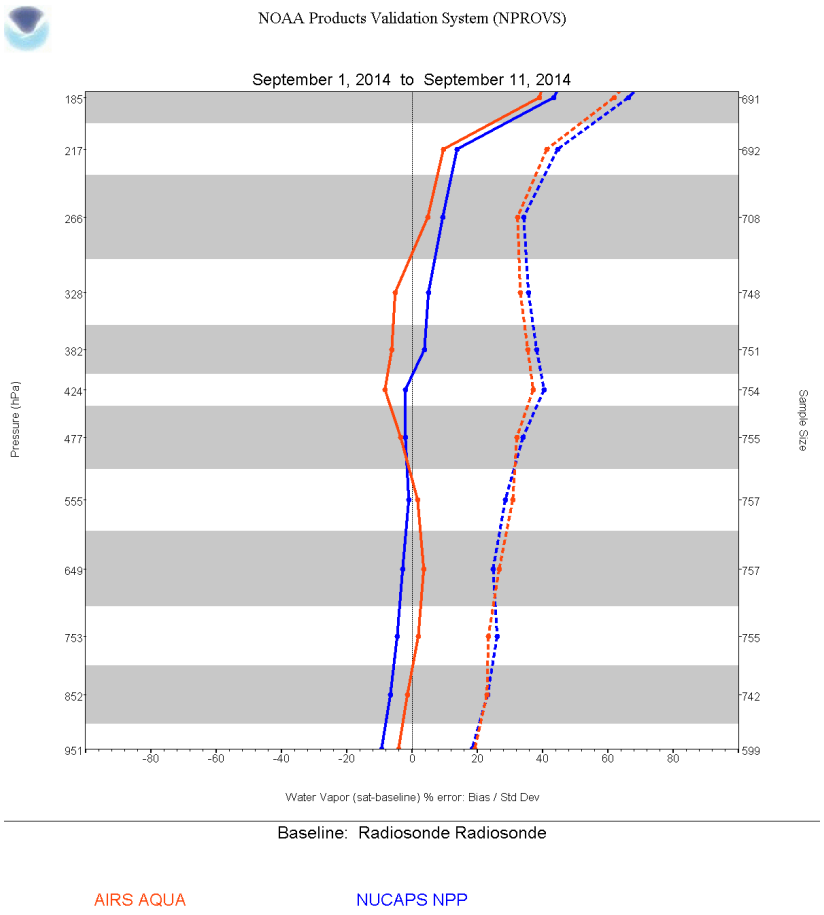
- 1–11 Sep 2014
- **RS92 and RS41 sondes**
- Single-closest FOR
- **Space-time window 2**
  - **–1–0 h before overpass**
  - **75 km**
- **Sample size 2**
  N = 39

NDE-OPS NUCAPS and AIRS versus NPROVS Collocated Conventional RAOB: Sample 1

AVTP (BIAS and RMS)

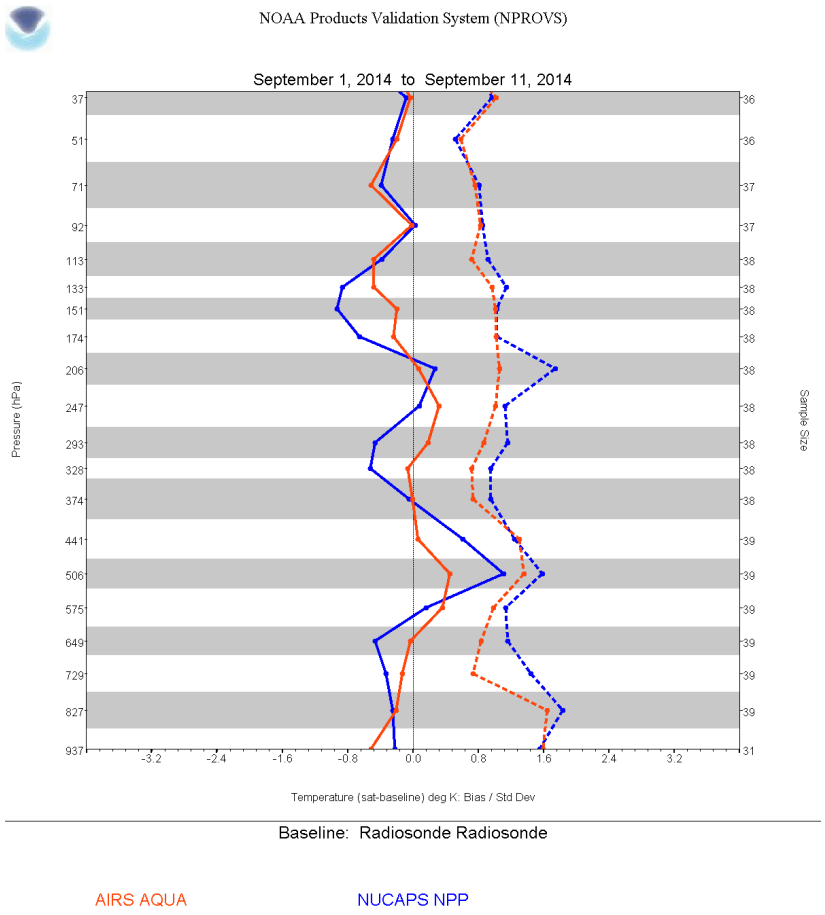


AVMP (BIAS and RMS)

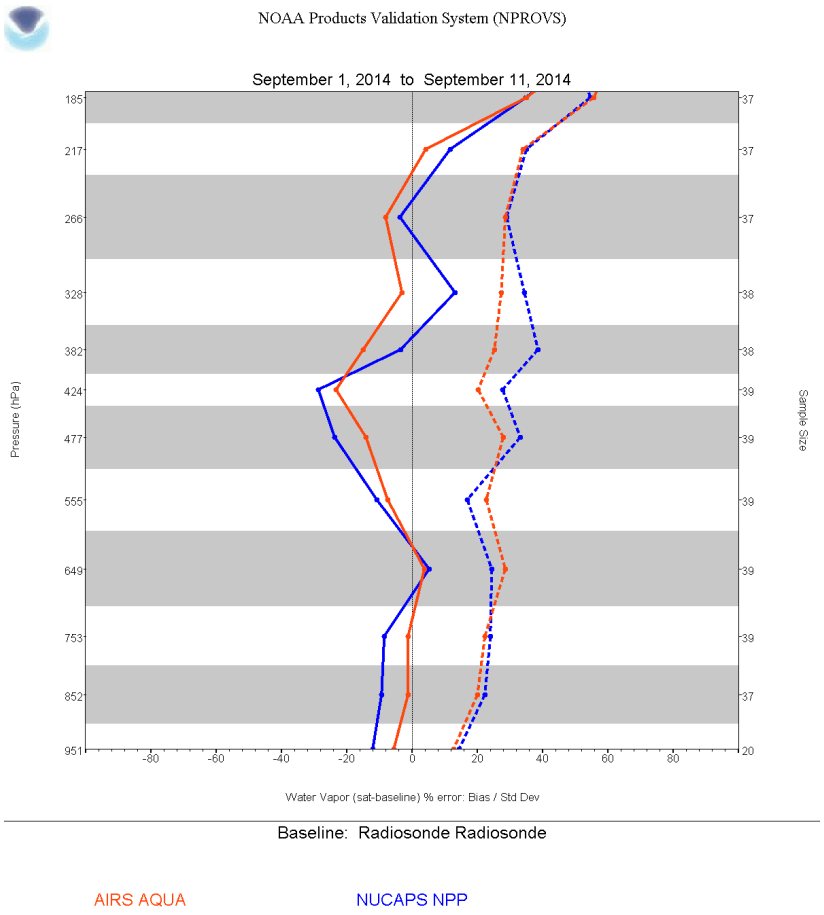


NDE-OPS NUCAPS and AIRS versus NPROVS Collocated Conventional RAOB: Sample 2

AVTP (BIAS and RMS)



AVMP (BIAS and RMS)

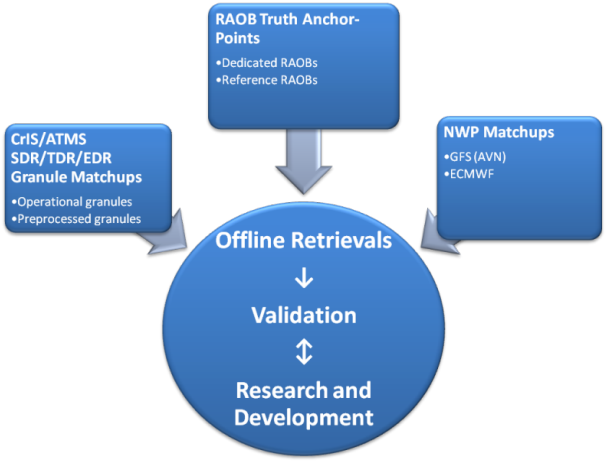


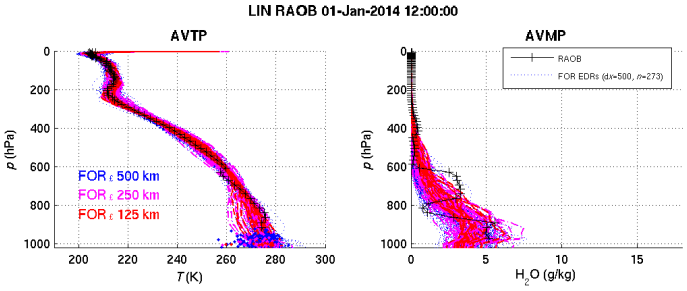
Validation Archive (VALAR) Dedicated/Reference RAOB

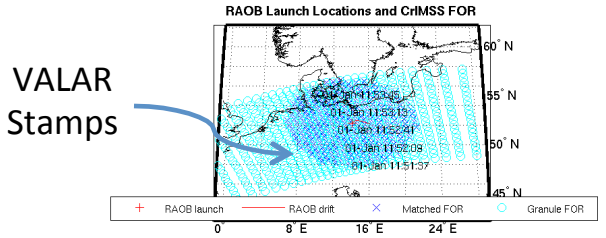
Granule "Stamp" Collocations

- A **Validation Archive (VALAR)** has been designed for satellite sounder validation, research and development (viz., CrIS/ATMS, IASI), intended to serve as a go-to archive for the life of the SNPP mission
- **VALAR data consist of:**
  - **High-quality RAOB Anchor Points** (dedicated and reference sondes)
    - Reduced 100 RTA layers (i.e., **correlative truth**)
    - GRUAN Reference RAOB matchups acquired via **NPROVS+**
  - **CrIS/ATMS SDR/TDR/EDR Granule "Stamps"**
    - A **VALAR "stamp"** is roughly defined as a granule file matched with a RAOB anchor point (the **minimal ingredients** needed for **offline retrievals** and validation)
    - SDR/TDR/EDR stamps consist of 4-scan line granules within ±1 minute of overpass (≈500 km radius, usually 4-5 granules centered on RAOB)

VALAR Concept and Objectives



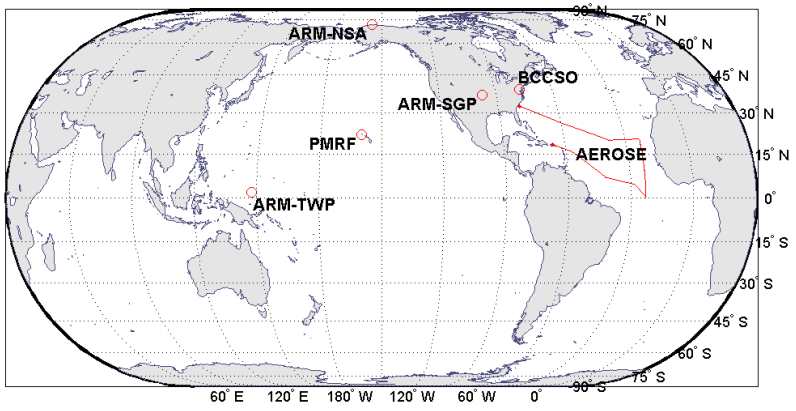




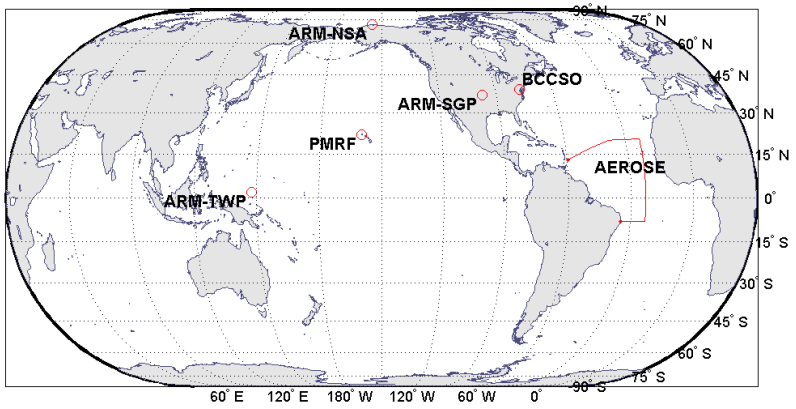
VALAR Dedicated and Reference RAOBs

JPSS S-NPP Dedicated

S-NPP CrIMSS EDR ICV Dedicated RAOB Sites (Year 1)

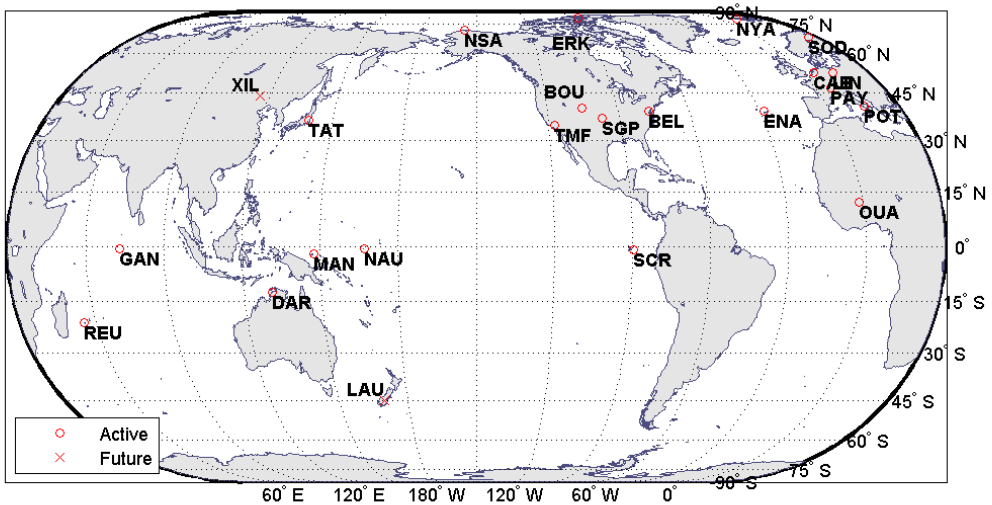


S-NPP CrIMSS EDR ICV Dedicated RAOB Sites (Year 2)



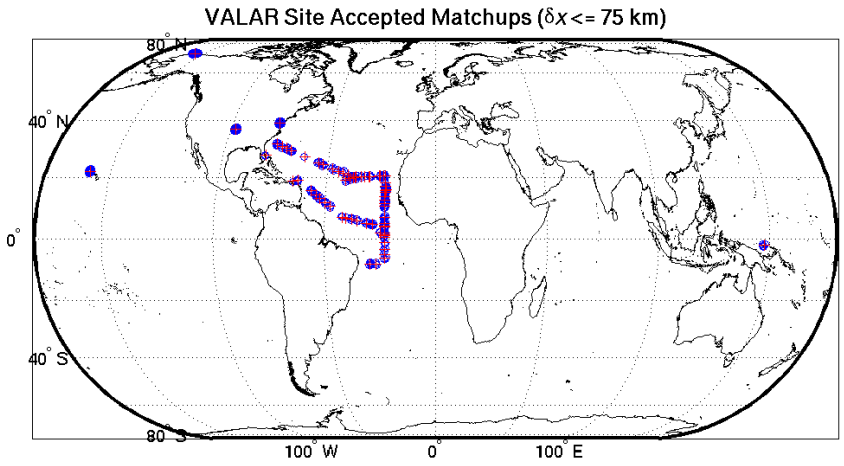
GRUAN Reference Sites (NPROVS+ Collocation)

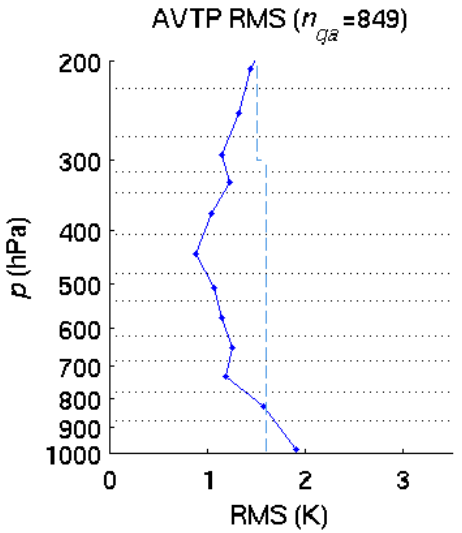
GRUAN RAOB Sites for Sounder EDR ICV

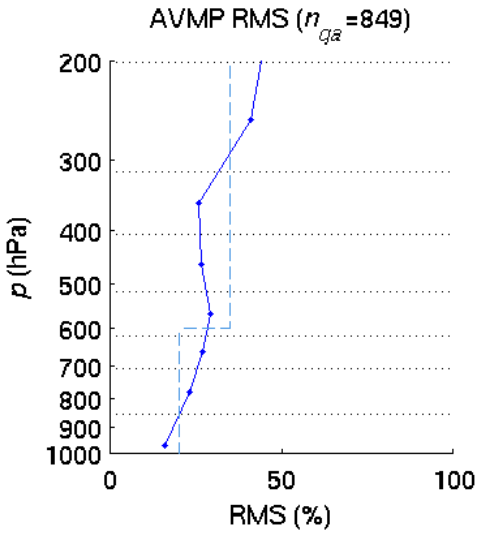


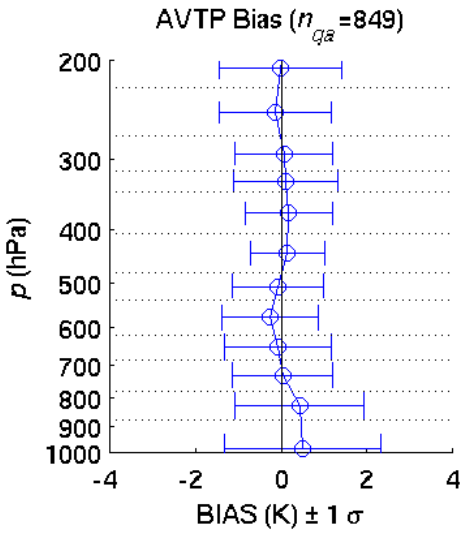
Offline NUCAPS IR+MW AVTP/AVMP versus VALAR Dedicated RAOB Stage-1 Validated Maturity Highlight

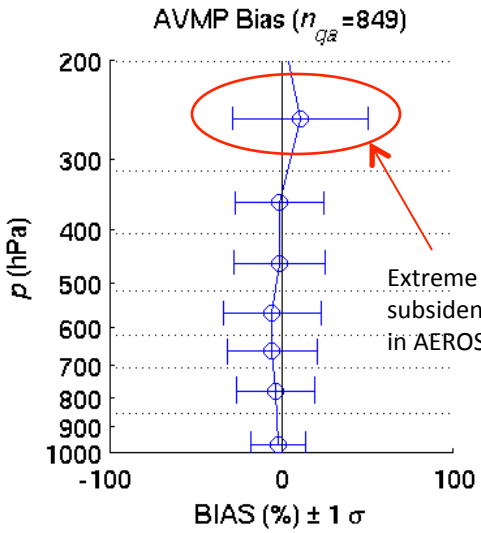
Year-1 ARM, PMRF, BCCSO
Year-1 and -2 GRUAN-Corrected AEROSE





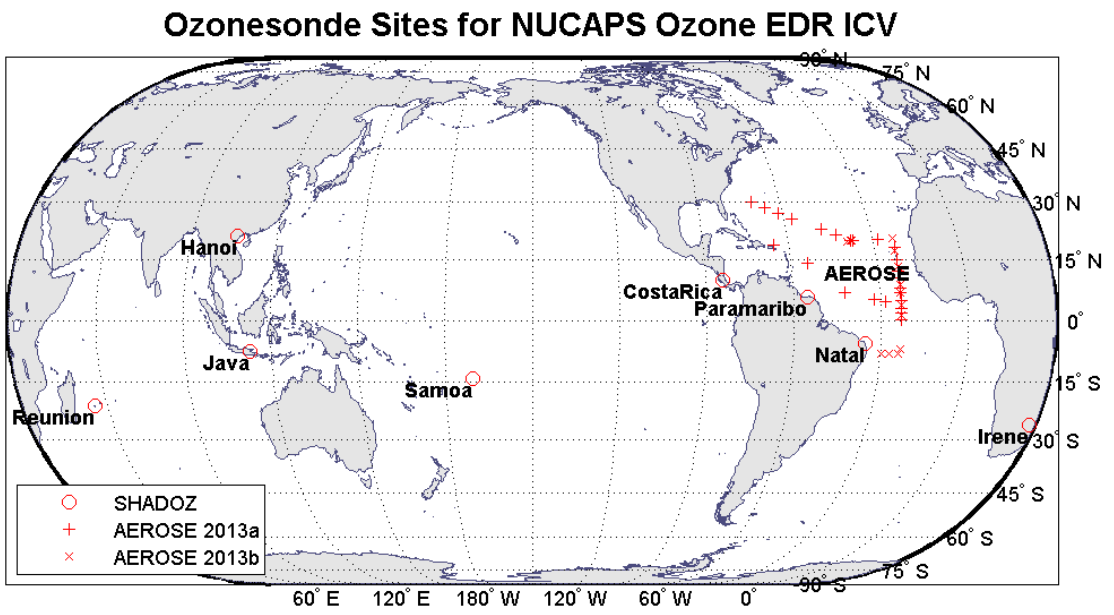






Future Work: VALAR Trace Gas Validation

- **Validation of NUCAPS Trace Gases** will be performed against **available *in situ* truth datasets:**
  - **Collocated ozonesondes** for **O_3 (ozone) profile EDR**
    - **SHADOZ sites**
    - **AEROSE** and **CalWater2** dedicated ozonesondes
  - **Collocated aircraft** data for **CO, CO_2, O_3**
    - **MOZAIC**
    - Additional sites currently being acquired
- **Comparisons of NUCAPS CO and O_3** can also be performed against models (e.g., WRF-CHEM Model , *Smith and Nalli,* 2014) (i.e., Step 1 of Validation Hierarchy)



Future Work

Acknowledgments

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