NUCAPS Operational Product Validation

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Outline

- **Introduction and Background**
  - Importance of Validating Sounder EDRs
  - CrIS/ATMS (CrIMSS) Sounder EDR Validation
  - CrIS/ATMS EDR L1 Requirements
  - Validation Methodology Overview
    - Validation Hierarchy
    - Assessment Methodology
- **Validation Archive (VALAR)**
  - VALAR Concept and Objectives
  - VALAR Data
- **NUCAPS Validation Highlight**
  - AVTP and AVMP (Stage-1 Highlight)
  - Ozone Profile (Preliminary)
- **Future Work**

The Importance of Validating Sounder EDRs

- **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
- EDR validation enables development/improvement of algorithms
- 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)
- 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)

CrIS/ATMS (CrIMSS) Sounder EDR Validation

- **CrIMSS Operational EDR Algorithms**
  - **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)
    - Superseded by NUCAPS as operational algorithm in Sep 2013
    - Transition to NUCAPS validation ongoing over past year
  - **NOAA Unique CrIS/ATMS Processing System (NUCAPS)**
    - 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)
    - Operational algorithm starting Sep 2013
    - **Stage-1 Validated Maturity achieved in Sep 2014**

- **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*)

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

Validation Methodology Hierarchy – Overview

1. **Numerical Model (e.g., ECMWF, NCEP/GFS) Global *Comparisons***
   - Large, 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 (viz., NPROVS) *Assessments***
   - Conventional 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
   - Limitations:
     - Skewed distribution toward NH-continental sites
     - Significant mismatch errors, potentially systematic at individual sites
     - Non-uniform, less-accurate and poorly characterized radiosonde types used in data sample

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, Vaisala RR01 under development
     - 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 aircraft IR sounder (e.g., NAST-I, S-HIS) underflights
   - Detailed performance specification; state specification; SDR cal/val; EDR "dissections"
   - E.g., **AEROSE**, J**CalWater2**, AIVEX, WAVES, AWEX-G, EAQUATE,

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.

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

$$\mathrm{RMS}(\Delta q_{\mathfrak{L}}) = \sqrt{\frac{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}(\Delta q_{\mathfrak{L},j})^2}{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}}}, \qquad \text{water vapor weighting factor, } W_{\mathfrak{L},j},$$

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

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

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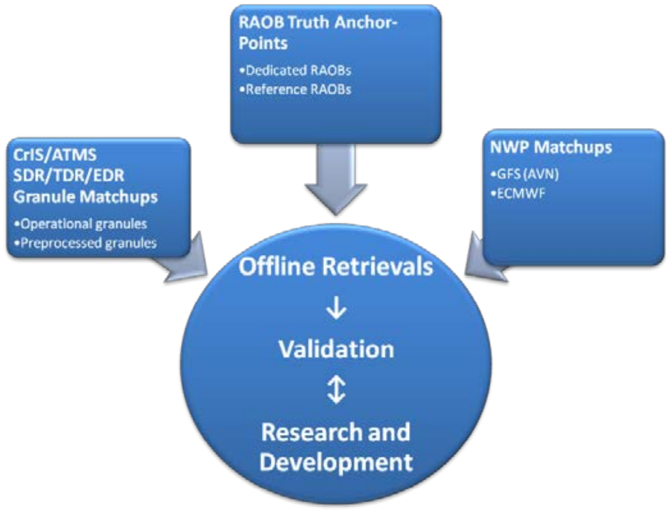
VALIDATION ARCHIVE (VALAR)

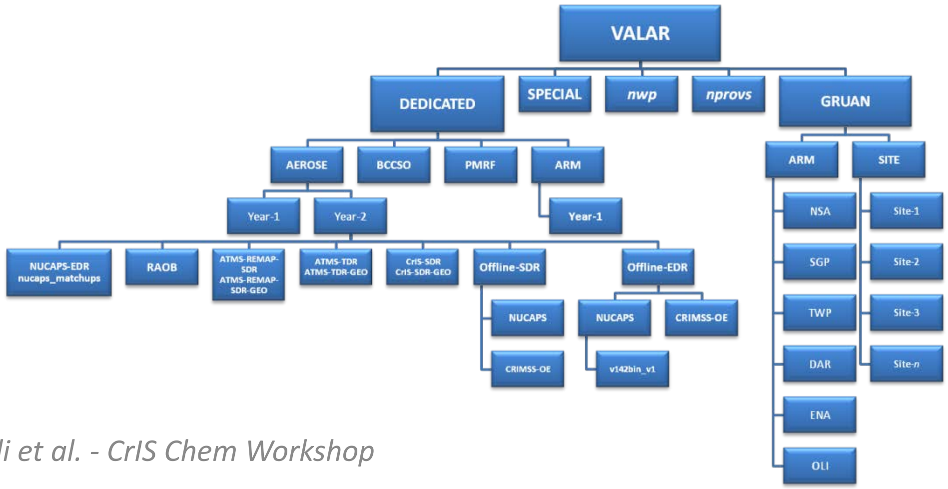
Validation Archive (VALAR) Concept

- A **Validation Archive (VALAR)** has been designed for satellite sounder validation, research and development (viz., CrIS/ATMS, IASI)
- **VALAR** is intended to serve as a go-to archive for the life of the SNPP mission to **directly support validation and development**

VALAR Concept and Objectives



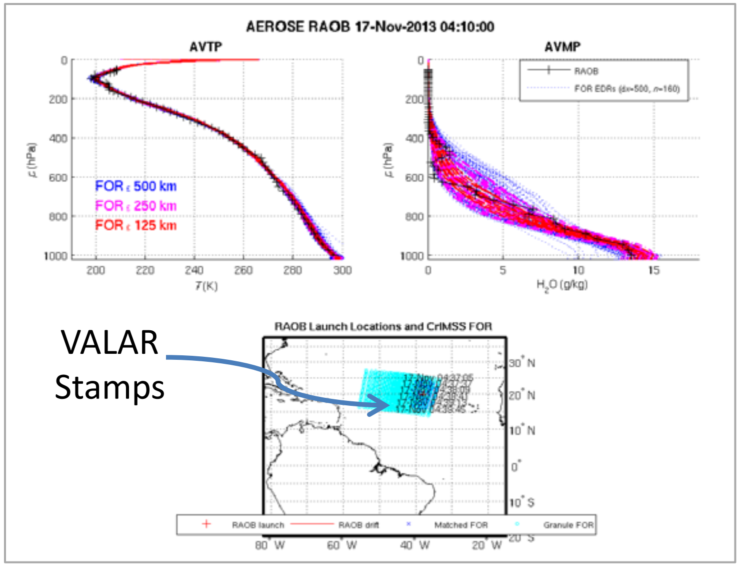
VALAR Data Organization

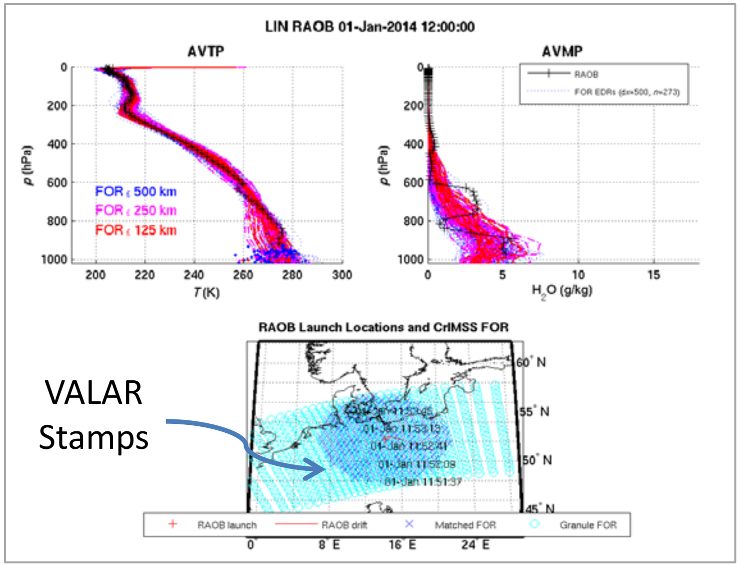


VALAR Data

- **High-quality RAOB Anchor Points** (dedicated and reference sondes)
  - Original native files "untouched" at full resolution
  - Reduced 100 RTA layers (i.e., **correlative truth**)

- **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)

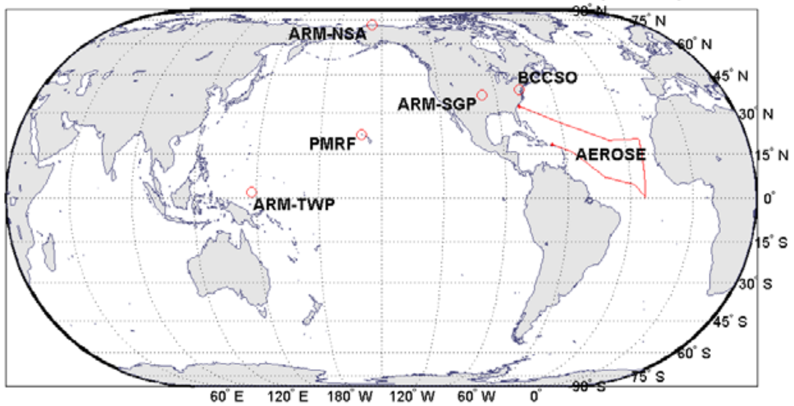




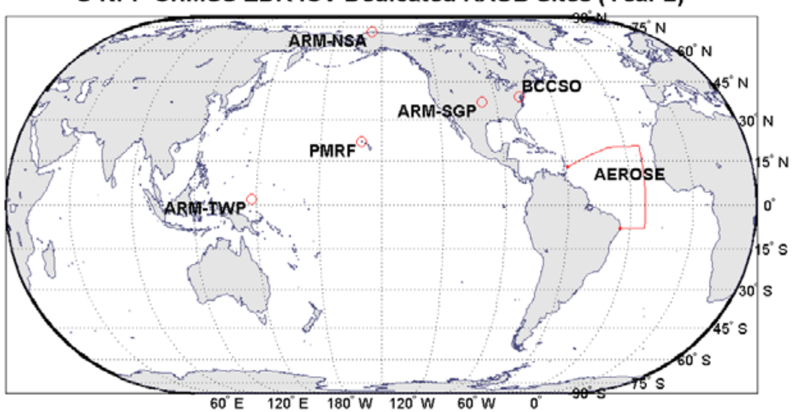
VALAR Dedicated and Reference RAOBs

JPSS S-NPP Dedicated

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

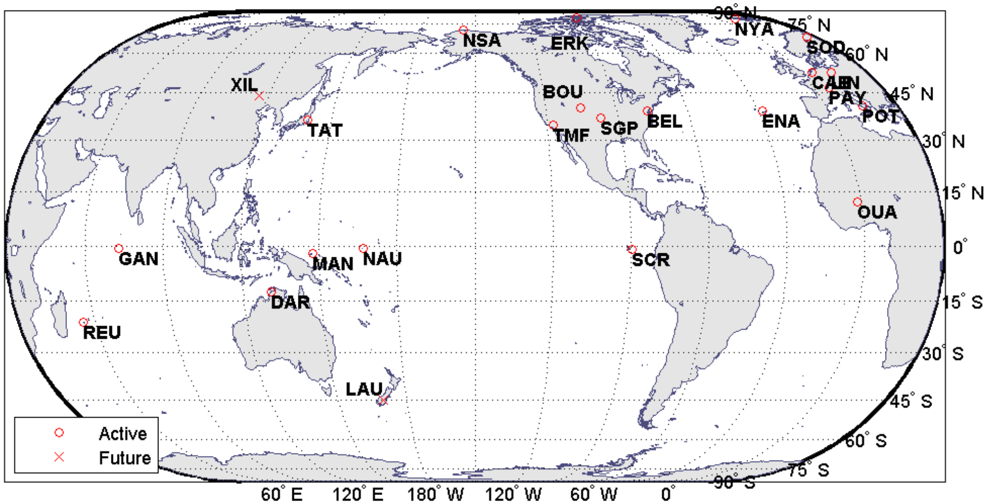


S-NPP CrIMSS EDR ICV Dedicated RAOB Sites (Year 2)



GRUAN Reference Sites (NPROVS+ Collocation)

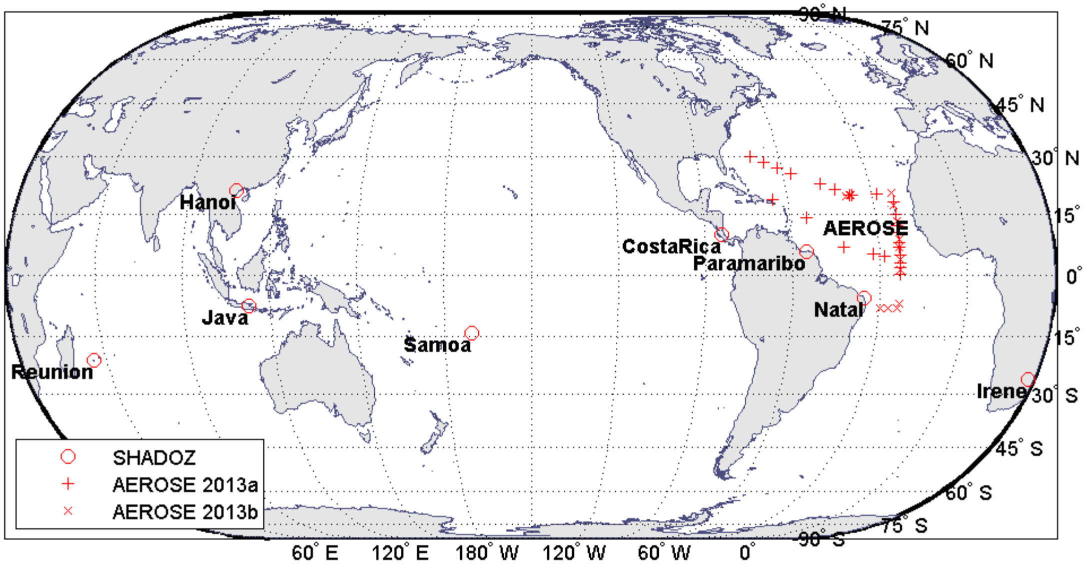
GRUAN RAOB Sites for Sounder EDR ICV



VALAR Trace Gas Truth Datasets

- **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**
- **Comparisons of NUCAPS CO and O_3** can also be performed against **WRF-CHEM Model** (e.g., *Smith and Nalli,* 2014) (i.e., Step 1 of Validation Hierarchy)

Ozonesonde Sites for NUCAPS Ozone EDR ICV



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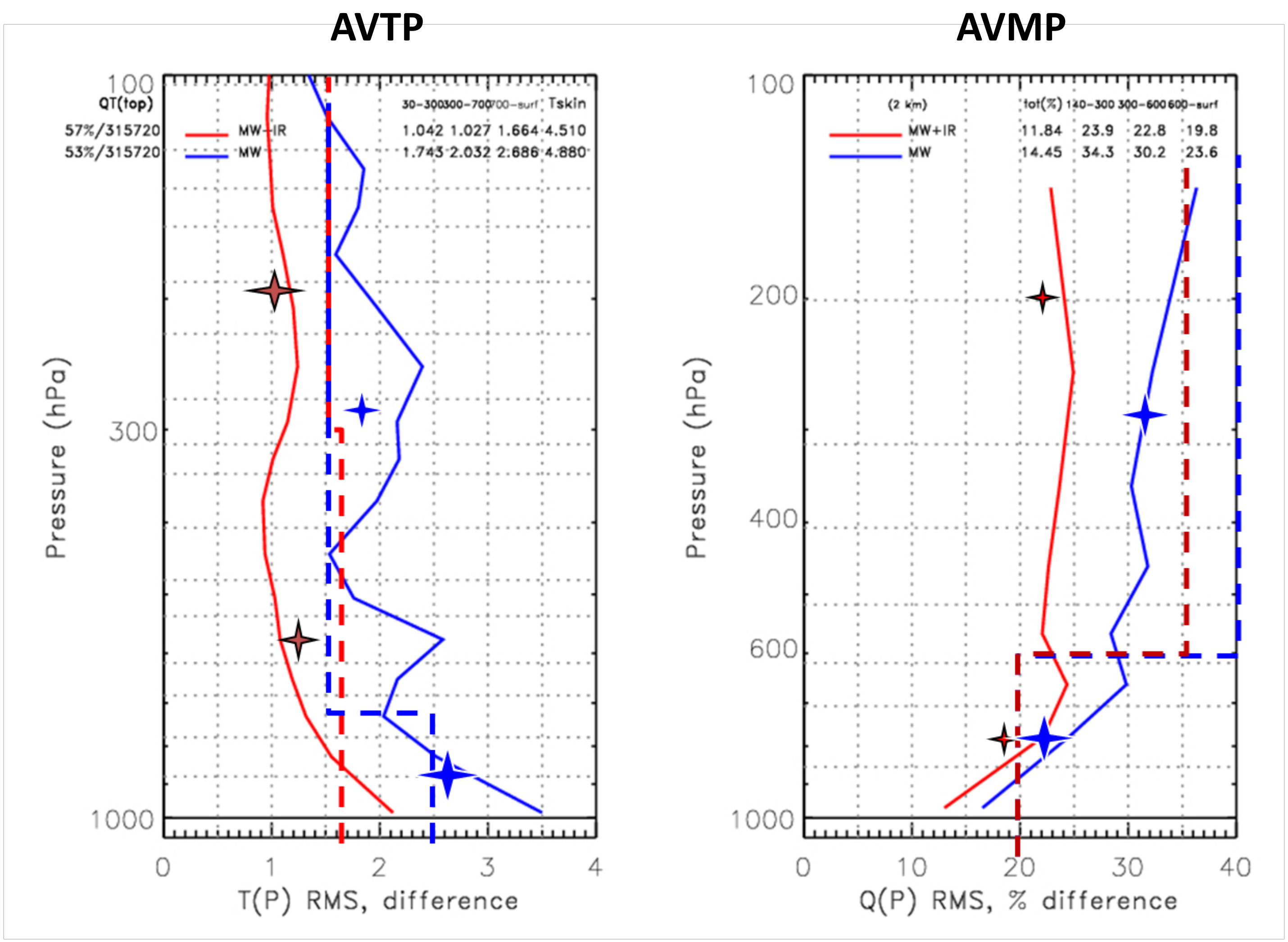
NUCAPS VALIDATION HIGHLIGHT

NUCAPS AVTP/AVMP versus Global ECMWF Analysis

Focus Day 15 May 2012, Land+Ocean

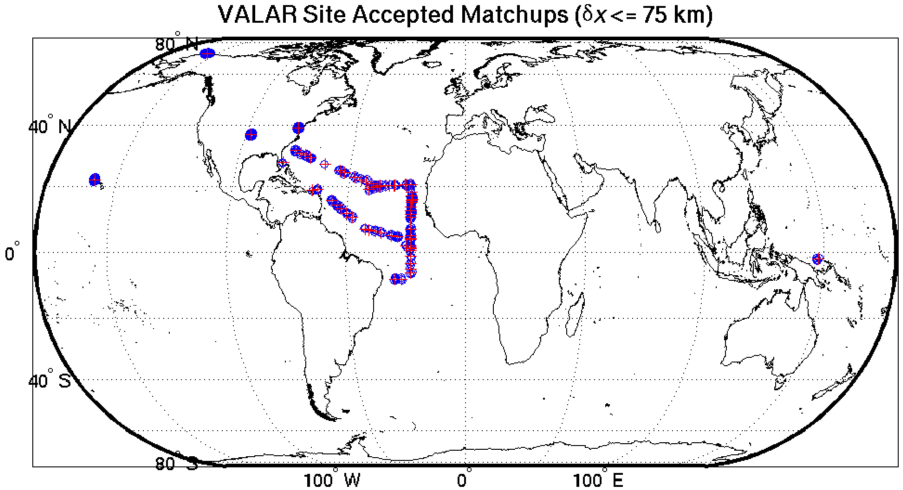
Stage-1 Validated Maturity Highlight

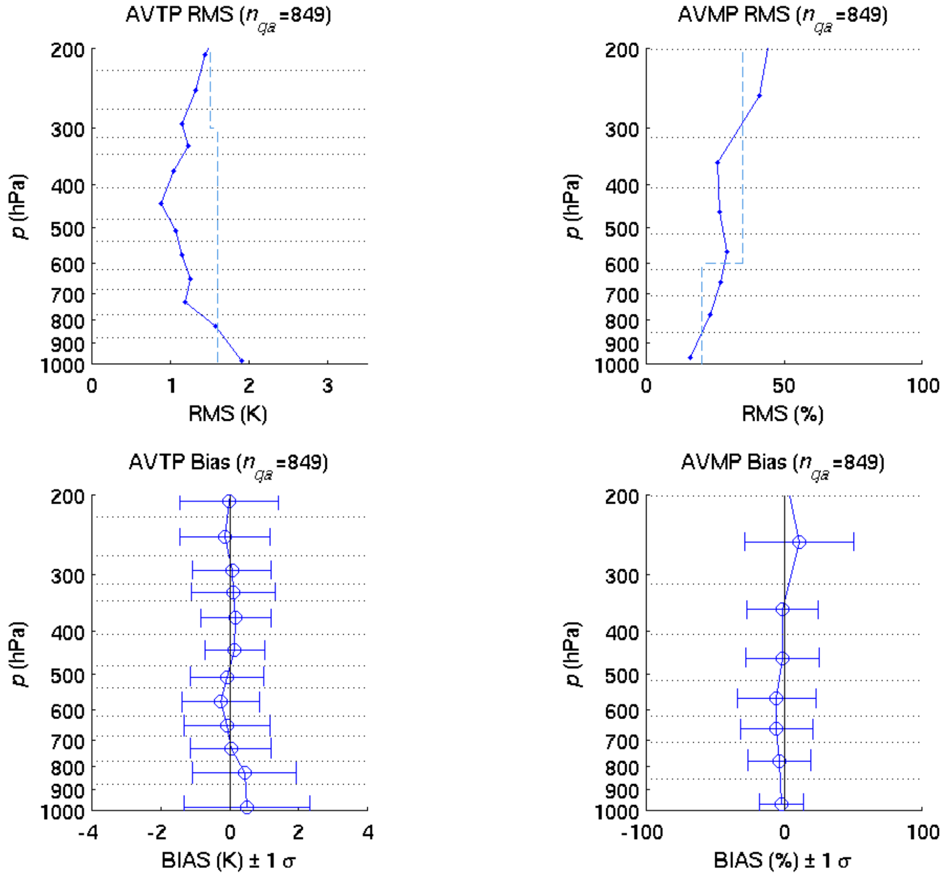


Red = MW+IR (Partly Cloudy)

Blue = MW Only (Cloudy)

NUCAPS AVTP/AVMP versus VALAR Dedicated RAOBs
Stage-1 Validated Maturity Highlight

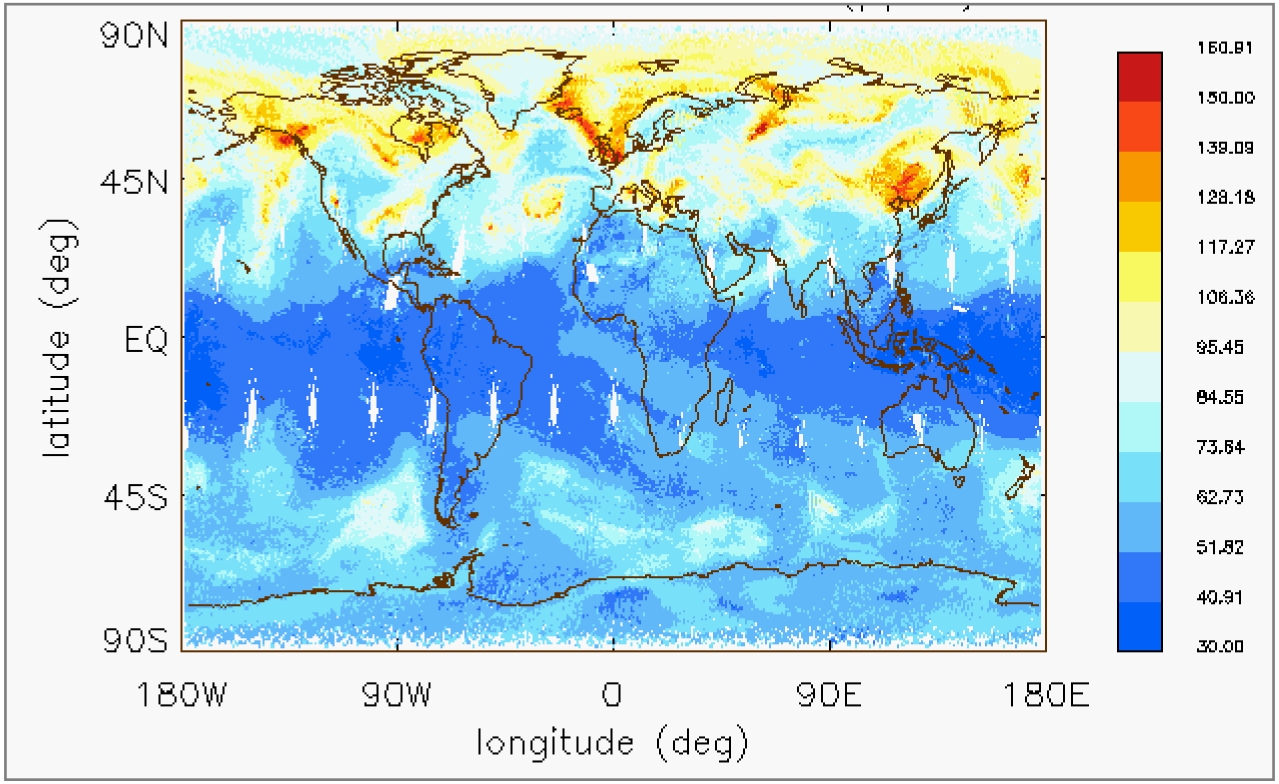




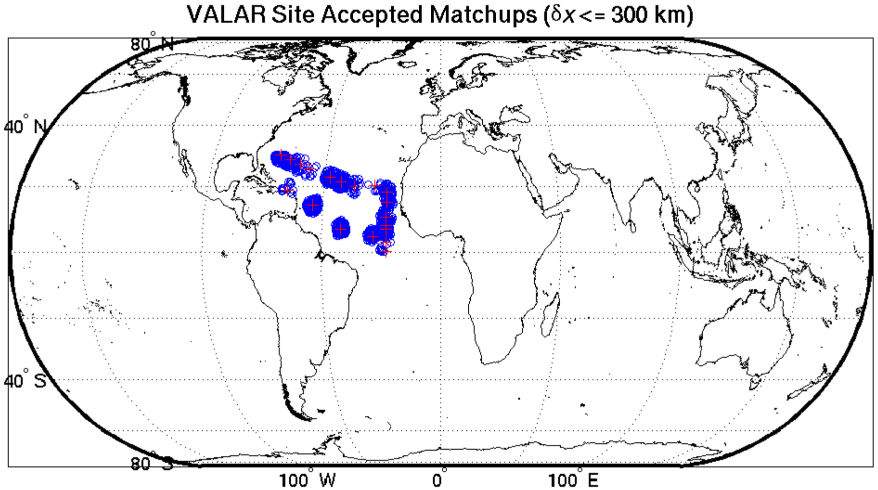
Preliminary Ozone Validation

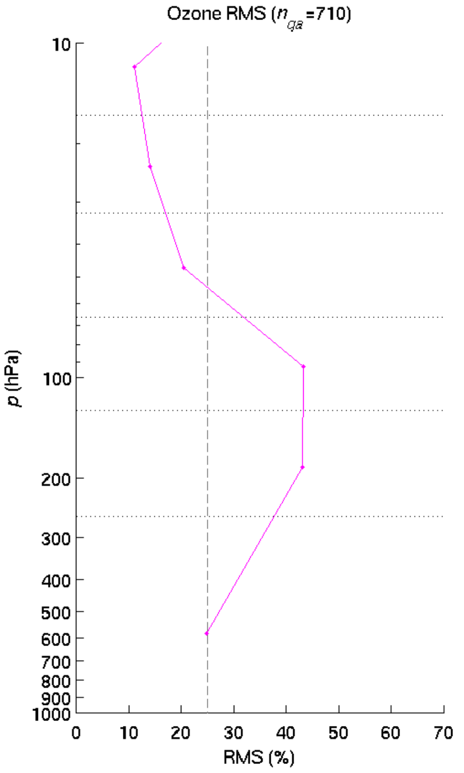
NUCAPS Ozone retrieval 450 hPa

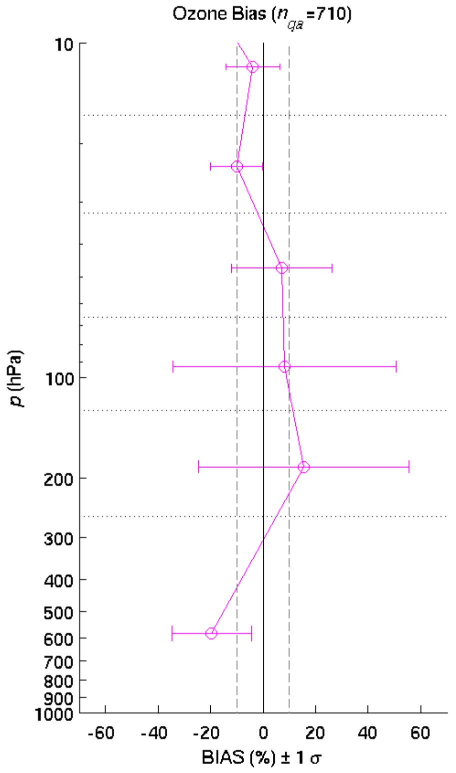
15 May 2012 Focus Day



NUCAPS Ozone First Guess – VALAR AEROSE Year-1 Dedicated Ozonesondes







Future Work

- **SNPP NUCAPS Stages 2-3 Validated Maturities**
  - NUCAPS AVTP and AVMP EDRs were recommended for Stage 1 Validated Maturity on 5 September 2014
  - Support short-term NUCAPS algorithm updates/improvements

- **Intensive Cal/Val (ICV)** and **Long Term Monitoring (LTM)** of **NUCAPS EDRs**
  - VALAR growth, development and enhancements
    - Support CalWater2 (early 2015) and future AEROSE campaigns
    - ARM dedicated RAOBs
    - GRUAN reference RAOBs
  - AVTP and AVMP validation for operational and offline code versions
    - Coarse-layer ensemble statistical analyses versus dedicated, reference and conventional RAOB truth
  - **Trace gas profile EDR (e.g., O_3, CO) validation**
    - Ozonesondes (e.g., AEROSE, SHADOZ)
    - WRF-CHEM modeling (e.g., *Smith and Nalli,* 2014)
  - GRUAN reprocessing of RS92 RAOB data (e.g., AEROSE)
  - Apply averaging kernels in NUCAPS error analyses, including ozone profile EDR
  - calc − obs (e.g., CCR) analyses
  - Skin SST EDR validation
  - Support long-term NUCAPS EDR algorithm development
    - *A priori*
    - AVTP/AVMP uncertainty estimates

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NUCAPS Operational Product Validation

EXTRA SLIDES

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 then RTA layer quantities, e.g.,

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

Assessment Methodology: Use of Averaging Kernels (AKs)

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

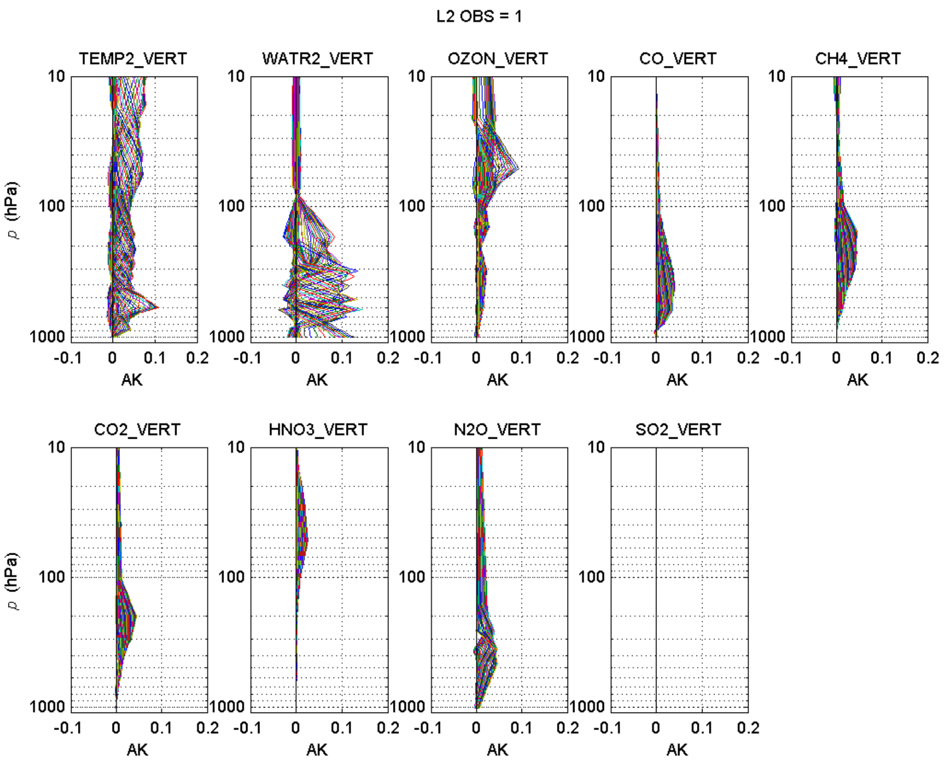
$$\mathbf{A} \equiv \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}}$$

- 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

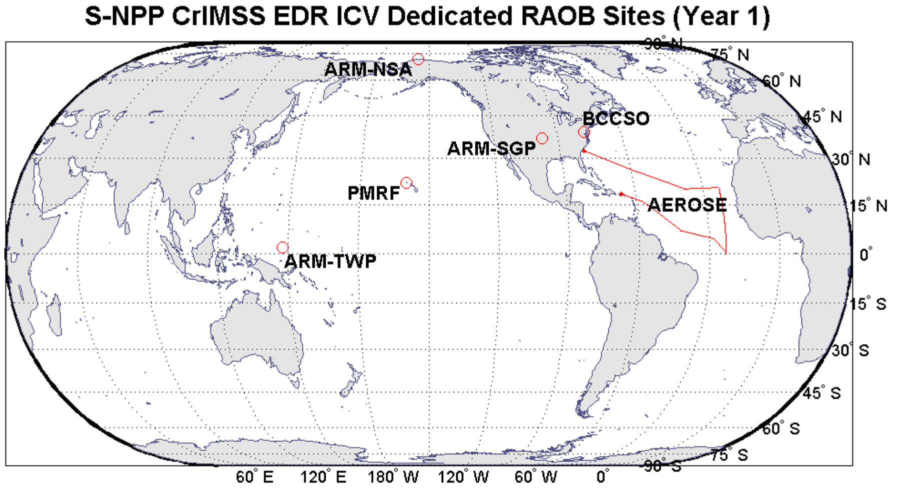
$$\mathbf{x}_s = \mathbf{A}(\mathbf{x} - \mathbf{x}_0) + \mathbf{x}_0$$

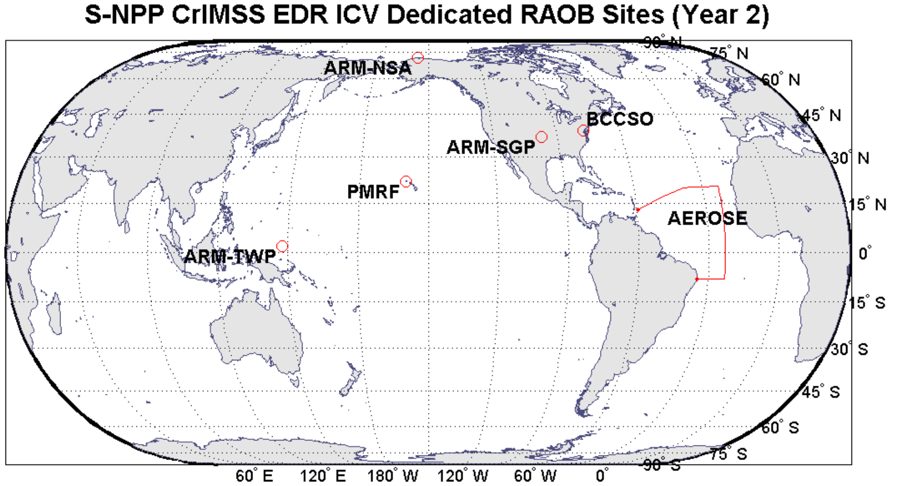
NOAA-Unique IASI Averaging Kernels



JPSS SNPP Dedicated RAOB Truth

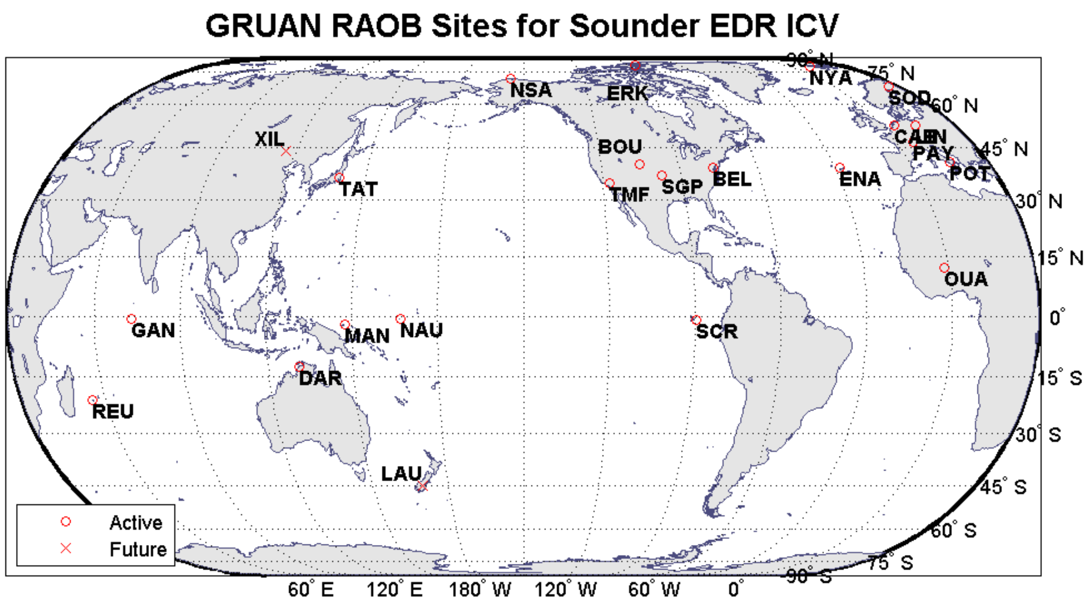
- **PMRF** (Kauai, Hawaii)
  - 2012 SNPP testbed site
- **BCCSO** (Beltsville, MD)
  - Howard University
  - Continent, urban
- **ARM Sites** (*Tobin et al.,* 2006)
  - TWP (Manus Island)
  - SGP (Oklahoma)
  - NSA (Alaska)
- **AEROSE Campaigns** (*Nalli et al.,* 2006, 2011)
  - Tropical Atlantic Ocean
  - Dust/smoke aerosols, Saharan air layers
  - Dedicated Ozonesondes
  - Truly independent dataset





Reference RAOB Truth

- GRUAN reference RAOB (*Seidel et al.*, 2009) collocations (00:00 and 12:00 UTC) are currently being acquired via the **NPROVS+** system (e.g., *Reale et al.*, 2012)
  - Traceable reference measurements
- NPROVS+ collocations support development of the **STAR Validation Archive (VALAR)**



VALAR and NPROVS+

NPROVS+

- 7-day delay GRUAN and dedicated RAOB collocation
- Nearest-FOR Operational-EDR Collocation Files
- Nearest-FOR Reprocessed-EDR Collocation Files
- User Interface Tools: PDISP, NARCS and ODS
- **Routine ICV and LTM**

VALAR

- Reduced 100 layer collocated RAOB
- SDR/TDR/EDR Granule Stamps
- Host Offline Retrievals
- Reprocessed EDR Granule Stamps
- **Research ICV and LTM**
- Facilitate Algorithm Research/Development