Status of the NOAA Unique Combined Atmospheric Processing System (NUCAPS) Trace Gas products

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2017 JPSS Annual Meeting – Trace Gas Session

[1]STC; [2] IMSG; [3] NOAA/NESDIS/STAR; [4]UMBC; [5]NOAA JPSS

Outline of this talk

Part I.

Introduction on the NUCAPS system

Part II.

Overview of the NUCAPS Full Spectral Resolution (FSR) upgrades relevant to trace gas retrievals

- SARTA RTA upgrades and bias corrections
- CrIS FSR trace gases channel selection

Part III.

Current activities, future plans

N as in NUCAPS

NOAA	NOAA's mandate: ensuring highest computational efficiency and state of art inversion methods to maximize utilization of large volumes of data for a weather ready nation
Unique	A mathematically sound, globally applicable (land/ocean, day/night, all season, all sky, TOA-surface) hyperspectral retrieval code
Combined	… that can fully exploit all available satellite assets: infrared, microwave, visible
Atmospheric	… to generate a full suite of retrieval products: cloud cleared radiances, skin temperature, vertical profiles of temperature, water vapor, O3, CO, CH4, HNO3, N2O, SO2, CO2 (future: HN3)
Processing	… by the use of a modular design compatible with multiple platforms: Aqua, MetOp, SNPP, JPSS, EPS-SG
System	NUCAPS has been running operationally at NOAA since 2004. it is now in AWIPS II. It has been installed in CSPP DB.

Nominal vs Full Spectral Resolution CrIS

- **The Cross-Track Infrared Sounder (CrIS)** is a Fourier spectrometer covering the longwave (655-1095 cm^{-1}, "LW"), midwave (1210-1750 cm^{-1}, "MW"), and shortwave (2155-2550 cm^{-1}, "SW") infrared spectral regions.

- **Past operations (NUCAPS Phase 1-3):**
  - Maximum geometrical path *L* of 0.8 cm (LW), 0.4 cm (MW) and 0.2 cm (SW)
  - Nyquist spectral sampling (*1/2L*): 0.625 cm^{-1}, 1.25 cm^{-1} and 2.5 cm^{-1}

- **Experimental since 2013 – Operational in August 2017 (NUCAPS Phase 4):**
  - Maximum geometrical path *L* of 0.8 cm in all three bands
  - Nyquist spectral sampling (*1/2L*): 0.625 cm^{-1} in all three bands

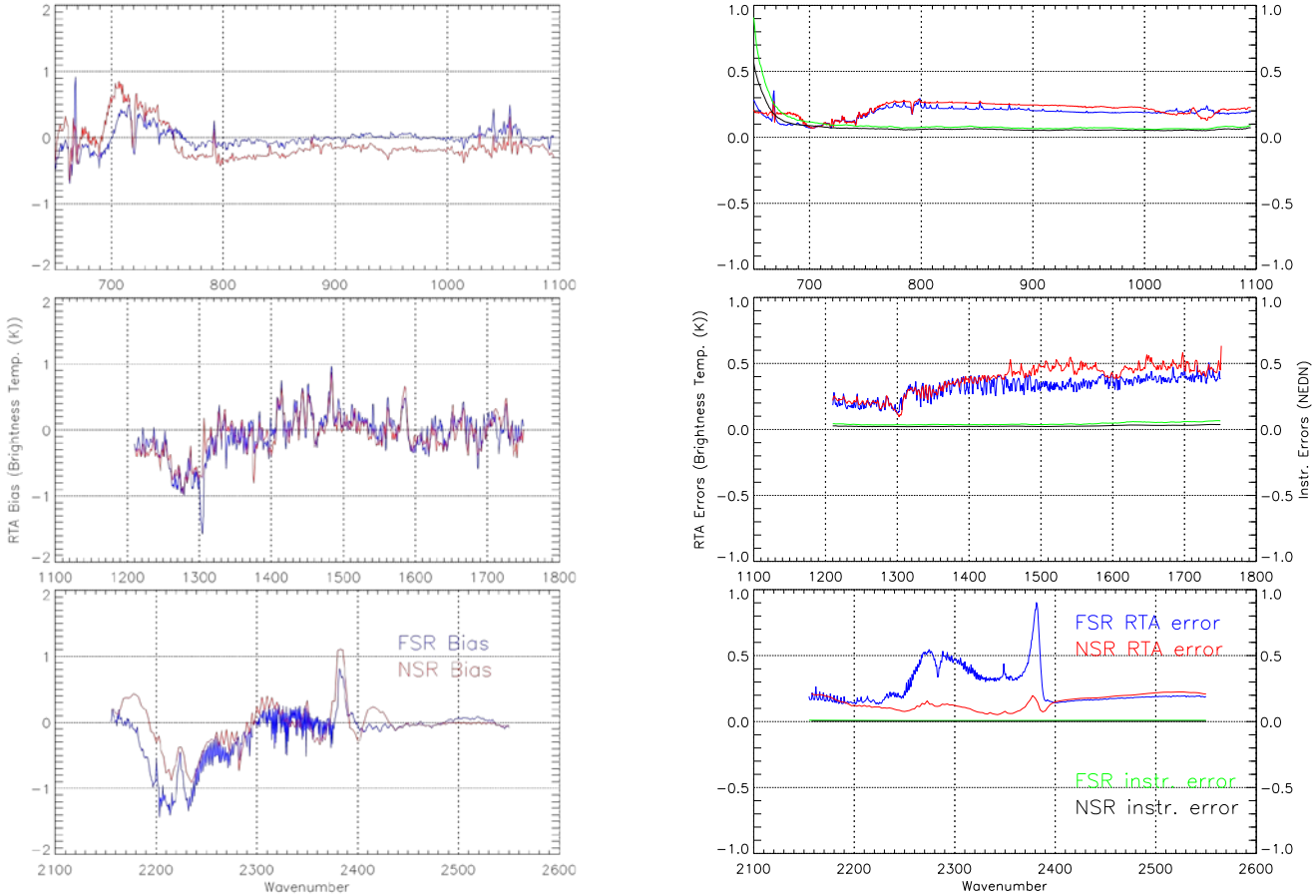
CrIS Full Spectral Resolution (FSR) SARTA Rapid Transmittance Algorithm (RTA)

Upgrades in the CrIS FSR SARTA RTA (L. Strow's talk in the today's session)

- CrIS high-resolution ILS
- HITRAN 2012 (vs 2008 in original CrIS RTA)
- LBLRTM Line Mixing for CO2 and CH4, H2O continuum
- UMBC line-by-line for water vapor
- Improved reflected thermal component for high secant angles
- Tested on 750+ profiles (from ECMWF selected subset), regressed on 49 profiles
- Error covariance estimates available from 750+ profile testing

CrIS FSR SARTA bias tuning and sdev

Bias | Standard deviation



CH4 and CO2 profiles from JAMSTEC atmospheric chemistry-transport model (ACTM) as truth.
CO profiles from MOPITT retrieval as truth. Selection of clear CrIS FOVs was performed using collocated VIIRS cloud mask IPs. (1) only confident clear pixels; (2) satellite view angle less than +/-30 degrees; (3) set multi-thresholds to screen out outliners.

Channel Selection Methods: two schools of thoughts

Jacobians method aka "Physical Approach"

- Selection methodology metrics:
  - Channel spectral purity

- Current operational users (to cite a few)
  - AIRS science team [1,3]
  - NOAA (AIRS, IASI, CrIS) [1,2]
  - ECMWF (IASI) [4]
  - Meteo UK (IASI) [4]
  - Meteo France (IASI) [4]
  - LATMOS (AIRS, IASI, CrIS) [5]
  - ULB (AIRS, IASI, CrIS)[5]

- List of references
  - (1) Susskind, Barnet, Blaisdell, IEEE 2003
  - (2) Gambacorta and Barnet, IEEE 2013;
  - (3) Susskind, Blaisdell, Iredell, JARS, 2014
  - (4) Martinet, Levananat, Fourrie, Gambacorta, 2014
  - (5) Crevoisier, Chedin, Scott, QJRM, 2003

Rodgers Method

- Selection methodology metrics:
  - Channel information content

- Current operational users (to cite a few)
  - ECMWF [1,2,3,4]
  - Meteo UK [1,2,3,4]
  - Meteo France [1,2,3,4]

- List of references
  - (1) Rodgers, 1997
  - (2) Fourrie *et al*. 2002;
  - (3) Rabier *et al*., 2002
  - (4) Collard and McNally, 2007

Physical Method vs Rodgers Method

Jacobians or Physical method

- A physically-based methodology where channels are selected upon their spectral properties.
- For each atmospheric species, we perform a spectral sensitivity analysis and retain the spectrally purest channels and reject channels carrying confounding signals.
- Other than spectral purity, priority is given to vertical sensitivity properties, low instrumental noise and RTA errors.
- The method is algorithm independent in that both simultaneous and sequential inversion algorithms benefit from channels that can discriminate between atmospheric species. Details to be explained ahead.

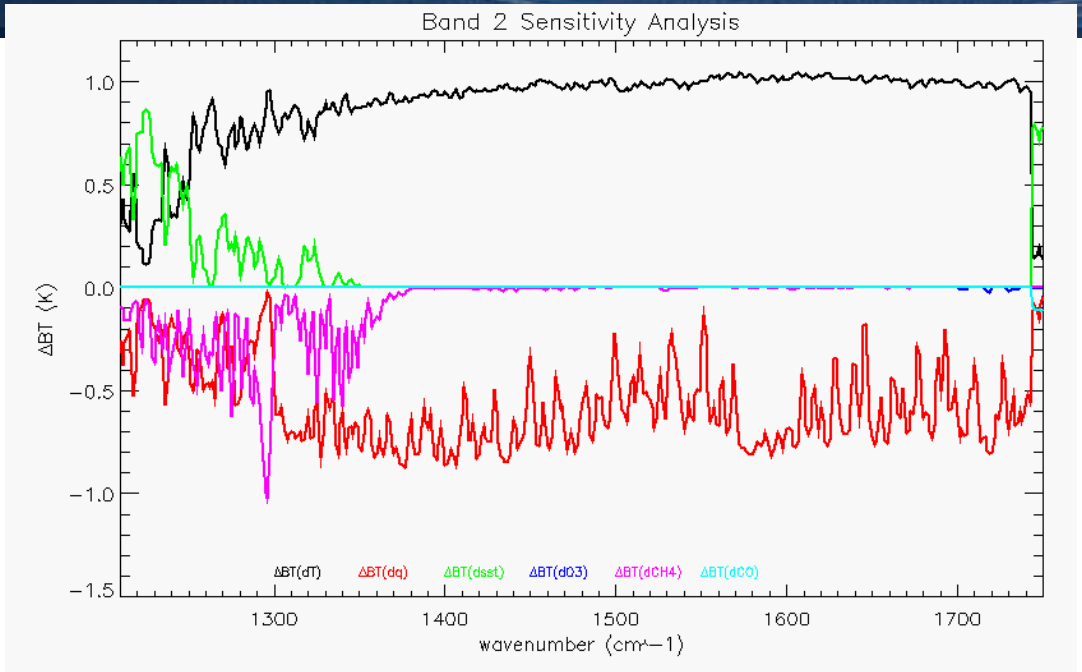
Rodgers method

- Follows a statistical iterative approach where channels are incrementally added after being tested for increased degrees of freedom.
- This methodology is more suited for simultaneous optimal estimation retrieval techniques.
- Can be automated by establishing fixed thresholds.

Both methods:

- a constant channel selection is normally used, which is derived as an average from multiple optimal selections computed over different geophysical regimes (polar, mid latitudes, tropical, land, ocean, desert).

CrIS FSR Channel Selection



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)
- **unique spectral features** (to capture atmospheric variability, maximize vertical resolution)

REF: A. Gambacorta and C. Barnet., Methodology and information content of the NOAA NESDIS operational channel selection for the Cross-Track Infrared Sounder (CrIS), IEEE, Vol. 51, Issue 6, 2013

Why do we use the Jacobian method

- NUCAPS required list of retrieval products (all sky, all seasons, all surface types)
  - Cloud cleared radiances
  - Cloud top pressure and fraction
  - Surface temperature
  - Vertical temperature
  - Water vapor
  - Trace gases: O_3, CH_4, CO, CO_2, SO_2, N_2O, HNO_3
- Future candidates:
  - NH_3 (Ammonia), HCO_2H (Formic Acid), $CH_3COOONO_2$ ("PAN")
- A "**trace gas"** is a gas which makes up less than 1% of the volume of the Earth's atmosphere.
- Trace gas radiative signals are in the range of the instrument noise.
- Most channels are largely contaminated by clouds, temperature and water vapor signals.
- <u>Answer</u>: *Spectral purity is essential to improve signal to noise for the retrieval of the full list of NUCAPS required products, particularly for trace gases, under all sky conditions.*
- This methodology, being *physically based*, is applicable to *ALL* retrieval schemes. It is particularly suited for sequential retrieval approaches. See next slide.

REF: A. Gambacorta and C. Barnet., Methodology and information content of the NOAA NESDIS operational channel selection for the Cross-Track Infrared Sounder (CrIS), IEEE, Vol. 51, Issue 6, 2013

Why do we use the Jacobian method

Summary of current NUCAPS retrieval products

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*

Potential additions

How do we maximize linearity?

- **Sequential OE** (solves each state variable separately) **vs simultaneous OE** (solves all parameters simultaneously) **approach**

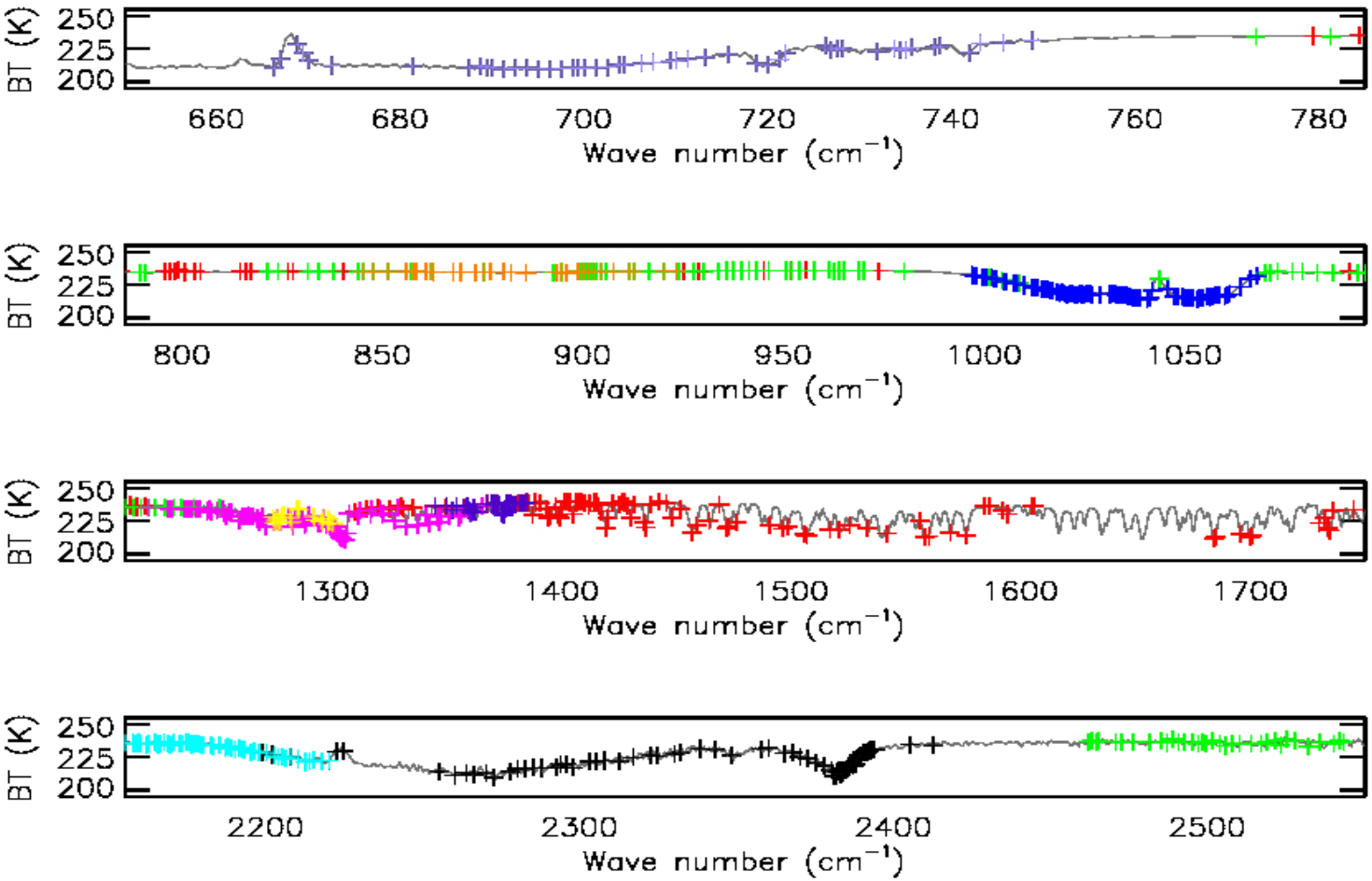
$$R_n^{obs} - R_n(\vec{X}) \simeq K_{n,i}^1 \cdot \Delta\vec{T}_i + e_n$$

$$\begin{aligned} e_n &= K_{n,i}^2 \cdot \delta\vec{q}_i \\ &+ K_{n,i}^3 \cdot \delta\vec{O}_i \\ &+ K_{n,i}^4 \cdot \delta\vec{C}O_i \\ &+ \ldots + \epsilon_n \end{aligned}$$

- Careful analysis of the physical spectrum will show that many components are physically separable (spectral derivatives are unique).
- Select channels within each step with large K and small e_n
- This makes the solution more linear with respect to the simultaneous OE approach.
- State matrices are small and covariance matrices of the channel subsets are quite small. This has significant implications for operational execution time.

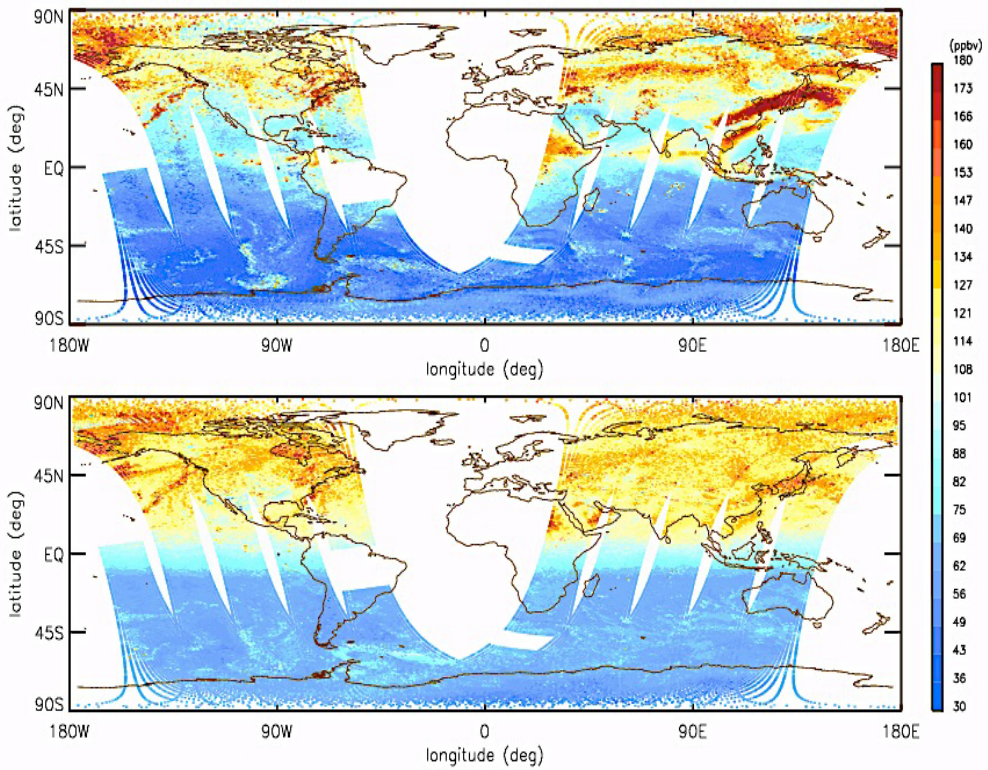
NUCAPS Operational FSR CrIS channel selection (610 channels)

EDR	#chns
Temp	116
Surf	136 (62)
HO2	123 (62)
O3	77
CO	52
CH4	84
N2O	21
SO2	31
HNO3	30
CO2 (& Temp)	50 (T LW)

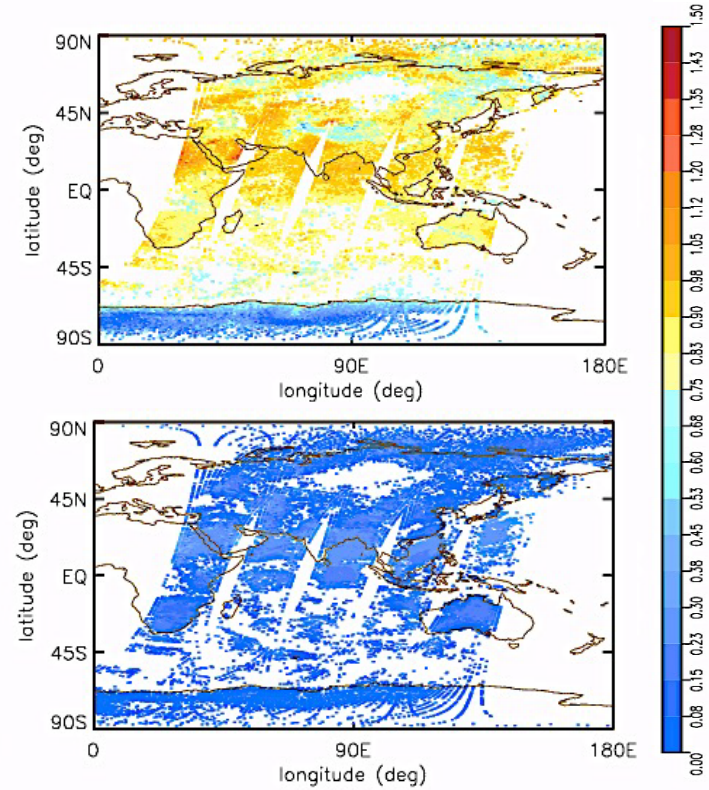


August 2013: Preliminary demonstration of FSR NUCAPS CO (top) vs NSR NUCAPS CO (bottom) using 5 test FSR orbits and ~2008 FSR RTA

NUCAPS CO retrieval (~450mb)



NUCAPS CO DOF



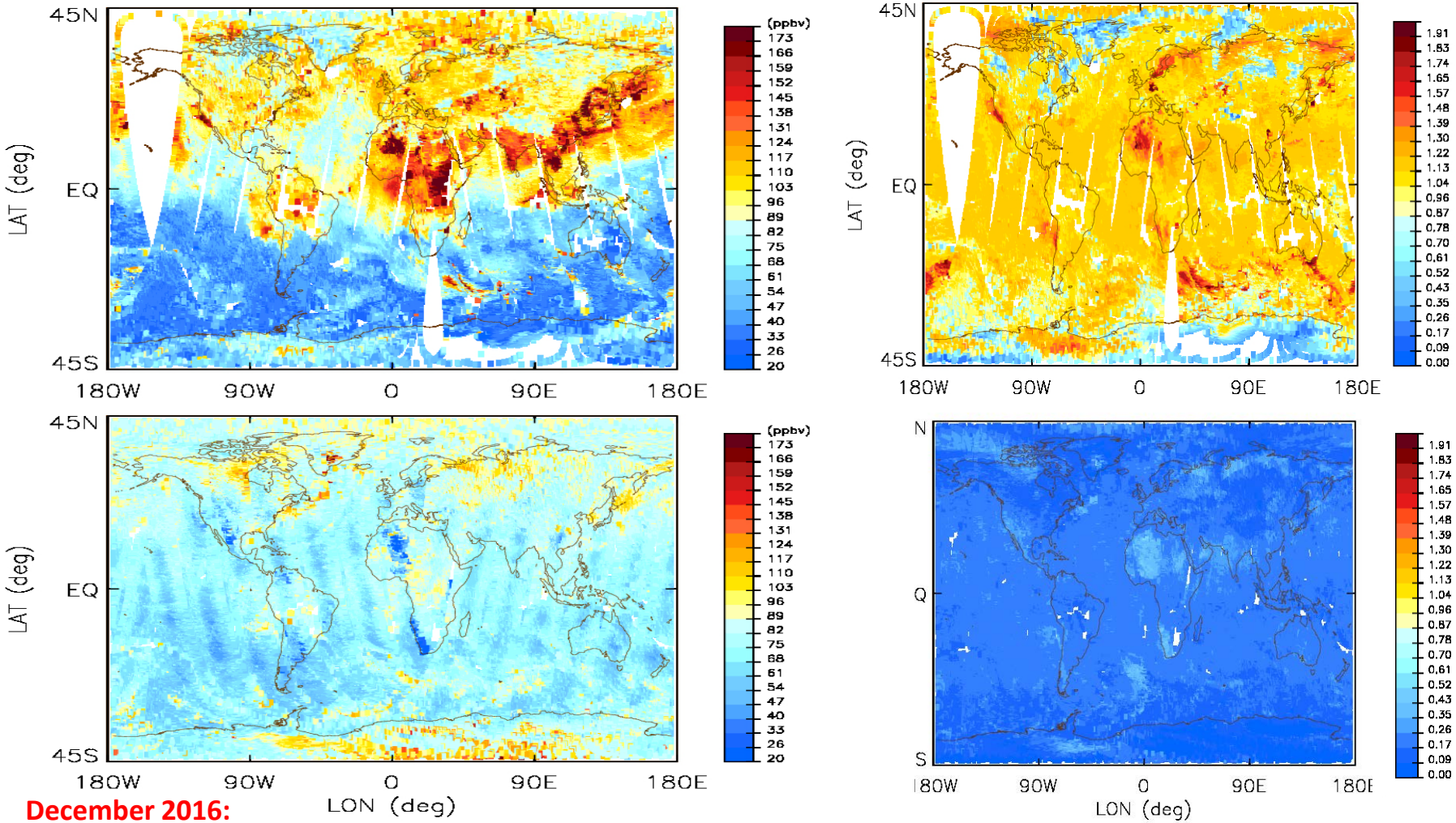
- The higher information content enables a larger departure from the a priori, hence the increased spatial variability observed in the high spectral resolution map (top left) compared to the low resolution (bottom left).
- **August 2013**: this was a demonstration experiment in support for the need of high spectral resolution CrIS measurements using 5 experimental orbits from March 2013. Top is FSR NUCAPS; Bottom is NSR NUCAPS.

Ref.: Gambacorta et al., "An experiment using CrIS high spectral resolution measurement for trace gas retrievals: CO retrieval impact study", IEEE Transactions on Geoscience and Remote Sensing Letters, 2014.

December 2016: Preliminary demonstration of FSR NUCAPS CO (top) vs NSR NUCAPS CO (bottom) using Operational FSR RTA and Chn. Selection

NUCAPS CO retrieval (~450mb)

NUCAPS CO DOF

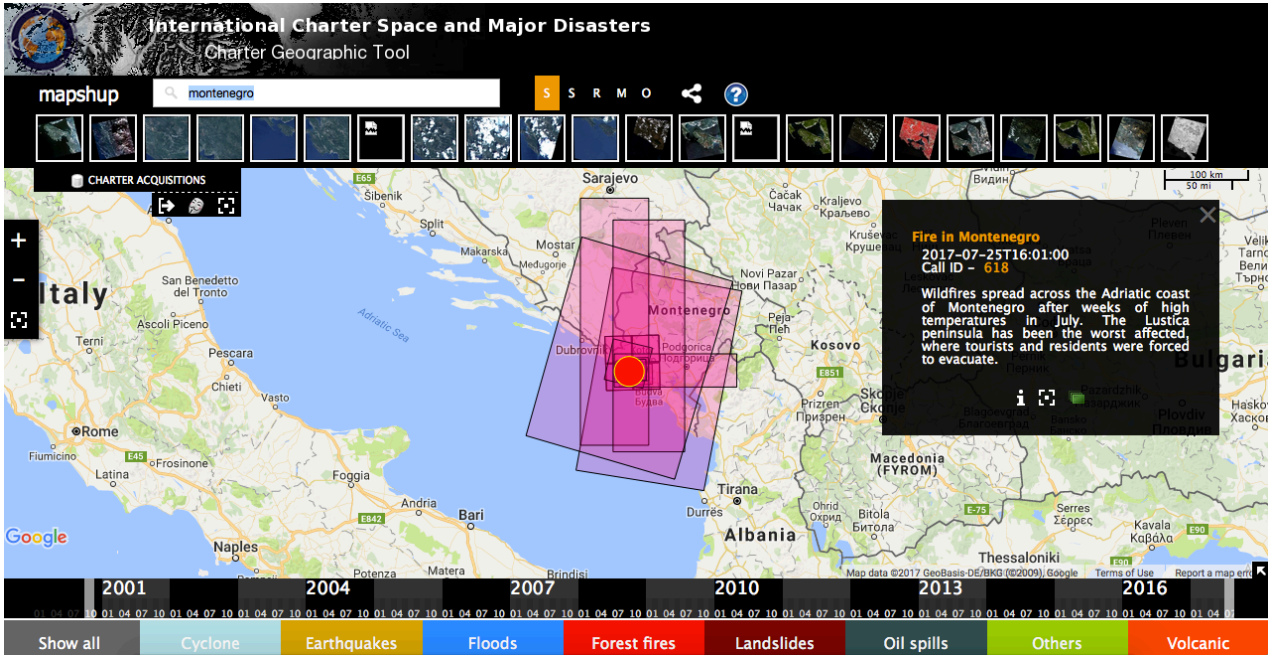


December 2016:

TOP: FSR NUCAPS/CLIMCAPS CO retrieval results (focus day 2015-02-17)

BOTTOM: NSR NUCAPS/CLIMCAPS CO retrieval results (focus day 2015-02-17)

July 2017 – Montenegro Fire



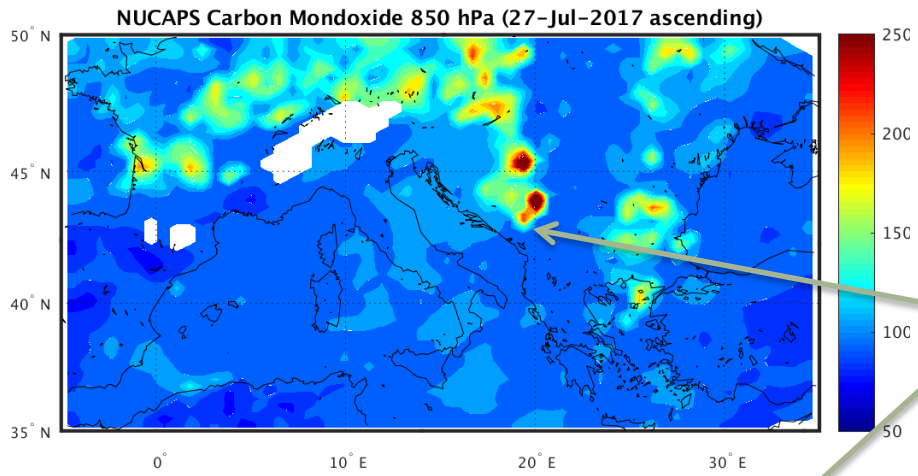
- The International Charter aims at providing a unified system of space data acquisition and delivery to those affected by natural or man-made disasters through Authorized Users.
- Each agency member has committed resources to support the provisions of the Charter and thus is helping to mitigate the effects of disasters on human life and property.
- https://disasterscharter.org/web/guest/home

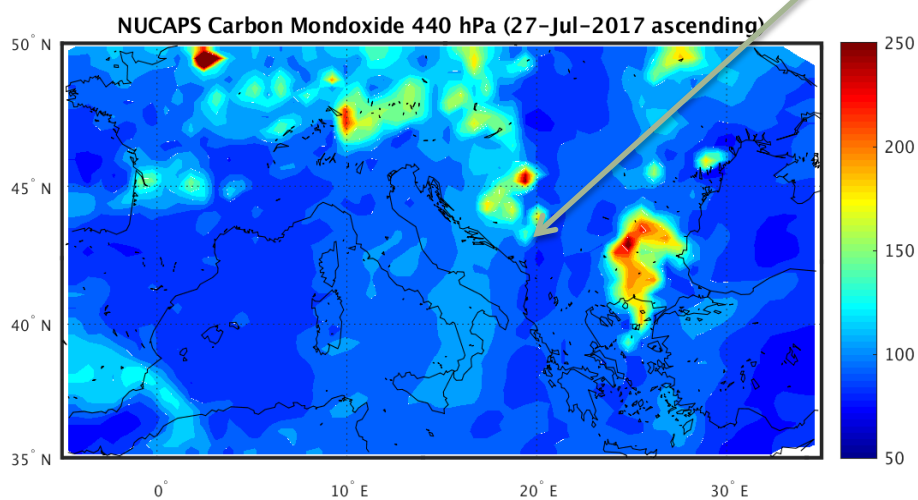
July 2017 – Croatia and Montenegro Fires

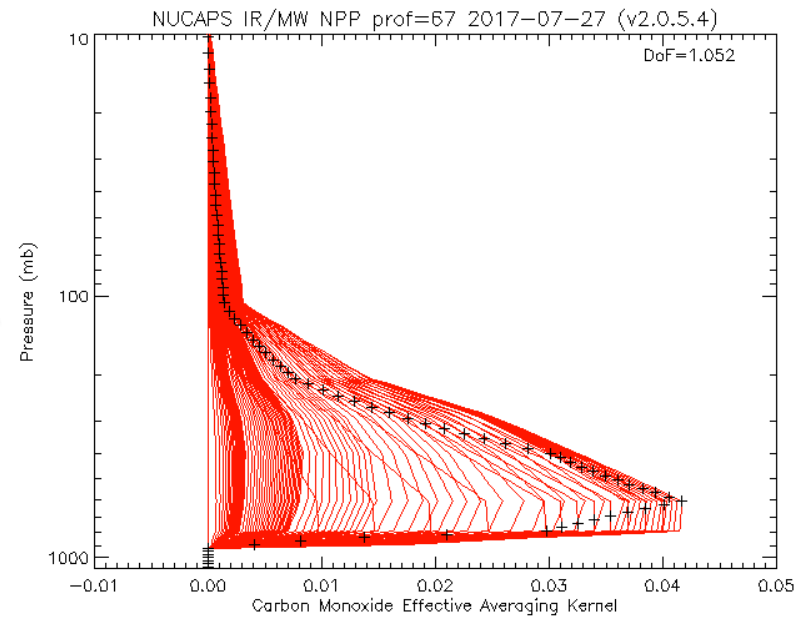
Left: Smoke and flames rise from a fire in the village of Podstrana, near the Adriatic coastal town of Split, on July 18, 2017. Montenegro asked for international help to fight wildfires on the Lustica peninsula on the country's Adriatic coast, while forest fires in neighboring Croatia spread to suburbs of the coastal city of Split.

Right: NASA image courtesy NASA MODIS Rapid Response Team
https://www.nasa.gov/image-feature/goddard/2017/nasa-sees-smoke-from-fires-in-croatia-and-montenegro

NUCAPS FSR CO retrieval skills: July 27 2017 – Croatia and Montenegro Fires







NUCAPS FSR CO Aks

Near Podgorica, LAT: 42.7583 LON: 19.1978

Current NUCAPS trace gas JPSS funded initiatives

This is not validation in the traditional sense, it is developing new users applications.

1. **Carbon Monoxide and Methane product evaluation** (NESDIS/STAR & OAR/ESRL/CSD).

Scope: Models are used to interpolate the sparse aircraft observations to the satellite temporal, spatial, and vertical sampling characteristics for detailed validation. NUCAPS (and AOD from VIIRS) will be used within IDEA (Infusing Satellite Data into Environmental Air Quality Applications)

I. PI Greg Frost: "Understanding emissions and tropospheric chemistry using NUCAPS and VIIRS"

II. PI Brad Pierce: "High Resolution Trajectory-Based Smoke Forecasts using VIIRS Aerosol Optical Depth and NUCAPS Carbon Monoxide Retrievals. "

- References:
  - Songnex: http://esrl.noaa.gov/csd/projects/songnex/
  - SENEX: http://www.esrl.noaa.gov/csd/projects/senex/
  - IDEA: http://www.star.nesdis.noaa.gov/smcd/spb/aq/

2. Use of NUCAPS Ozone in hurricane extra-tropical transition applications (SPoRT)

Scope: Migrate AIRS/SEVIRI product to NUCAPS O_3 with VIIRS RGB. To conduct a product demonstration and assessment with the NHC, WPC and OPC forecasters

I. PI Emily Berndt: "investigation of NUCAPS T(p), q(p), and O3(p) to study extra-tropical transition of hurricanes"

- Reference:
  - https://nasasport.wordpress.com/2016/10/05/nucaps-soundings-and-hurricane-matthew/

Few lessons learned on users needs in preparation for the next field campaign (FIREX 2018)

- Users need to know spatial and vertical error covariance
  - Many of the signals we see have seasonal or spatial variability in the information content.
  - Trace gas retrievals are sensitive to stratospheric-tropospheric exchange. Broad vertical weighting functions tend to mix stratospheric and upper tropospheric contributions together. Averaging kernels should become an integral part of the operationally distributed products.
  - We are working on submitting a formal user request to have NUCAPS averaging kernels operationally distributed.

- Users need reprocessing capability to study long-term stability of an 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)

- Users need user-friendly data formats (netcdf4 is generally preferred)
- Users need more sophisticated QCs than what is used in current operations
  - Original QC was developed to demonstrate that we meet requirements
  - Some "green" scenes are bad, some "red" scenes are good
  - We need to develop QCs specifically tailored for trace gas applications

- Users need near real time access to NUCAPS high resolution operational products (essential for applications involving fire trajectories and air quality).
  - FSR NUCAPS soon to be installed in the NOAA DB.
  - This is in preparation of the future NOAA FIREX 2018 campaign (http://www.esrl.noaa.gov/csd/projects/firex/).

Future upgrades and conclusions remarks

Coming next

- We are working on a formal request for a NUCAPS NH_3 product.
- What defines the need for a trace gas operational product?
  - Just because we can retrieve a product, it does not mean that we should do it.
  - 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.

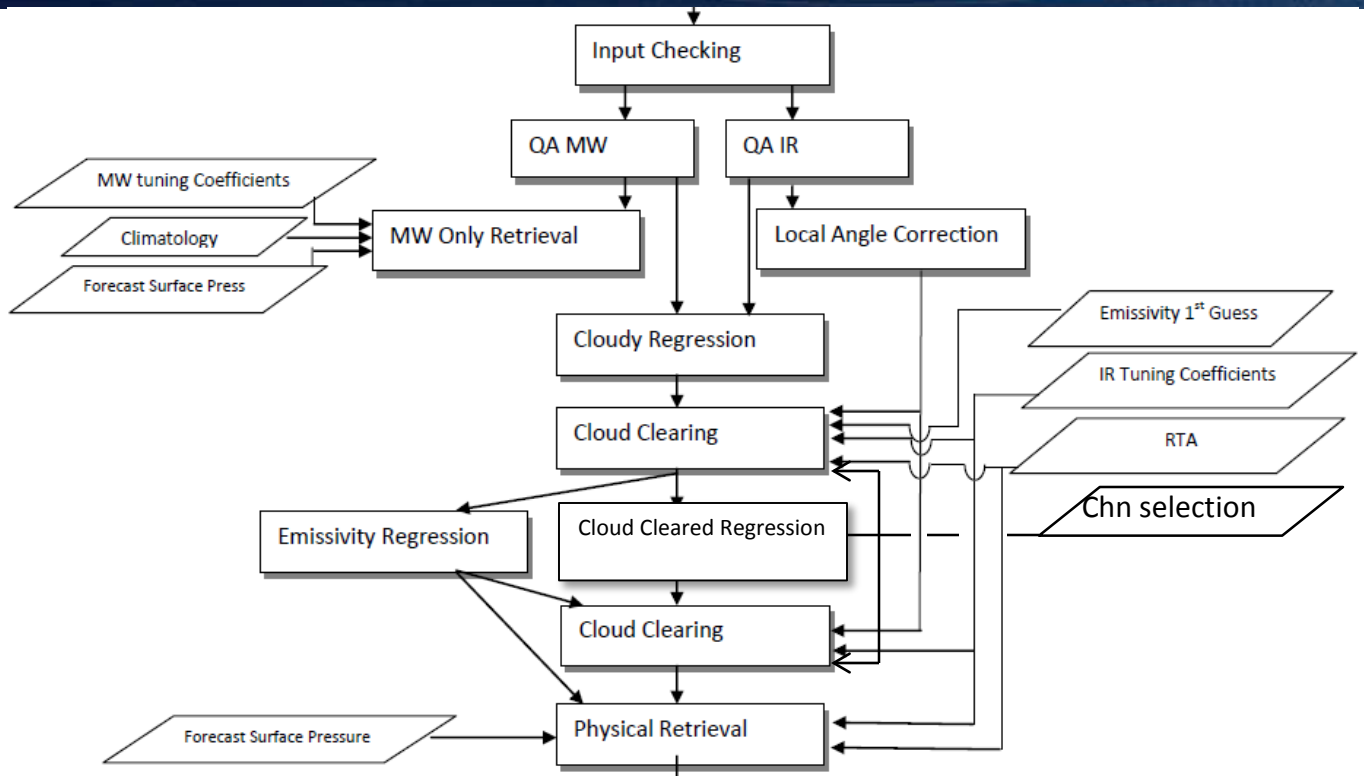
Conclusion remarks

- 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 <u>user requirement</u> to justify the effort of**
  - **maintaining and improving current and**
  - **developing new**

  trace gas operational products.

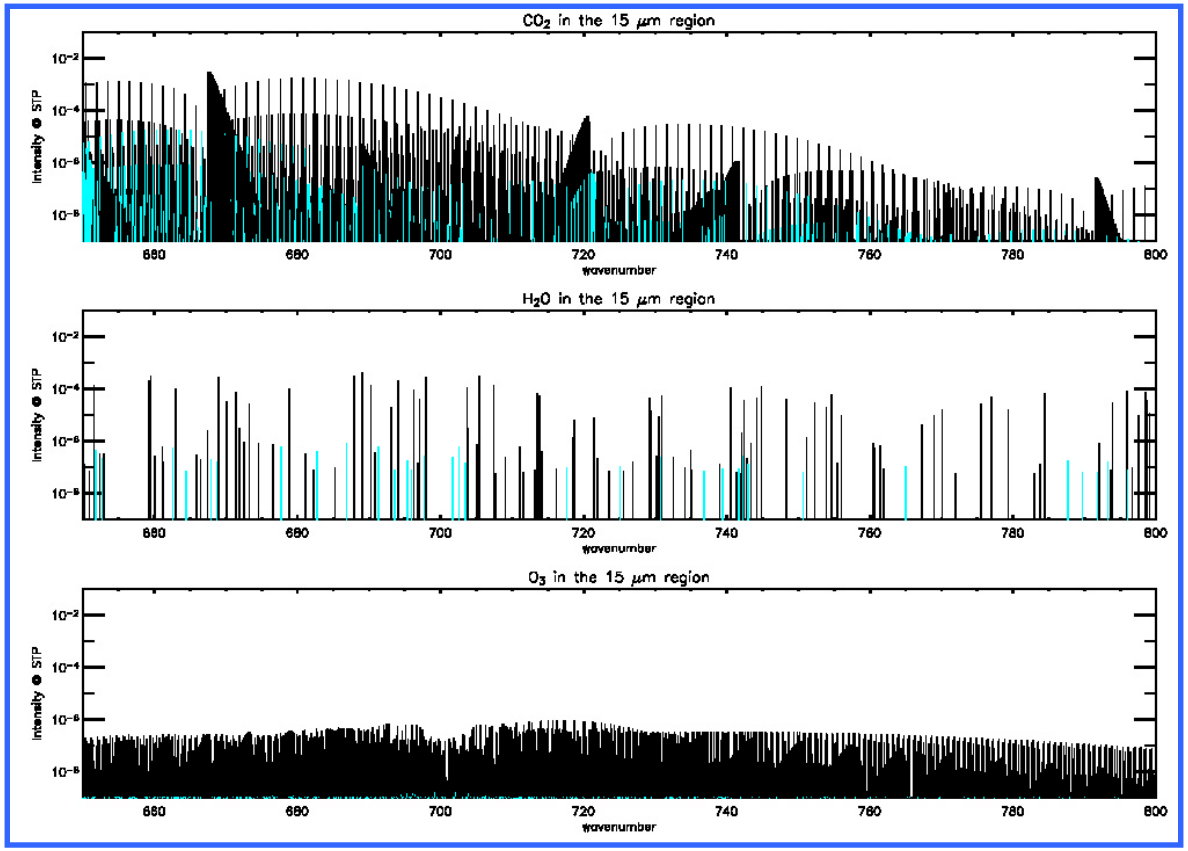
Back ups

NUCAPS Retrieval Algorithm Flow Chart



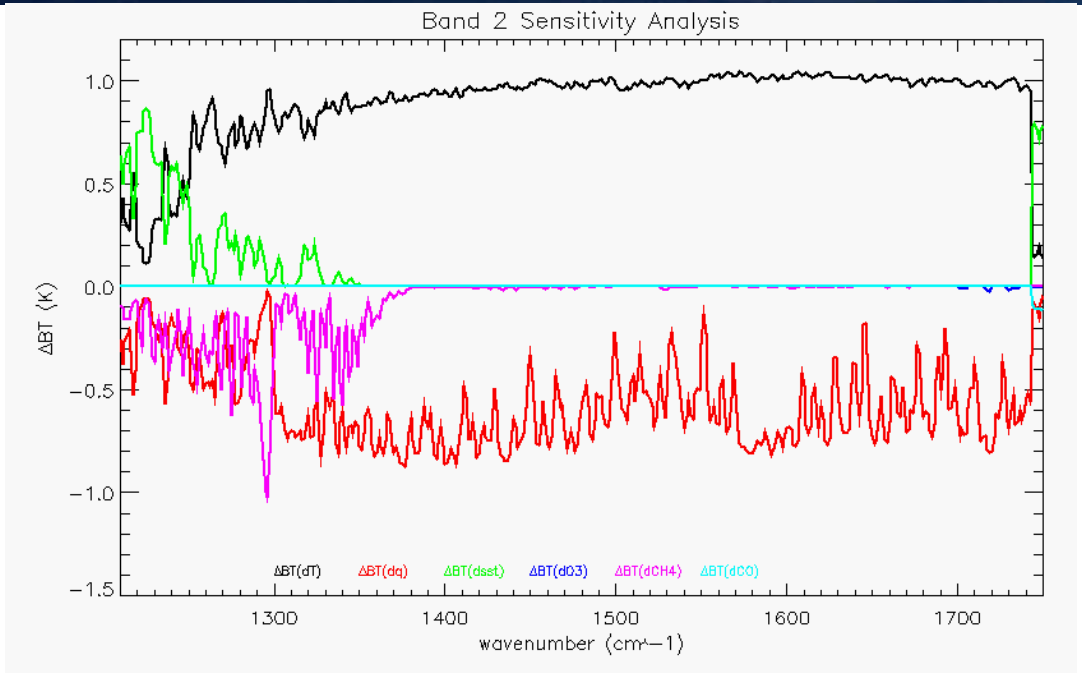
- **I. A microwave retrieval module** which computes Temperature, water vapor and cloud liquid water (Rosenkranz, 2000)
- **II. A fast eigenvector regression** retrieval that is trained against ECMWF and all sky radiances which computes temperature and water vapor (Goldberg et al., 2003)
- **III. A cloud clearing module** (Chahine, 1974)
- **IV. A second fast eigenvector regression** retrieval that is trained against ECMWF analysis and cloud cleared radiances
- **V. The final infrared physical retrieval** based on a regularized iterated least square minimization: temperature, water vapor, trace gases (O_3, CO, CH_4, CO_2, SO_2, HNO_3, N_2O) (Susskind, Barnet, Blaisdell, 2003)

Definition of "Spectral Purity"



- The finite spectral resolution of the instrument does not allow for *spectral purity*. Specifically, in the infrared domain, the signal associated with a given channel of nominal frequency ν is, in reality, the result of multiple molecular rotovibrational transitions whose spectral range of occurrence falls in within the spectral resolution Δν of the channel.

NUCAPS: a sequential, iterated, linearized, weighted, regularized least square fit



Perturbation Applied

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

$$\Delta R_n = K^i_{n,L} \Delta X^i_{n,L} + \varepsilon_n$$

$$\varepsilon_n = NEDT_n + \delta R_{CCR} + \delta RTA_n + \sum_{j \neq i} K^j \delta X^j$$

$$X_L = X^a_L + \left[K^T_{L,n} \cdot S^{-1}_{\epsilon n,n} \cdot K_{n,L} + S^{-1}_{aL,L} \right]^{-1} \cdot K^T_{L,n} \cdot S^{-1}_{\epsilon n,n} \cdot (R_n - K_{n,L} \cdot X^a_L) \pm \delta X$$

NUCAPS FSR CO DOFs