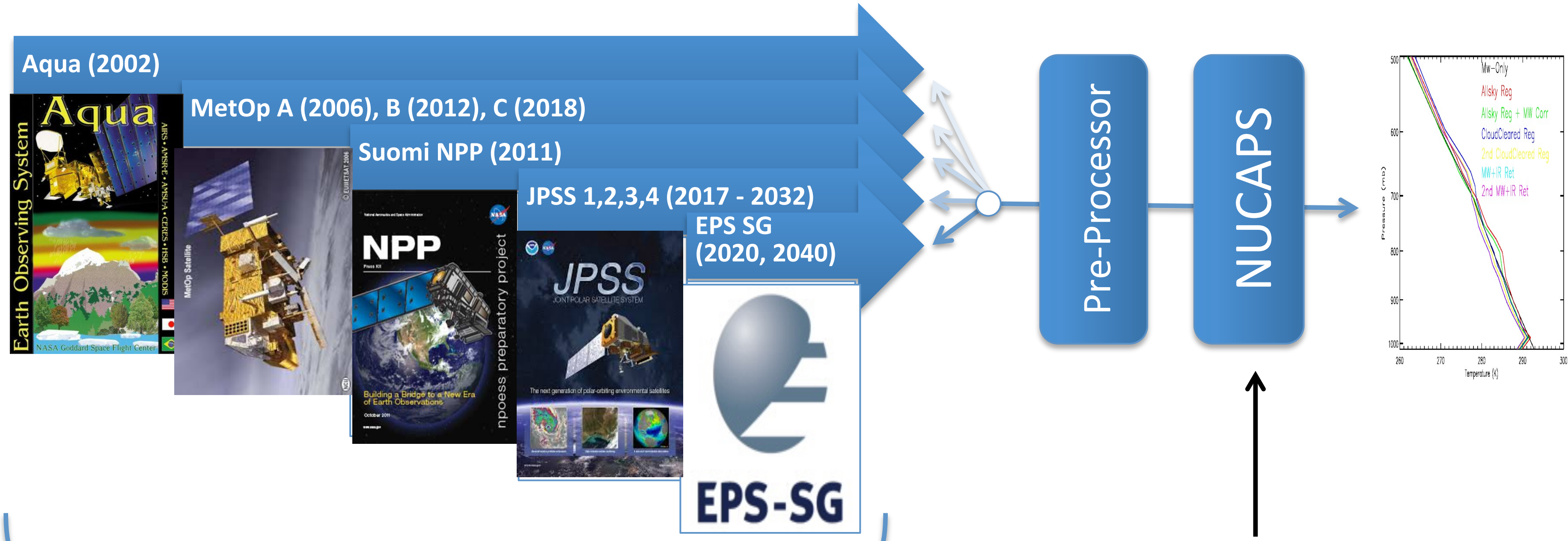
NOAA Long-term Strategy of trace gases from hyper-spectral thermal sounders

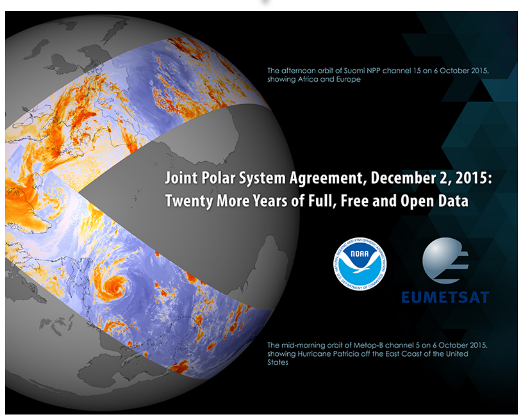
Antonia Gambacorta [1], Chris Barnet [1], Nadia Smith (1), Jonathan Smith (1), Walter Wolf (2), Mark Liu (2), Tony Reale (2), Tom King (2), Michael Wilson (2), Letitia Suillard (2), Nick Nalli (2), Bomin San (2), Kexin Zhang (2), Changyi Tan (2), Flavio Iturbide-Sanchez (2), Xiaozhen Xiong (2), Mitch Goldberg [3]

3rd JPSS Annual Meeting
August 11, 2016

1. Science and Technology Corporation, STC
2. NOAA NESDIS STAR
3. NOAA JPSS Project Scientist

NOAA long-term strategy of trace gases from hyper spectral sounders





The NOAA Unique Combined Atmospheric Processing System (NUCAPS)

Same exact executable

Same underlying Spectroscopy

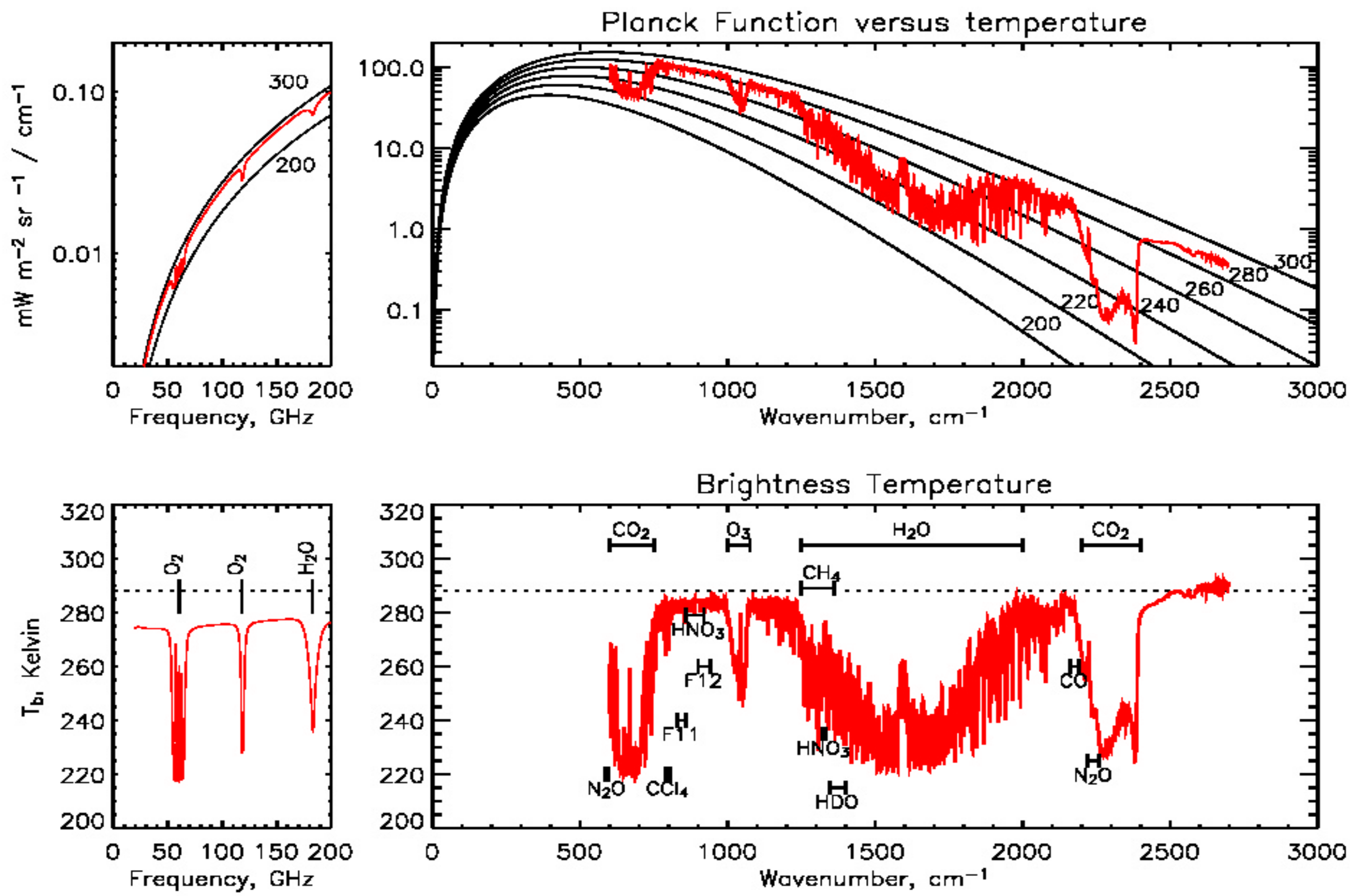
Same look up table methodology for all platforms

Philosophy of NUCAPS

- **The challenge**: high computationally efficiency and sophisticated inversion methods to maximize utilization of large volumes of data for real time weather and long-term climate applications

- **Philosophy of NUCAPS**: developing a mathematically sound and globally applicable (land/ocean, day/night, all season, all sky, TOA-surface) retrieval algorithm that can fully exploit all available satellite assets (infrared, microwave, visible) to retrieve the full suite of surface temperature and vertical profiles of temperature, moisture and trace gases. These are among the essential metrics defining a modern, physical and independent data record of atmospheric variables, suitable for both weather and climate applications.

Hyper spectral sounders sensitivity to trace gases



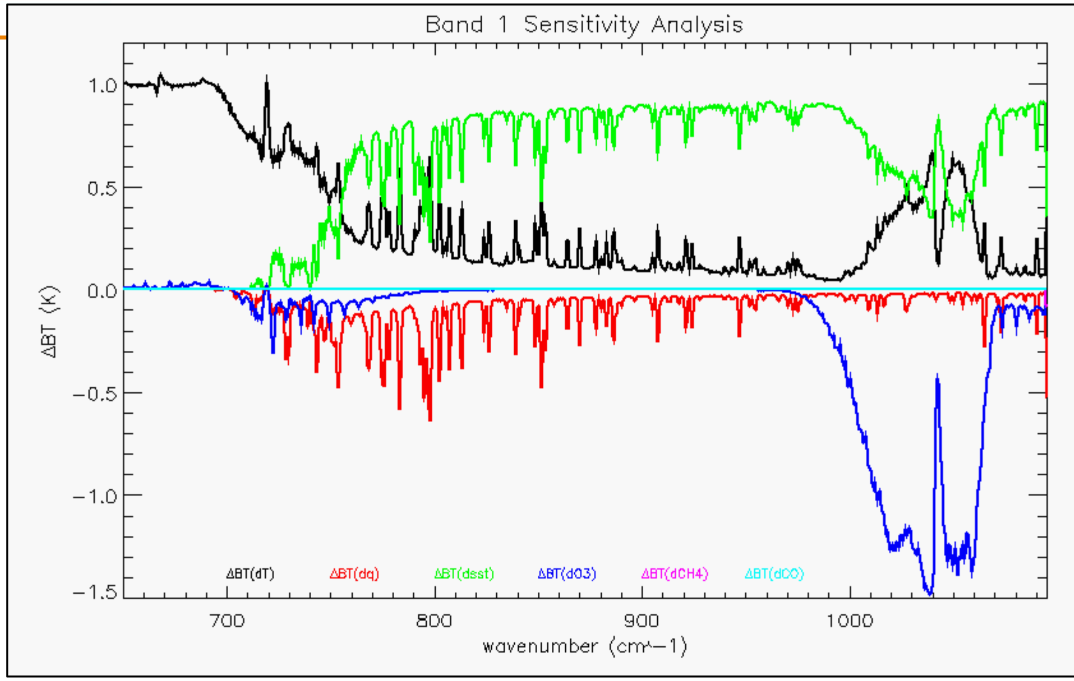
Summary of products from NUCAPS

gas	Range (cm^{-1})	Precision	d.o.f.	Interfering Gases
T	**650-800** **2375-2395**	**1K/km**	**6-10**	**H2O,O3,N2O** **emissivity**
H_2O	**1200-1600**	**15%**	**4-6**	**CH4, HNO3**
O_3	**1025-1050**	**10%**	**1+**	**H2O,emissivity**
CO	**2080-2200**	**15%**	**≈ 1**	**H2O,N2O**
CH_4	**1250-1370**	**1.5%**	**≈ 1**	**H2O,HNO3,N2O**
CO_2	**680-795** **2375-2395**	**0.5%**	**≈ 1**	**H2O,O3** **T(p)**
Volcanic **SO_2**	**1340-1380**	**50% ??**	**< 1**	**H2O,HNO3**
HNO_3	**860-920** **1320-1330**	**50% ??**	**< 1**	**emissivity** **H2O,CH4,N2O**
N_2O	**1250-1315** **2180-2250**	**5% ??**	**< 1**	**H2O** **H2O,CO**
$CFCl_3$ (F11)	**830-860**	**20%**	**-**	**emissivity**
CF_2Cl (F12)	**900-940**	**20%**	**-**	**emissivity**
CCl_4	**790-805**	**50%**	**-**	**emissivity**

The challenge of trace gas retrievals from hyper spectral sounders

- Retrieving trace gases from hyper spectral sounders is a highly non linear and ill-conditioned problem
- Trace gas signals are small and characterized by strong spatial and seasonal variability
- In some cases trace gases are physically correlated with other geophysical variables – for example in respiration of soil CO_2 is correlated with surface temperature; Ts/CH_4; CO/CH_4/O_3;
- Most of geophysical correlations in nature are non-linear.
- With trace gases geophysical *a-priori* information is limited.
- Lack of information content is problematic especially in presence of cloudy, cold, isothermal scenes.
- Trace gases are highly spectrally correlated (CO_2,O_3,H_2O in 15 um band, etc.)
- Errors in spectroscopy and geophysical state.
  - All trace gases dependent on temperature profile.
  - CO_2 and temperature are intimately correlated since CO_2 absorption is used to derive temperature
  - CO_2 can be correlated with clouds both in the retrieval and geophysical sense.
- Stitching satellite instruments together with different
  - Spatial sampling,
  - Spectral sampling, and
  - Noise characteristics
- Ground truth
  - Need full atmospheric state – up to ≥ 30 km.

Spectral Sensitivity Analysis (LW band)



Perturbation Applied

SST	1K
T	1K
H2O	10%
O3	10%
CH4	2%
CO	1%

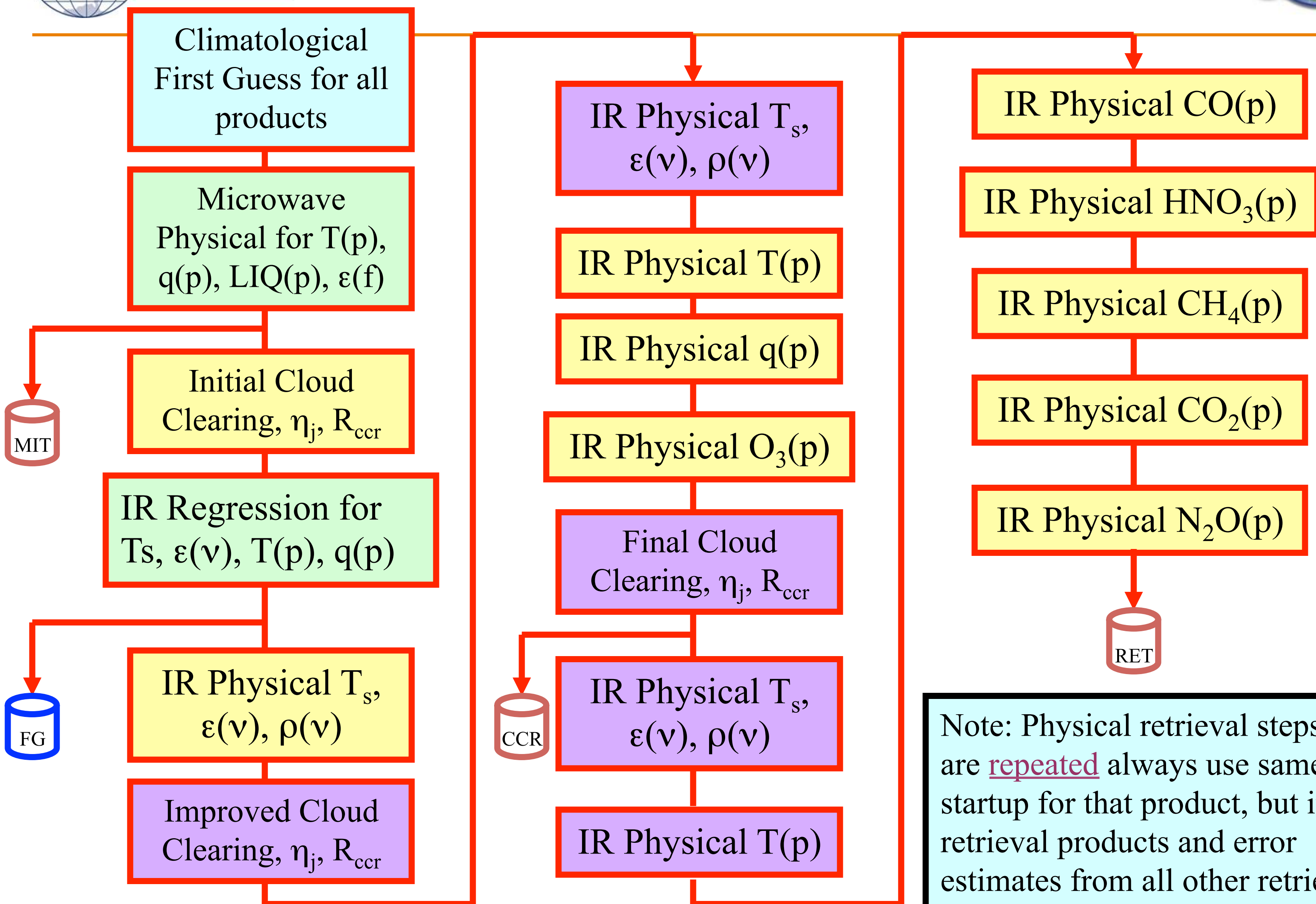
Brightness temperature difference (ΔBT) terms represent the sensitivity of each channel to a given perturbation species and are indicative of the degree of "spectral purity" of each channel.

- For each atmospheric species, we select channels with:
  - the highest degree of spectral purity (the highest sensitivity to the species of interest and the lowest sensitivity to all other interfering species).
  - the lowest noise sources (NEDT, calibration & apodization corr., RTA errors. See ahead.)
  - unique spectral features (to capture atmospheric variability, maximize vertical resolution)

NUCAPS long-term strategy of trace gases from hyper spectral sounders

- A minimum dependence on the geophysical a priori and full exploitation of the measurement and knowledge of the physics of radiative transfer.
  - Channel selection aimed at maximizing spectral purity and information content.
  - Spectral correlation, cloud clearing errors and instrument noise used as terms of the measurement error covariance in a weighted least square minimization
- A sequential approach, solving for most linear (including cloud clearing) or high S/N parameters first and a formal error propagation from one step to the next
- A retrieval is a signal averaging process over many channels and only makes changes where we have information content. Vertical averaging kernels, $A_{j,j}$, define where the instrument has skill.
- Users need to know vertical and spatial error covariance and vertical weighting functions.
  - Many of the "signals" we see have seasonal or spatial variability in the information content.
  - Broad vertical weighting functions tend to mix stratospheric and upper tropospheric contributions together.
    - Trace gas retrievals are sensitive to stratospheric-tropospheric exchange.
- Reprocessing capability to study long-term stability of algorithm.
  - All archived data ("granule" processing)
  - Global "gridded" data sub-sets (for rapid evaluation of algorithm modifications)
  - All validation datasets (including radio-sonde, aircraft match up datasets)

NUCAPS Flow Diagram



Note: Physical retrieval steps that are repeated always use same startup for that product, but it uses retrieval products and error estimates from all other retrievals.

The path forward

- We have built a retrieval system aimed at making the best use of hyper spectral data.
- Previous validation efforts have proven that we can meet requirements.
- With temperature and water vapor, users are clearly identifiable.
- What defines the operational need for these trace gas products instead?
  - Just because we can do it, it does not mean that we shall do it.
  - We would like to support any project supported by the NOAA AC4 Program to engage new potential users and gain insights on the applicability of our products. This will ultimately lead to a user requirement to justify the effort of transitioning products into operations.
  - NOAA JPSS is funding an unprecedented list of Proving Ground and Risk Reduction (PGRR) initiatives to demonstrate the operational need of our products. This is not validation in the traditional sense, it is developing new user's applications.
- What defines a trace gas operational user?
  - We need a real time, vetted, institutional user: EPA, National Forest Service, DOA, etc.
  - We need users that need archived consistent products: NUCAPS CO2 might serve as forecast climatology for the National Weather Service.

Main goal of this session

- This session should discuss what trace gases should be explored in a research sense and what trace gases should be distributed operationally.

- NASA and NOAA have different research mandates, goals and intended users.
  - NASA's focus is primarily on new instrument concepts and fundamental research.
  - NOAA leverages on NASA's research to develop a real time, operational and archival product, intended for specific end users applications of societal benefits.

- We are now looking for those user applications that will (1) verify the applicability of our trace gas products, (2) educate us on the need for new or improved products, QCs and formatting, (3) justify new efforts for algorithm improvements and transition to operations.

- The ultimate result is a continued and intelligent use of hyper-spectral trace gas products, both for real time and long-term applications.

Back Up slides

Why are CO_2 averaging functions broad while T(p) functions have profile information?

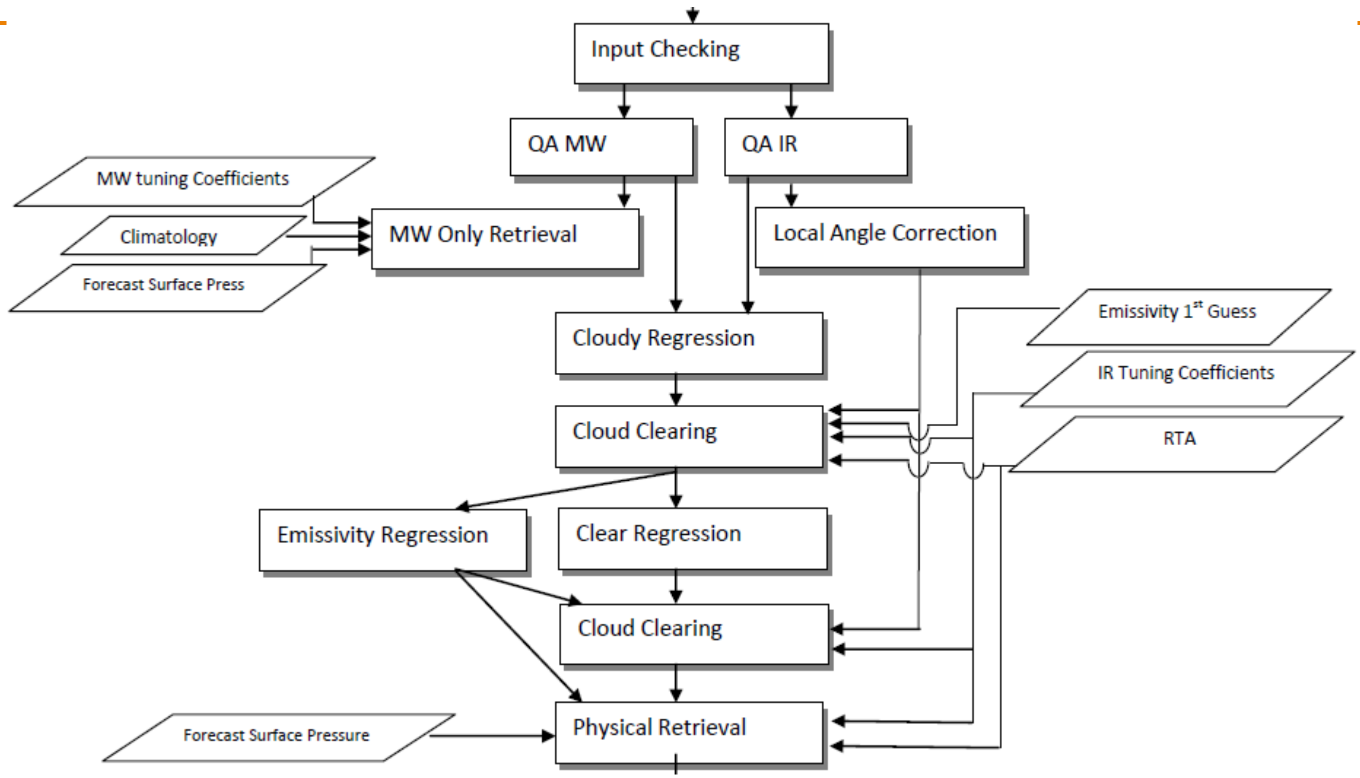
- Spectroscopy: The CO2 lines are strong narrow lines. Temperature affects the width (and hence the channel transmittance) while # of CO2 molecules affects the strength. Once the line is saturated (near the surface, where p is large) we loose sensitivity.

$$\kappa_i(\nu, p, T, \theta) \simeq \sum_{j=1}^{J} \frac{N_i \cdot S_{ij}}{\pi} \frac{\gamma_{ij}}{(\nu - \nu_{ij})^2 + (\gamma_{ij})^2} \cdot \sec(\theta) \qquad \gamma_{ij} \simeq \gamma_{ij}^0 \cdot \frac{p}{P_0} \cdot \sqrt{\frac{T}{T_0}}$$

- Radiative transfer: The temperature enters both in the absorption coefficient and in the Planck function.

$$R_n(\vec{X}) \simeq \int_\nu \Phi_n(\nu) \int_p B_\nu(T(p)) \cdot \frac{\partial \exp\left(-\int_{z'=\infty}^{z(p)} \sum_i \kappa_i(\vec{X}, p, \ldots) dz'\right)}{\partial p} \cdot dp \cdot d\nu$$

NUCAPS Flow Chart



- **I. A microwave retrieval module** which computes Temperature, water vapor and cloud liquid water (Rosenkranz, 2000)
- **II. A fast eigenvector regression** retrieval that is trained against ECMWF and CrIS all sky radiances which computes temperature and water vapor (Goldberg et al., 2003)
- **III. A cloud clearing module** (Chahine, 1974)
- **IV. A second fast eigenvector regression** retrieval that is trained against ECMWF analysis and CrIS cloud cleared radiances
- **V. The final infrared physical retrieval** based on a regularized iterated least square minimization: temperature, water vapor, trace gases (O3, CO, CH4, CO2, SO2, HNO3, N2O) (Susskind, Barnet, Blaisdell, 2003)