Composition Products from Hyperspectral Thermal Sounders

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At the

2020 JPSS/GOES Proving Ground / Risk Reduction (PGRR) Summit

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STC Team: Nadia Smith, Rebekah Esmaili

Other Developers: STAR NUCAPS Team, NASA JPL, and NASA GSFC

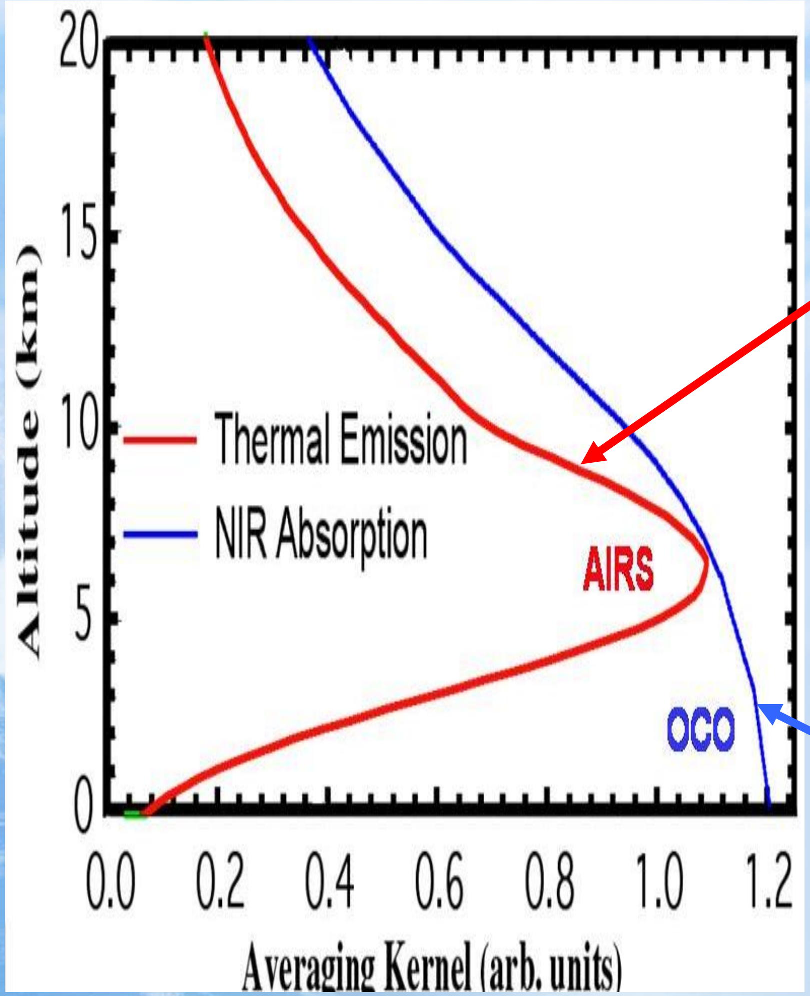
Past Developers: Wallace McMillan, Eric Maddy, Antonia Gambacorta …

Measurement Approaches

	Passive-Thermal	Passive-Solar	Active
Source Function	Planck Function	Sun	LASER
Measures	Mid-trop column	Total Column	Total Column/Profile
Sampling	Global, Day & Night	Global, Daytime	TBD
Interference	Strong interaction with T(p), q(p)	Weak interaction with T(p), q(p)	Very weak interference
Data availability	20+ years, launch almost guaranteed	Research grade, 2-3 mission, no follow-on	Future missions

- An excellent overview of instruments, methods, and status by Dave Crisp et al. “A constellation architecture for monitoring carbon dioxide and methane from space”
- http://ceos.org/document_management/Virtual_Constellations/ACC/Documents/CEOS_AC-VC_GHG_White_Paper_Version_1_20181009.pdf

Utilization of thermal product requires knowledge of vertical averaging



- Thermal instruments measure mid-tropospheric column
  - Peak of vertical weighting is a function of clouds, lapse rate and water and ozone content.
  - Age of air is on the order of weeks or months.
  - Significant horizontal and vertical displacements of the trace gases from the sources and sinks.
- Solar/Passive instruments (*e.g.*, SCIA, OCO) & laser approaches measure a total column average.
  - Mixture of surface and near-surface atmospheric contribution
  - Age of air varies vertically.

Space-borne operational hyperspectral *thermal sounders* to be discussed today

- We have 5 operational thermal sounder suites at this time

Satellite	Instruments	Overpass	Launch dates
Aqua	AIRS, AMSU	1:30 **	2002
Metop	IASI, AMSU, MHS	9:30	2008, 2012, …
S-NPP, JPSS	CrIS, ATMS	1:30	2011, 2017, …

- There are numerous differences in these sounding suites
  - **Instruments are different**
    - Spectra resolution, sampling and noise
    - Spatial sampling
    - Degradation over time
  - **Algorithm differences**
    - NOAA algorithms became operational ~1-2 year after launch and have asynchronous maintenance schedules (e.g., training datasets are different)
    - 9:30/1:30 orbits co-location w/ in-situ is different (affects tuning/regression training and makes validation more difficult)
  - **Sensitivity to a-priori assumptions**
    - Sensitivity to meteorology (e.g., clouds at 9:30 vs 1:30 am/pm)
    - Sensitivity to seasonal and climate changes (e.g., 8% increase in CO_2, 2002-2017)

Trace Gas products were not the primary design criteria of the modern satellite sounding suite

** in early 2022 Aqua will drop out of A-train // begins a 6 year drift to 5:30

At STC, we are attempting to bridge NASA and NOAA sounding development efforts

- Operational products are not as much fun as you think.
  - With limited funding we are attempting to satisfy all users with “one” algorithm.
- What we are doing: NASA AIRS v5.9 → R2O → NUCAPS → O2R → CLIMCAPS → R2O ?? → *NECAPS(GFS or HRRR)*

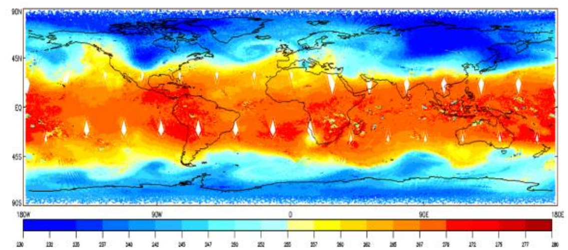
	NASA/CLIMCAPS	NOAA/NUCAPS
A-priori	Merra-2	Global regression (i.e.,model independent)
Error propagation	2-D covariance	Diagonal
Supported systems	S-NPP NSR & FSR running (4.5 years are done) NOAA-20 has begun Aqua begins this summer	Metop –A, -B, -C S-NPP, NOAA-2x Aqua (non-op, post A-train proposal by NASA/NOAA)
Latency	~1 month f/ MERRA	Real time (~30 minutes)
Averaging Kernels?	YES – fully supported	Not operational, but can provide via science code

Operational and experimental retrieval products

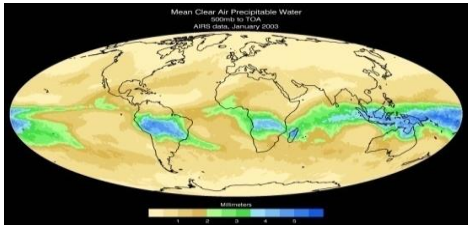
Supported profile products

Retrieval Product	Spectral Region(s)
Lower stratosphere / Upper Trop Ozone, $O_3(p)$	990 – 1070 cm^{-1}
Mid-tropospheric Carbon Monoxide, CO(p)	2155 – 2220 cm^{-1}
Mid-troposphere Methane, $CH_4(p)$	1220 – 1350 cm^{-1}
Mid-troposphere Carbon Dioxide, $CO_2(p)$	660 – 760, 980, 2200 – 2400 cm^{-1}

500 hPa Temperature



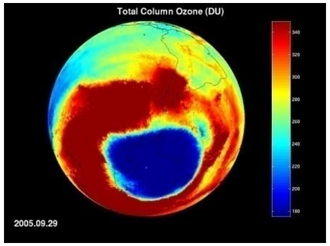
500 hPa Water Vapor



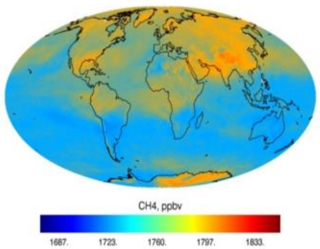
Experimental profile products

Mid-troposphere Nitric Acid, $HNO_3(p)$	760 – 1320 cm^{-1}
Lower-stratosphere Nitrous Oxide, $N_2O(p)$	1290 – 1300 cm^{-1} 2190 – 2240 cm^{-1}
Volcanic mid-tropospheric Sulfur Dioxide, $SO_2(p)$	1343 – 1383 cm^{-1}

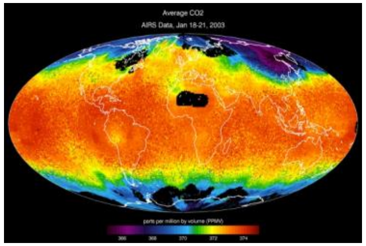
Ozone



Methane



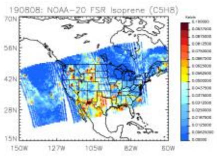
Carbon Dioxide



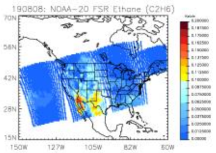
Noise filtered S-FOV detection flags

Isoprene (C5H8)	893.8 cm^{-1}
Ethane (C2H6)	822.5 cm^{-1}
Propylene (C3H6)	911.9 cm^{-1}
Ammonia (NH3)	966.25 + 928.75 cm^{-1}

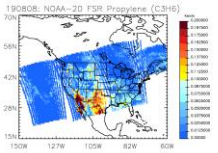
Isoprene



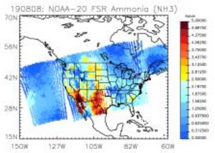
Ethane



Propylene



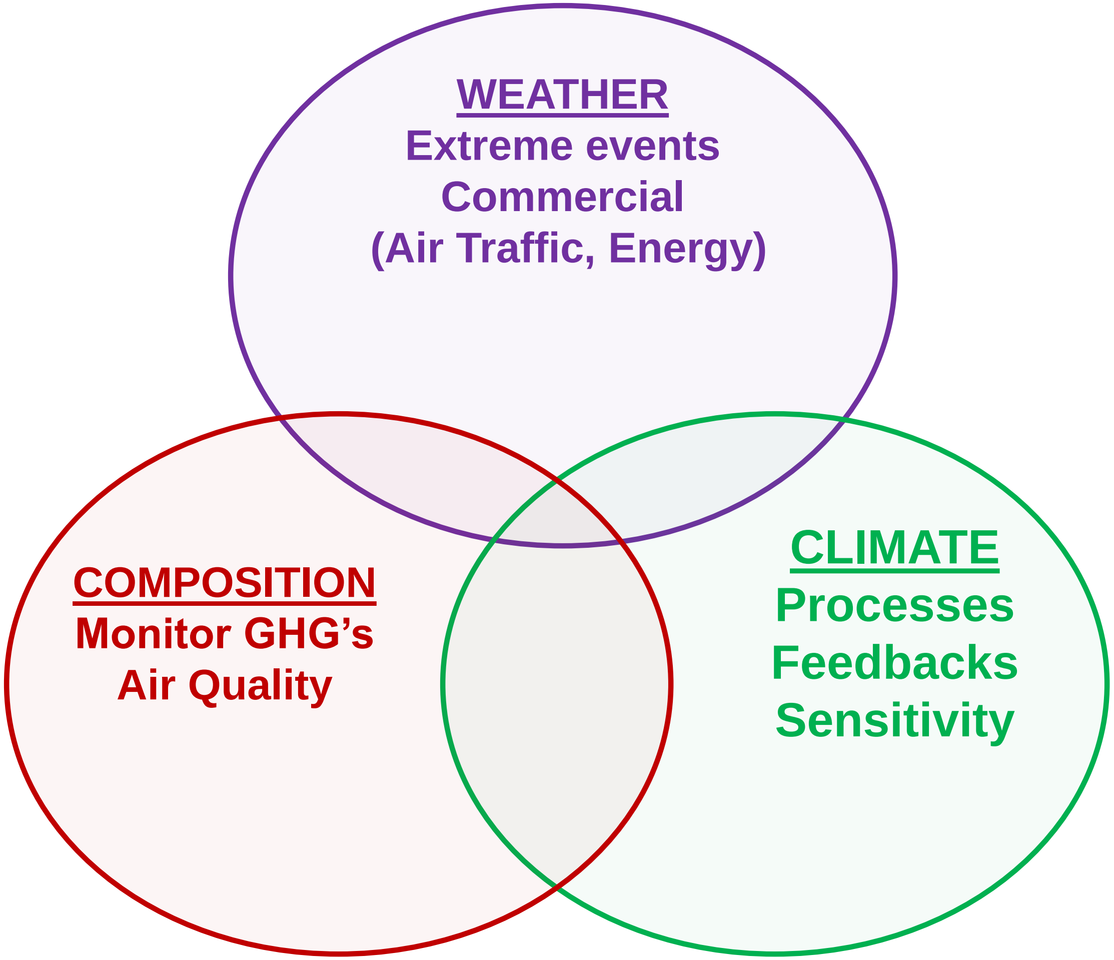
Ammonia



Relevant ROSES-TASNPP funded research activities at NASA – began 1.5y ago

- Larrabee Strow (UMBC) Climate anomalies of CO2, CH4, N2O, etc. from CrIS and AIRS
- Helen Worden (UCAR): Extend MOPITT Carbon Monoxide from CrIS + TROPOMI
- Karen Cady-Pereira (AER) and David Henze (U.Colorado): Ammonia retrieval and inverse modeling from CrIS
- Vivienne Payne: Peroxyacetyl Nitrate (PAN) retrievals from CrIS

Together these algorithms can ***contribute*** to the needs of three communities



Applications we are **NOT** targeting with NUCAPS & CLIMCAPS.

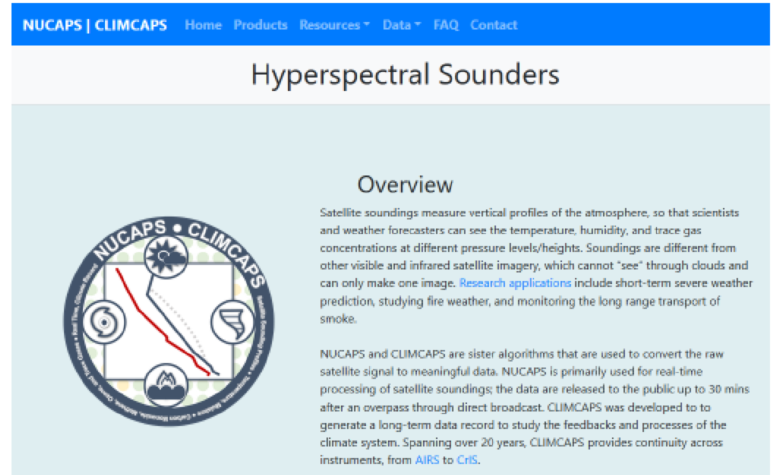
Topic	Potential applications for thermal sounding products
Long term trends	For GHG-relevant gases we have very low information content. We relax to a-priori assumptions so we only see ~50% of the signal. Large cross-talk between CO2/T, N2O/T, CH4/q, etc. Recommend using Larrabee Strow's radiance anomaly product for trends
GHG Monitoring	We have very low (and variable) sensitivity in the boundary layer. Need passive solar or active sensors to
High spatial resolution approaches	Clouds are still a major obstacle for infrared sounding. NU/CLIMCAPS are intended as global quick look products NU/CLIMCAPS can be used as "triggers" for more advanced algorithms could launch algorithms that are computationally expensive (e.g., NASA TASNPP or AC4 funded algorithms, MUSES, etc.)

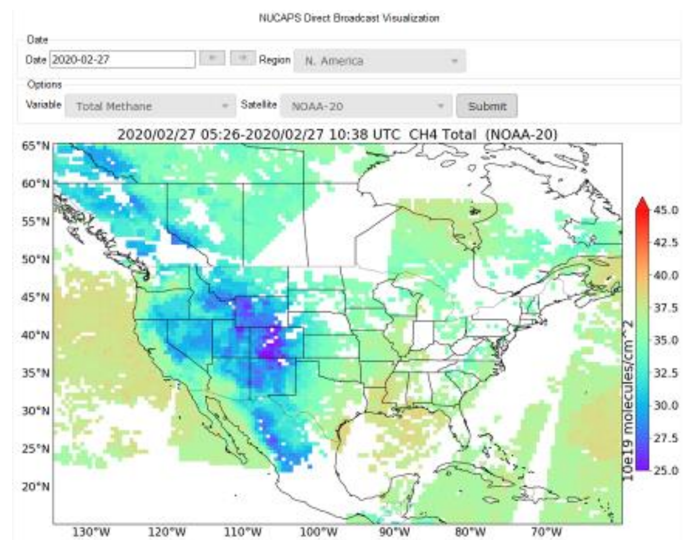
Applications we are targeting with NUCAPS & CLIMCAPS.

Topic	Potential applications for thermal sounding products
T(p), q(p) sounding and data assimilation	We require knowledge of CO2, O3, HNO3, N2O etc. to derive T(p) We require knowledge of CH4 to derive q(p)
GHG Monitoring	We enhance the boundary layer sensitivity of passive solar or active methods.
Ozone	Ozone hole; Intrusions and mid-trop O3 (Langford 2018 Atmos. Env); LS O3 trends (Ball 2018 ACP, Wargan 2018 GRL); CO/O3 ratio (Anderson 2016 Nat.Comm)
Carbon Dioxide (CO2)	Contribute to discussion of seasonal cycle amplitude (Barnes 2016 JGR), clear bias and diurnal “rectifier” effects (Corbin 2008 JGR), and stratospheric/troposphere CO2 gradient. Evaluation of transport models (mixing into mid-trop, etc.). Note that separability of T/CO2 is significantly improved with use of Merra-2 a-priori and with AMSU/ATMS O2 bands for T(p)
Carbon Monoxide	Long-term trends of CO (Worden 2013 ACP). Impact on OH (Gaubert 2017 GRL), Seasonal cycle (Park 2015 JGR) and CO/CO2 emission factors (Wang 2009 ACP)
Methane (CH4)	Monitoring of Amazon CH4 (Bloom 2016 ACP), Changes to Arctic emissions (Shakhova 2010 Science, Thornton 2016 GRL)
Other trace gases	Nitric Acid, Nitrous Oxide, Sulfur Dioxide, Isoprene, PAN, Acetylene, Methanol, etc Potentially useful as tracer-tracer correlations, emission ratios (errors tend to cancel), source type identification, etc.

More information

- Rebekah Esmaili and Emily Berndt (NASA/SPoRT) created a NUCAPS & CLIMCAPS landing site: https://weather.msfc.nasa.gov/nucaps
  - Product descriptions, data access, FAQ's and more
- Rebekah created a direct broadcast (real time) visualization page for selected NUCAPS products from CSPP: http://sigma.umd.edu/resmaili/nucaps.html
  - T, q, O3, CO, CH4, d.o.f., etc.



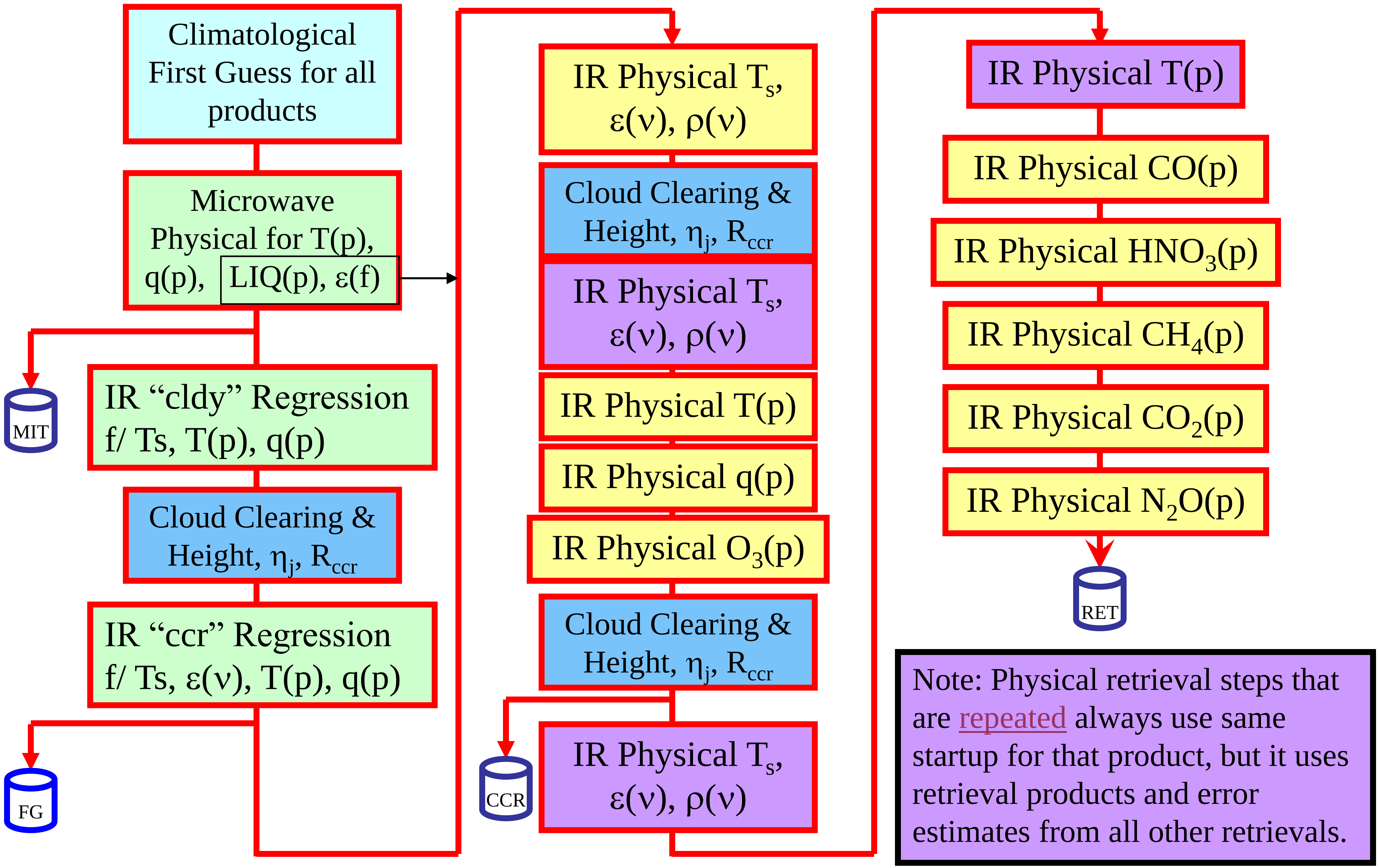


HOW WE TRY TO ADVANCE COMPOSITION PRODUCTS

- We have actively sought out partners to help us explore and characterize the value (or lack of value) of specific products (e.g., O3, CO, CH4)
  - Need user feedback on a-priori choices
- JPSS funds a project to characterize all NUCAPS trace gases (PI: Frost)
- I personally find scientific field campaigns the most valuable:
  - We learn about user-specific needs.
  - Users gain experience of our products and caveats.
  - Burst of development.
  - We can tailor our products to application needs.

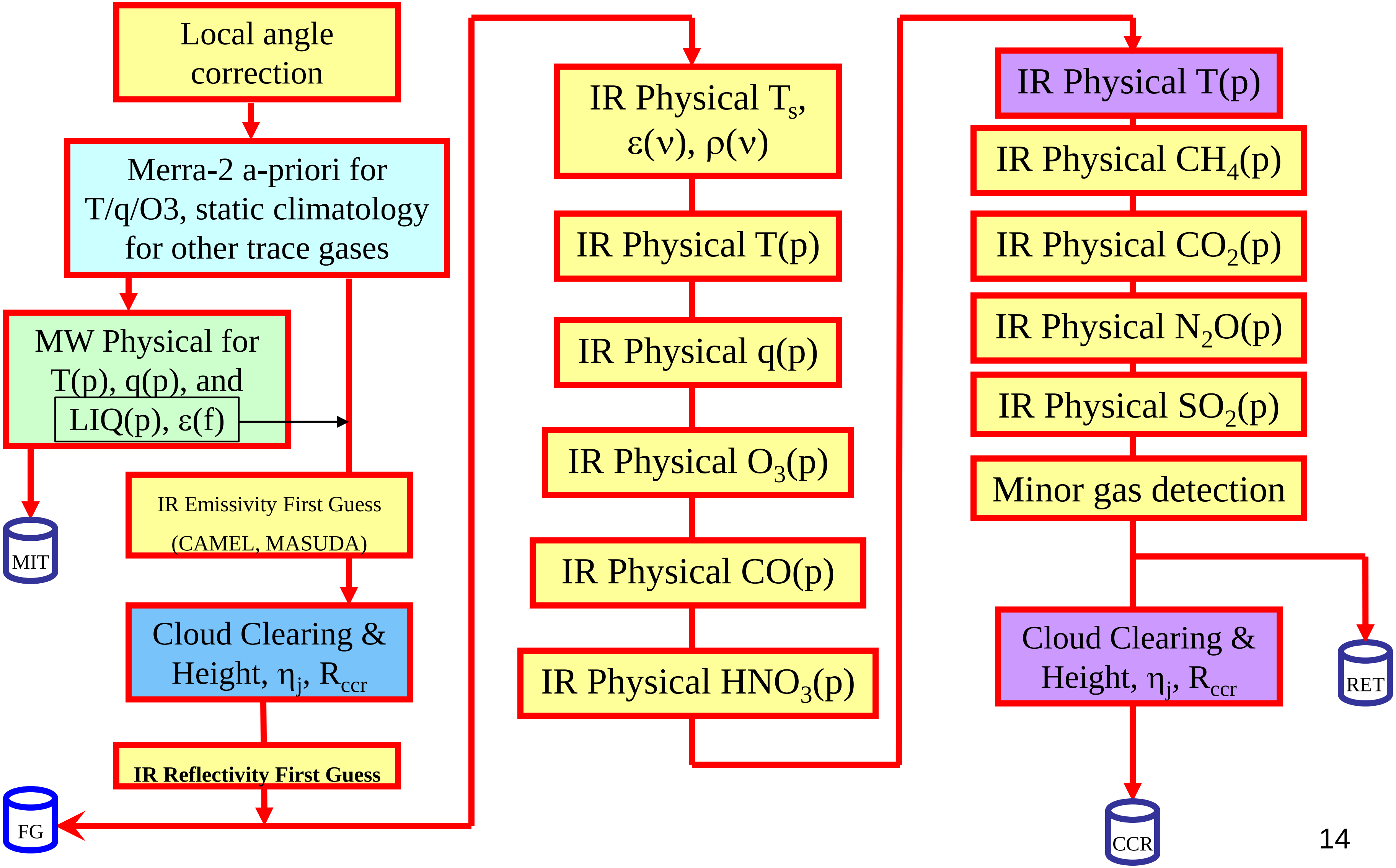
Link to CLIMCAPS algorithm paper:
https://www.mdpi.com/2072-4292/11/10/1227

Simplified Flow Diagram of the NUCAPS Algorithm (based on AIRS v5.9)

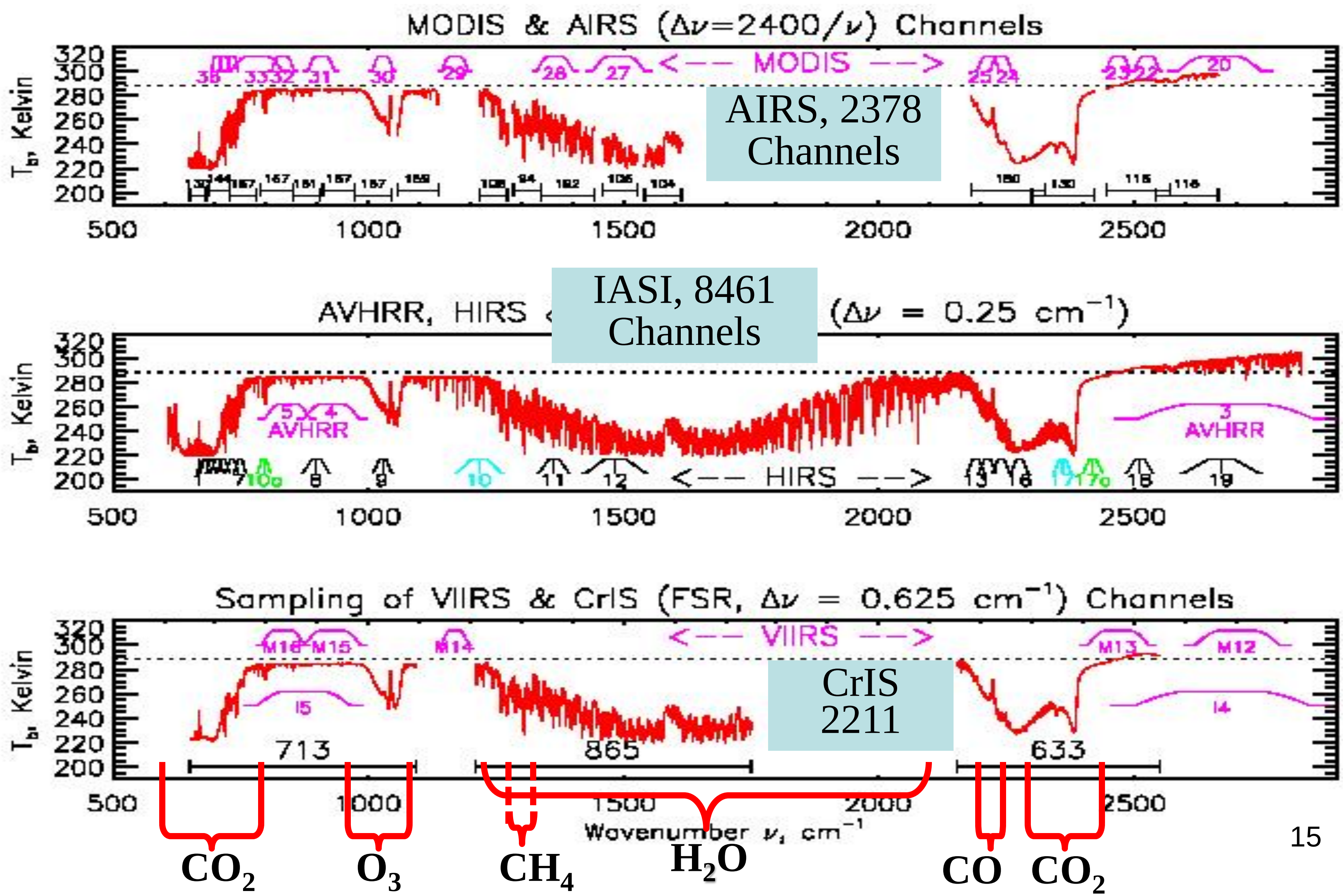


<u>Simplified</u> Flow Diagram of the CLIMCAPS Algorithm

Note: <u>Repeated</u> steps use same a-priori, w/ updated error estimates from other steps.

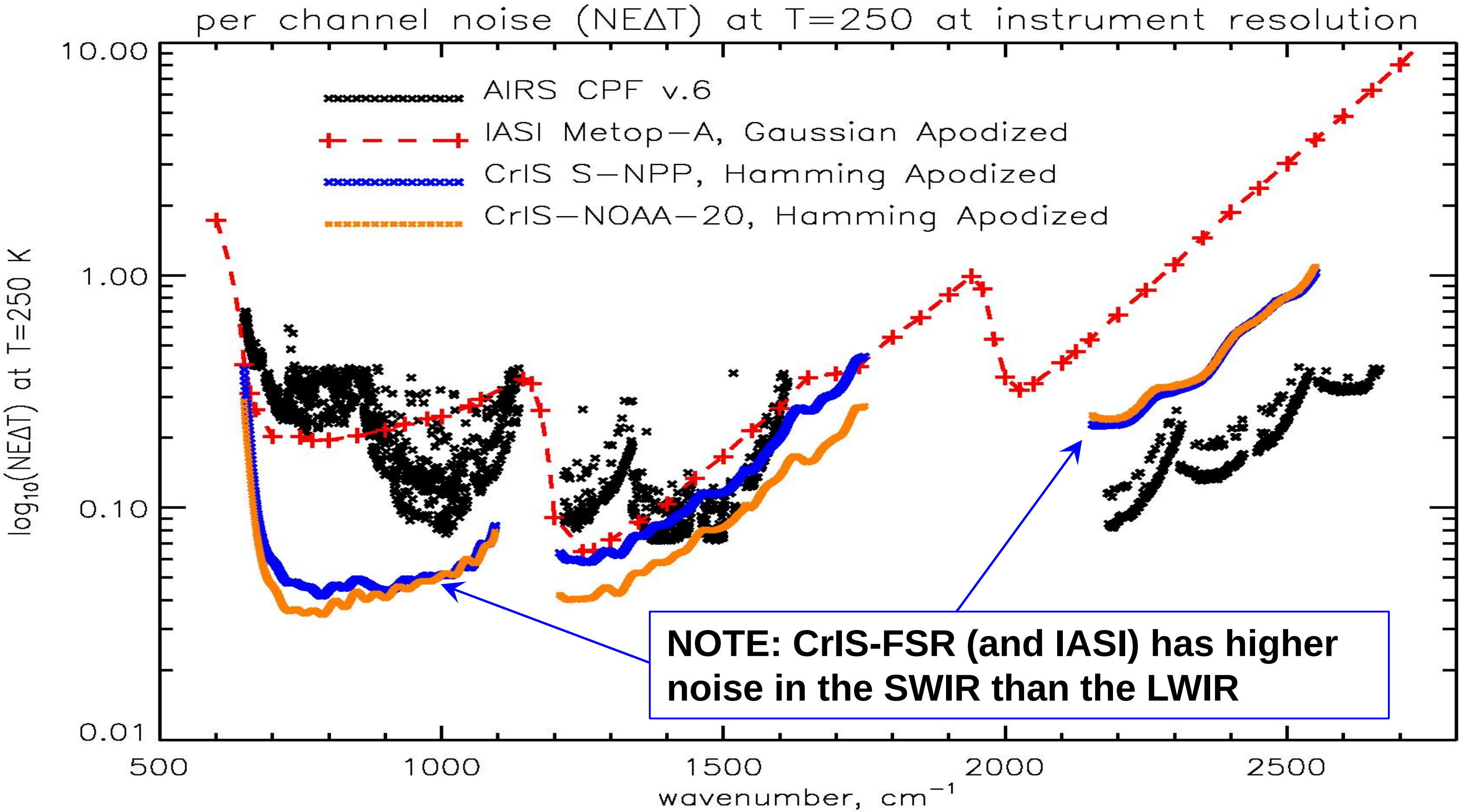


Spectral Coverage of Thermal Sounders & Imagers (Aqua, Metop-A,B,C, Suomi-NPP, NOAA-20+)



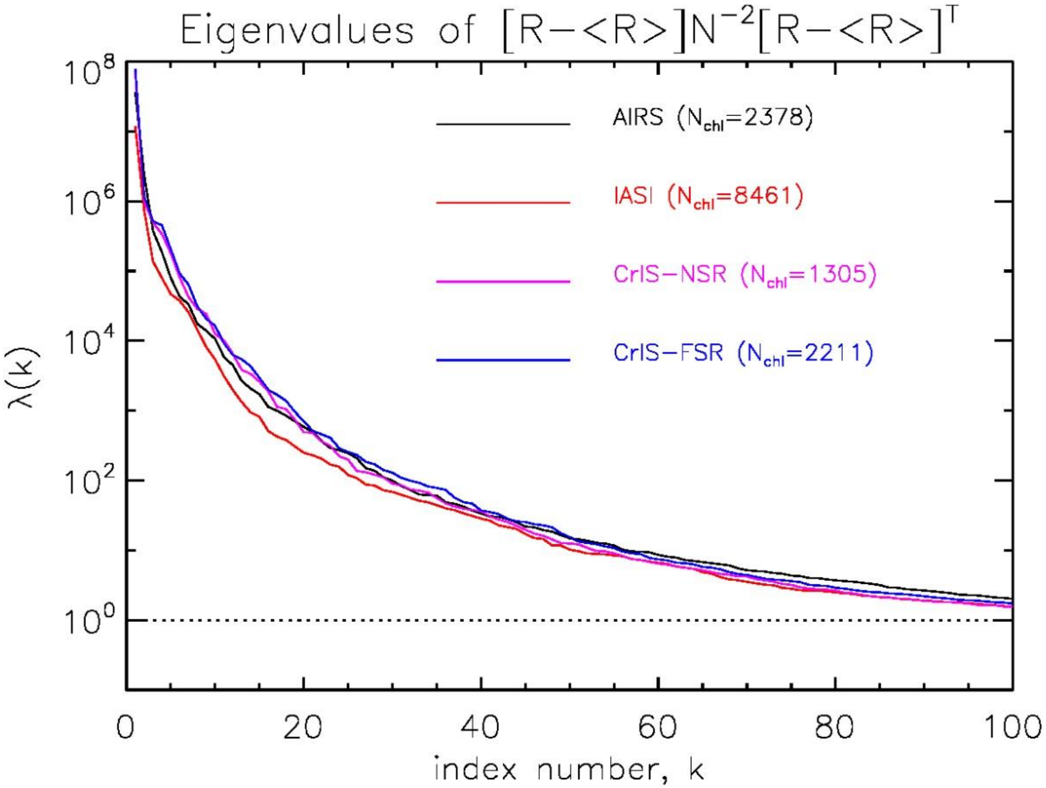
What is important for sounding is signal to noise

Per channel noise is shown as noise equivalent delta temperature (NEΔT) at a cold scene temperature (T=250 K)



The information content of modern sounding instruments is ***amazingly*** similar

- AIRS, IASI, and CrIS each have ~100 degrees of freedom
- Even though AIRS, IASI, and CrIS have different number of channels, ILS, noise, etc.



The 1st 100 significant eigenvectors of radiance covariance for a set of focus days normalized at λ(k=200)

Choosing the cross-over points for Aqua, S-NPP, NOAA-20 and beyond