Calcon Workshop: Current Challenges in the Remote Sounding of the Earth

1. Introduction to Remote ***Sounding***

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Topics for Today

- Workshop will have 3 sections
  1. Introduction to Remote Sounding
  2. Example of operational sounding: NUCAPS, CLIMCAPS, and NECAPS
  3. Applications and future sounders.
- Each section will consist of
  - ~40 minute lecture
  - ~15 minutes Q&A
  - ~5 minute bio break

A comment on the presentation itself.

- These slides have a lot more information on them than I plan to discuss.
- In addition, there are many slides that I will skip over today.

Why?

- This is a complex topic and I believe you need to approach it in multiple passes.
- My presentation will be the 1st pass.
- The slides are available when you are interested and ready for the 2nd pass.

And I have detailed ***notes*** for when you are ready for the 3rd pass

NOTES, used in teaching at UMBC: Remote Sounding (phys741) and Computational Physics (phys640, sections on apodization & least squares)

~/rs_notes.pdf (~17.5 MB)

~/phys640_s04.pdf (~8.8 MB)

These are ***living*** notes, or maybe even a scrapbook

– they are not textbooks.

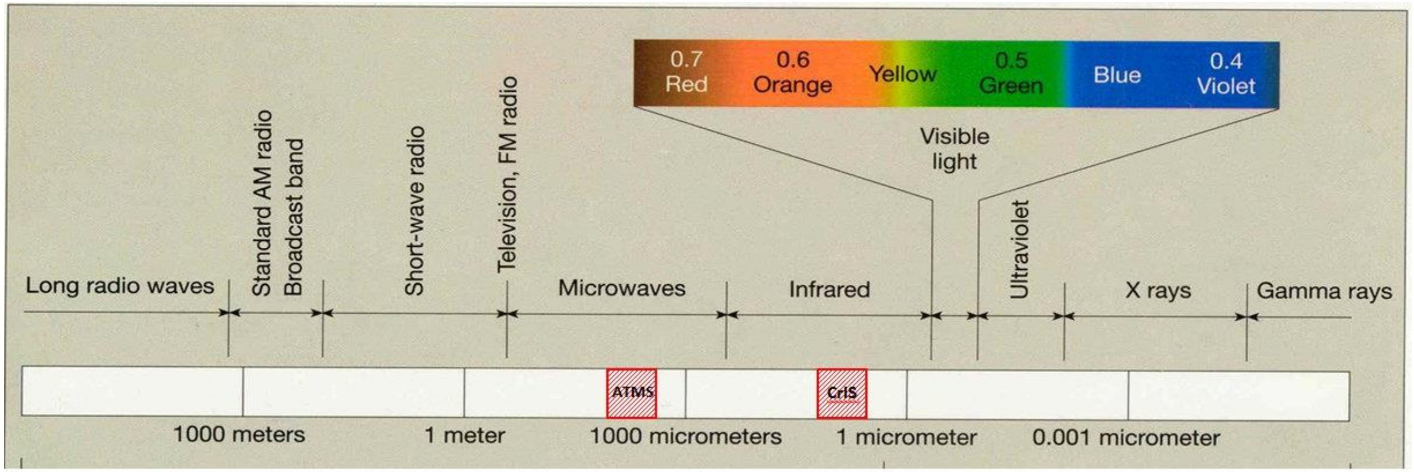
Available at this Google drive short link: **http://goo.gl/twuRtW**

What do *I mean* by Satellite Sounding?

- Remote ***sensing***: looking at something
- Remote ***sounding***: looking through something to infer its contents – analogy to sonar.
- A satellite ***active*** sounding instrument carries its own energy source (LASER, etc.) and "pings" the atmosphere.
- A satellite ***passive*** sounding instrument measures the top of atmosphere (TOA) radiance (energy) through the atmosphere using the Earth radiation (*thermal*) or reflected *solar* radiation.
- A satellite "sounding" is the literal ***inversion*** (a.k.a. *retrieval*) of the satellite measurements

Review: Infrared and microwave frequency scales

- Infrared traditionally measured in wavenumbers in inverse centimeters: $\nu(\text{cm}^{-1}) = 10000/\lambda(\mu\text{m})$
  - $\nu \equiv f/c$
    - f = frequency in Hertz (or s^{-1})
    - c = speed of light = 2.9979×10^{10} cm/s
- Microwave tends to be measured in frequency units (GHz = 10^9 Hertz): $f(\text{GHz}) = 300/\lambda(\text{mm})$



Micrometer = μm

Millimeter = mm

Rotational **Vibrational** **Electronic** **Nuclear**

Review: The Planck Function

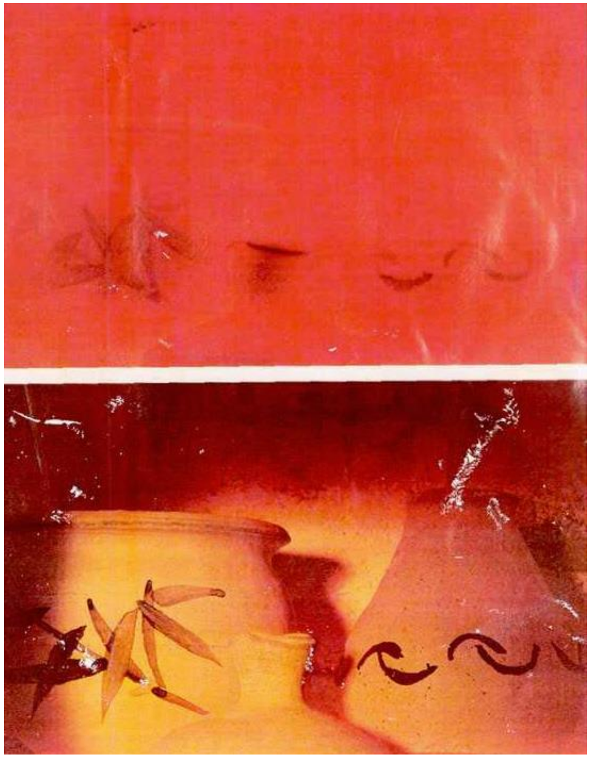
- The Planck function represents the radiance as a function of frequency from an object or gas at a given temperature in local *thermodynamic equilibrium (LTE)*

$$T_{kinetic} = T_{radiative} = T_{vibrational} = T_{rotational}$$

- It can be written in terms of wavenumber, υ, or wavelength, λ , as

$$B_\nu(T) = \frac{2 \cdot h \cdot c^2 \cdot \nu^3}{e^{\frac{h \cdot c \cdot \nu}{k \cdot T}} - 1}$$

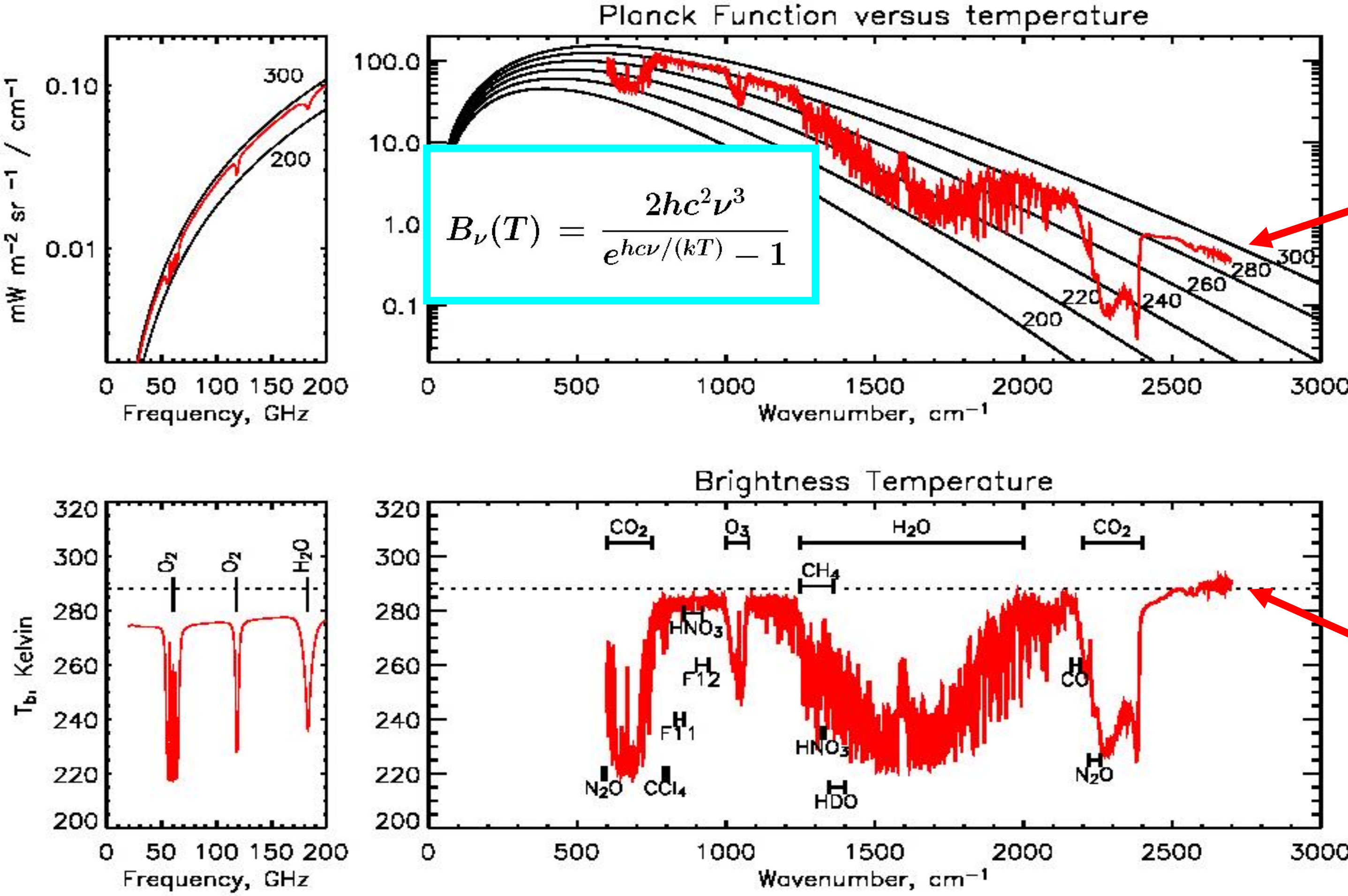
$$B_\lambda(T) = \frac{2 \cdot h \cdot c^2}{\lambda^5 \cdot \left(e^{(hc/\lambda kT)} - 1\right)}$$



Example of pottery in a kiln, lower panel, at low T, is not in thermal equilibrium.
Upper panel, at high T, is nearing thermal equilibrium.

Review: Instruments measure radiance

(energy/time/area/steradian/frequency-interval)



$$B_\nu(T) = \frac{2hc^2\nu^3}{e^{h c \nu/(kT)} - 1}$$

This is what we measure and how we use the data.

This is how we usually show it.

Convert to Brightness Temperature = Temperature that the Planck Function is equal to measured radiance at a given frequency.

Radiative equilibrium is an extremely important concept

- It means we can infer molecules hitting your skin (and other molecules, $T_{kinetic}$) from measurements of how the molecules are vibrating, $T_{vibrational}$ and rotating ($T_{rotational}$).
- In equilibrium they are all equal.
- How we feel is also a function of the moisture content. Why?
  - Moisture affects the down-welling radiation.
  - Which we can measure by discriminating water vibrations from other gas vibrations (e.g., CO_2, N_2O) and rotations (O_2 at 57 GHz).

How does sounding differ from data assimilation (DA)?

- Both DA and retrievals measure what is happening in the here and now and aid forecasting what will happen in the near future.
  - We are trying to measure things like temperature, moisture, UV-B radiation, and many other things that impact our daily lives.
- DA uses a collection of measurements and models of dynamics (conservation of energy, momentum, and continuity) to *forecast* the geophysical state into the near future.
  - It is a blending of model and *all* measurements – including multiple satellites, multiple instrument types and also in-situ observations
  - Requires parameterization of complex geophysical processes (e.g., convection, cloud condensation, etc.).
- In sounding, we use exactly the same equations as the DA *analysis* but we attempt to *invert* the measurements directly to the geophysical state without knowledge of underlying dynamics.
  - We require observations to be co-located in time and space
  - Both DA and Sounding require the ability to model the radiative transfer – i.e., the forward model (a.k.a. observation operator).

Data Assimilation versus Retrieval

Data Assimilation	Sounding
In practice, a spectral subset (10%), spatial subset (5%), and clear subset (5%) of the hyperspectral infrared observations are made.	All instrument channels can be used to minimize a larger number of parameters (T, q, O_3, CO, CH_4, CO_2, clouds, etc.)
Instrument error covariance is usually assumed to be diagonal. For apodized radiances (*e.g.* IASI) adjacent channels must be avoided.	Retrieval can be done in stages (most linear first). Product error covariance has vertical, spatial, and temporal off-diagonal terms.
Require very fast forward model, and derivative of forward model.	Most accurate forward model is used with a model of detailed instrument characteristics.
Tendency to weight the instrument radiances lower (due to representation error) to stabilize the model. Use correlation lengths to stabilize model horizontally, vertically, and temporally.	Retrieval can exploit a-priori information in the forward model and minimize assumptions about geophysical a-priori. Representation error is zero since retrieval is along slant path.
On any given iteration the satellite radiances have a small impact. Assumption is that the satellite observations will continually knudge the system towards the correct state.	Retrieval maximizes the utilization of the radiances of a single satellite. Promotes better understanding of the potential value of that satellite.

Remote Sounding: Estimating the Geophysical State from the Radiances

Excellent Textbooks on this topic are:

1. **Rodgers, C.D. 2000. Inverse methods for atmospheric sounding: Theory and practice. World Scientific Publishing 238 pgs.**
2. **Hanel, R.A., B.J. Conrath, D.E. Jennings and R.E. Samuelson 1992. Exploration of the solar system by infrared remote sensing. Cambridge University Press 458 pgs.**

How Do We Invert a Spectrum

Two types of sounding algorithm approaches

Regression

- Analogous to how we learn: our instinct, first impressions, pattern recognition, etc.
- Fast, can use all the information.

Physical

- Analogous to analyzing or understanding of the problem.
  - Reasoning, comparison to spectroscopic or geophysical models.
- Computationally intense.

But these two approaches are really mimicking how the human brain works.

- humans rely on instinct and experience
- but we temper that with objective reasoning.

Example of Catching a Ball

- When you learn to catch a ball, you are training your neural network.
  - It takes many hours to “learn” how to catch a ball.
- Imagine building a robot to catch a ball.
  - Requires programming equations of motion, gravity, and friction (drag) into a forward model.
    - Need to teach the robot human concepts like gravity, inertia, momentum, and conservation of energy.
  - The robot’s detectors (or radiances) are the eyes, but these are never perfect.
    - Optical illusions, glare, dust, shadows, etc.
    - And in baseball, it needs to sense what the pitcher is going to do to the ball (curve ball, etc.).

Quick Review of *my* notation for Linear Algebra

- Matrices will be written with dimensions, as subscripts to help in explanation: for example, $K_{n,j}$ is a 2-dimensional matrix of *n* rows and *j* columns, *K(n,j)*
- The transpose($K_{n,j}$) is written as $K_{j,n}^T$, and is a matrix of *j* rows and *n* columns, *K(j,n)*

- The order of multiplication is by columns then rows such that the products are

$$X_{j,j} = K_{j,n}^T \cdot K_{n,j} \quad or \quad Y_{n,n} = K_{n,j} \cdot K_{j,n}^T$$

- *A weighted, W(n,n), vector, y(n), can have two forms: a scalar or a covariance*

$$J = y_n^T \bullet y_n \quad or \quad C_{n,n} = y_n \bullet y_n^T$$

Review: Traditional Least Squares

- A linear system of *n* equations of an observable, y_n, and a model, $K_{n,j}$, can be expressed as follows

$$\boldsymbol{y}_n = \boldsymbol{K}_{n,j} \cdot \boldsymbol{x}_j + \boldsymbol{\epsilon}_n$$

- An unconstrained least squares fit, when $n > j$, can be found by simple inversion of $K_{n,j}$

$$\boldsymbol{x}_j = \boldsymbol{K}_{j,n}^{-1} \cdot \boldsymbol{y}_n$$

- Where the inverse of an asymmetric matrix is given by:

$$\begin{aligned} \boldsymbol{K}_{n,j} \cdot \boldsymbol{K}_{j,n}^{-1} &= \boldsymbol{I}_{n,n} \\ \boldsymbol{K}_{j,n}^{T} \cdot \left(\boldsymbol{K}_{n,j} \cdot \boldsymbol{K}_{j,n}^{-1}\right) &= \boldsymbol{K}_{j,n}^{T} \cdot \boldsymbol{I}_{n,n} \\ \left(\boldsymbol{K}_{j,n}^{T} \cdot \boldsymbol{K}_{n,j}\right) \cdot \boldsymbol{K}_{j,n}^{-1} &= \boldsymbol{K}_{j,n}^{T} \end{aligned}$$

$$\boldsymbol{K}_{j,n}^{-1} = \left[\boldsymbol{K}_{j,n}^{T} \cdot \boldsymbol{K}_{n,j}\right]^{-1} \cdot \boldsymbol{K}_{j,n}^{T}$$

Example of LSQ #1: Polynomial
(see *phys640_s04.pdf* Chap.13 for more details)

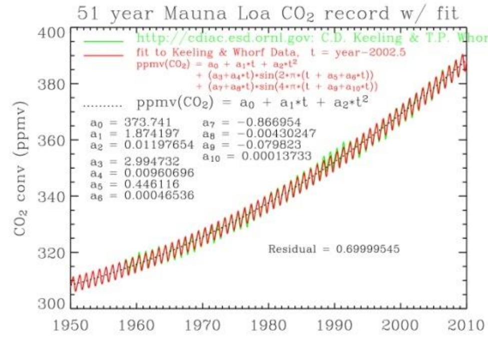
- For example, if the desired fitting equation (i.e., model) is a polynomial given by

$$y_n(t_n) = x_0 + x_1 \cdot t_n + x_2 \cdot t_n^2 + \ldots$$

- Then $K_{n,j}$ is given by

$$K_{n,j} = \begin{pmatrix} 1 & t_1 & t_1^2 & \ldots \\ 1 & t_2 & t_2^2 & \ldots \\ \ldots & \ldots & \ldots & \ldots \\ 1 & t_n & t_n^2 & \ldots \end{pmatrix}$$

Example of LSQ #2: Polynomial + sine function (see *phys640_s04.pdf* Chap.13 for more details)



- Suppose we wanted to fit an oscillating function (e.g., the Mauna Loa measurement of $CO_2(t)$). The fitting function could be given by

$$\begin{aligned} y_n(t_n) &= x_0 + x_1 \cdot t_n + x_2 \cdot t_n^2 + b_0 \cdot \sin\left(b_1 \cdot t_n + b_2\right) \\ &= x_0 + x_1 \cdot t_n + x_2 \cdot t_n^2 + x_3 \cdot \sin\left(b_1 \cdot t_n\right) + x_4 \cdot \cos\left(b_1 \cdot t_n\right) \\ & \quad \text{where} \quad x_3 = b_0 \cdot \cos(b_2) \quad \text{and} \quad x_4 = b_0 \cdot \sin(b_2) \end{aligned}$$

- And $K_{n,j}$ is given by

$$K_{n,j} = \begin{pmatrix} 1 & t_1 & t_1^2 & \sin(b_1 \cdot t_1) & \cos(b_1 \cdot t_1) \\ 1 & t_2 & t_2^2 & \sin(b_1 \cdot t_2) & \cos(b_1 \cdot t_2) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & t_n & t_n^2 & \sin(b_1 \cdot t_n) & \cos(b_1 \cdot t_n) \end{pmatrix}$$

$$b_0 = \sqrt{x_3^2 + x_4^2} \quad \text{and} \quad b_2 = \tan^{-1}\left(\frac{x_4}{x_3}\right)$$

Details of Statistical Retrievals

(a.k.a., regression, neural networks, interpretable machine learning)

Regression:

- A regression is where we attempt to derive a relationship from the observations themselves

$$X = f\{R\}$$

- We usually do this by taking a large training ensemble of J scenes, that represents everything we expect to see.

$$X(j,L) = f\{R(j,n)\}$$

- We need to know the “truth” of the L items we want to retrieve for each case of N observations R(j,n)

Statistical Regression Retrievals
(see Goldberg et al. 2003)

- Statistical eigenvector regression uses J_e observed spectra (on a subset of M "good" channels) to compute eigenvectors.
- We usually use signal to noise, $\theta_{m,j} = R_{n(m),j}/NEDN_{n(m)}$ to improve numerical accuracy and stability
- The spectral radiance for scene j, the radiance, $R_{n(m),j}$, can then be represented as principal components, $P_{k,j}$

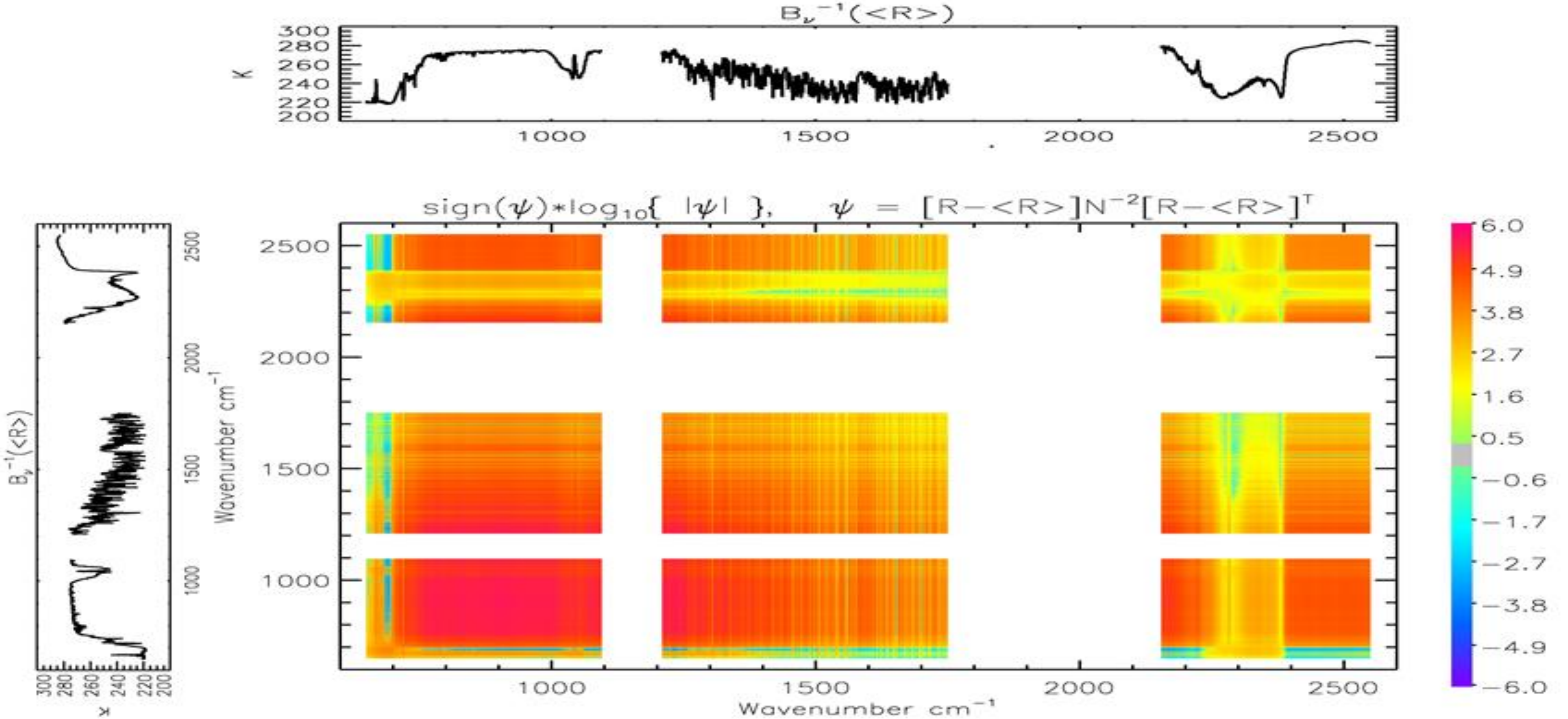
$$\Delta\tilde{\Theta}_{m,j} \equiv \frac{R_{n(m),j}}{\mathrm{NE\Delta N}_{n(m)}} - < \tilde{\Theta}_{m,j} >_{J_e}$$

$$P_{k,j} = \frac{1}{\sqrt{\lambda_k}} \cdot E_{k,m} \cdot \Delta\tilde{\Theta}_{m,j}$$

- Where the eigenvectors are determined using a couple of days of satellite (cloudy) radiances by solving for $\lambda_k \equiv \mathrm{trace}(\lambda_{kk})$ and $E_{m,k}$

$$\lambda_{kk} = E_{k,m} \cdot (\Delta\theta_{m,j} \Delta\theta^T_{j,m}) \cdot E^T_{m,k}$$

Example of the computation of $<R_{n(m)}>_j$ and $R \cdot R^T$ for a large <u>global</u> ensemble



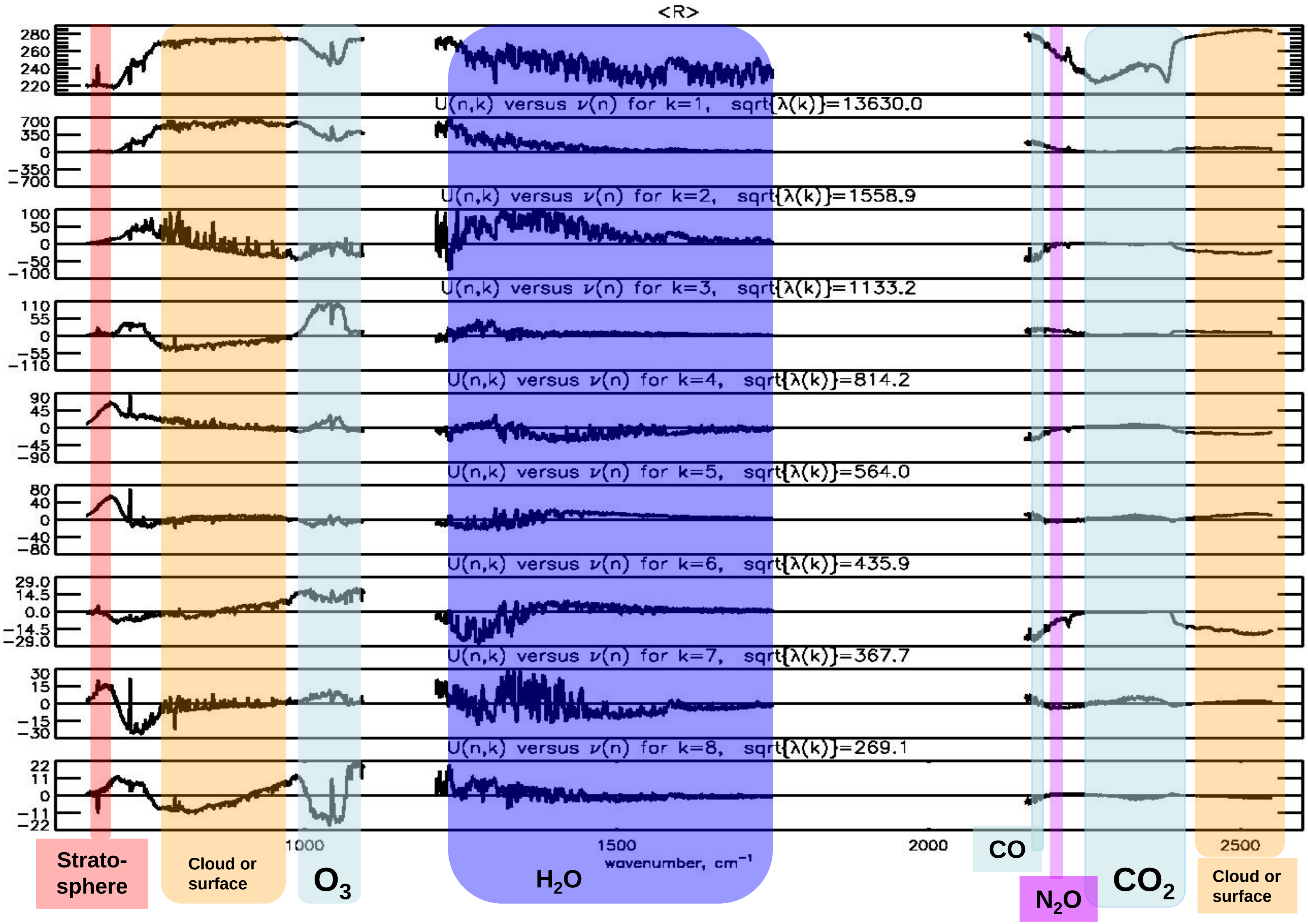
"Checkerboard" pattern results from spectroscopic redundancy within the spectrum (lines that sample same vertical region or gas)

667 cm^{-1} (stratospheric) is anticorrelated with tropospheric channels – this is meteorology, not spectroscopy

15 μm band (680-720 cm^{-1}) and 4.3 μm band (2390-2410 cm^{-1}) covary (measure same thing)

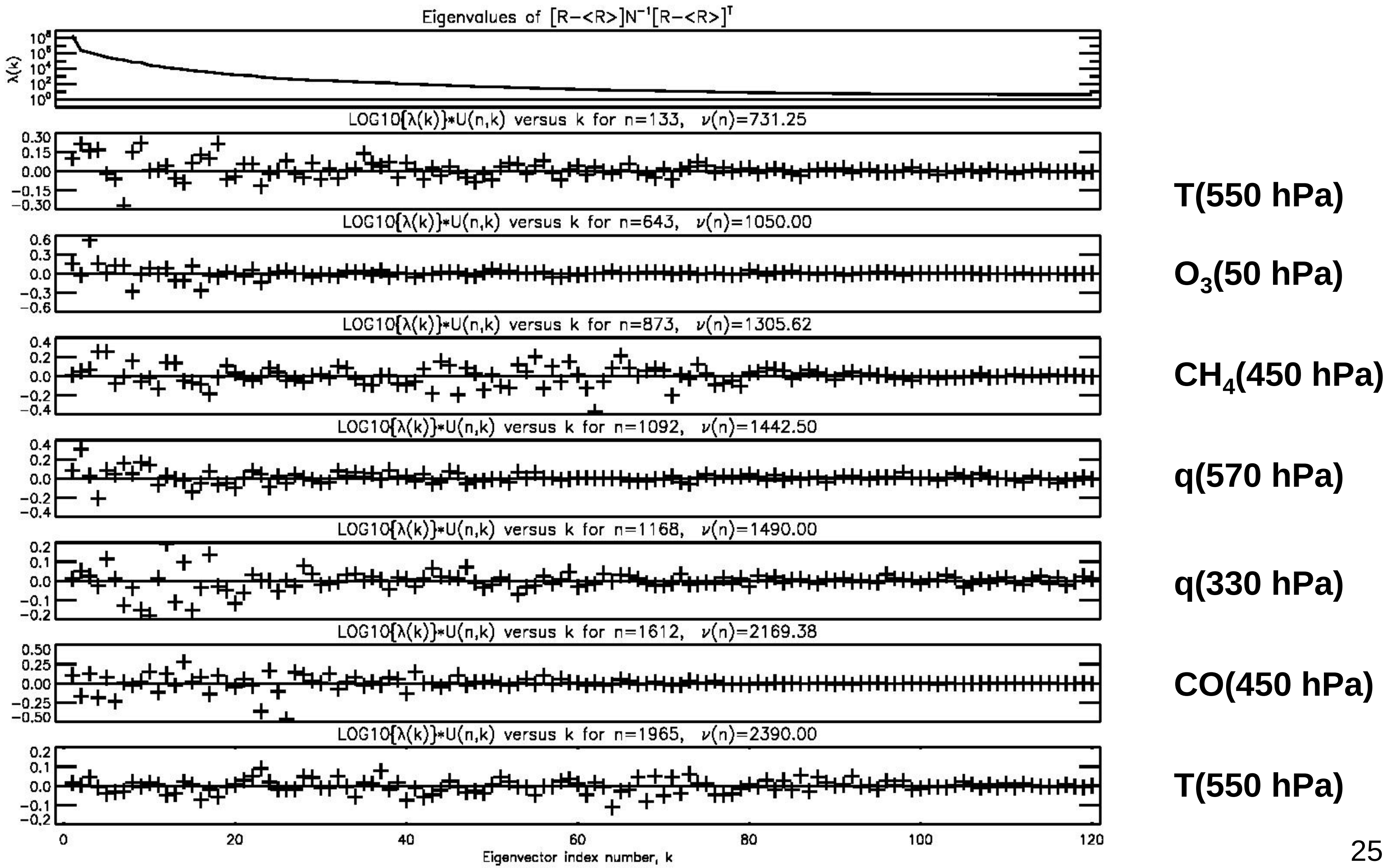
$E_{k,m}$ vs. $\upsilon(m)$ for k=1, 8

(see 200511npp_fsr_all_new_eig_plot.pdf for k=1,160)

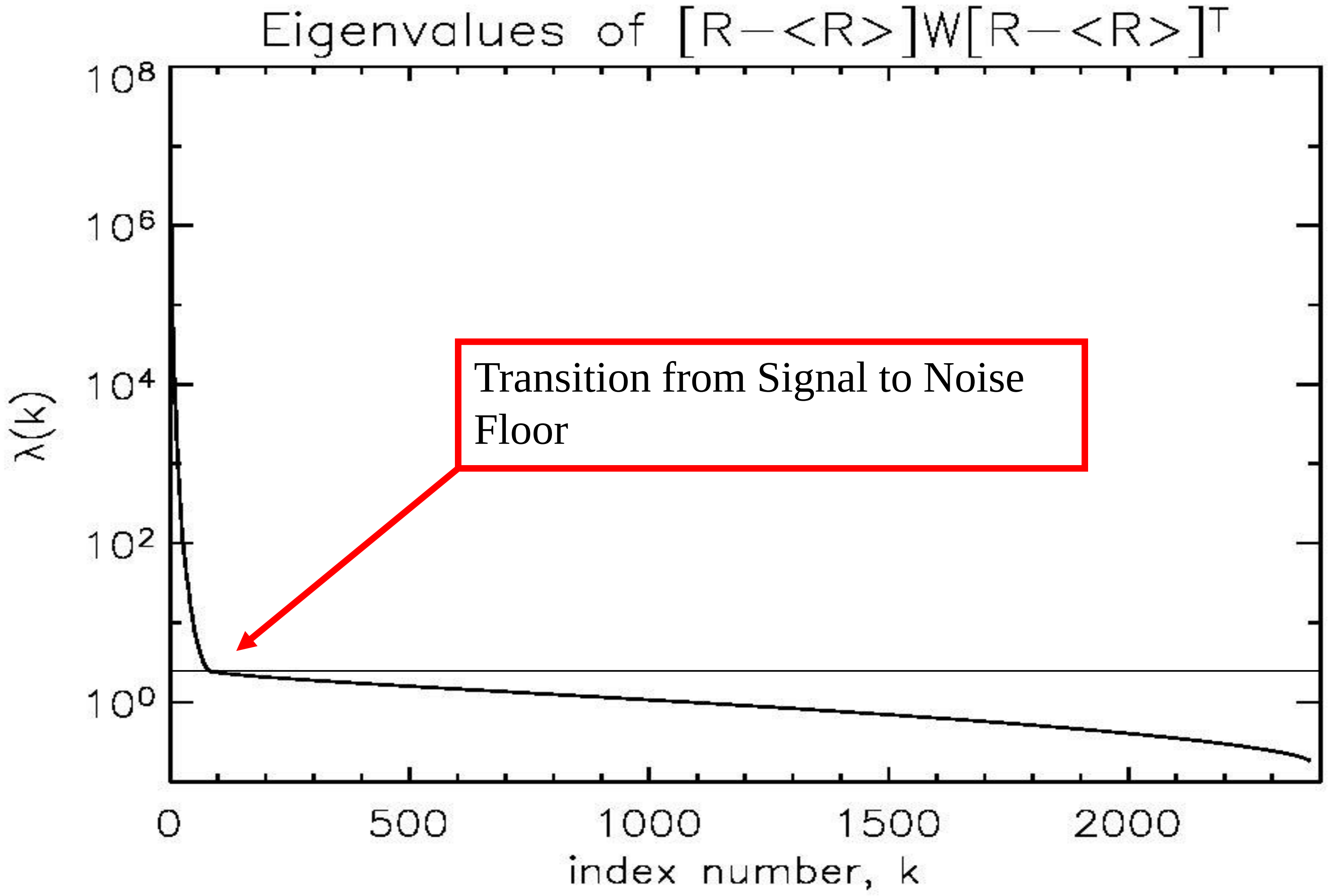


E_{km} vs k for selected channels

NOTE: scaled by *log10(λ(k))* to highlight high *k* values

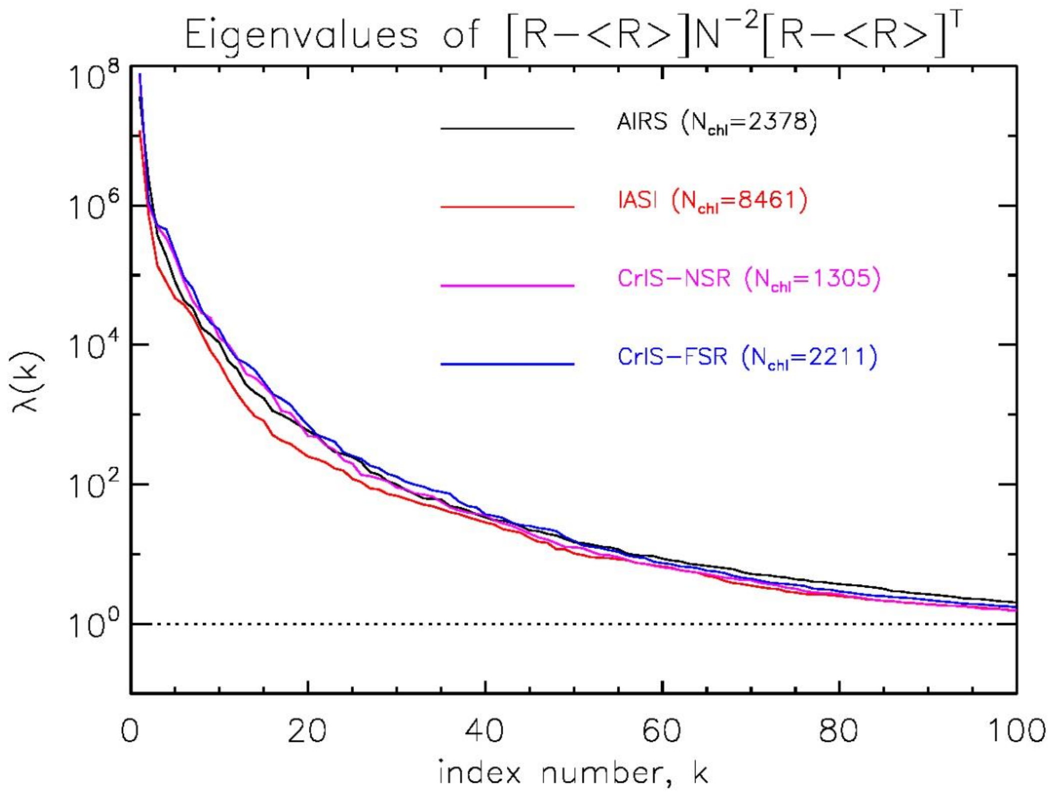


Information Content of AIRS (N = 2378): Eigenvalues of RR^T



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 channel and different noise.



The 1st 100 significant eigenvectors from the operational NUCAPS regression training normalized at $\lambda(k=200)$

Statistical Regression Retrievals (continued)

- A regression, $A_{i,k}$, between a "truth" state parameter ***i***, $\boldsymbol{X_{i,j}}$ (e.g., ***T(i), log(q(i))***, and principal components (centered about mean of ensemble) can be computed.

$$X_{i,j} = < X_{i,j} >_{J_r(v,L)} + A^v_{i,k} \cdot \Delta P_{k,j}$$

- Truth states for scene(s), ***j***, are difficult to come by. We can use models (e.g., ECMWF), radiosondes, etc.
- The equation above is solved by linear least squares.
  - Since it uses a truncated set of principal components (AIRS Science Team Approach uses 85/1600) the inversion has removed observational noise and is "regularized"
- $\boldsymbol{A^v_{i,k} \bullet P_{k,j}}$ can be interpreted as empirical channel weighting functions for parameter group ***i*** and scene ***j***
  - Its inverse is the spectral fingerprint of a parameter $\boldsymbol{X_{i,j}}$

Pro's and Con's Of Statistical Regression Retrievals

Pro's	Con's
Does not require a radiative transfer model for training or application.	Training requires a large number of co-located "truth" scenes for every possible state of the atmosphere.
Application of eigenvector & regression coefficients is VERY fast and for hyper-spectral instruments it is very accurate.	The regression operator cannot provide meaningful error estimates and will degrade rapidly for scenes not in training.
If real radiances are used the regression implicitly handles many instrument calibration (e.g., spectral offsets) issues. This is a huge advantage early in a mission and can provide early diagnostics.	The regression answer builds in correlations between geophysical parameters. For example, anything that co-varies with the radiances – including things we cannot not measure.
Since clouds are identified as unique eigenvectors, a properly trained regression tends to "see through" clouds.	Very difficult to assess errors in a regression retrieval without the use of a physical retrieval.

Lessons Learned About Regressions

1. We initially tried regressions for trace gases.
   - Ozone (O_3) worked great, ***too great***.
   - Upon analysis (interrogation of the coefficients) we learned ozone was mostly derived from carbon monoxide and tropopause sensitive channels.
     - Ozone is created by CO, CH_4 emissions – SOMETIMES!
     - Ozone is also affected by dynamics (tropopause height).
2. In 2003 the Etna volcano erupted and caused dramatically bad results.
   - The regression had never "seen" sulfur dioxide, SO_2.
     - T(p) and q(p) regressions extrapolated its training to ***dramically physically implausible*** results.

Physical Retrievals

(a.k.a., optimal estimation, 1D-VAR)

What is a physical retrieval.

Think about when you go into the city to an event.

- Maybe you talk with friends or check out google maps before go (this is a-priori information)
- But then you want to update that with traffic information, road closures, etc. (observations)
- Finally you get there, and you look signs, people dressed a certain way, etc. (a mixture of a-priori expectations and observations).
- You are *iterating* towards a solution.
  - But sometimes, you fail to find your destination (wrong information, etc.). You need to be able to adjust your thinking for next time.

Quick Review: Unconstrained Least Squares (LSQ) retrieval

- For non-linear LSQ $K_{n,j}$ is a function of the state parameters, x_j

$$\begin{aligned}(y_n - K_{n,j}\cdot x_j) &= \frac{\partial y_n}{\partial x_j}\cdot \Delta x_j \\ &= K_{n,j}\cdot \Delta x_j\end{aligned}$$

- We can weight the observations

$$\begin{aligned}W_{n,n}\cdot(y_n - K_{n,j}\cdot x_j) &= W_{n,n}\cdot K_{n,j}\cdot \Delta x_j \\ K_{j,n}^T\cdot W_{n,n}\cdot(y_n - K_{n,j}\cdot x_j) &= K_{j,n}^T\cdot W_{n,n}\cdot K_{n,j}\cdot \Delta x_j\end{aligned}$$

- The solution can be written in an iterative form

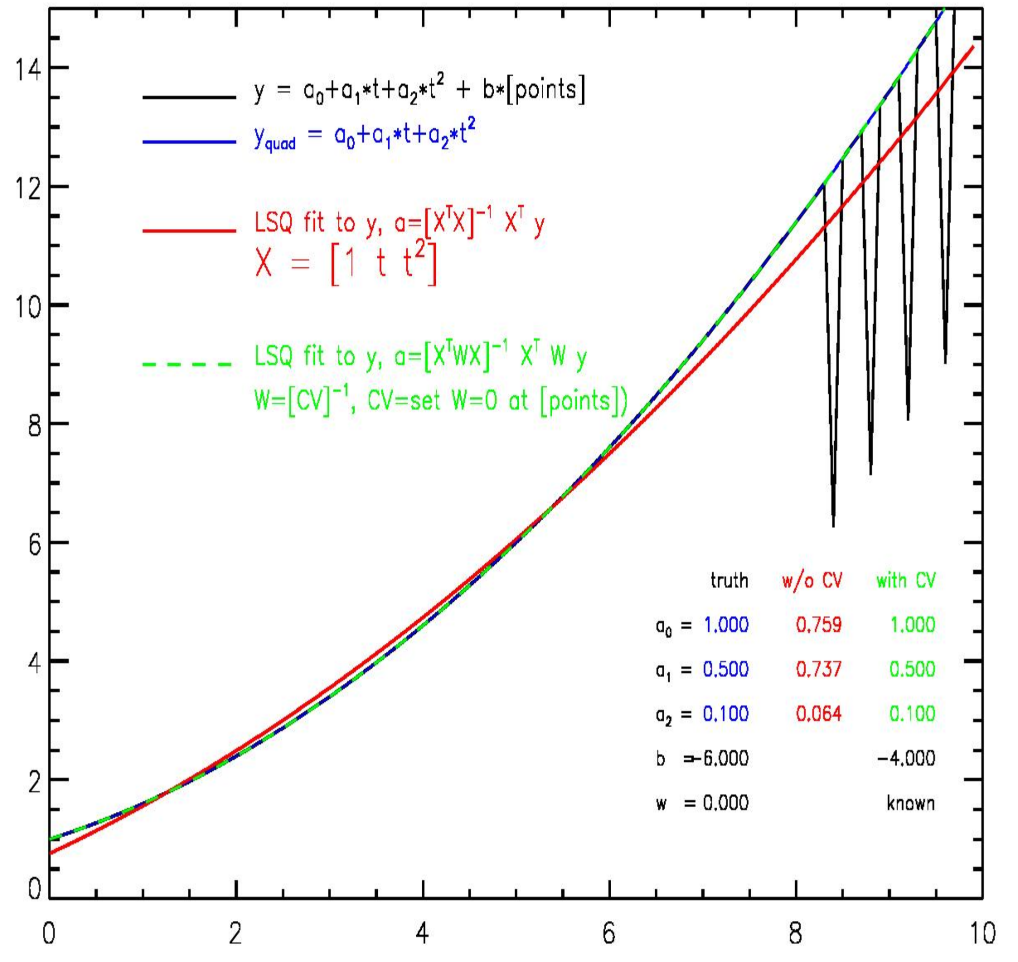
$$\begin{aligned}\Delta x_j &= \left[K_{j,n}^T\cdot W_{n,n}\cdot K_{n,j}\right]^{-1}\cdot K_{j,n}^T\cdot W_{n,n}\cdot(y_n - K_{n,j}\cdot x_j) \\ x_j^{i+1} &= x_j^i + \left[K_{j,n}^T\cdot W_{n,n}\cdot K_{n,j}\right]^{-1}\cdot K_{j,n}^T\cdot W_{n,n}\cdot(y_n - K_{n,j}\cdot x_j^i)\end{aligned}$$

- The linear algebra solution can be derived and is identical to minimization of a cost function *without any constraint*:

$$J = \left(y_n^{obs} - y_n^{calc}\right)^T\cdot W_{n,n}\cdot\left(y_n^{obs} - y_n^{calc}\right)$$

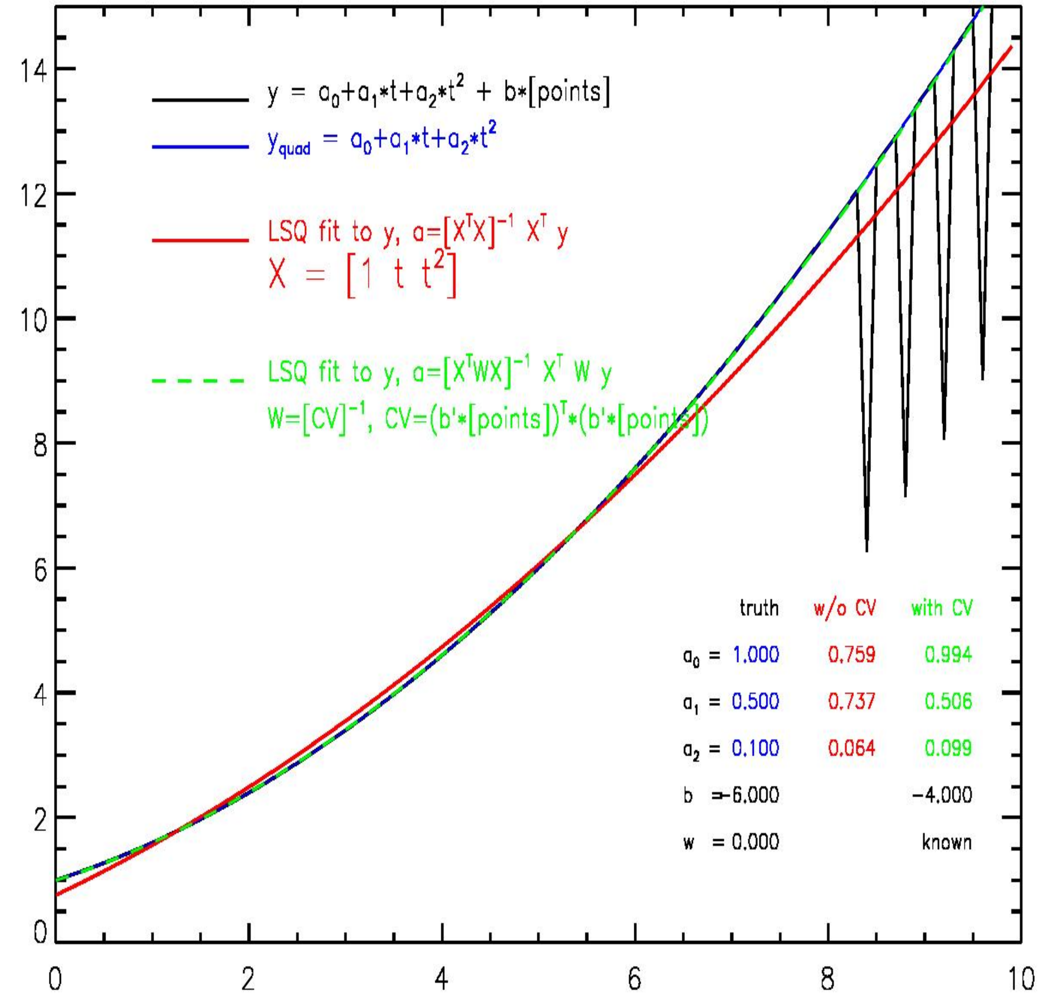
An example of making retrieval a insensitive to an interfering gas

- Black curve is a quadradic polynomial plus large spectral features.
  - Quadratic is an analogy for retrieval of T(p)
  - Spikes represent a spectra of an known gas (we know location of lines, but not amplitude).
- Red curve is fit with *W(n,n)* = 1.0 and no off-diagonals
- Green dashed curve is solution with *W(n,n)* = 0 for interfering lines locations.



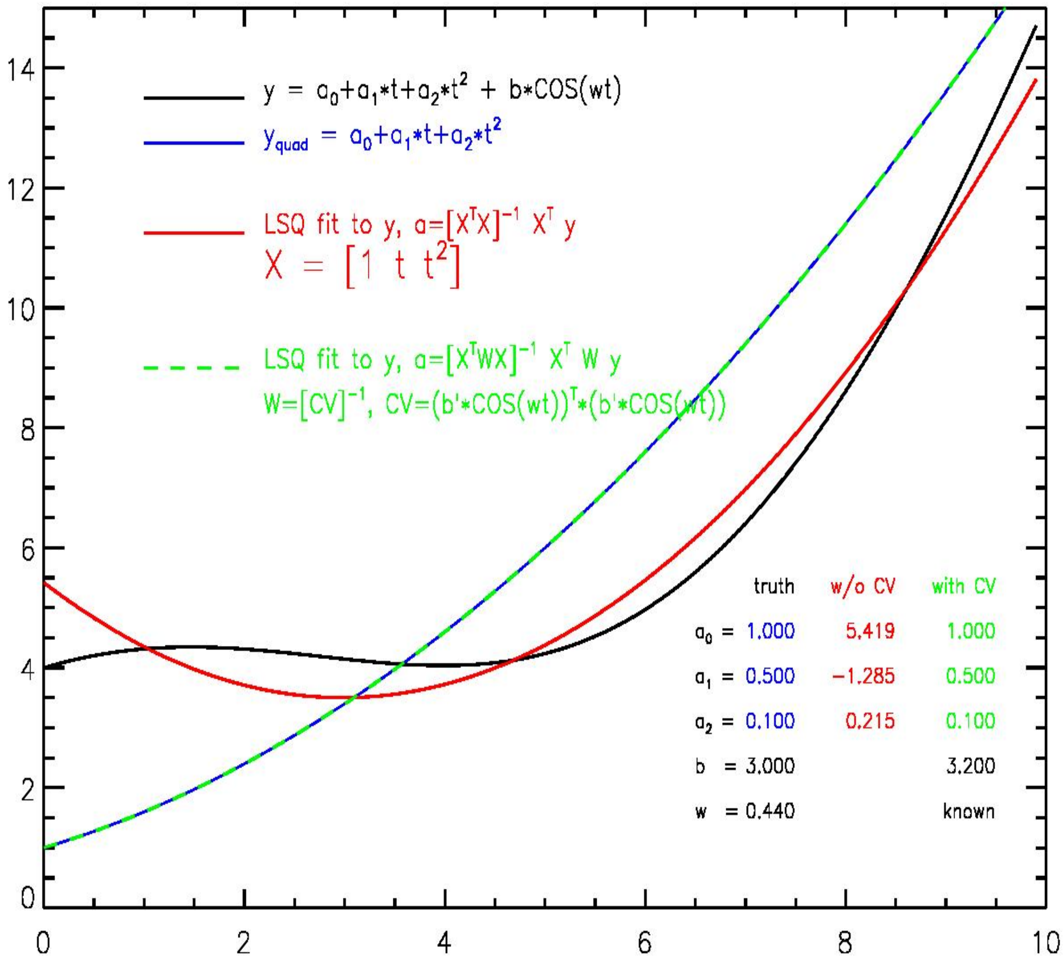
A better way: Use off diagonal elements of W(n,n) to estimate interference

- Same curves as previous figure, but *W(n,m)* is an estimate (had 50% error) of the strength of the lines (assuming perfect knowledge of the location of the lines).
- Fit is reasonable good even with poor estimate of strength of lines.



Off-diagonal terms in W are very important – allow you to "*see through*" errors

- Example at right is an analogy for ***T(p)*** when a "unknown" smooth interference is imposed (cloud or surface error).
- Black line is the "truth"
- Blue line (under dashed green) is quadradic component of the "truth"
- Red line is quadradic fit to the black line. It is in error due to the sinusoidal term.
- Dashed green is LSQ fit using off-diagonal *estimate* of the error. We can "see through" the sinusoidal component and fit the quadradic component.



What we learn from using LSQ analysis of hyper-spectral radiances

- Linear variables are more stable
  - For example, *log(q)* is more linear than *q*
- Weighting can mitigate geophysical channel interactions

$$W_{n,n} = N_{n,n}^{-1}$$

$$N_{n,n} \simeq \mathrm{NE\Delta N}^2 + \sum_j \left[\frac{\partial R_n}{\partial x_j} \cdot \left(\frac{\partial R_n}{\partial x_j} \right)^T \right]$$

- We minimize "null space" error by selecting unique (*i.e.,* non-interacting) geophysical parameters
- Error in retrieved products can be estimated (and propagated from step to step)

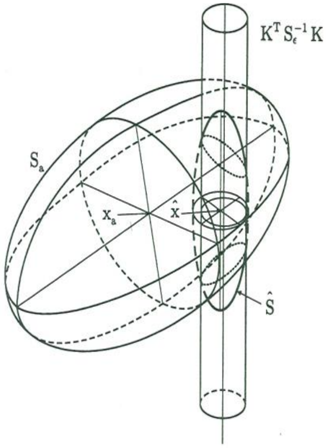
$$dx dx^T \simeq J(min) \cdot \left[K_{j,n}^T \cdot W_{n,n} \cdot K_{n,j} \right]^{-1}$$

Physical retrieval is a minimization of a *constrained* cost function

Covariance of observed minus computed radiances: includes instrument noise model and spectral spectroscopic sensitivity to components of the state, X, that are held constant (these are spectral "fingerprints" using radiative transfer).

$$J = \left(R_n^{obs} - R_n\left(X_j^{i-1}\right)\right)^T \cdot N_{n,n}^{-1} \cdot \left(R_n^{obs} - R_n\left(X_j^{i-1}\right)\right) + \left(X_j^{i-1} - X_j^A\right)^T \cdot C_{j,j}^{-1} \cdot \left(X_j^{i-1} - X_j^A\right)$$

- Covariance of products (*e.g.*, *T(p)*, *q(p)*, $CO_2(t)$) can be used to optimize minimization of this underdetermined problem.
- Application dictates desired *amount of a-priori*.
  - For weather products one can use a minimum variance ($C = \lambda I$) approach to eliminate inducing unintended correlations.
  - For climate, some combination of simple climatologies or re-analysis products are most likely desired



The solution of *J* is a weighted average of observations and a-priori knowledge

- adapted from Houghton 1986, pg. 129-130
  - See rs_notes.pdf section 8.12.1 for full derivation
- The cost function represents a weighted average of observations and the a-priori
- The best weight is the one that minimizes the standard deviation (SDV) of the result.
  - For average of 2 numbers: If x_1 has a SDV σ_1 and x_2 has a SDV σ_2 then minimum SDV is $\sigma^2_1 + \sigma^2_2$

    $$x = (1/\sigma^2_1 + 1/\sigma^2_2)^{-1} (x_1 / \sigma^2_1 + x_2 / \sigma^2_2)$$

  - Our cost function is the same idea, but for vectors we weight by the covariance

The Inverse Solution: Hyper-spectral Instruments

$$\Delta X_j = [K^T_{j,n} \cdot N^{-1}_{n,n} \cdot K_{n,j} + C^{-1}_{j,j}]^{-1} \cdot [K^T_{j,n} \cdot N^{-1}_{n,n} \cdot \Delta R_n + C^{-1}_{j,j} \cdot \Delta X^a_j]$$

$x_1 \rightarrow [K^T N^{-1} K]^{-1} \bullet K^T N^{-1} \Delta R$ $\quad x_2 \rightarrow \Delta X^a$

$\sigma_1 \rightarrow COV(x_1) = [K^T N^{-1} K]^{-1}$ $\quad \sigma_2 \rightarrow C$

$$K^{i-1}_{n,j} = \frac{\partial R_n \left(\vec{X}^{i-1}\right)}{\partial X_j}$$

Hyper spectral radiances have high information content (IC) in the spectrum:

Inverse methods can exploit this high IC by using fast derivatives of the forward model, $K_{n,j}$ for all parameters *held constant.*

Iterative Solution to the Cost Function has many forms

- Optimal estimation can “pivot” off of the *a-priori* state.

$$X_j^i = X_j^A + \left[K_{j,n}^T \cdot N_{n,n}^{-1} \cdot K_{n,j} + C_{j,j}^{-1}\right]^{-1} \cdot K_{j,n}^T \cdot N_{n,n}^{-1} \cdot \left[R_n^{obs} - R_n(X^{i-1}) + K_{n,j} \cdot \left(X_j^{i-1} - X_j^A\right)\right]$$

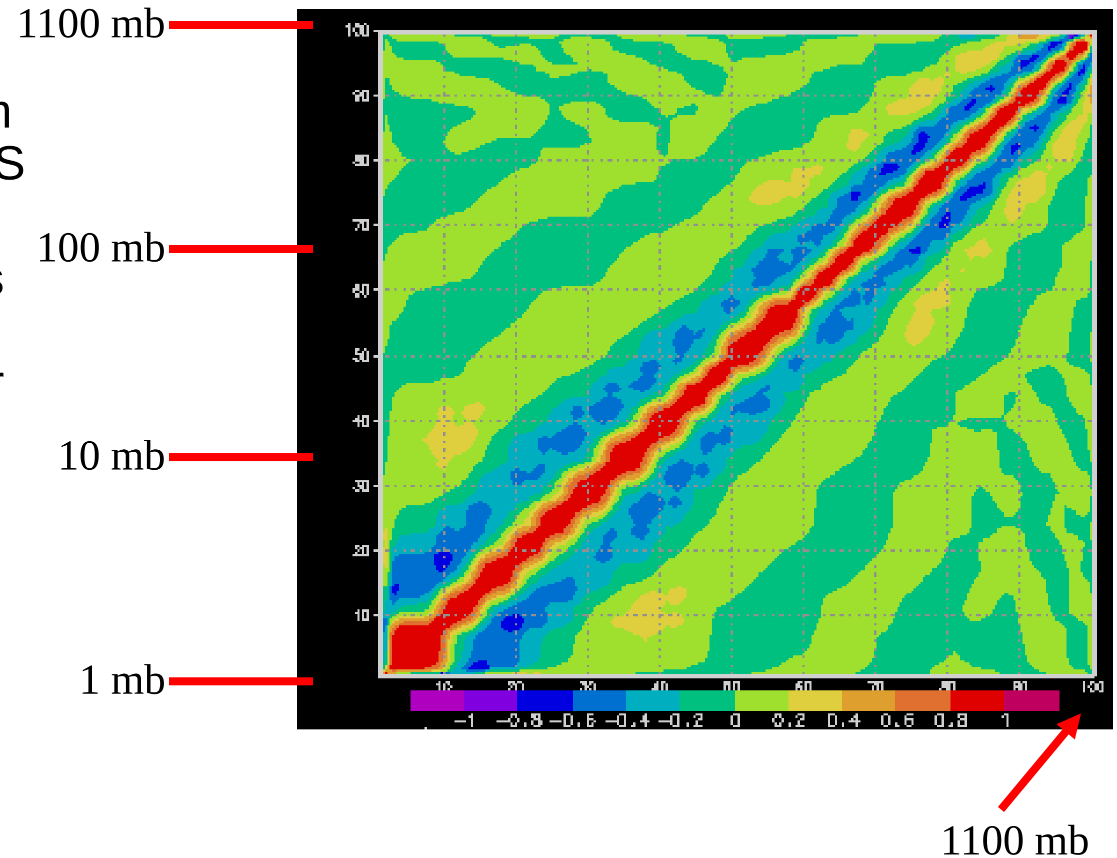
- An is equivalent to “pivoting” from the previous iteration:

$$X_j^i = X_j^{i-1} + \left[K_{j,n}^T \cdot N_{n,n}^{-1} \cdot K_{n,j} + C_{j,j}^{-1}\right]^{-1} \cdot \left[K_{j,n}^T \cdot N_{n,n}^{-1} \cdot \left(R_n^{obs} - R_n(X^{i-1})\right) - C_{j,j}^{-1} \cdot \left(X_j^{i-1} - X_j^A\right)\right]$$

  - The “background term” modifies the obs-calc’s to converge to a regularized solution.
  - The background term prevents believing what was held back on previous iterations such that *a-priori* information is retained

Example of temperature retrieval error covariance

- An example of temperature retrieval correlation (minimum variance method) for the AIRS instrument
- Top of atmosphere radiances (TOA) are used to invert the radiative transfer equation for T(p).
- This results in a correlation that is a vertical oscillatory function.
  - TOA radiances are minimized, but
  - An error in one layer is compensated for in other layer(s).



Error *covariance* matrices are very difficult to construct and global matrices tend to be large and under-damp the solution whereas regional matrices are smaller and solution can become unstable if extremes occur.

Another approach: Think about the retrieval as a physics problem, not a statistical problem

$$R_n^{obs} - R_n(\vec{X}) \simeq K_{n,j} \cdot \Delta\vec{X}_j + \epsilon_n$$

- Linear minimization of a cost function is equal to expanding Obs-calc's into a Taylor expansion and minimizing with constrained LSQ fitting.
  - In a linear operator, the different components of geophysical space can be separated into separate retrievals.

$$\begin{aligned} R_n^{obs} - R_n(\vec{X}) \simeq\ & K_{n,i}^1 \cdot \Delta\vec{T}_i \\ +\ & K_{n,i}^2 \cdot \Delta\vec{q}_i \\ +\ & K_{n,i}^3 \cdot \Delta\vec{O}_i \\ +\ & K_{n,i}^4 \cdot \Delta\vec{C}O_i \\ +\ & \ldots + \epsilon_n \end{aligned}$$

$$K_{n,j} = \frac{\partial R_n(\vec{X})}{\partial X_j}$$

Simultaneous versus sequential retrieval trade-offs

Simultaneous OE	Sequential OE (NUCAPS)
Solve all parameters simultaneously.	Solve each state variable (*e.g*., T(p)), q(p), O_3(p), … HNO_3) separately.
O-C error covariance can be simpler (does not require propagation of errors from one step to another)	O-C error covariance is computed for all *relevant* state variables that are held fixed in a given step. Retrieval error covariance *must be* propagated between steps.
Each parameter is derived from <u>all</u> channels used (*e.g*., can derive T(p) from CO2, H2O, O3, CO, … lines).	Each parameter is derived from the best channels for that parameter (*e.g.,* derive T(p) from CO2 lines, q(p) from H2O lines, etc.). More linear.
A-priori must be rather close to solution, since state variable interactions can de-stabilize the solution. Covariance must contain all cross-terms (e.g., dT/dq, dT/dO3) – which are difficult to determine.	*A-priori* can be simple (and global) for hyperspectral and, therefore, more signal can be derived from the radiances. Do not need regional or ad-hoc covariance terms.
Has larger state matrices (all parameters solved) and O-C covariance matrices (all channels used). Inversion of large matrices is computationally expensive (i.e., *C(n,n)* inversions scale as n^3).	State matrices are small (largest is ≈30 T(p) parameters) and O-C covariance matrices of the channel subsets are quite small. Very fast algorithm. Encourages using more channels in relevant steps.
Has never been done for full state vector – so simultaneous usually refers to T/q/clouds and maybe <u>*some*</u> *trace* gases.	Solve for full state vector (T, q, all trace gases). This approach is so fast it can be used a quick-look and then target simultaneous approach for more in-depth retrievals, if so desired.

Some Final Thoughts on Remote Sounding Approaches

- Simultaneous versus sequential retrieval discussion isn't new. It has been going on for more than 30 years!
- It really boils down to *Physics* versus *Statistics* – although in the modern era this distinction has been blurred.
  - Regression and Neural Network approaches are used as first guesses.
  - Use of regional geophysical covariances allows tweaking results.
- See the discussion in Rodgers, C.D. 1977. "Statistical principles of inversion theory." in "Inversion Methods in Atmospheric Remote Sounding" (ed. A. Deepak) p.117-138.
  - This discussion is also transcribed in Section 23.2 of my notes (reference/rs_notes.pdf).
- As in all things, the answer may lie in the middle ground. We are exploring adding some *a-priori* statistics to help in certain geophysical domains (*e.g.*, lower boundary layer T(p), etc.) and we can explore some simultaneous retrievals (T(p) and emissivity, etc.) to improve certain products.

Questions?

More information at:
http://goo.gl/twuRtW

~/rs_notes.pdf
- Radiative transfer
- Derivations
- Details about instruments

~/phys640_s04.pdf
- Mathematical methods
- Linear and non-linear Least Squares
- FFT's and Apodization

References for this session

- The mathematics of sounding: Rodgers, C.D. 2008. Inverse methods for atmospheric sounding: Theory and practice. World Scientific Publishing 240 pgs.
- An excellent introduction to sounding of the planets: Hanel, R.A., B.J. Conrath, D.E. Jennings and R.E. Samuelson 1992. Exploration of the solar system by infrared remote sensing. Cambridge University Press 458 pgs.
- A good general introduction to sounding: Houghton, J.T., F.W. Taylor and C.D. Rodgers 1986. Remote sounding of atmospheres. Cambridge University Press 310 pgs   ISBN: 9780521310659
- A good introduction to regularization: Twomey, Sean 1996. Introduction to the mathematics of inversion in remote sensing and indirect measurements. Dover Publ. Inc. 243 pgs. ISBN: 9781483289564, used copies available on Amazon
- A nice historical reference with discussions by many of the earl sounding pioneers: 1977: "Inversion methods in atmospheric remote sounding" - Deepak (Ed.), ISBN: 978-0-12-208450-8

Calcon Workshop: Current Challenges in the Remote Sounding of the Earth

2. Example of operational sounding: NUCAPS, CLIMCAPS, *and NECAPS*

Chris Barnet

NOAA/JPSS Senior Advisor for Atmospheric Sounding

NASA S-NPP Sounder Discipline Lead

Science and Technology Corporation (STC) Senior Scientist

Monday Aug. 30, 2021

Topics for Today

- Workshop will have 3 sections
  1. Introduction to Remote Sounding
  2. Example of operational sounding: NUCAPS, CLIMCAPS, and NECAPS
  3. Applications and future sounders.
- Each section will consist of
  - ~40 minute lecture
  - ~15 minutes Q&A
  - ~5 minute bio break

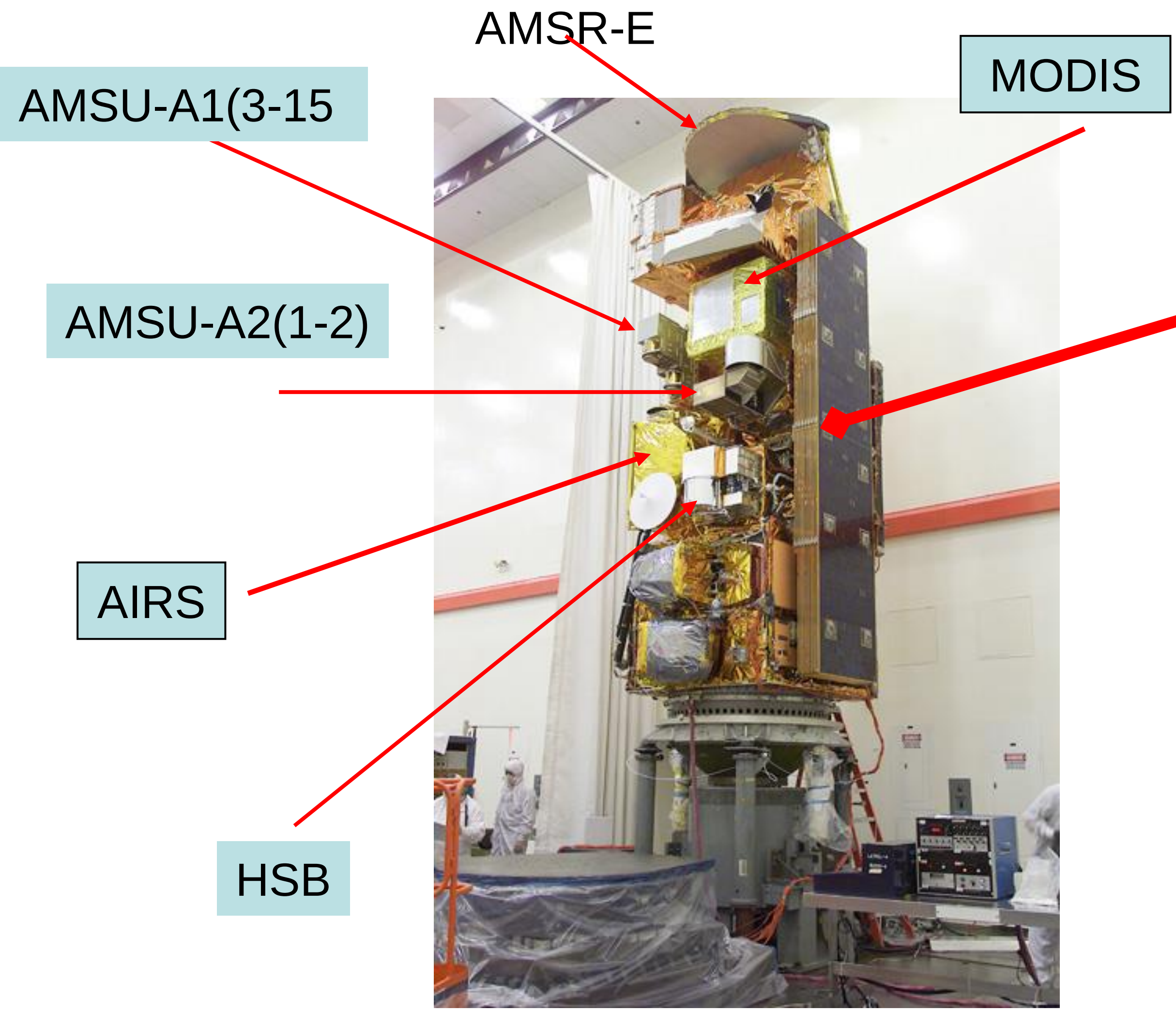
Quick Overview of the Instruments We Will Discuss Today

AIRS and AMSU on Aqua

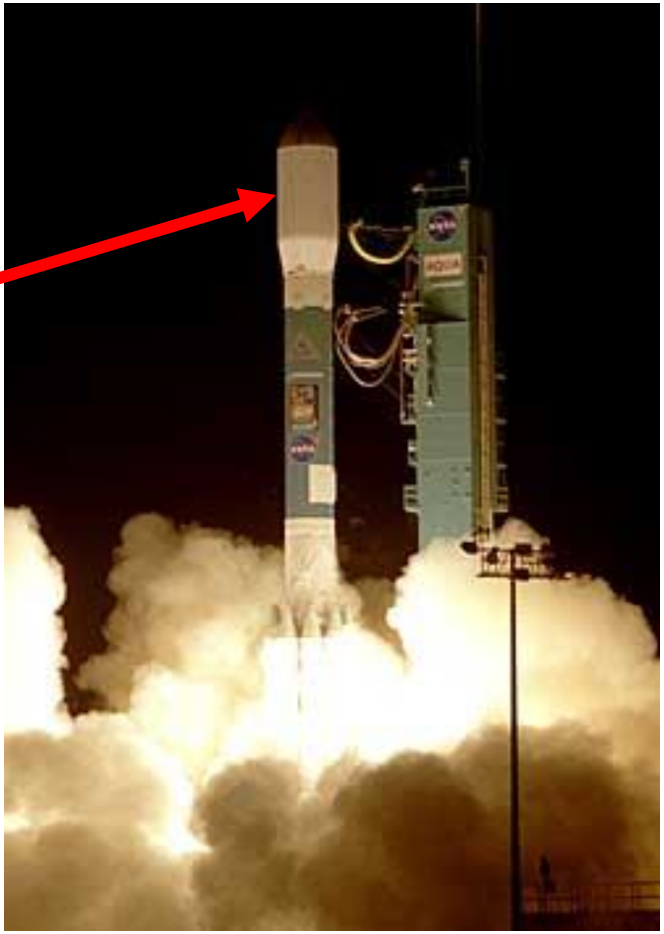
IASI, AMSU, and MHS on Metop-A, -B, -C

CriS and ATMS on Suomi-NPP, NOAA-20, JPSS-2,3,4

AIRS, AMSU, & HSB were launched on the EOS Aqua Platform May 4, 2002



Aqua Acquires 325 Gb of data per day



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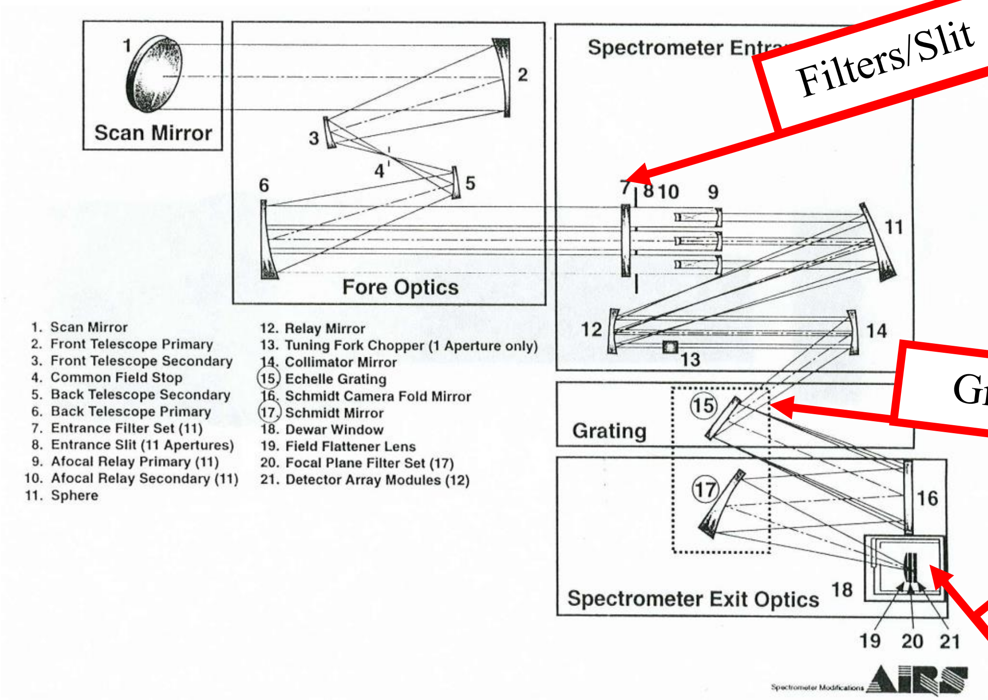
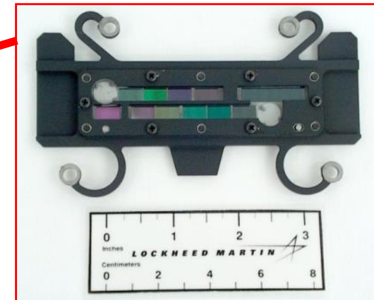
AIRS Optical Diagram

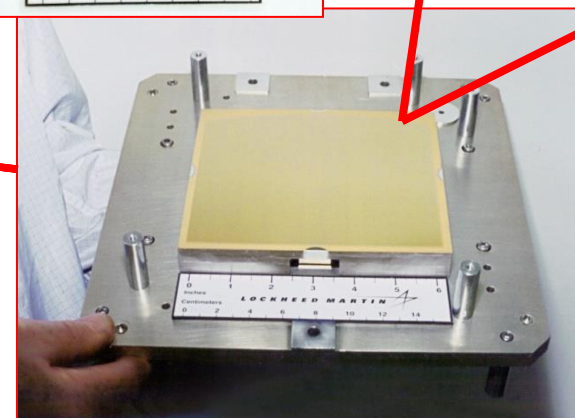


Filters/Slit

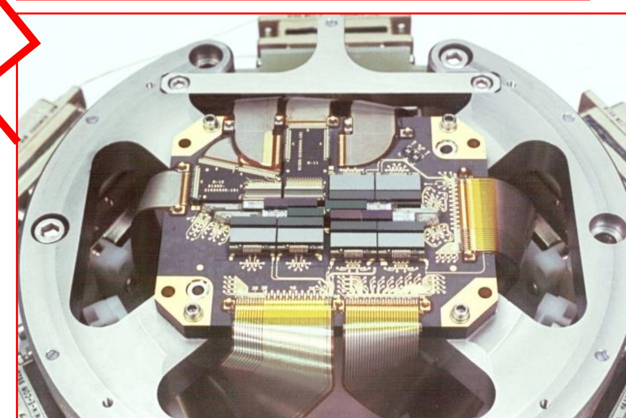


12.8 lines/mm

Grating



Detectors

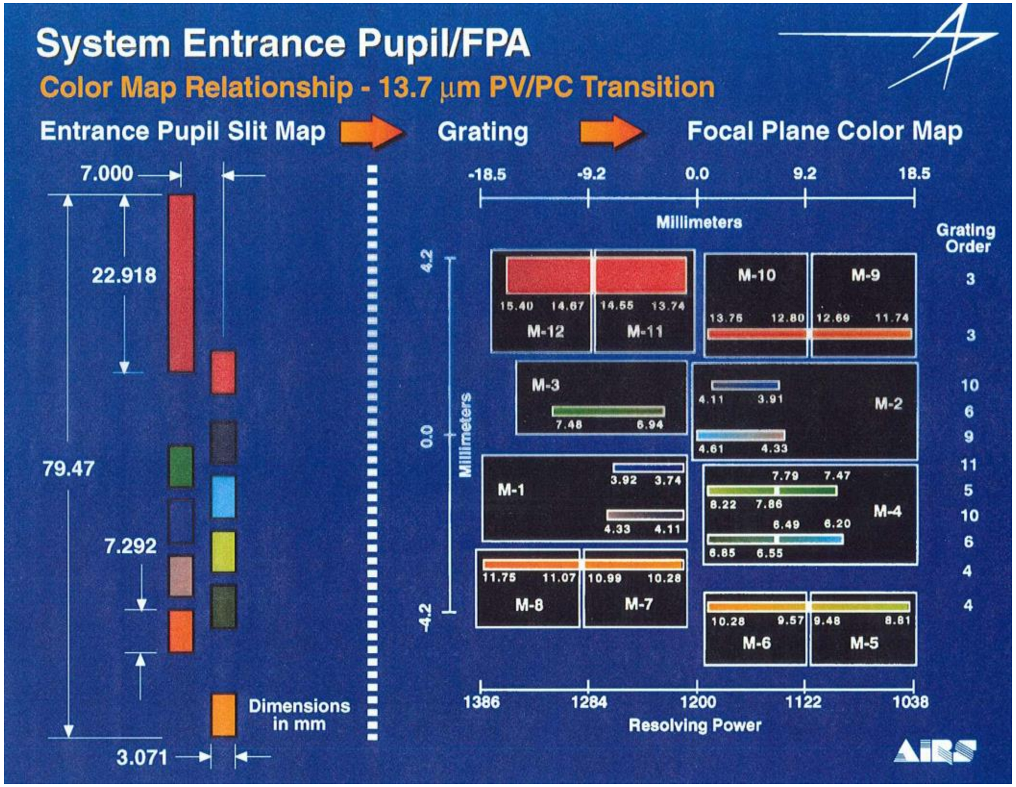


Only moving parts on AIRS are

1. Scan mirror
2. Sterling Cooler Pistons (no shown) (mechanical cooler required to cool & control focal plane at 58K)

AIRS Instrument (continued)

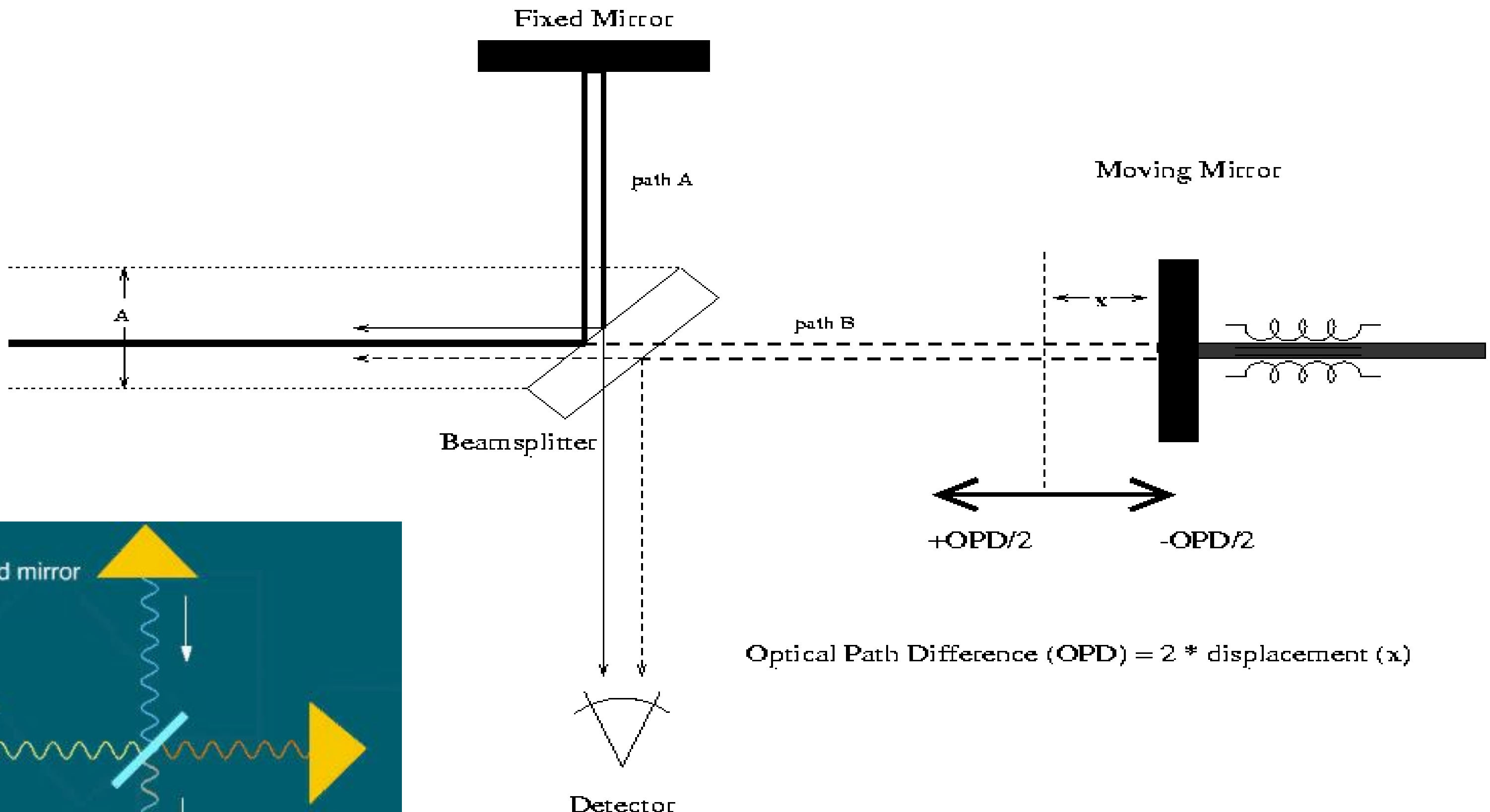
- Entrance Slits, with interference filters to select grating order and to remove stray light, are used to map spectral regions onto focal plane linear arrays.
- Optical design is “pupil imaging” to eliminate spatial sensitivity within a FOV
- Resolving Power is inversely related to slit width R_{AIRS}=1200

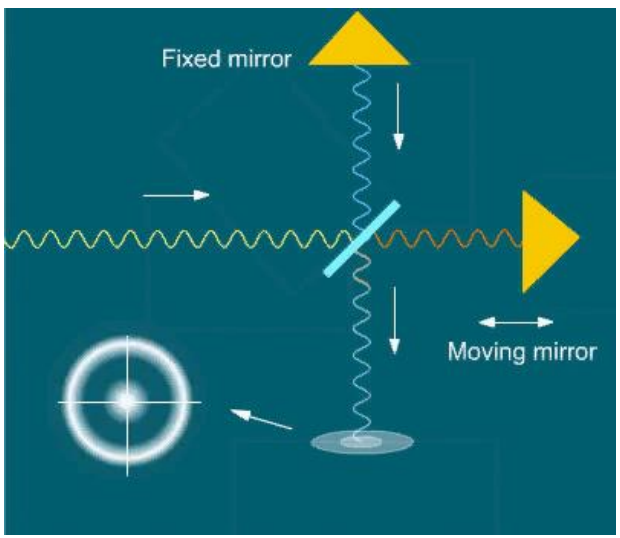


NOTE: Each detector is ≅ 50 μm

$R = (FL/W)*\tan(\theta) = 227/3*\tan(85^o)$

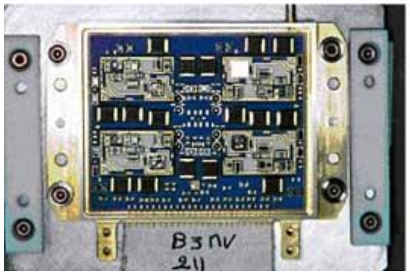
IASI (and CrIS) use an Interferometer
(graphic shows a simplified Michelson Interferometer)

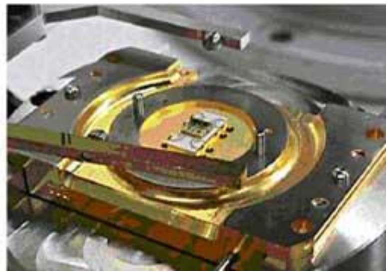


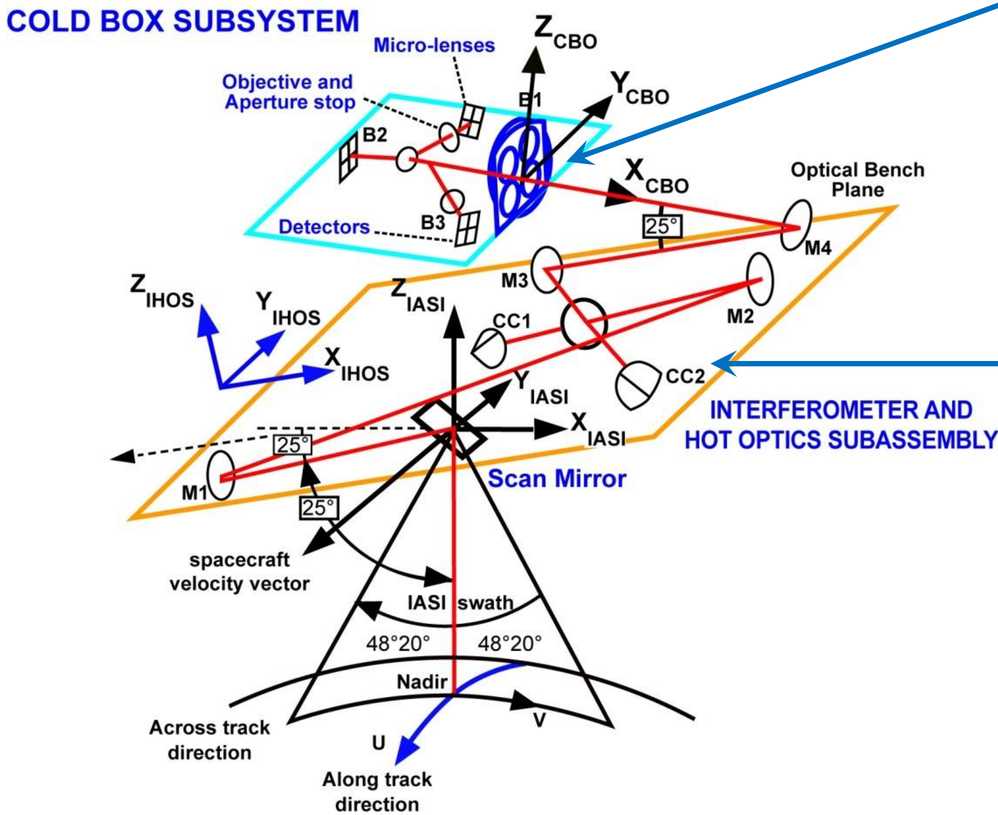


NOTE: A handful of detectors can be used to sample multiple scenes simultaneously. Each detector can be Fourier transformed into many "channels" in the infrared

IASI Optical Diagram







IASI has 4 FOV's measured simultaneously

Aperture stop is common to all 3 bands

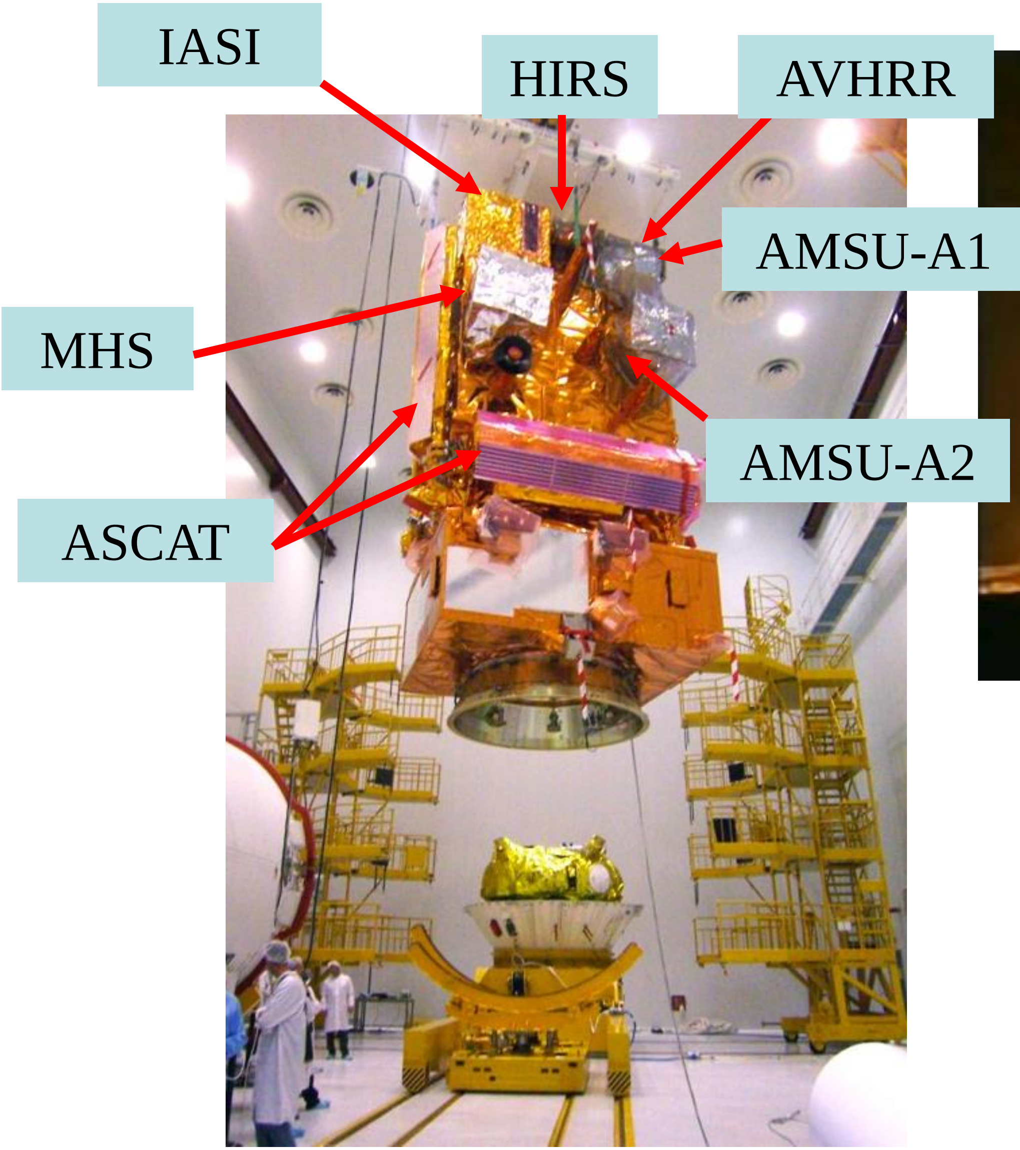
Small number of detectors allows a passive cooler (90 K) can be used.

Corner cubes are used to maintain alignment in space environment.

Moving parts in IASI:

1. Scan mirror
2. Corner Cube (CC1)

The 1st IASI/AMSU/MHS was launched on the MetOp-A Satellite on Oct. 19, 2006

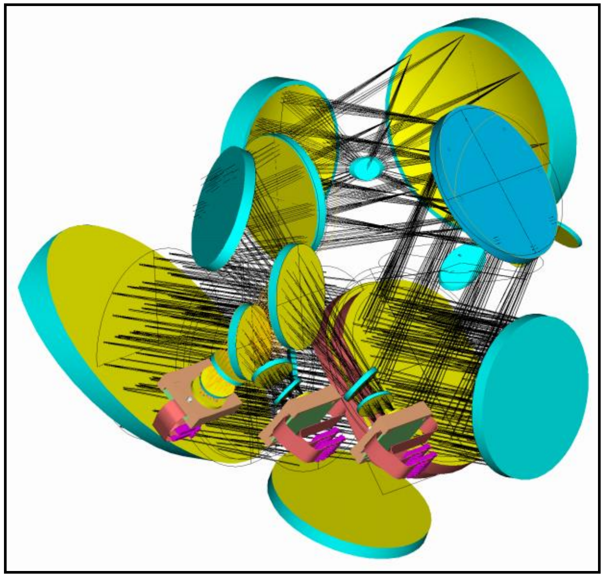


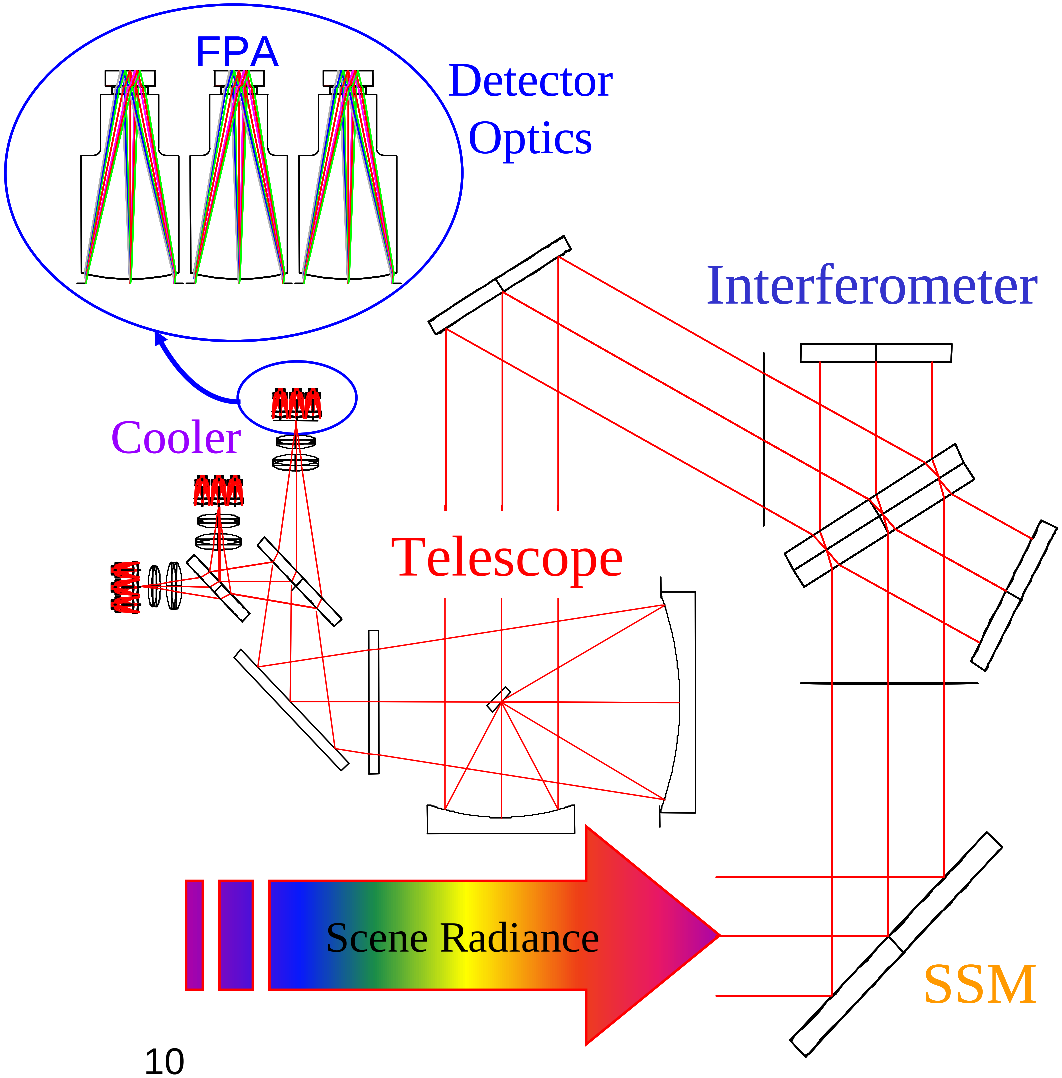
Soyuz 2/Fregat launcher,

Baikonur, Kazakhstan

A Real Instrument: the CrIS Optical System

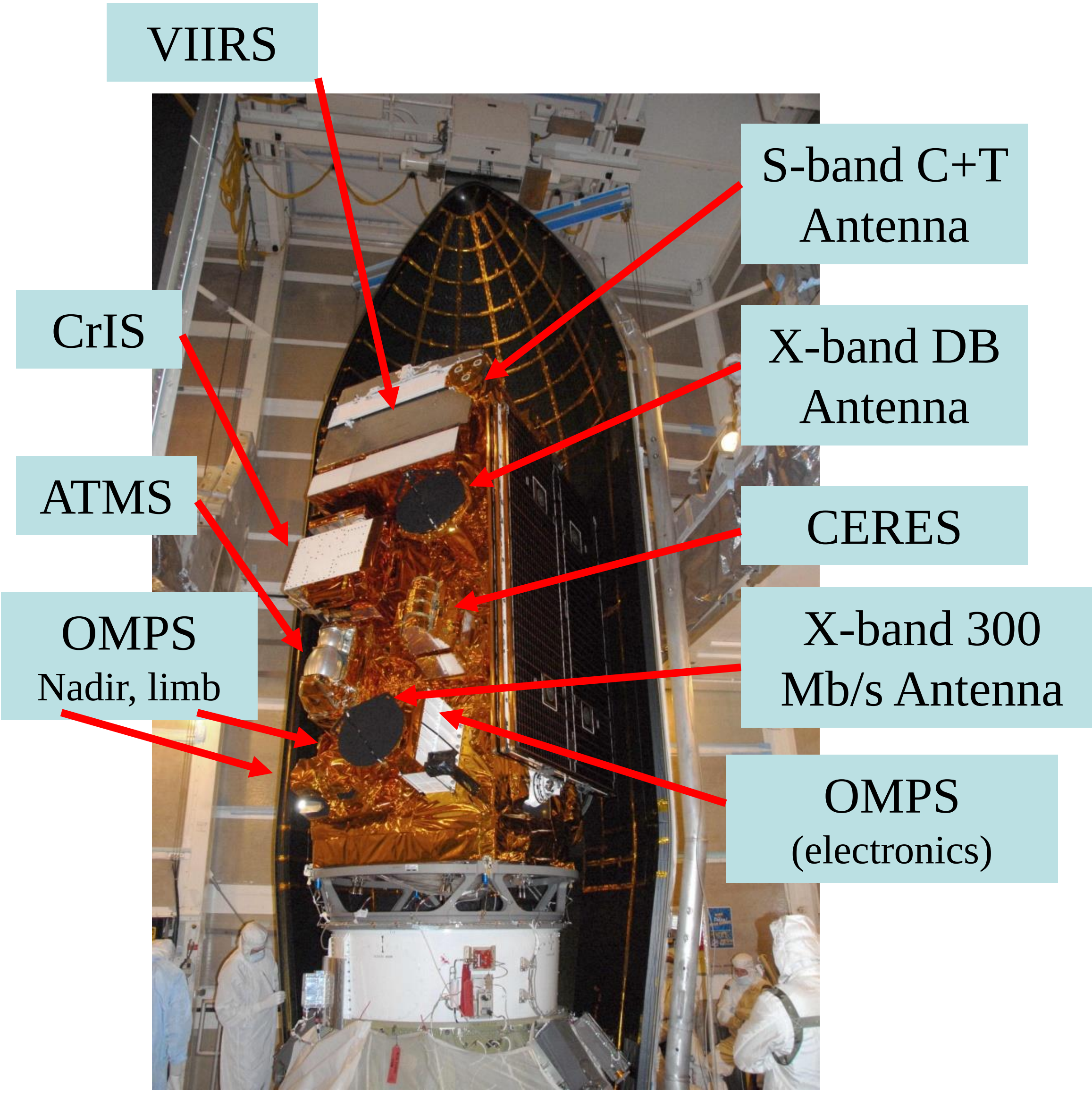
- Extremely Compact
- Large Aperture
- Excellent Image Quality
- Fully Wedged / Tilted
- Athermalized Design
- Pupil Imaging System





Slide courtesy of Joe Predina
ITT/Exelis, May 6, 2009

The 1st CrIS/ATMS was launched on the NPP Satellite on Oct. 28, 2011



Delta-II-7920

Vandenburg AFB

Space-borne operational hyperspectral *thermal sounders*

- There are 5 operational thermal sounder suites at NASA or NOAA

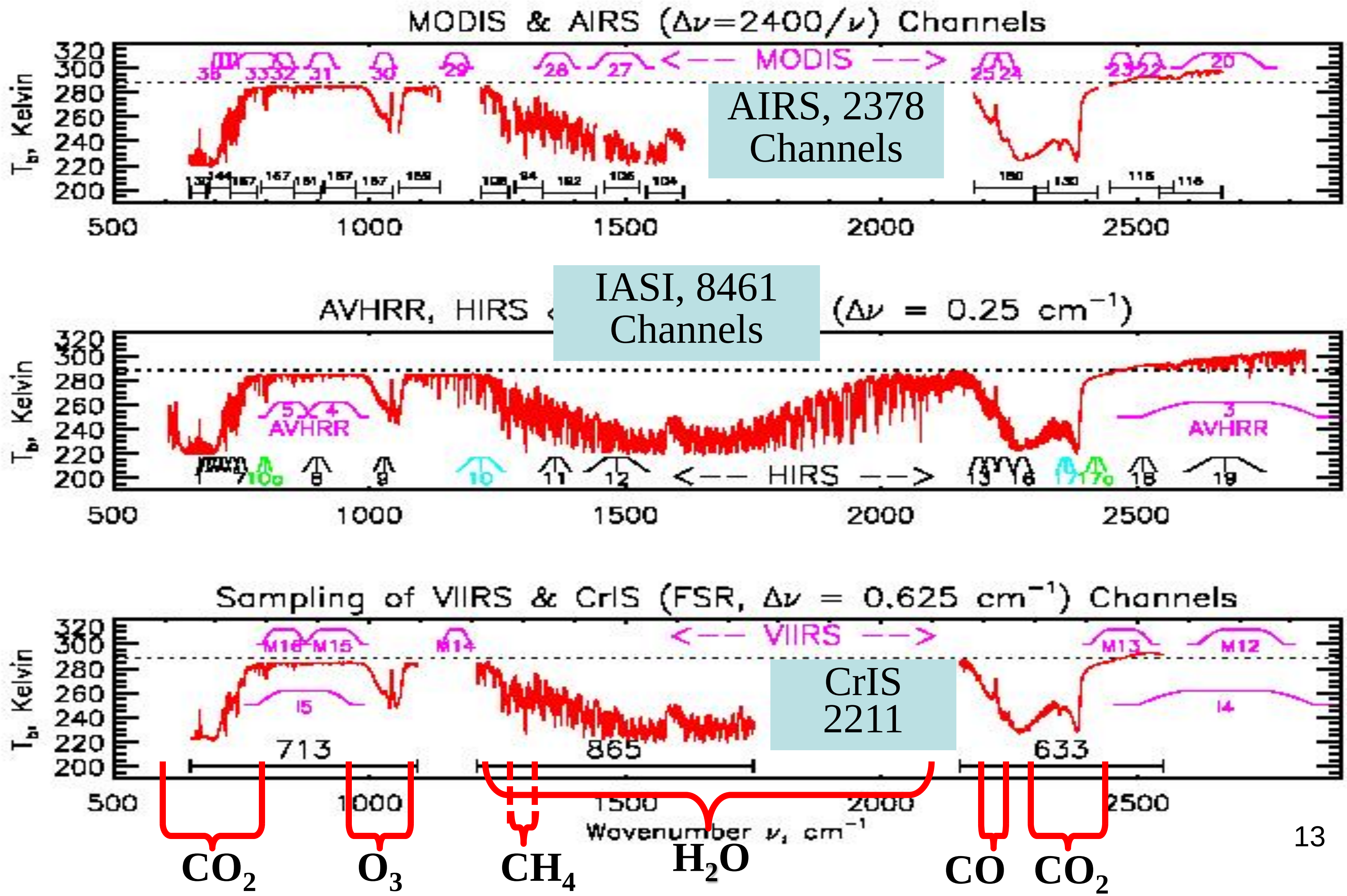
Satellite	Instruments	Overpass	Launch dates
Aqua	AIRS, AMSU	1:30 **	2002
Metop	IASI, AMSU, MHS	9:30	2006, 2012, 2018
S-NPP, JPSS	CrIS, ATMS	1:30	2011, 2017, …

- 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., 10% increase in CO_2, 2002-2020)

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

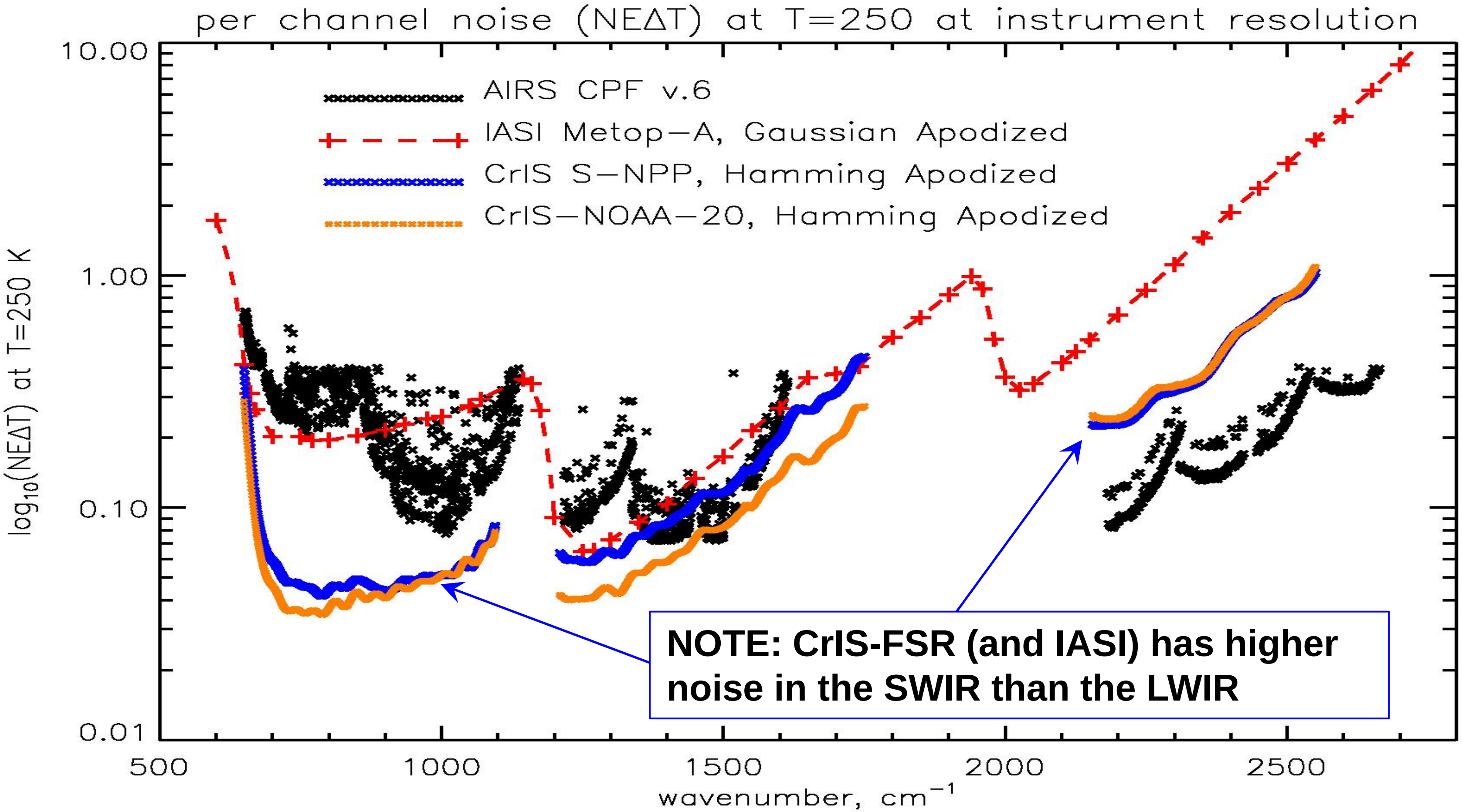
** in early 2022 Aqua will move out of A-train // begins a 6 year drift to 5:30

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



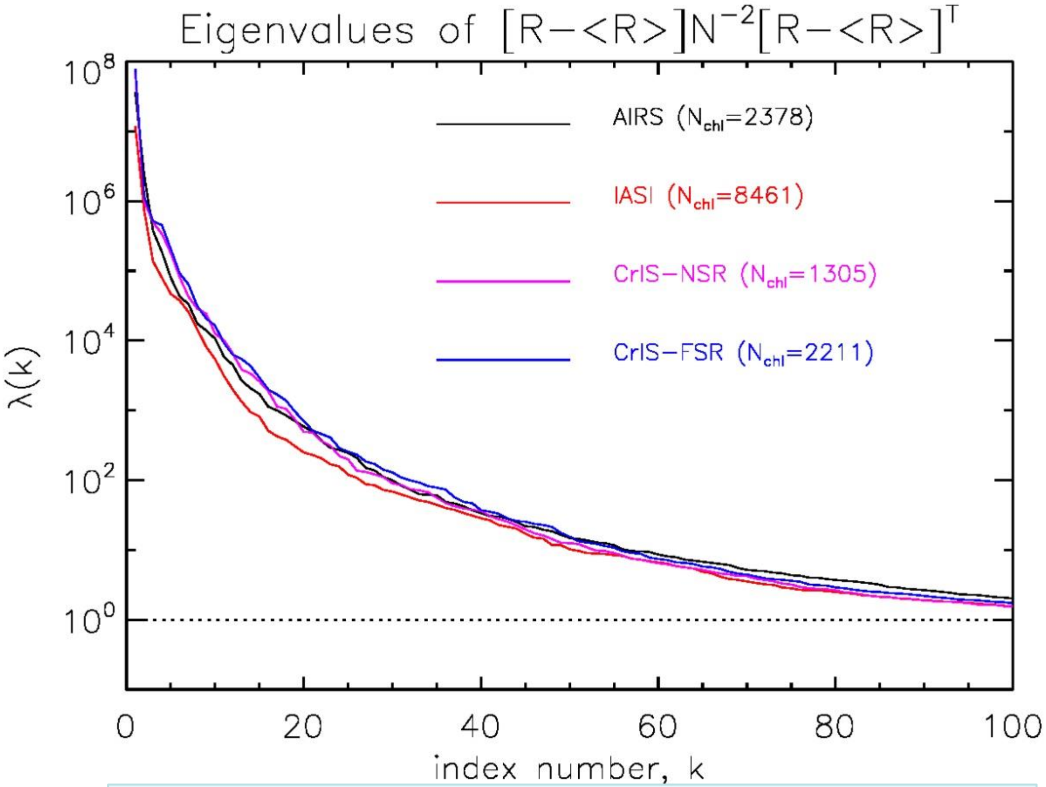
Signal to noise is important for sounding https://doi.org/10.5194/amt-13-4437-2020

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



The information content of AIRS, IASI, CrIS is similar
https://doi.org/10.5194/amt-13-4437-2020

- Single pixel of 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)

https://doi.org/10.5194/amt-13-4437-2020

But level-2 products can differ for other reasons than spectral information content

- Orbit: 9:30 orbits has different meteorology than 1:30
    - clouds tend to have less contrast at 9:30
    - Smaller lapse rate at 9:30 – less vertical contrast
    - Day vs. night differences are larger at 1:30
- Instrument
    - – IASI SW-band has higher noise than CrIS or AIRS
    - – IASI 4 FOV has less cloud contrast than 9 FOV
    - – CrIS's 3 spectral bands has spatial co-registration error
        - AIRS has spatial co-registration errors between individual channels – known as C_{ij} – for some channels error is large
        - IASI has common aperture, so its 3 bands are co-registered
    - – IASI and CrIS pixel-to-pixel radiometric errors with FOR

What Kind of Products Can Thermal Instruments Provide

NASA and NOAA synergy for weather sounding applications

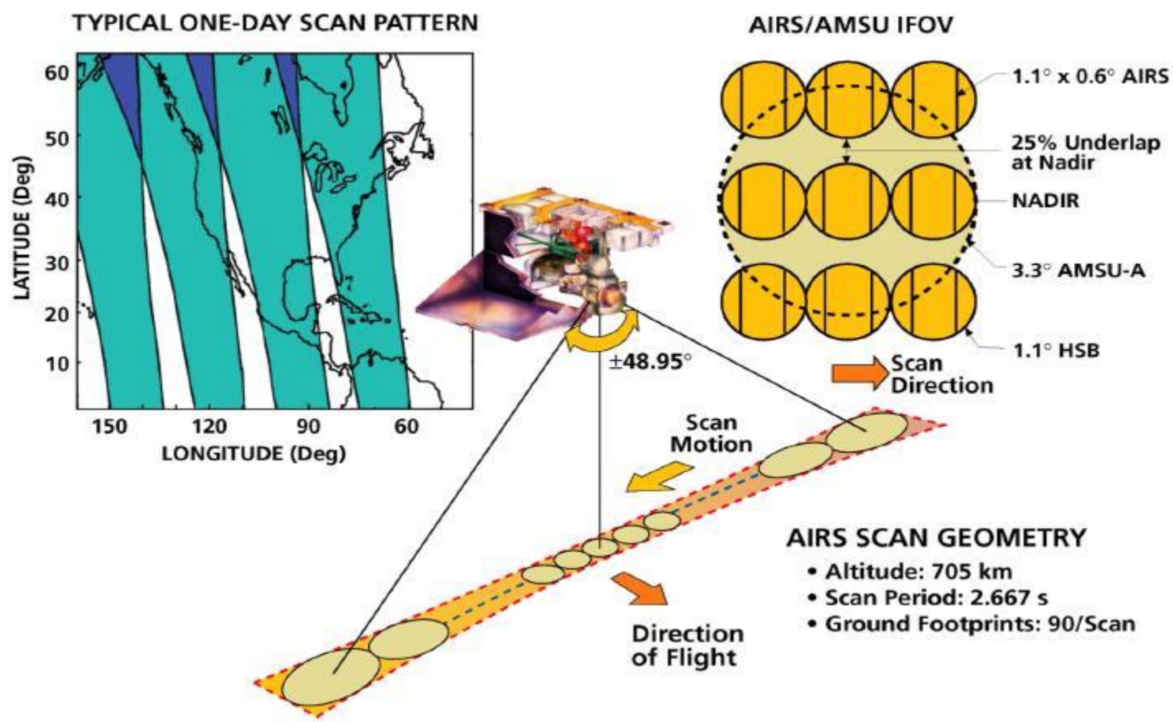
- 1995 NASA AIRS science team (AST) led the early algorithm development and science applications for hyperspectral infrared sounders.
    - Merged three algorithm types into one algorithm
    - Used regression operator as first guess: used all channels, very fast
    - Used sequential physical approach with built-in information content analysis.
- 2003 NOAA adopted the AIRS Science Team methodology for their sounding applications --- called NUCAPS
    - Extremely low latency, model independent products for forecasting.
    - Provides guidance for optimal use of infrared within NWP models.
- 2014 NOAA JPSS Sounding Initiatives began funding application-relevant research for sounding applications within NOAA.
    - NASA SPoRT has played a unique role in the transitioning of AST science to operational applications at NOAA.
        - Training, user guides, develop and demonstrate new applications.
- 2014 NASA funded CLIMCAPS, a climate version of this algorithm
    - 2019 re-processed full missions of S-NPP and NOAA-20 with CrIS and ATMS
    - 2020 re-process full mission of Aqua AIRS+AMSU and AIRS-only

AIRS Science Team: Authors of the Algorithm Components

- Phil Rosenkranz (MIT)
  - Microwave (MW) radiative transfer algorithm
  - Optimal estimation algorithm for T(p), q(p), LIQ(p), MW emissivity(f), Skin Temperature
- Larrabee Strow (UMBC)
  - Infrared (IR) radiative transfer algorithm
- Larry McMillin (NOAA)
  - Cloud Clearing, Local Angle Correction (LAC) algorithm
- Mitch Goldberg (NOAA)
  - Eigenvector regression operator for T(p), q(p), O_3(p), IR emissivity(υ), and Skin Temperature
- Joel Susskind (GSFC) & Chris Barnet
  - Cloud Clearing Algorithm
  - Physical retrieval using SVD for T(p), q(p), O_3(p), Ts, ε_{IR}, CTP, Cloud Fraction
- Chris Barnet (NOAA)
  - Physical Retrieval (currently using SVD and O-E) for CO(p), CH_4(p), CO_2(p), HNO_3(p), N_2O(p), SO_2

Sounding Strategy in Cloudy Scenes: Co-located Thermal & Microwave (& Imager)

- **Sounding is performed on 50 km a field of regard (FOR).**
- **FOR is currently defined by the size of the microwave sounder footprint.**
- **IASI/AMSU has 4 IR FOV's per FOR**
- **AIRS/AMSU & CrIS/ATMS have 9 IR FOV's per FOR.**
- **ATMS is spatially over-sampled can emulate an AMSU FOV.**



AIRS, IASI, and CrIS all acquire 324,000 FOR's per day

Operational sounding products using the AIRS, CrIS, IASI (& AMSU, ATMS)

	NASA AST, NOAA NUCAPS	NASA CLIMCAPS
A-priori	Global regression for T(p),q(p) (i.e.,model independent)	MERRA-2 for T(p), q(p), O3(p)
Error propagation	1-D diagonal w/ specified vertical "oscillation"	Eigenvector expansion of full 2-D covariance
Supported systems	• ASTv.7/Aqua & NUCAPS/Aqua • NUCAPS/Metop –A, -B, -C • NUCAPS/SNPP FSR • NUCAPS/NOAA-20	• Aqua full mission, 2002- • SNPP NSR full mission, 2012-21 • SNPP FSR full mission, 2015-21 • NOAA-20 full mission, 2016-
Latency	Real time (~30 minutes)	~1 month (wait f/ MERRA)
Averaging Kernels?	Not operational in NUCAPS Operational in AST v6 & v7	YES – fully supported

AST vx.x = AIRS Science Team algorithm, currently v7.0
NUCAPS = NOAA-Unique Combined Atmospheric Processing System ~= AST v5.7
CLIMCAPS = Community Long-term Infrared Microwave Coupled Atmospheric Product System

For more details see https://airs.jpl.nasa.gov/data/products/retrieval-systems/ and/or
https://docserver.gesdisc.eosdis.nasa.gov/public/project/AIRS/Overview_of_the_AIRS_Mission.pdf

Operational and experimental sounding products from AST, NUCAPS & CLIMCAPS

Core profile products

Retrieval Product	Key Spectral Region (cm^{-1})
Temperature	650-750, 2380-2410
Water vapor	1200-1600
Ozone, O_3	990 – 1070
Carbon Monoxide, CO	2155 – 2220
Methane, CH_4	1220 – 1350
Carbon Dioxide, CO_2	660 – 760 2200 – 2400

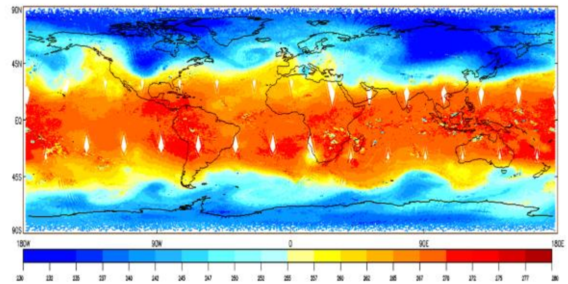
Experimental trace gas products

Nitric Acid, HNO_3	760 – 1320
Nitrous Oxide, N_2O	1290 – 1300 2190 – 2240
Volcanic Sulfur Dioxide, SO_2	1343 – 1383

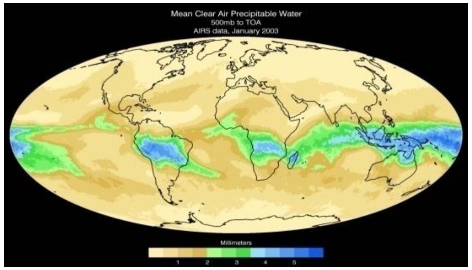
Single-FOV detection flags (CLIMCAPS)

Isoprene (C_5H_8)	893.8
Ethane (C_2H_6)	822.5
Propylene (C_3H_6)	911.9
Ammonia (NH_3)	966.25 + 928.75

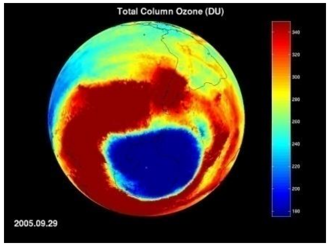
500 hPa Temperature



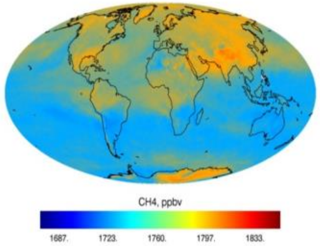
500 hPa Water Vapor



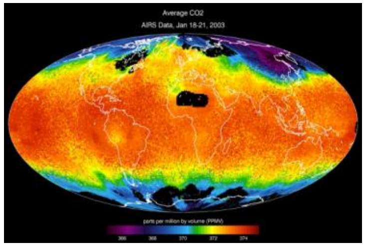
Ozone



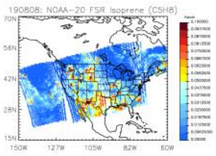
Methane



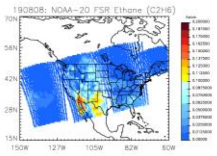
Carbon Dioxide



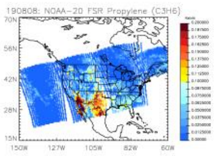
Isoprene



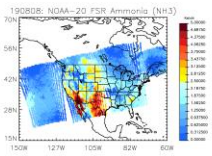
Ethane



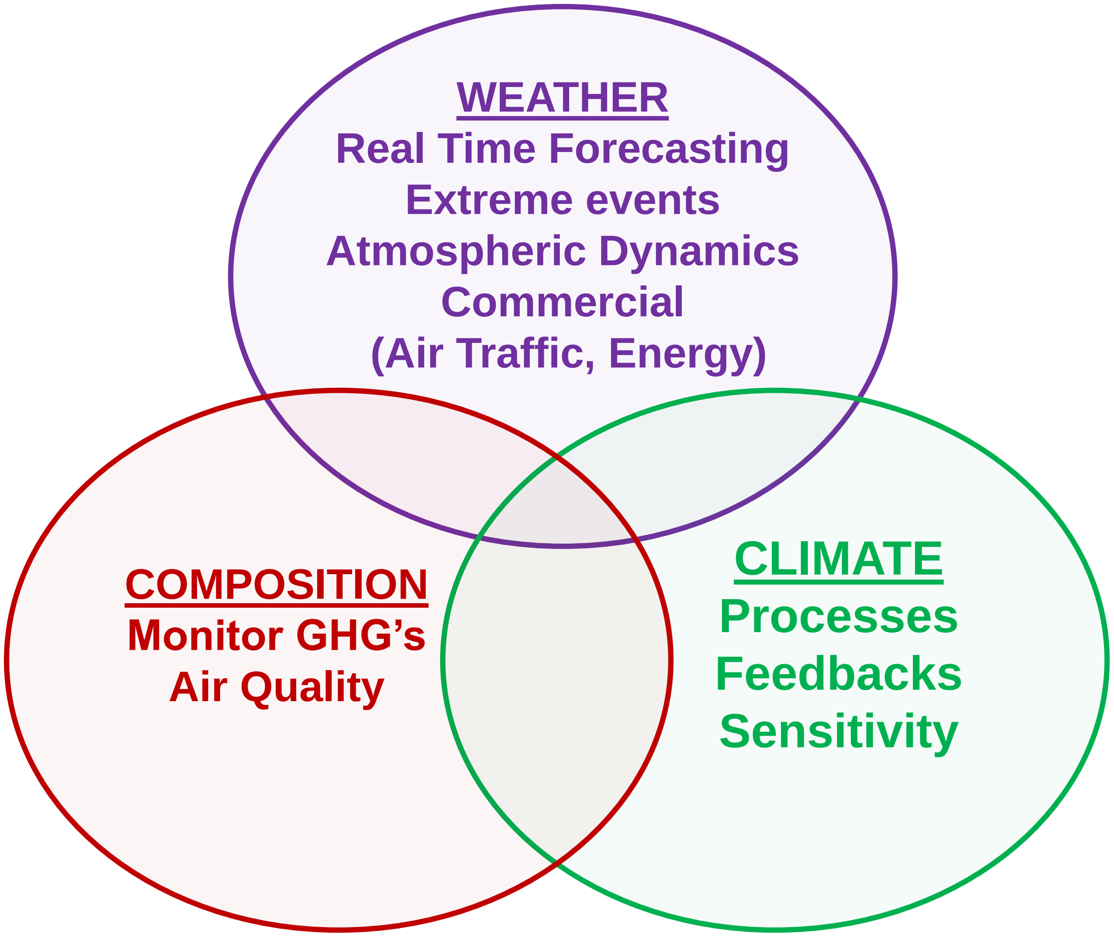
Propylene



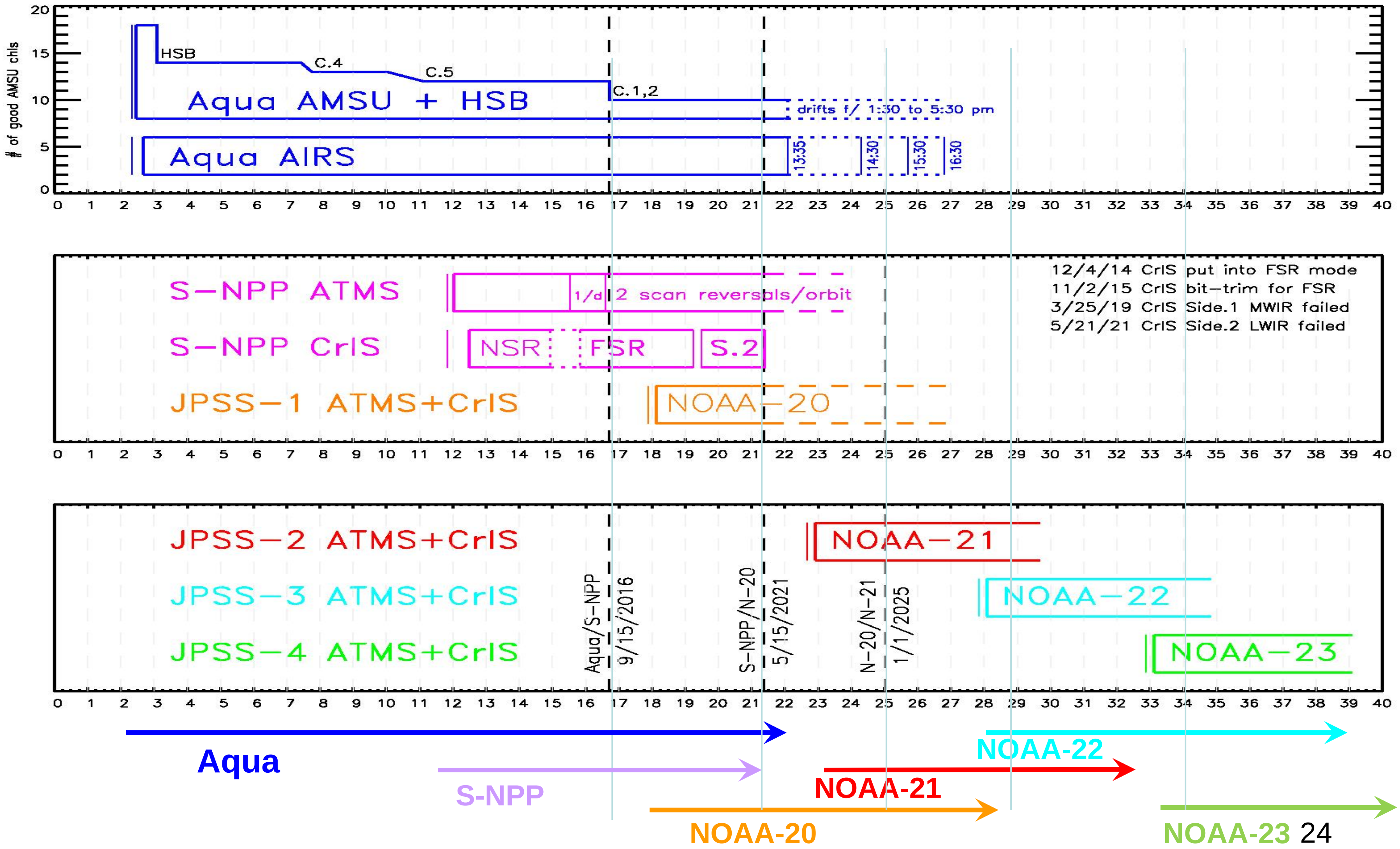
Ammonia



Together these algorithms are *contributing* to the needs of three communities



With CLIMCAPS we have achieved the continuity of Aqua, S-NPP, JPSS-0x records



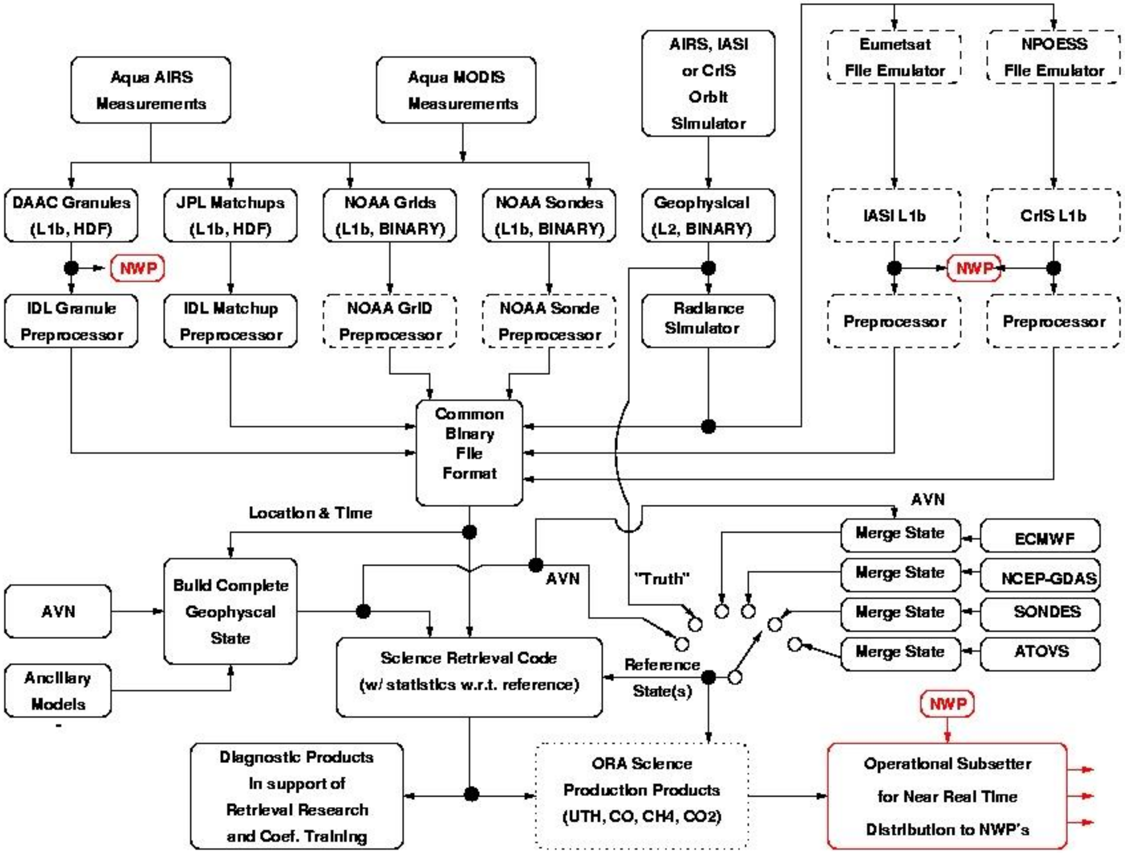
ALLCAPS is both an R2O and an O2R engine

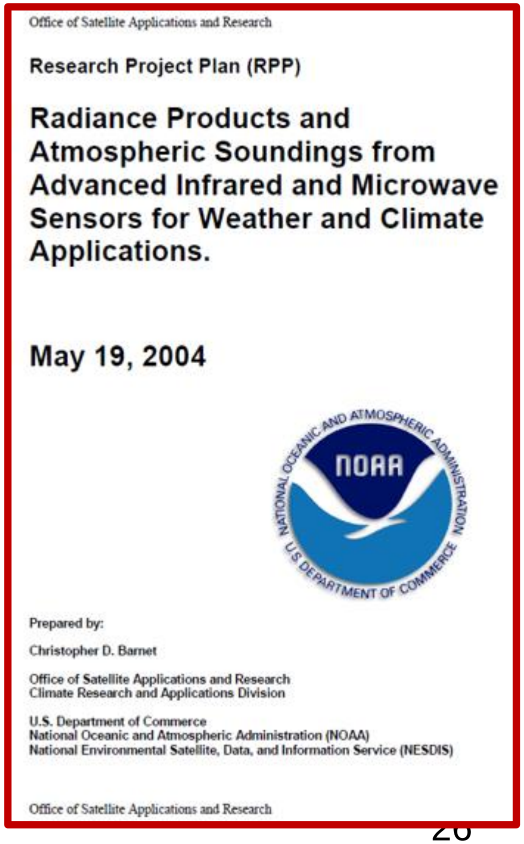
- NUCAPS is based on AIRS Science Team (AST) methodology (version 5.9) and leverages a NASA research investment to support NOAA operations (R2O)
  - NUCAPS-Metop has been operational since 2008
    - 2008 to present Metop-A/IASI+AMSU+MHS + AVHRR
    - 2012 to present Metop-B/IASI+AMSU+MHS
  - NUCAPS/S-NPP went operational in early 2013
  - NUCAPS/NOAA-20 will be operational soon (in DB now)
  - *NUCAPS/Aqua is in development to support post A-train Aqua*
  - NUCAPS has many operational users (T, q, O_3, CO, and CH_4)
- CLIMCAPS leverages NUCAPS & AST development (O2R)
  - We are exploring a NOAA Experimental system: NECAPS
    - NOAA requires diurnal continuity of Metop/S-NPP/NOAA-2x

CLIMCAPS has benefited from NUCAPS O2R investment
NECAPS can benefit from CLIMCAPS R2O investment

Enterprise approach for NUCAPS and CLIMCAPS was built in from the beginning

– Leveraged NASA AIRS science team research
– Made the retrieval algorithm sensor agnostic




Office of Satellite Applications and Research

Research Project Plan (RPP)

Radiance Products and Atmospheric Soundings from Advanced Infrared and Microwave Sensors for Weather and Climate Applications.

May 19, 2004

Prepared by:

Christopher D. Barnet

Office of Satellite Applications and Research
Climate Research and Applications Division

U.S. Department of Commerce
National Oceanic and Atmospheric Administration (NOAA)
National Environmental Satellite, Data, and Information Service (NESDIS)

Office of Satellite Applications and Research

ALLCAPS: Algorithm Philosophy, 1/3

- Operational code should be identical to the science code with diagnostics turned off.
- Algorithm should function on all operational *modern* hyperspectral and *advanced* microwave sounder space-borne instruments
  - Minimize instrument dependent features
  - Exploit the full information content of the measurements
    - Ability to discriminate between physical correlations (e.g., climate sensitivity of $\delta q/\delta T$) and spectral correlations induced by measurements (e.g., $\delta q/\delta T$ induced by spectroscopy)

ALLCAPS: Algorithm Philosophy, 2/3

- Minimize dependence of things we don't know well.
  - Minimize sensitivity to clouds
    - Exploit microwave information
    - IR cloud forward models are still not robust enough (in my opinion, but some day this will be false)
    - Sensitivity of infrared radiances to cloud parameters (particle sizes and shapes, vertical density) are highly non-linear
    - cloud parameters are not well constrained by infrared or microwave sounder measurements alone
  - Minimize Sensitivity of products to interfering signals
    - dT, dq, dT_{skin} co-varies with cloud signals
    - dT co-varies w/ dCO_2, dN_2O and interference with dq, dO3, ...
      - Microwave has unique dT from O2 band --
    - dq co-varies w/ dT, dCH4, dSO2, ... for IR
      - dq in the microwave is significantly more linear
    - If ignored, this “spectral” covariance can confound measurement of natural correlations (*i.e.*, Earth physical correlations)

ALLCAPS: Algorithm Philosophy, 3/3

- Desire a global, all season, all sky, all regions, retrieval
  - Avoid regional or highly tailored a-priori terms.
  - Avoid datasets that are not available or not skillful in remote regions.
- Derive formal and traceable error estimates
  - Provide either averaging kernels or error covariance output for each product (NOTE: they can be derived from each other).
  - The algorithm should fully characterize inter-correlation of products induced by retrieval.
- Desire a real time (weather) and re-processing (climate) capability
  - Avoid algorithms that are computationally intensive (either in CPU or memory requirements) if they do not add sufficient skill.
  - For weather applications avoid datasets with high latency.

Introduction to Physical Retrievals

Using operational

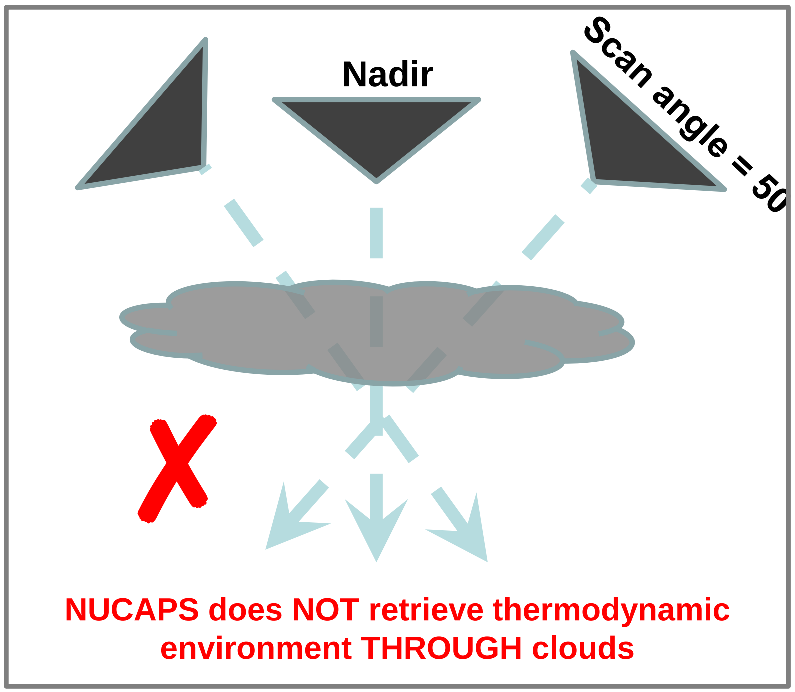
NUCAPS and CLIMCAPS
as an example

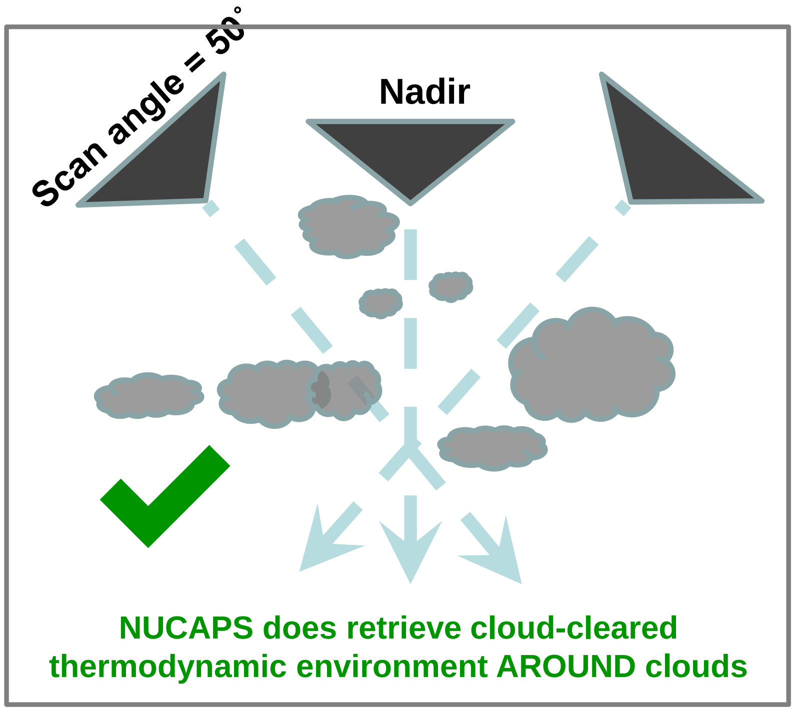
Is there a better way to deal with clouds?

To an Infrared Sounder (AIRS, IASI or CrIS) even a small amount of cloud is an obstacle.

NUCAPS performs "cloud clearing" to increase the yield of quality soundings

The goal is to provide soundings in difficult meteorological situations ….. and ….. as close to the surface as possible





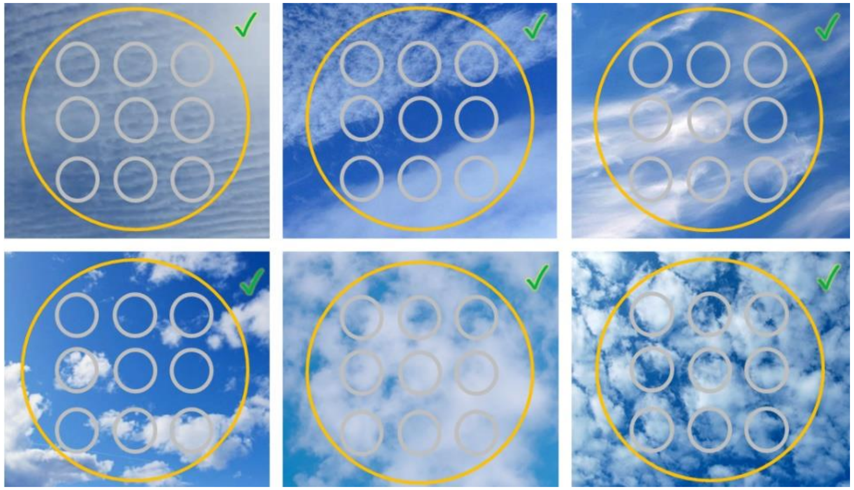
NUCAPS uses cloud clearing to retrieve soundings in partially cloudy scenes

Cloud Clearing succeeds when NUCAPS FOR has cloud variability; i.e. when the FOV's have variable cloud fractions

~2% probability a FOV is clear
~5% probability a FOR is clear

But ~70-80% of scenes can be cloud cleared
→ even if no single FOV is clear

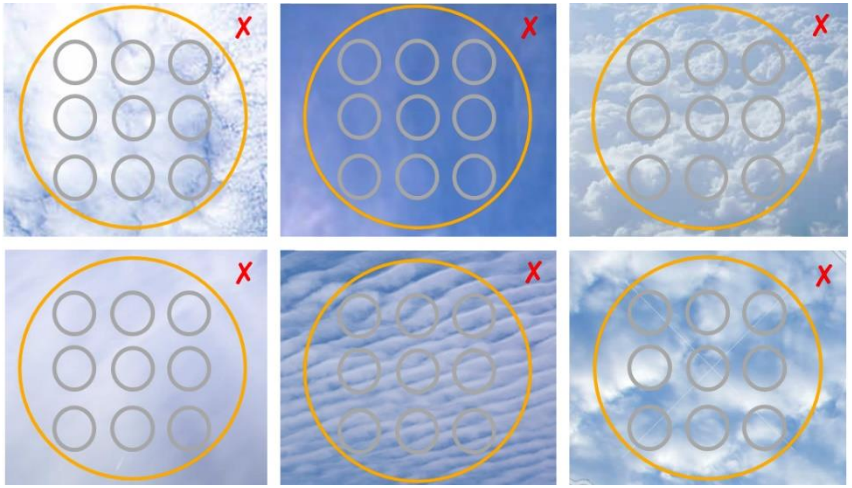
NUCAPS field of regard (FOR)
with a set of 9 field of view (FOV)



Cloud Clearing FAILS when NUCAPS FOR is uniformly cloudy, *i.e*. when each FOV has the same cloud fraction

Scene does not have to be overcast

Even a small amount of *uniform* clouds needs to be rejected
- Can use microwave to reject these



Spatial variability in scenes is used to correct radiance for clouds.

- We use a sub-set (≈ 50 chl's) of computed radiances from the a clear estimate (microwave helps here), $R_n = R_n(X)$ and 9 sets of cloudy infrared radiances, $R_{n,j}$ to determine a small set of extrapolation parameters, η_j.

$$\hat{R}_n = < R_{n,j} >_j + (< R_{n,j} >_j - R_{n,j}) \cdot \eta_j$$

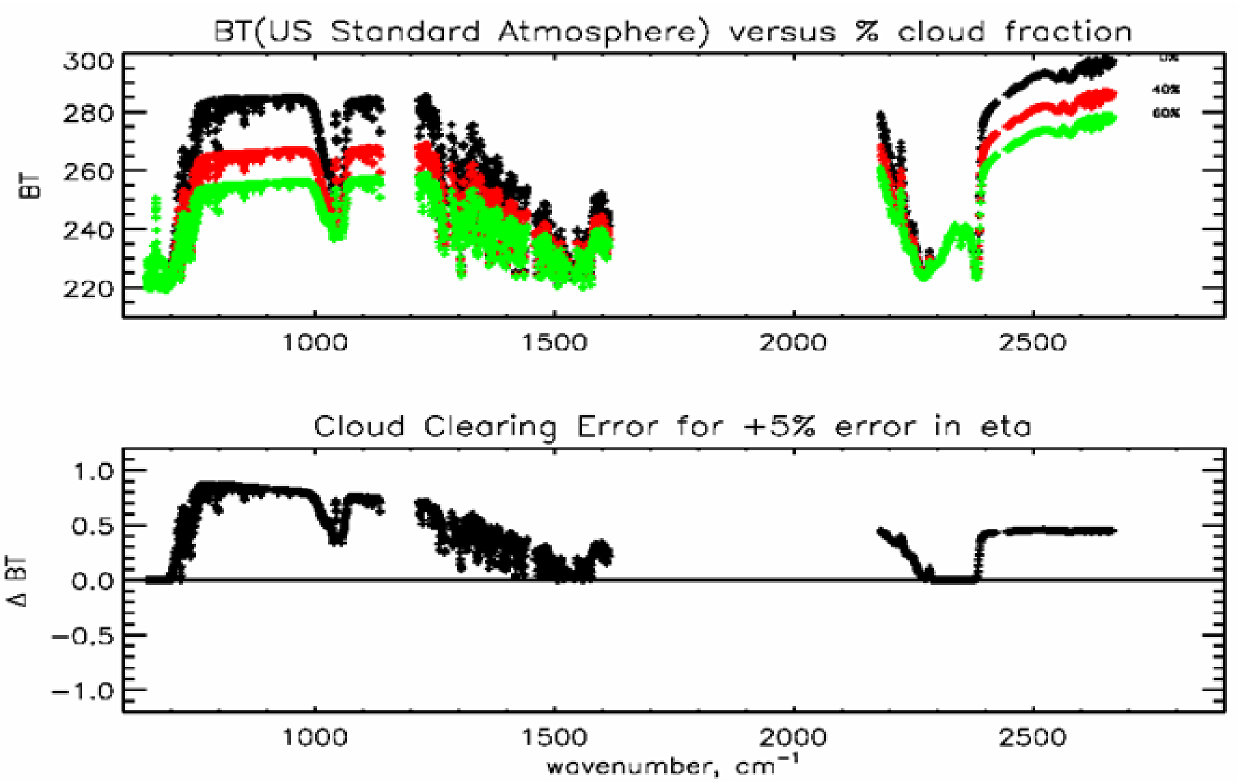
- Solve this equation with a constraint that $\eta_j \leq 4$ degrees of freedom (cloud types) per FOR
  - Same equation used to compute cloud cleared radiances, $\boldsymbol{R_{CCR}}$
- A small number of parameters, η_j, can remove cloud contamination from thousands of IR channels.
  - Does not require a model of clouds and is not sensitive to cloud spectral structure (this is contained in radiances, $\boldsymbol{R_{n,j}}$)
  - Complex cloud systems are handled with by the multiple η_j
  - $\delta\eta\delta\eta^T$ & $\boldsymbol{R_{n,j}}$ used to compute $\delta R_{CCR} \bullet \delta R^T_{CCR}$ – fully off-diagonal

Example of cloud clearing correlated error from AIRS Cloudy Spectra

Example AIRS spectra for a scene with
α= 0% clouds (black),
α=40% clouds (red) and
α=60% clouds (green).

Can use a small subset of channels in 15 μm region to determine clearing parameters, η_j

Note that cloud clearing produces a strongly spectrally correlated error, $\delta R_{CCR} \cdot \delta R^T_{CCR}$, but we know it well



In this 2 FOV example, the cloud clearing parameters, η_j, is equal to $\frac{1}{2}\langle\alpha\rangle/(\alpha_j-\langle\alpha\rangle)$

Pro's and Con's Of Cloud Clearing versus solving for cloud parameters

Pro's/Con's of cloud clearing	Pro's/Con's of parameter retrieval
Pro: Does not require a radiative transfer model for clouds.	Pro: Derives cloud particle types, optical depth, and other cloud information.
Pro: ~4 linear parameters can remove complex cloud formations (multiple cloud types, strong scattering, etc.)	Pro: Does not modify the instrument radiance. Theoretically can fit radiances to level of the instrument noise.
Con: Does not work when clouds are uniform on the ~50 km scale. Must use microwave to reject these cases	Con: Infrared does not constrain the plethora of parameters necessary to describe clouds.
Con: Sacrifices spatial resolution, but … Pro: retain spectral information for all other geophysical parameters.	Pro: can operate at full spatial resolution (~15 km for AIRS, IASI, CrIS)
Con: Radiances have highly variable noise that can be spectrally correlated. Pro: Error is well characterized.	Con: Cloud forward model errors are very large and induce large and unknown errors into the clear radiance.

Physical Retrievals

a.k.a., optimal estimation

This section picks up where session #1's slides ended

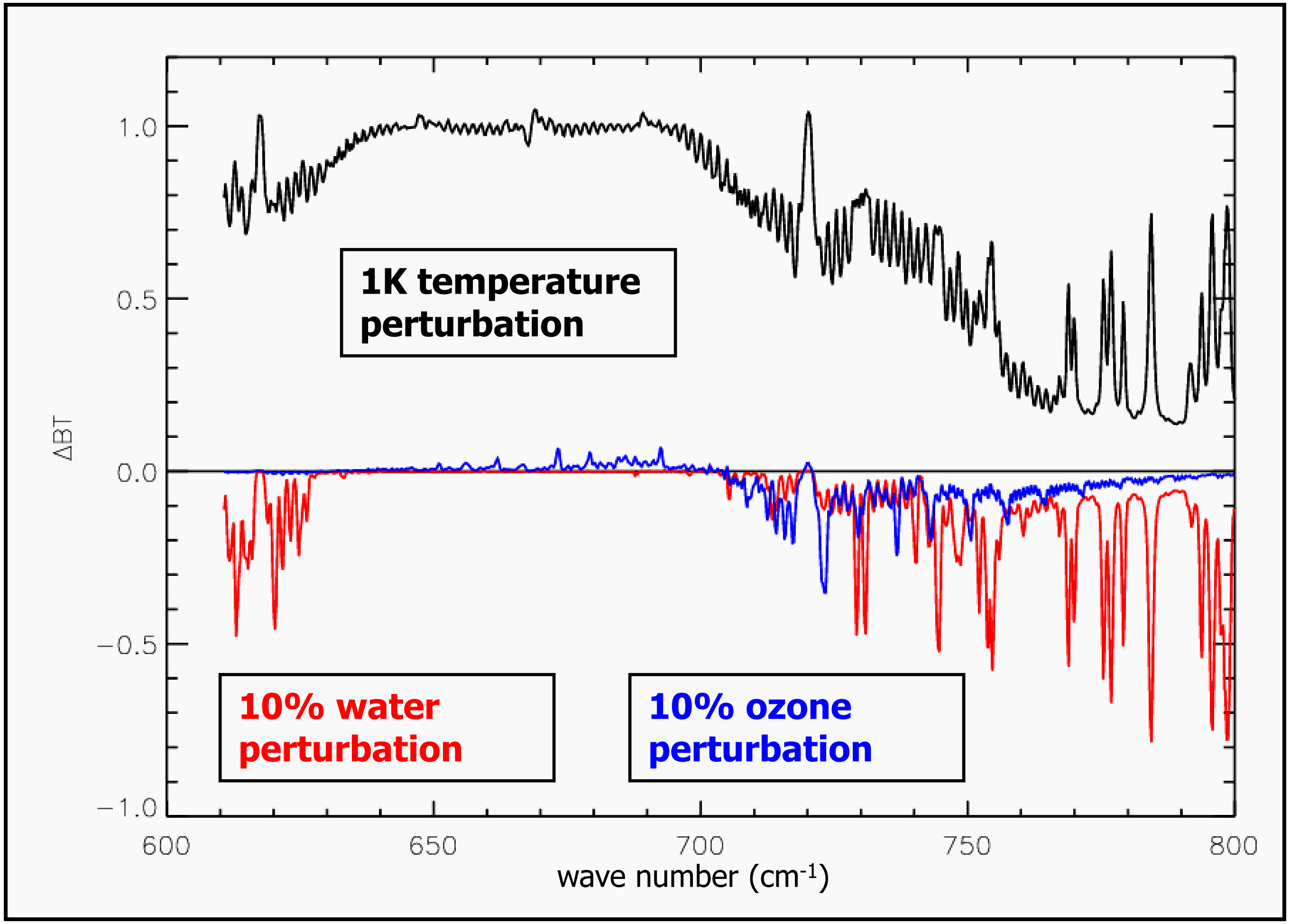
The Problem is Physical and Can be Solved by Parts

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

- 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 solution more stable.
- And has significant implications for operational execution time.

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

Sensitivity Analysis for Temperature Retrieval in 15 μm Band



Select channels for T(p) retrieval that have strong sensitivity to T(p)

Ignore channels with high interference to H2O, O3, etc. – i.e., weight = 0

Channels with strong sensitivity to T(p) and weak interference: add interference in N(n,m)

Step 1: *Temperature* Solution

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

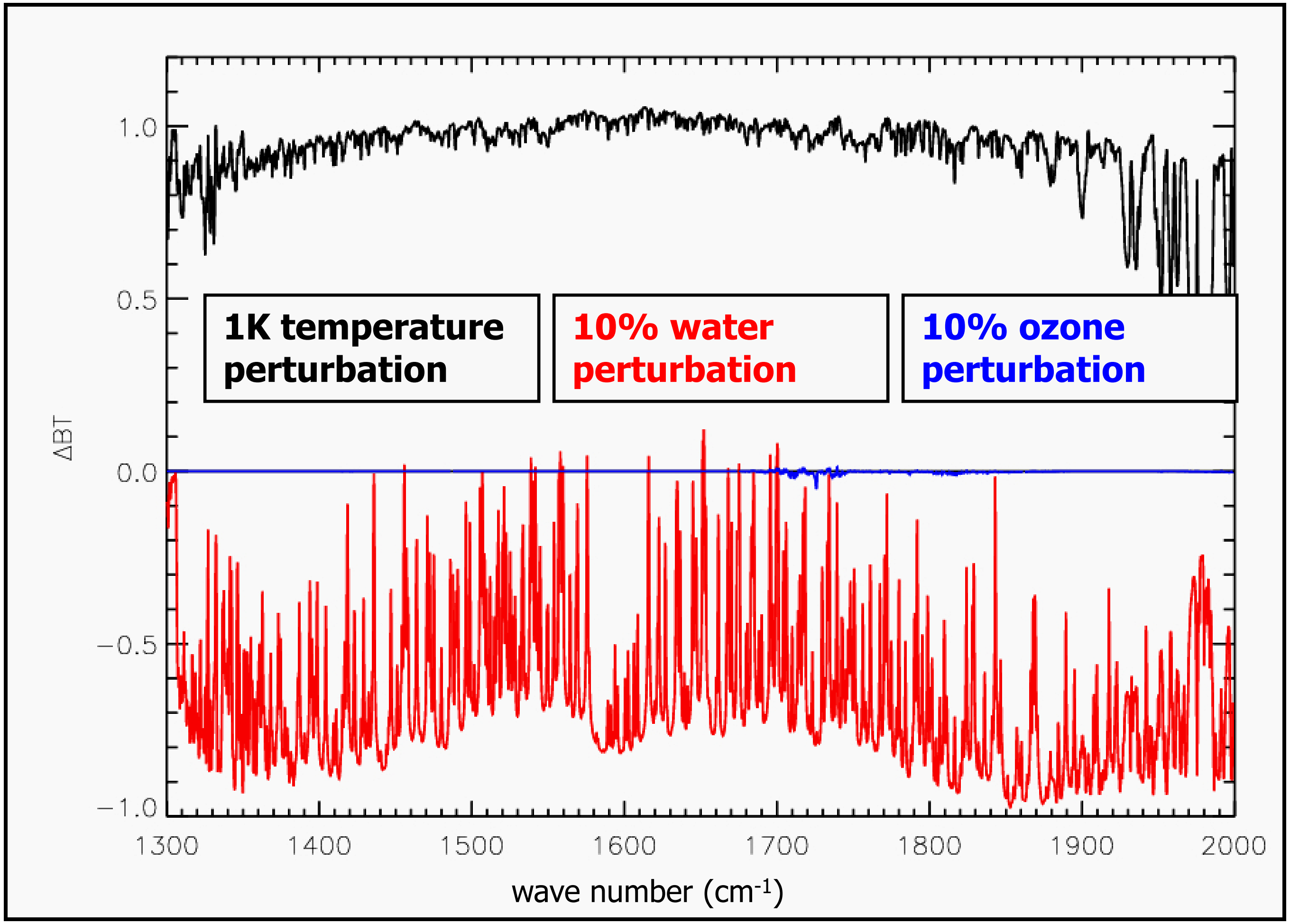
$$e_n = K_{n,i}^2 \cdot \delta\vec{q}_i + K_{n,i}^3 \cdot \delta\vec{O}_{3i} + K_{n,i}^4 \cdot \delta\vec{C}O_i + \ldots + \varepsilon_n$$

$$\Delta T_i = [K^{1^T}_{i,n} \cdot N_{n,n}^{-1} \cdot K^1{}_i + C_{i,i}^{-1}]^{-1} \cdot \left[K^{1^T}_{i,n} \cdot N_{n,n}^{-1} \cdot \Delta R_n + C_{i,i}^{-1} \cdot \Delta T_i^a\right]$$

$$N = \delta R_{CCR} \delta R_{CCR}{}^T + K^2 \delta q \delta q^T K^{2^T} + K^3 \delta O_3 \delta O_3{}^T K^{3^T} + \ldots$$

If δR_{CCR}, δq and δO_3 are small and their spectral fingerprint (K^2, K^3) is different than K_1, then we can "see through" the interference

Sensitivity analysis for water vapor retrieval in 6.7 μm band



Select channels with strong q(p) and weak interference from O3, CH4, SO2, etc

Ignore channels with strong interference.

Add interference to N(n,m) off-diagonal.

Note that T(p) is a strong interference, so we want errors as low as possible.

Step 2: *Water vapor* solution

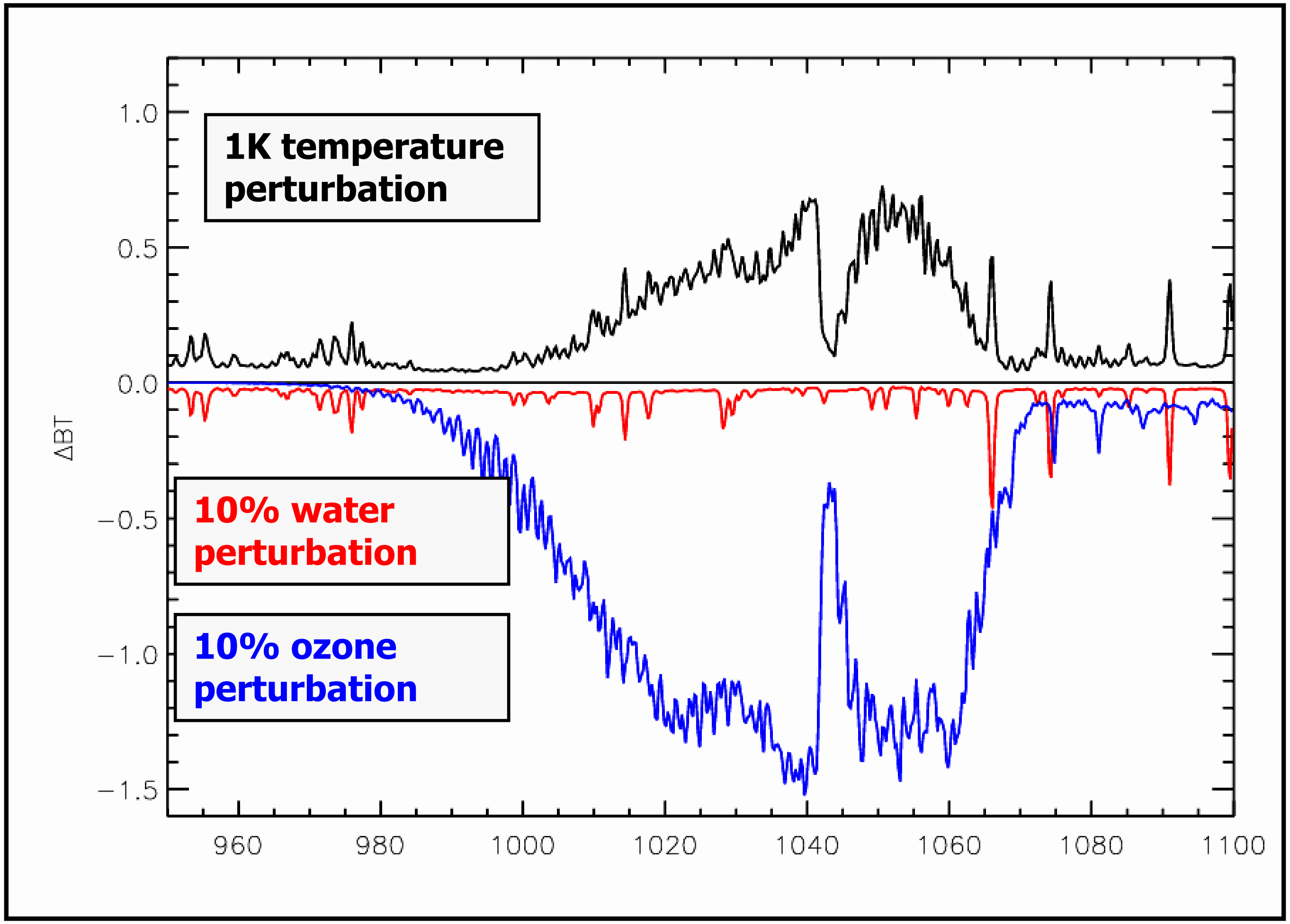
$$R_n^{obs} - R_n(\vec{X}) \approx K^2_{n,i} \cdot \Delta\vec{q}_i + e_n$$

$$e_n = K^1_{n,i} \cdot \delta\vec{T}_i + K^3_{n,i} \cdot \delta\vec{O}_{3_i} + K^4_{n,i} \cdot \delta\vec{C}O_i + ... + \varepsilon_n$$

$$\Delta q_i = [K^{2^T}{}_{i,n} \cdot N^{-1}_{n,n} \cdot K^2{}_i + C^{-1}_{i,i}]^{-1} \cdot \left[K^{2^T}{}_{i,n} \cdot N^{-1}_{n,n} \cdot \Delta R_n + C^{-1}_{i,i} \cdot \Delta q^a_i\right]$$

$$N = \delta R_{CCR} \delta R_{CCR}{}^T + K^1 \delta T \delta T^T K^{1^T} + K^3 \delta O_3 \delta O_3{}^T K^{3^T} + ...$$

Sensitivity analysis for ozone retrieval in 9.6 µm band



Select channels with strong O_3(p) and weak interference from q(p), emissivity, etc

Ignore channels with strong interference.

Add interference to N(n,m) off-diagonal.

Note that T(p) is a strong interference, so we want errors as low as possible.

Step 3: *Ozone* solution

$$R_n^{obs} - R_n(\vec{X}) \approx K_{n,i}^3 \cdot \Delta\vec{O}_{3i} + e_n$$

$$e_n = K_{n,i}^1 \cdot \delta\vec{T}_i + K_{n,i}^2 \cdot \delta\vec{q}_i + K_{n,i}^4 \cdot \delta\vec{C}O_i + \ldots + \varepsilon_n$$

$$\Delta O_{3_i} = [K^{3^T}{}_{i,n} \cdot N_{n,n}^{-1} \cdot K^3{}_i + C_{i,i}^{-1}]^{-1} \cdot \left[K^{3^T}{}_{i,n} \cdot N_{n,n}^{-1} \cdot \Delta R_n + C_{i,i}^{-1} \cdot \Delta O_{3_i}^{\,a}\right]$$

$$N = \delta R_{CCR} \delta R_{CCR}{}^T + K^1 \delta T \delta T^T K^{1^T} + K^2 \delta q \delta q^T K^{2^T} + \ldots$$

Problem in ill-determined: choice of a-priori is critical

See https://www.mdpi.com/2072-4292/11/10/1227 for more details

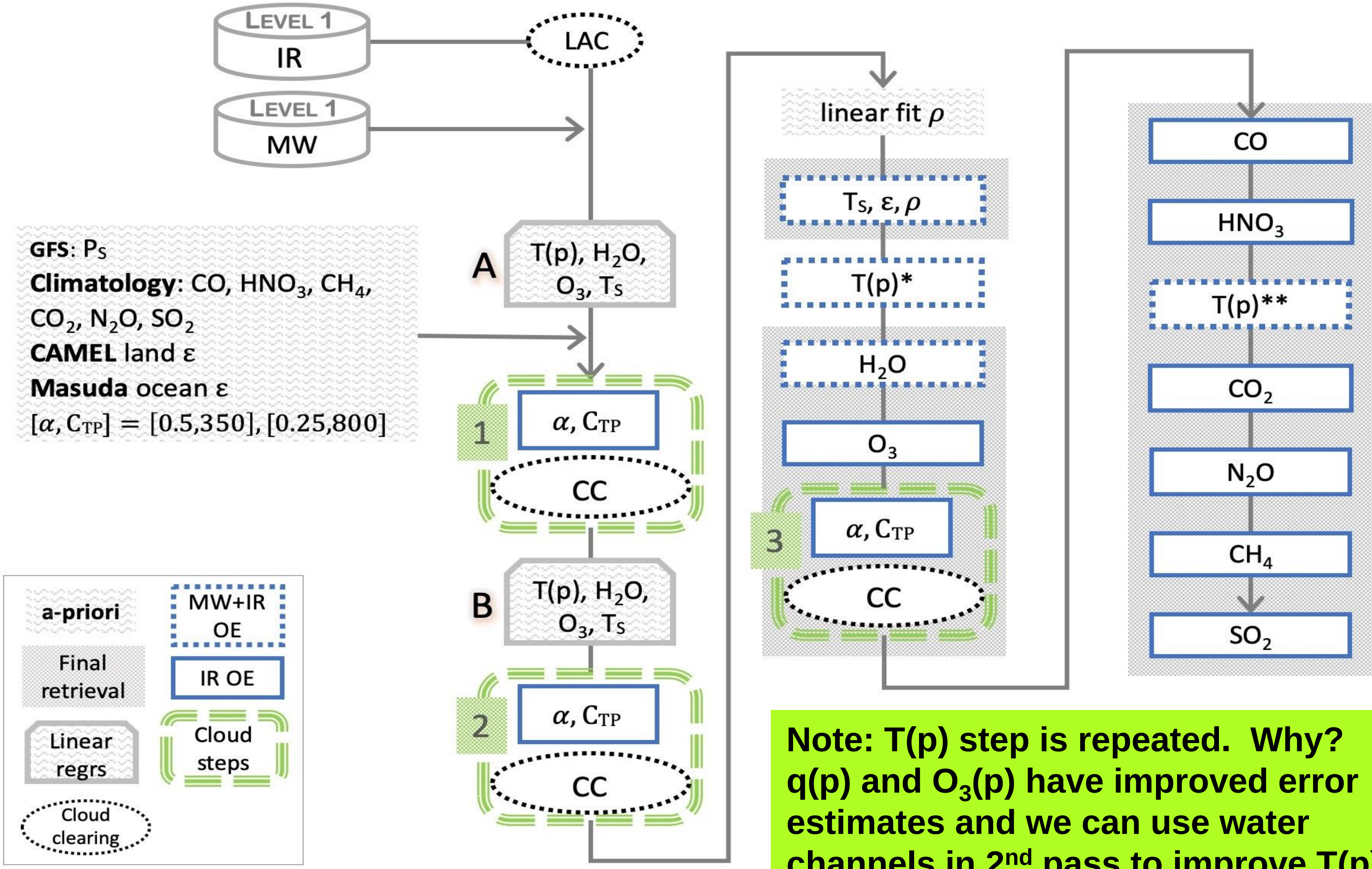
Regression-based

- Advantage it uses all spectral information and it is very fast and easy to implement.
- Training is limited by capability of single instrument and its space and time sampling.
  - Can propagate instrument specific biases.
  - Responds poorly to instrument calibration changes or aging that is outside its training domain.
  - Can induce spurious spatial structure due to sensitivity to cloud contamination or other signals that were not in the training.
- Amplifies scene dependent errors because information is used twice.
- Introduces correlations in the geophysical products that may or may not be real (e.g., CO/O3, q/SO2, T/CO2, T/N2O).

Reanalysis-based

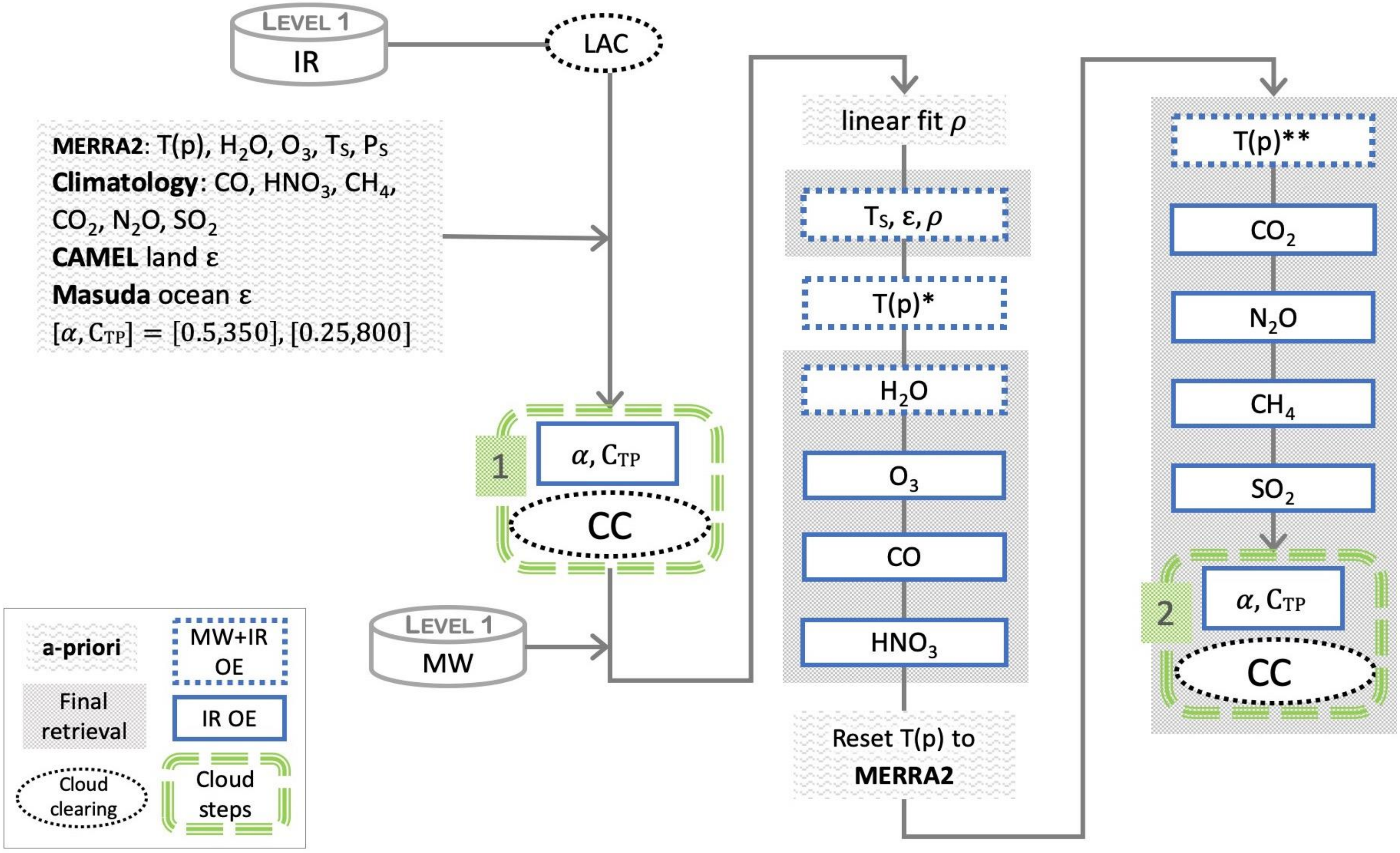
- Reanalysis is optimal-estimation of a suite of independent instruments.
  - We can benefit from full suite of in-situ and space-borne instruments (e.g., all AMSU, ATMS, CrIS, MLS(O3), OMI(O3)).
  - Our scene has been used in the assimilation (i.e., information used twice); however,
    - Obs are spatially and spectrally thinned.
    - Only uses cloud insensitive channels.
    - Overall weight of our instrument for this specific scene is extremely low.
    - We will study this and if it is an issue we can request a MERRA product that excludes our instruments.
  - Captures atmospheric variations at multiple space-time scales.
    - Blends observations of our specific instruments at other times and locations.
- MERRA-2 homogenizes the long-term EOS-era record
  - Model physics ensures scenes satisfy conservation of energy, momentum, and continuity (i.e., thermal wind equation).
  - MERRA mitigates biases induces by changing climate and trace gases.

Simplified NUCAPS Flow Diagram



Note: T(p) step is repeated. Why? q(p) and O_3(p) have improved error estimates and we can use water channels in 2nd pass to improve T(p).

Simplified CLIMCAPS Flow Diagram



Questions?

More information at:
http://goo.gl/twuRtW

~/rs_notes.pdf

- Radiative transfer
- Derivations
- Details about instruments

~/phys640_s04.pdf

- Mathematical methods
- Linear and non-linear Least Squares
- FFT's and Apodization

For More Information

AIRS Project Page:

https://airs.jpl.nasa.gov/

NUCAPS and CLIMCAPS Landing Page:

https://weather.msfc.nasa.gov/nucaps

Product descriptions, Training guides, Data access, FAQs

Access Publications

(Smith and Barnet 2019 Remote Sensing) CLIMCAPS Algorithm paper

https://www.mdpi.com/2072-4292/11/10/1227

(Smith and Barnet 2020 Atm. Meas. Tech.) CLIMCAPS Information Content

https://www.atmos-meas-tech-discuss.net/amt-2020-71/

(Esmaili et al. 2020 Remote Sensing) NUCAPS Hazardous Weather Applications

https://www.mdpi.com/2072-4292/12/5/886

Calcon Workshop: Current Challenges in the Remote Sounding of the Earth

3: Applications and future sounders

Chris Barnet

NOAA/JPSS Senior Advisor for Atmospheric Sounding

NASA S-NPP Sounder Discipline Lead

Science and Technology Corporation (STC) Senior Scientist

Monday   Aug. 30, 2021

Topics for Today

- Workshop will have 3 sections
  1. Introduction to Remote Sounding
  2. Example of operational sounding: NUCAPS, CLIMCAPS, and NECAPS
  3. Applications and future sounders.
- Each section will consist of
  – ~40 minute lecture
  – ~15 minutes Q&A
  – ~5 minute bio break

Some Example Applications

With the JPSS Initiatives we have had a paradigm shift in communication

- In the past the sounding community has had a "build it and they will come" approach.
  - It did not work.
- In NOAA JPSS Initiatives we are working within the user community to meet their needs.

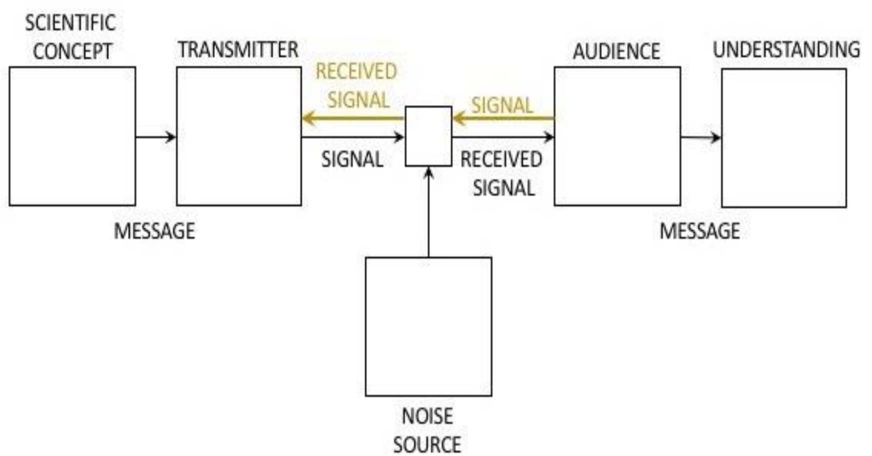
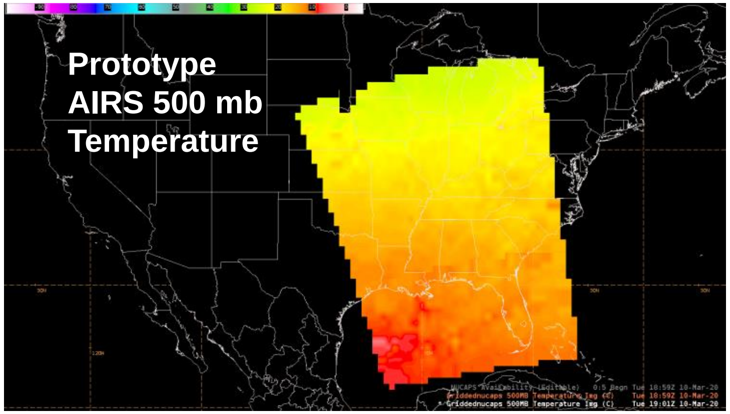


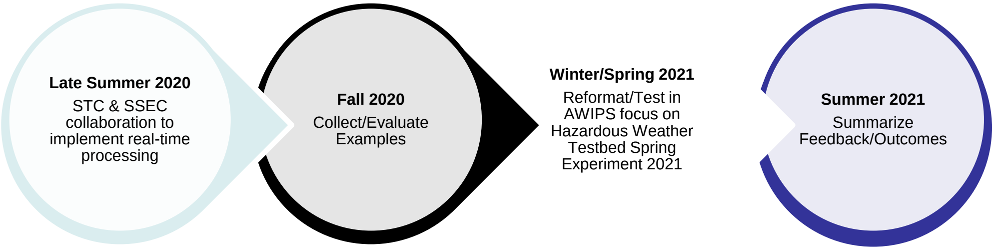
Fig. 2: Reinterpreting Fig. 1 with a focus on scientific communication

Smith, N., C.D. Barnet and K. Shontz 2018. What is a satellite measurement? Communicating abstract satellite science concepts to the world. AMS 14th Symposium on New Gen. Env. Sat., 3 pgs

Addition of NUCAPS/Aqua in AWIPS
PI’s: Emily Berndt (SPoRT), Nadia Smith (STC)

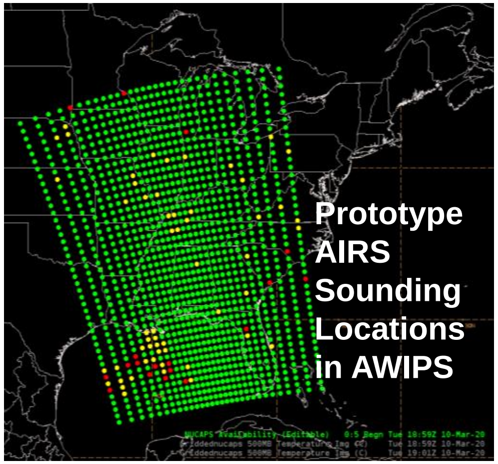
- **Goal:** Experimentally demonstrate the value of late afternoon orbits in NWS forecasting applications
- **2021:** Demonstrate real-time, low-latency NUCAPS/Aqua in AWIPS environment and characterize value w.r.t. NUCAPS/NOAA-20
- **2022-2025:** Demonstrate the value of hyperspectral infrared observations in the convective regime as Aqua’s orbit drifts from 1:30 to 5:30

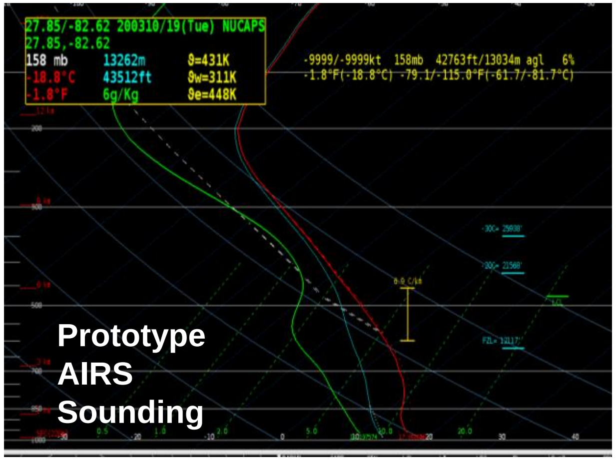




Sounding Science Questions:

- **What is the value of additional AIRS observations**
  - **Does NUCAPS/Aqua have same characteristics as NUCAPS/S-NPP and NOAA-20?**
  - **What does NUCAPS/Aqua provide that is unique?**
  - **Are there features that would have been missed with NOAA-20 alone?**
- **What are the challenges of sounding in the convective regime?**
- **What is the value of multiple satellite platforms that have diurnal continuity between pre-convective (JPSS-x) and convective regimes (Aqua)?**
  - **A low-cost path-finder for post-prime mission S-NPP and future SmallSat sounding missions**

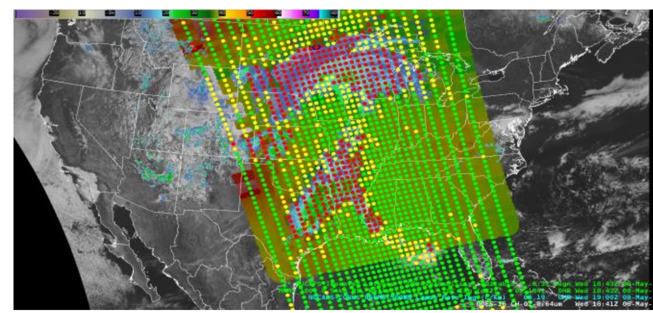




Hazardous Weather Testbed

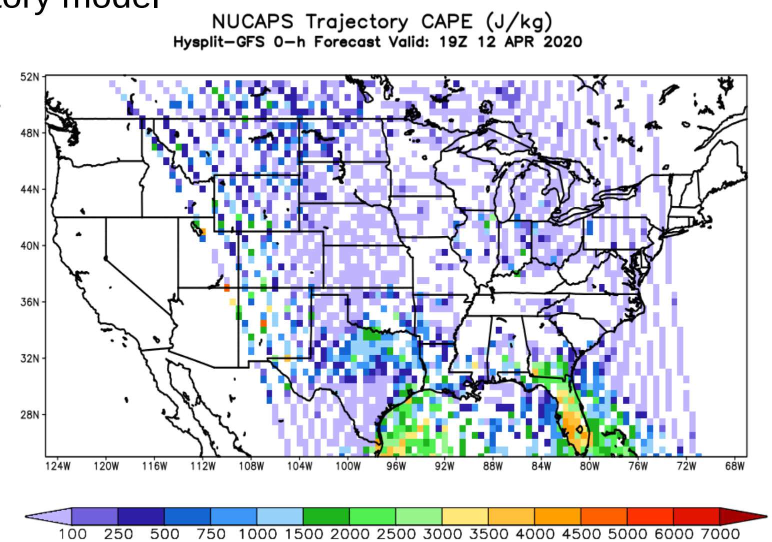
General Outcomes (so far):

- We had a successful spring experiment thanks to NASA/SPoRT
  - Supported 6 weeks of forecaster training.
  - Each week we had a group (4 to 5) NOAA forecasters and 1 media forecasters training on new products.
  - SOO from Des Moines, IA “We look for a dataset once or twice, but after that it’s dead to us.”
- The depiction of the boundary layer and low level instability calculations need to be improved for severe weather forecasting.
- Testing of new products: NUCAPS-FCST
  - Uses back-trajectories to “construct” a sounding in difficult regimes from previous soundings in less severe regions



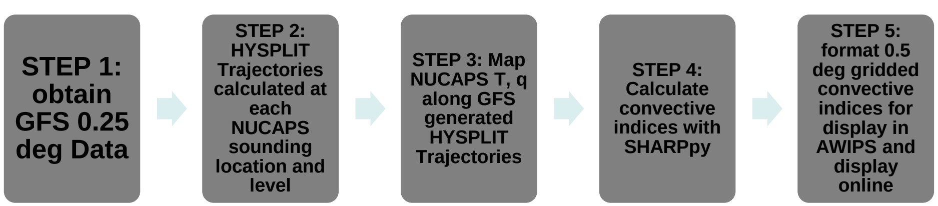
Expanding the time dimension
PI's: Kahn & Kalmus (JPL), Berndt (SPoRT)

- NUCAPS Soundings are advected forward in time (called NUCAPS-Forecast)
  - Developed by Peter Kalmus & Brian Kahn at JPL (Kalmus et al. 2019)
  - Assuming adiabatic parcel theory with the HYSPLIT trajectory model
  - 1 hour increments for a total of 6 hours
  - Output gridded for plan view displays of convective indices
  - Can utilize accepted soundings in storm environment to forecast soundings in regimes that are typically rejected.



- **Originally developed as a NASA AIRS project**
- **SPoRT operationalized research code to use near-real time NUCAPS and GFS model data, development of multi-node parallel processing to deliver AWIPS-compatible files**
- **Rapid conversion of science capabilities to demonstrate to forecasters at the Hazardous Weather Testbed**
- **Added capability to process both S-NPP and NOAA-20**
- **NUCAPS-Forecast is a capability to support scientific process studies and demonstrate the value of increased temporal & spatial coverage of hyperspectral infrared sounders**

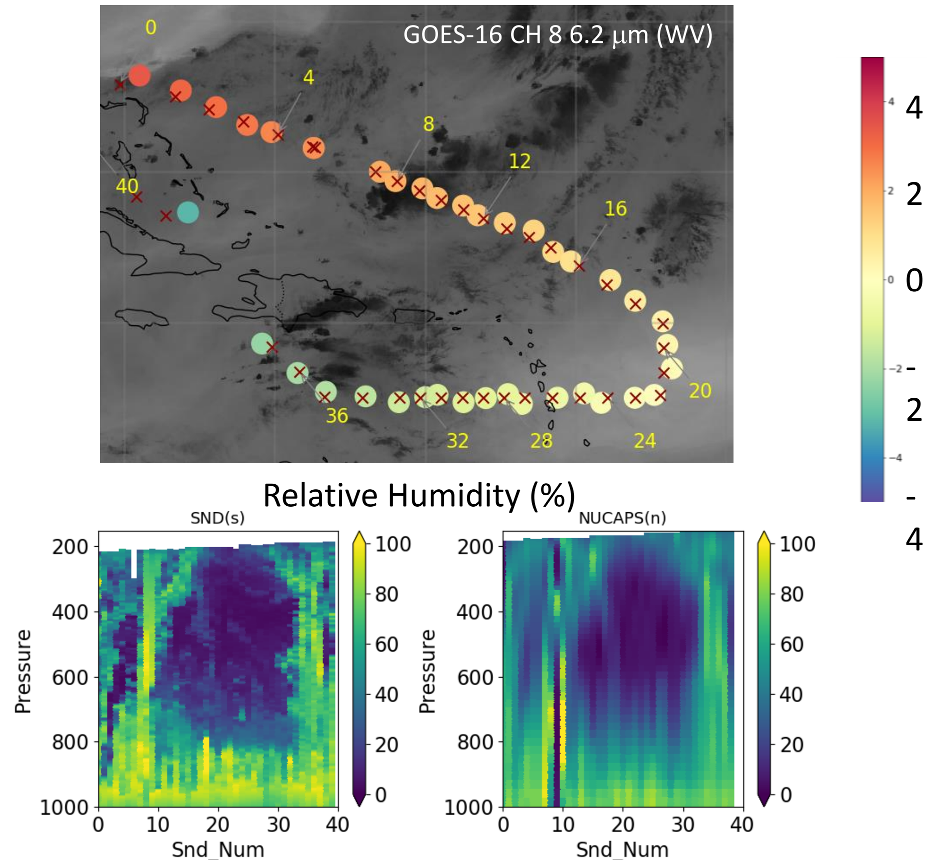
The gradients of CAPE are essential to diagnosing where convective initiation takes place. NUCAPSFCST not only provides gradients in space but also in time. ~forecaster HWT 2019



Kalmus 2019: Mon. Wea. Rev., doi: 10.1175/MWR-D-18-0055.1

Hurricane Field Program 2019

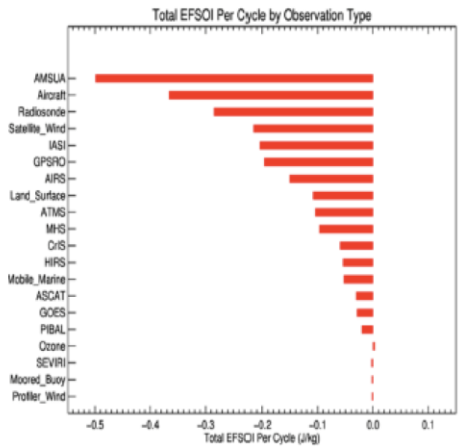
- Sample Saharan Air Layer (SAL) and tropical disturbances, particularly around/near Tropical Cyclone environment.
- Gulfstream-IV flight patterns and take-off times will be adjusted to sample targets that maximize temporal and spatial overlap with overpasses by the NOAA-20 and S-NPP.
- GPS dropsonde timed to be ≤1 hr and ≤50 km of collocated NUCAPS sounding granules.



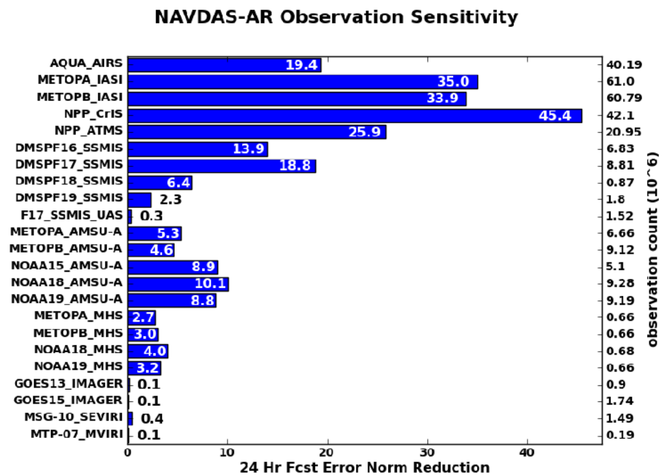
NOAA Sounding applications: DA

In Data Assimilation (DA) applications, hyperspectral infrared (IASI, AIRS, CrIS) and microwave (AMSU, MHS, and ATMS) sounders have high impact per instrument

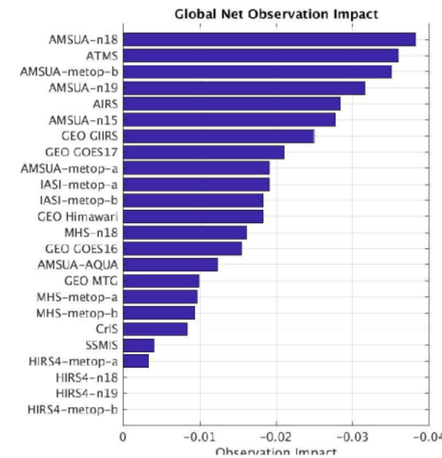
NCEP Global (Collard 2/2020)



NRL (Ruston 3/2020)



GMAO (McCarty 2/2020)

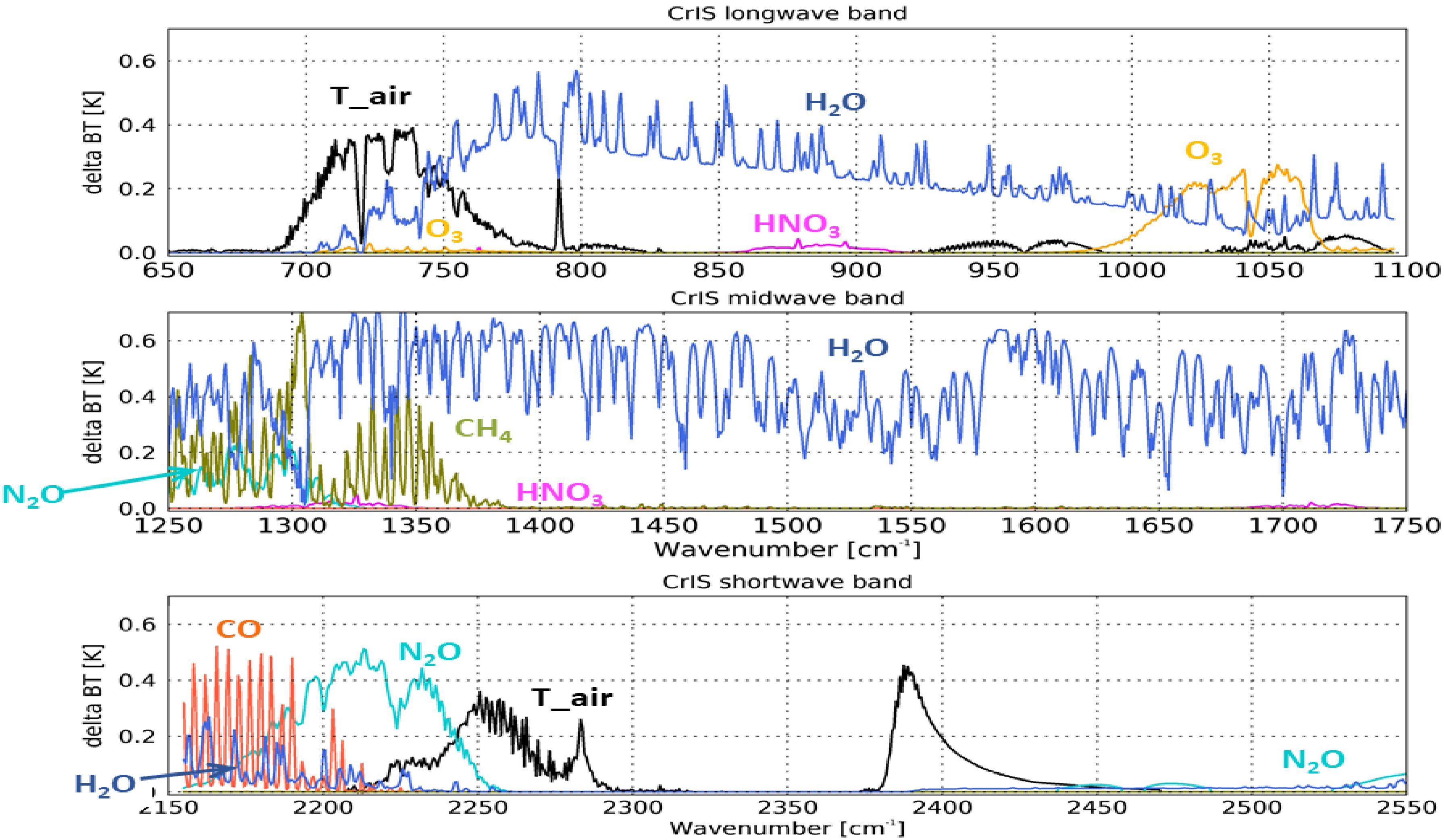


- Traditionally LWIR/VLWIR *infrared radiances* (15 um region) has been used.
- Recently NOAA/STAR has shown using real CrIS data that the MWIR (4.3 um) *radiances* has about the same skill as the LWIR/VLWIR in the NCEP system.

Data Assimilation versus Retrieval (discussed in talk #1)

Data Assimilation	Sounding
In practice, a spectral subset (10%), spatial subset (5%), and clear subset (5%) of the hyperspectral infrared observations are made.	All instrument channels can be used to minimize a larger number of parameters (T, q, O_3, CO, CH_4, CO_2, clouds, etc.)
Instrument error covariance is usually assumed to be diagonal. For apodized radiances (*e.g.* IASI) adjacent channels must be avoided.	Retrieval can be done in stages (most linear first). Product error covariance has vertical, spatial, and temporal off-diagonal terms.
Require very fast forward model, and derivative of forward model.	Most accurate forward model is used with a model of detailed instrument characteristics.
Tendency to weight the instrument radiances lower (due to representation error) to stabilize the model. Use correlation lengths to stabilize model horizontally, vertically, and temporally.	Retrieval can exploit a-priori information in the forward model and minimize assumptions about geophysical a-priori. Representation error is zero since retrieval is along slant path.
On any given iteration the satellite radiances have a small impact. Assumption is that the satellite observations will continually knudge the system towards the correct state.	Retrieval maximizes the utilization of the radiances of a single satellite. Promotes better understanding of the potential value of that satellite.

Sensitivity of CrIS radiances to T(p) and selected gases



Value of trace gases to NOAA applications.

- The infrared is sensitive to many trace gases.
- Temperature is derived from infrared using long-lived gases
  - Use carbon dioxide (CO_2) at both 15 and 4.3 μm
  - Use nitrous oxide (N_2O) at 4.5 μm
- Many trace gases affect the ability to retrieve T(p) and q(p).
  - Both CO_2 and N_2O vary in time and space and need to be known.
  - Ozone (O_3), volcanic sulfur dioxide (SO_2), methane (CH_4), and Nitric Acid (HNO_3) are interference gases that make sounding in BL more difficult.
- Sensitivity of an instrument to all of these gases is an implicit component of the T(p) & q(p) performance for modern sounding.
- But we are finding applications for the trace gases themselves.

Assessing Synoptic Scale Features (PI: Berndt, SPoRT)

- Originally developed as a NASA AIRS project.
  - Changes in mid-latitude cyclone and hurricane extratropical transition can be driven by interactions with stratospheric intrusions
- Transitioned to NOAA
  - NUCAPS 500 hPa Temperature and Relative Humidity can identify the upper-level trough and dry-conveyor belt
  - The Gridded NUCAPS Ozone Anomaly and Tropopause Level products can more precisely track the stratospheric intrusion location/depth

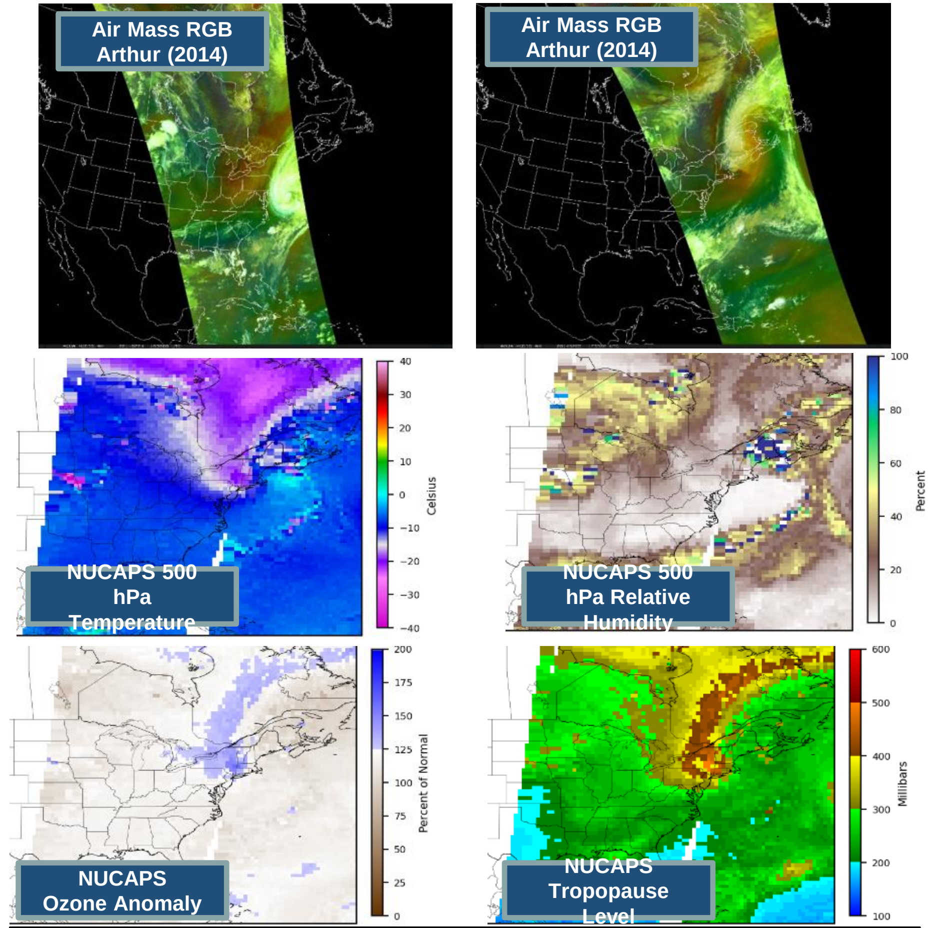
Ozone Anomaly (Percent of Normal)

- Stratospheric air can be identified where ozone values are at least 25% greater than the climatology (Van Haver et al. 1996)
- Product displayed in Percent of Normal 0-200%
- Shades of blue (values >= 125%) indicate stratospheric air and the ozone values are anomalous for the month and latitude (Ziemke et al. 2011)

Tropopause Level (Millibar)

- Ozone can be used to identify the tropopause level, use of a single value (e.g. 100 ppb) is misleading
- The seasonal variation of ozone at the dynamic tropopause (2 PVU) is described by Thouret et al. (2006)
  91 + 28 sin(pi*(month-2)/6)
- Tropopause level is found by matching the level where the ozone value is greater than or equal to the Thouret et al. (2006) value

Berndt et al. (2016); Berndt et al. (2020)



Gridded NUCAPS supports analysis of synoptic and dynamic features associated with the extratropical transition of Hurricane Arthur.

FIREX-AQ Field Campaign

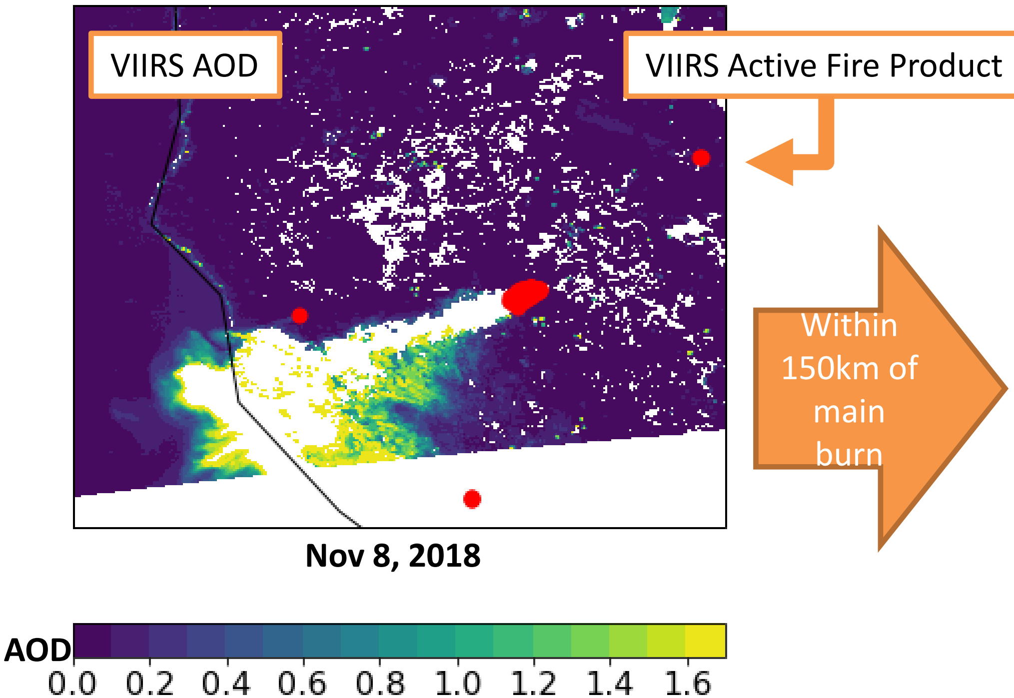
- **Event types**: Investigating wildfires, prescribed agricultural fires, prescribed forest service burns.
- **Science Goals**: Study composition, structure, fire progression

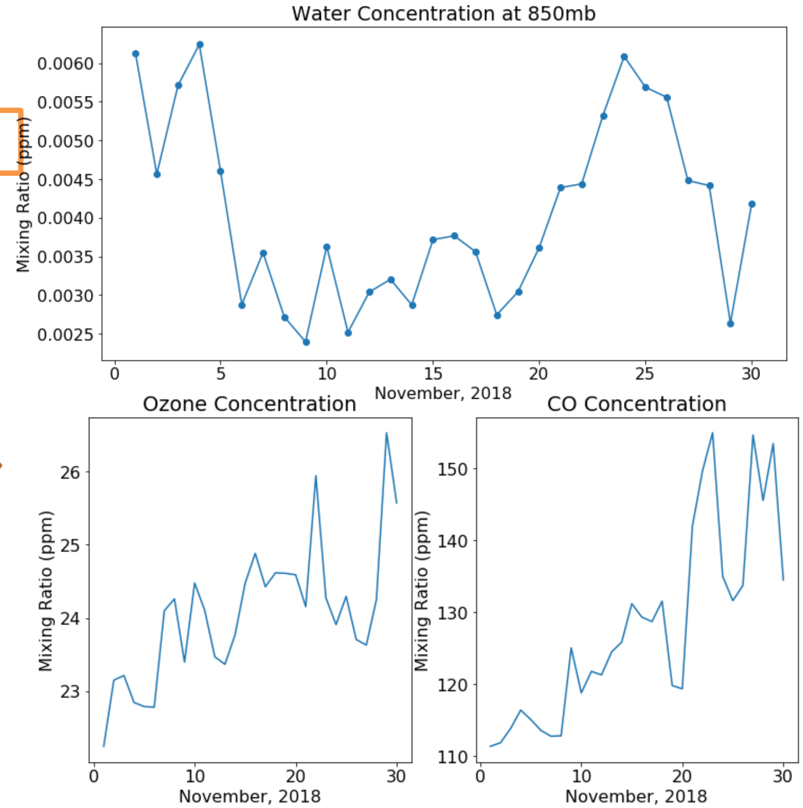
- We provided real-time (direct broadcast, ~20 latency) display of selected products to the field campaign (e.g., moisture, ozone, carbon monoxide, quality control):

  http://sigma.umd.edu/resmaili/nucaps.html

Camp Fire example

- A forest fire began on **Nov 8, 2018.** Caused by very low regional humidity due to strong gusting wind events and very dry surface.





The Future

Both DA and EDR applications require soundings in the most demanding of scenes

- Most valuable soundings are in rapidly evolving, convective weather where model parameterizations are failing.
  - Clouds and aerosols become a dominate error source in these regimes.
- Applications need high vertical resolution and accuracy in boundary layer (BL).
  - Atmospheric absorption features are naturally broadened by atmospheric pressure.
  - Water vapor absorption becomes significant – some spectral regions become opaque and other's water acts as a strong, non-linear, interference.
  - Errors in a top-of-atmosphere (TOA) sounding are compounded in the BL and vertical resolution necessary to resolve inversions, capping layers, etc. is not the major limitation.
- Validation in demanding scenes is extremely difficult.
  - It is difficult to demonstrate the performance of an instrument in these scenes.
    - Field campaign data is sparse in these environments
    - Operational radiosondes are typically 100's of km or hours away from these events.
      - Radiosondes do not represent the same scene as a sounding – different spatial and temporal sampling.
  - Simulated data is unrealistic in these scenes.
  - Global statistics are misleading – over-emphasize oceans and vast regions of stable scenes.

See https://www.mdpi.com/2072-4292/12/5/886 for an overview of the Hazardous Weather Testbed evaluation

Capabilities for sounder evaluation

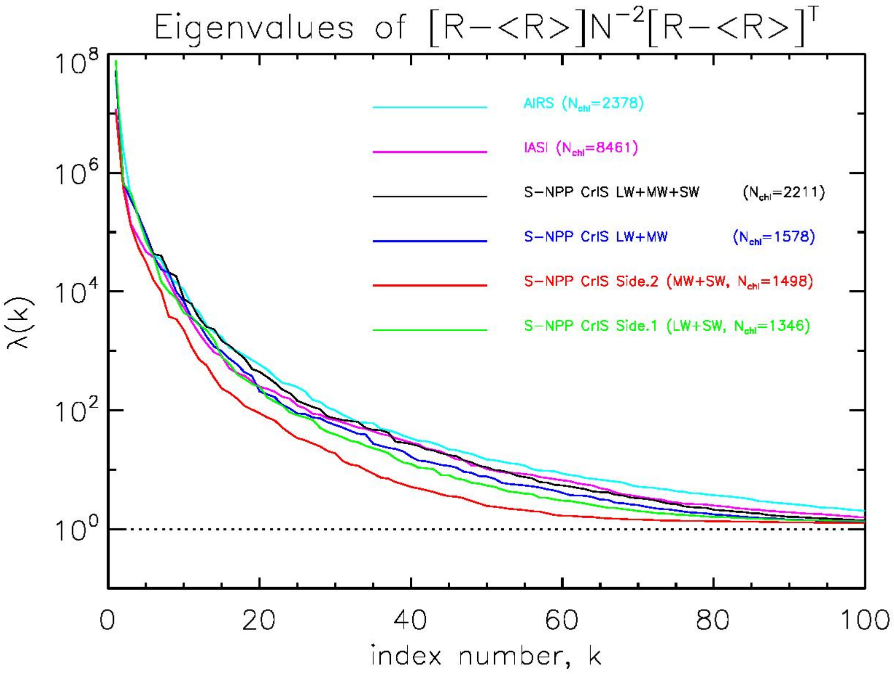
- We have been developing a capability to assess the performance of modern microwave and infrared sounders
  - Core system was developed for AIRS Science Team Simulations (circa 1995) and also the government assessment of CrIS vendor algorithms (circa 2001).
  - Recently used for used to test the early configurations of the JPL/CIRAS instrument.
- Components of this system are:
  - Theoretical: understanding the spectral properties of molecular species.
  - Statistical: empirical understanding the information content of the instrument.
  - Physical retrieval: ability to derive geophysical parameters for a given instrument configuration using real data with real world uncertainties.
    - Assess potential value of instrument in radiance assimilation.
    - Can test in specific applications: AWIPS pre-convective, cold air aloft, air quality applications (e.g., wildfire), winter weather, hurricane forecasting, etc.
- First, we will assess S-NPP CrIS in the LW+MW, MW+SW, LW+SW configurations.

Aging Instrument: Impact of the loss of bands on Suomi-NPP in NUCAPS

- Mar. 26, 2019 at 18:27 UTC (2:27 pm EDT) MW-band failed, CrIS turned off
- June 24, 2019 ~17:35 UTC S-NPP CrIS switched to Side-B, 18:52 UTC S-NPP CrIS switched to FSR mode
- May 21, 2021 15:42Z During Fairbanks contact 49561 (AOS 1552Z). CRIS Side.B LW band failed
- July 12, 2021 S-NPP CrIS switch back to Side-A, LWIR+SWIR is functional

Eigenvector decomposition of real data demonstrates expected performance

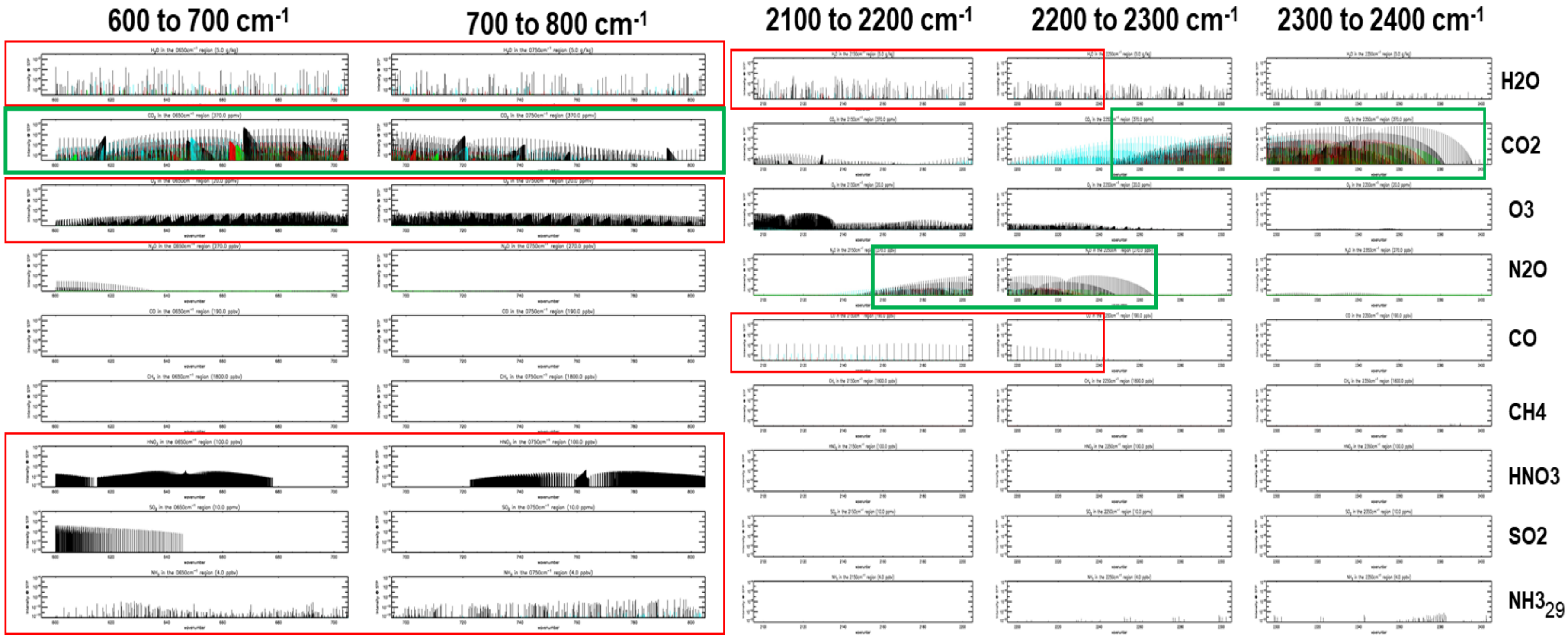
- We computed noise-normalized eigenvalues for the S-NPP CrIS radiances for all bands (black) and various subsets of the LW, SW, and MW bands.
- This approach informs us on how many independent degrees-of-freedom (d.o.f.) there are in each subset.
- It *does not tell us* what kind of information is contained in these subsets (looking at retrieval results in following slides; however, gives us reasonable clues).



Satellite	Spectral domain	Line in Figure	# of channels	d.o.f.
S-NPP / CrIS	LW + MW + SW	Solid black	2211	100
S-NPP / CrIS	LW + MW	Solid **blue**	1578	90
S-NPP / CrIS	MW + SW	Solid **red**	1498	65
S-NPP / CrIS	LW + SW	Solid **green**	1346	80
Aqua / AIRS	LW + MW + SW pristine	**Cyan**	~1500	110
Metop-B / IASI	LW + MW + SW	Magenta	8401	100

- **From an information content perspective, LW+SW is better than MW+SW**

Details of HITRAN for LW and SW bands used for T(p) sounding

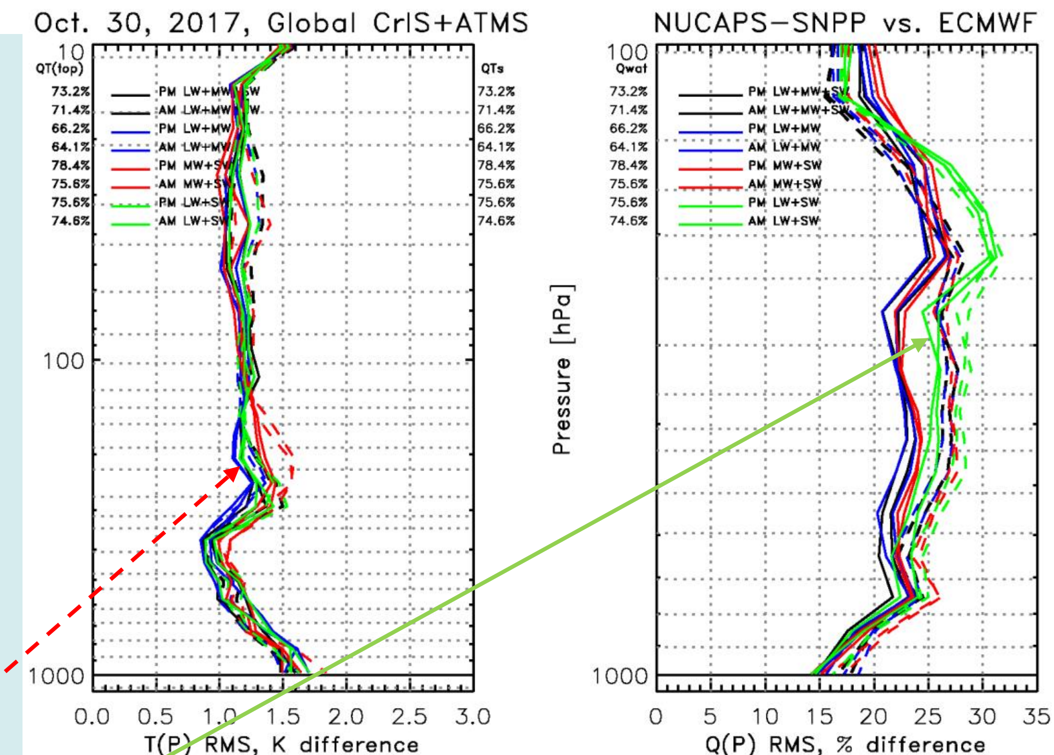


- LW (600- 800 cm^{-1}) T(p) sounding channels in **green**, boxes, interferences in **red**
- SW (2100-2400 cm^{-1}) T(p) sounding channels in **green**, boxes interferences in **red**
- **The 4.3 CO_2 R/P-branch, 2300-2400 cm^{-1}, has almost no interferences w.r.t. LW**
- **The N_2O υ3 band, 2150-2250 cm^{-1}, can also be used for T(p) sounding**

NUCAPS w/ CrIS configurations (ATMS used in REG and PHYS retrievals)

- **Black** lines are all-band system (LW+MW+SW+ATMS)
- **Blue** lines have SW band removed (LW+MW+ATMS)
- **Red** lines have LW removed (MW + SW + ATMS)   == S-NPP Side.B
- **Green** lines has MW removed (LW+SW+ATMS) == S-NPP Side.A

- Temperature is not significantly impacted by loss of MW band
  - Loss of MW chl's in pass.2 T(p) does degrade T(p) slightly
- MW+SW T(p) slightly degraded near the 200 hPa
- LW+SW q(p) RMS exceeds requirements by ~4% and is ~2-3% higher than LW+MW+SW
  - LW channels are used in q(p) retrieval.
  - A lot of the skill is from ATMS.



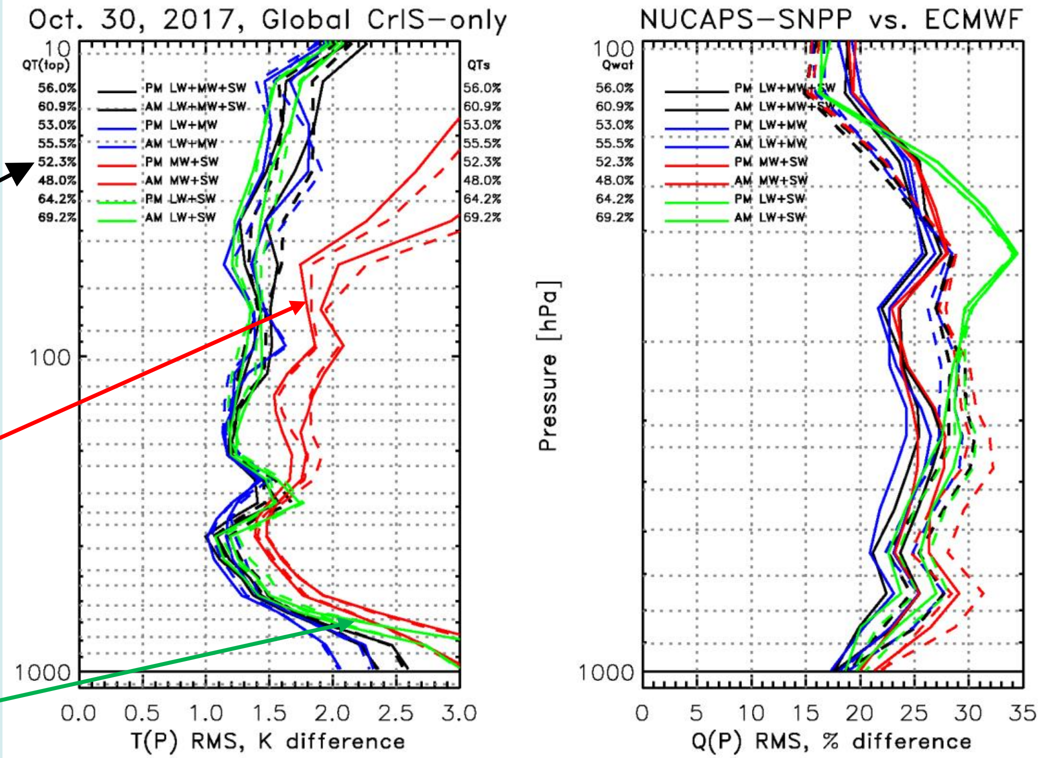
Notes:
- **AM and PM have separate statistics to see any day/night diff's**
- **Dashed lines are regression retrieval that uses cloud cleared radiances**
- **Solid lines are physical retrieval**

Same CrIS configurations, NO ATMS
(We have NOT recommended this operationally)

Same colors as previous slide

Results:

- Overall yield decreases from ~75% to ~55% due to loss of ATMS in regression and physical steps and poorer cloud clearing.
- MW+SW performance degrades in stratosphere due to loss of ATMS Chl's 14-15 and high-peaking channels at 665 cm-1.
- MW+SW and LW+SW lower troposphere degrades in both the regression and physical approaches which we attribute to more difficulty in the cloud clearing methodology.
- Water vapor degrades for all systems due to the loss of ATMS H2O sensitive channels in both REG and PHYS and poorer performance in T(p).



Notes:

- **AM and PM have separate statistics to see any day/night diff's**
- **Dashed lines are regression retrieval using cloud cleared radiances**
- **Solid lines are physical retrieval**

Summary of impact on CrIS soundings (Assumes ATMS is functional)

Product	Side.A: LW+SW	Side.B MW+SW
Temperature, T(p)	Minor degradation	~0.2 K degradation
Water vapor, q(p)	Can't meet requirements	Minor impact in PBL
Ozone	**No impact**	**Turn Off**
Carbon Monoxide	**WV displacement error**	**No impact**
Methane	**Turn Off**	**No impact**
Carbon Dioxide	**WV displacement error**	Significantly Degraded
Nitric Acid	Minor degradation	Significantly Degraded
Volcanic Sulfur Dioxide	**Turn Off**	**No impact**
Isoprene, Ammonia, PAN, Ethane, Propylene	**WV displacement error**	**Turn Off**

A water vapor (WV) displacement error is induced when converting from layer column density to volumetric mixing ratio (i.e., parts-per-million (or billion))

Potential Usage of CrIS bands

product	LW	MW	SW	ATMS
temperature	T(CO_2)	T(H_2O)	T(CO_2)	T(O_2)
			T(N_2O)	
Water,	q(PBL)	q(p)	-	q(p)
Ozone, (O3)	1050 cm^{-1}	-	-	183 GHz
Carbon Monoxide	-	-	Unique	-
Methane, (CH4)	-	Unique	-	-
Carbon Dioxide	Primary	-	Secondary	-
Nitric Acid, (HNO3)	Primary	Secondary	-	-
Nitrous Oxide (N2O)	-	Secondary	Primary	-
Sulfur Dioxide (SO2)	Secondary	Primary	-	-
Ammonia, (NH3)	868, 929 cm^{-1}	-	-	-
Ethane, (C2H6)	822.7 cm^{-1}	-	-	-
Propylene, (C3H6)	911.5 cm^{-1}	-	-	-
Isoprene, (C5H8)	893.8 cm^{-1}	-	-	-

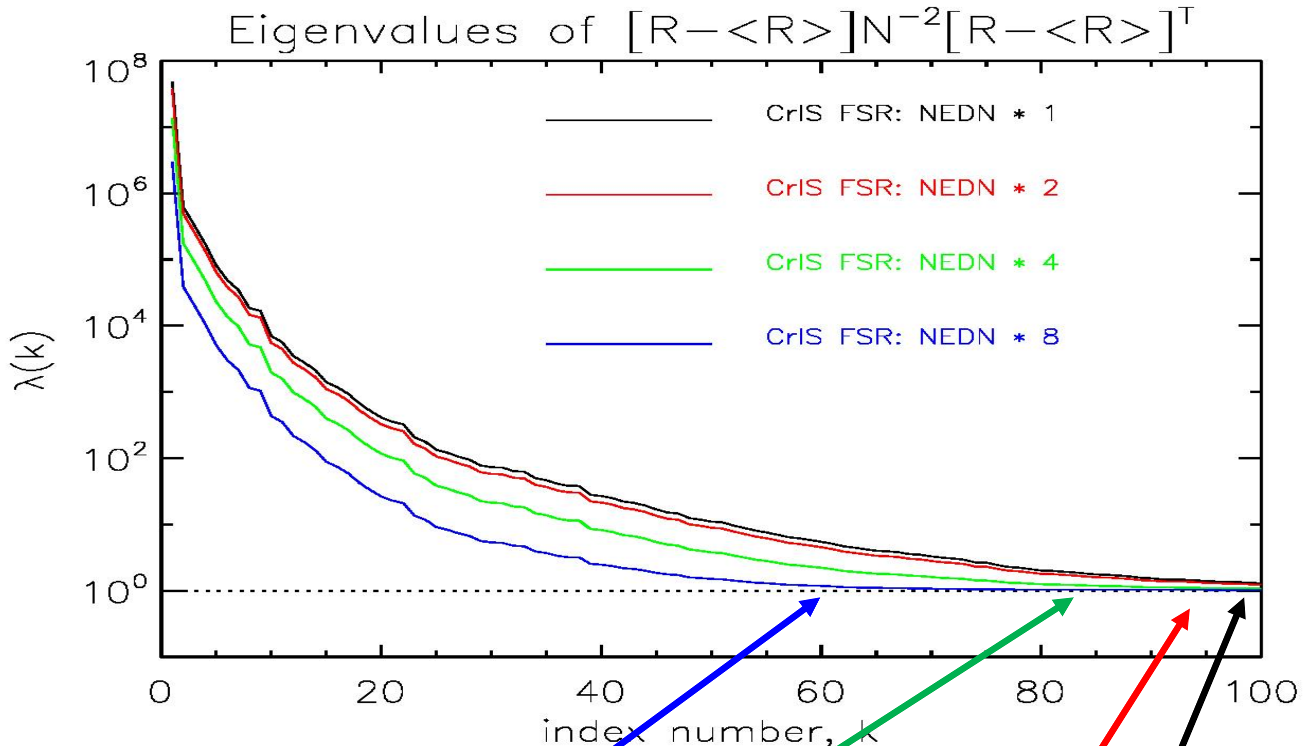
NOAA released BAA to study new sounder concepts: some personal thoughts.

- NOAA's target EDR requirements are essentially the JPSS CrIS+ATMS requirements
  - Strong focus is on data assimilation – however, this ignores some potential value to sounding capabilities.
  - NOAA/STAR has demonstrated that NUCAPS EDR's can meet this requirement using a hierarchical approach using a mix of model, operational radiosondes, other satellite products, in-situ trace gases, and dedicated research radiosondes. (Nalli 2013 JGR, Nalli 2018 IEEE TGARS)
- NOAA's future EDR requirements are more stringent (0.7 K/km, 10% q, 7 years) while simultaneously decreasing the spatial footprint area
  - But … performance is limited by physics, not the instrument, in most NOAA (and NASA) applications.
  - Demonstrating performance using simple analysis techniques (e.g., linear analysis and/or simulated data) is not adequate.
    - We will require a high spatial resolution OSSE with realistic clouds and convection in scenes that are unstable and evolving.

Statistical example: Information content (IC) as a function of added noise

Repeated the eigenvector analysis but added additional random noise to the observed radiances

Demonstrates the expectation that having instruments with noise ~4x CrIS noise will reduce the information content of the instrument.

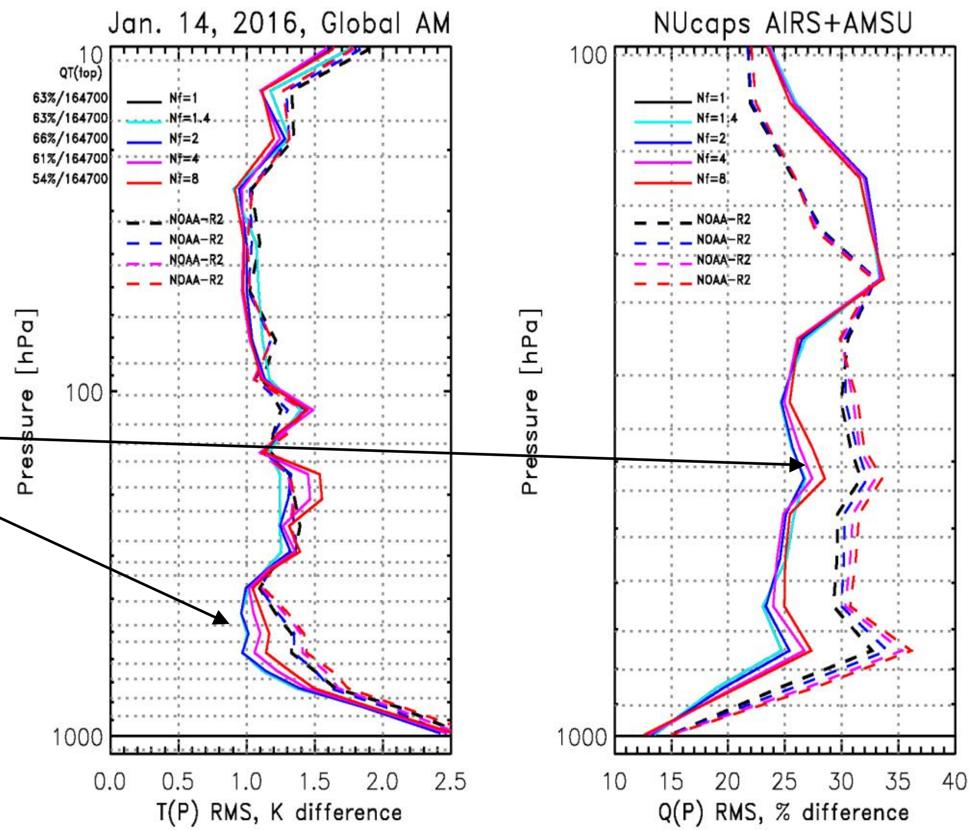


- ~60 dof for x8 noise (blue) with additional loss of S/N
- Loss of a few dof with x4 noise (green) but S/N is reduced for all eigen-vectors

- ~100 dof for LW+MW+SW (black)
- Doubling the CrIS noise does not significantly impact IC (red)

Another study: impact of random noise on NUCAPS-AIRS retrievals for a global ensemble

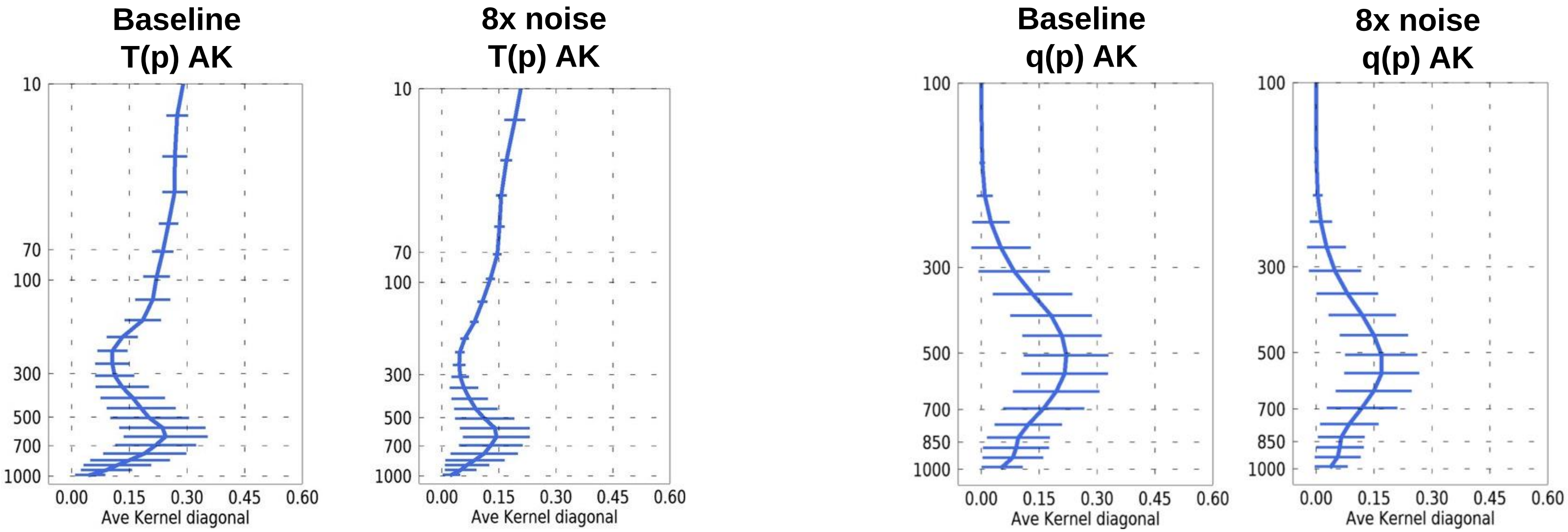
- AIRS is a grating design with very low correlated noise
- Ran NUCAPS/Aqua system and added additional random noise.
- Global T(p) and q(p) statistics show a monotonic decrease in performance as random noise is increased
  - x4 has ~0.1 K, 1% degradation in mid-troposphere
  - x8 has ~0.2K, 2% degradation
- Some of the loss in skill could be recovered if more channels are used (since noise is random we can get a SQRT(N) noise reduction in some spectral regions).



Notes:

1) **Dashed lines are the regression**
2) **Solid lines are physical**
3) **The black solid line is hidden under the cyan and blue lines.**

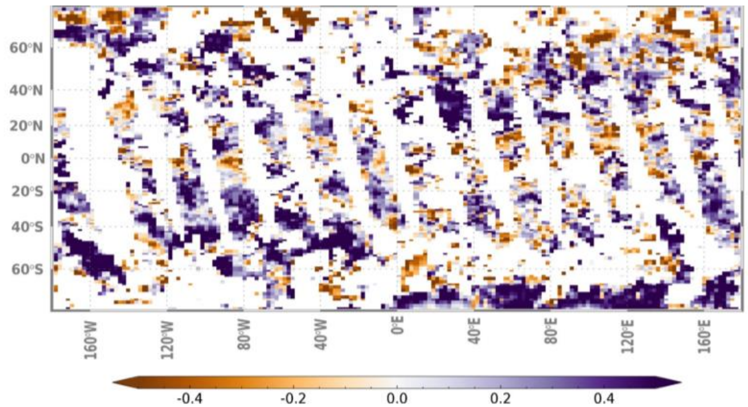
Additional random noise also degrades retrieval averaging kernels



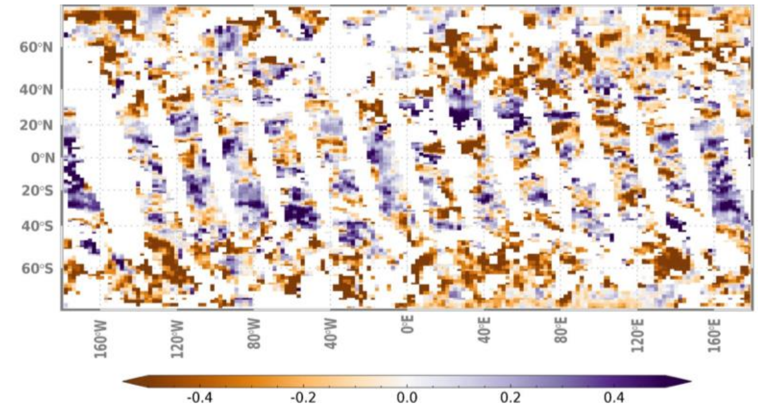
- Averaging kernels (AK’s) represent the amount of signal coming from the measurements. In the plots above we show both the average and variability (horizontal lines) of mid-latitude AK’s during daytime
- Increasing instrument by 8x causes information content to diminish at all vertical levels for T(p) and mostly mid-tropshere for q(p)

Impact of 4x *random* noise on AIRS retrievals at T(500 hPa)

AIRS(1x) – MERRA-2

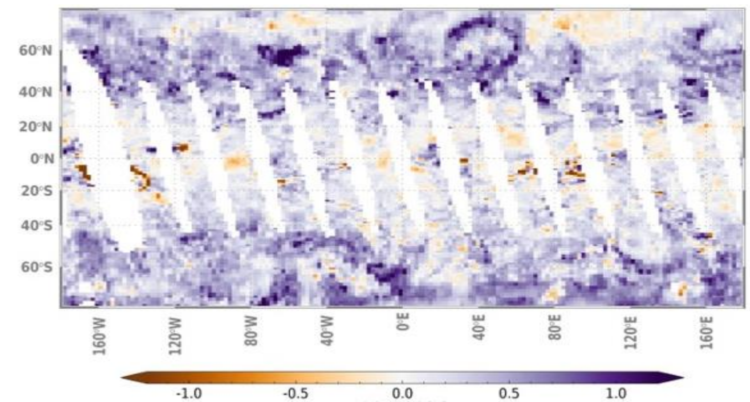


AIRS(4x) – MERRA-2



- Comparison with MERRA-2 shows AIRS with 4x noise is more susceptible to cloud contamination.
- There are stronger differences in polar regions and near edges of cloud systems

AIRS+AMSU(baseline) minus
AIRS(4x noise)+AMSU



For NOAA sounding applications, we are not instrument noise limited – Why?

- There are many *geophysical* error sources that impact soundings
  - Clouds and aerosols typically represent the largest errors
    - Cloud contamination can induce errors than are typically an order of magnitude larger than the instrument noise of modern instruments.
    - Lack of knowledge of cloud microphysics or ability to forward model clouds.
  - Lack of knowledge of trace gases (O3, HNO3, etc.) can impact T(p) and q(p).
  - Lack of knowledge of CO2 (and N2O) can induce errors in T(p).
- Forward model errors are larger than instrument noise.
  - Laboratory spectroscopy has large systematic and state-dependent errors.
  - Fast models have additional errors due to fitting assumptions.
- Retrievals are inherently non-linear and are sensitive to assumptions in the first guess (a.k.a. as regularization or null-space errors).
  - Retrievals can benefit from "better" first guess (e.g., use a model T/q as first guess)
  - But **many forecasters want model-independent retrievals**, which is significantly more difficult.
- In addition, data assimilation requires large *representation* errors (~0.5 K) to account for spatial and temporal co-location of observations.
- All of these errors have spectral or spatial correlations that are extremely difficult to model and expensive to implement in modern sounding applications.

Performance response to noise

- Retrievals, and by implication data assimilation (DA), will respond quasi-linearly to increases in an instruments *random* noise
  - Analysis on previous pages suggests that we can absorb a modest increase in instrument noise with the current systems
    - This is due to the larger errors induced by geophysical errors (e.g., clouds, forward model errors, etc) and representation errors (co-location, spatial scales).
  - Increases of instrument noise by ~4x over heritage noise will NOT result in noticeable degradation in performance for most applications.
- **Decreasing FOV size should be a significant improvement even if the noise is 2x or 4x larger that CrIS.**
  - In both retrievals and DA, smaller FOV’s require less cloud corrections.
    - Cloud contamination is spectrally correlated and is the largest error source.
  - In DA, representation error is larger for larger footprints
    - Representation error is usually larger than random instrument noise and can induce systematic biases due to aliasing of satellite overpass time and analysis synoptic time.
- Noise and spectral resolution are related
  - In sounding we are sensitive to the signal-to-noise of the observation.
  - If spectral resolution is higher, we can tolerate a larger noise because we have more channels to average. “Signal” could also be higher due to spectral purity.
  - Scaling the instrument noise to a common resolution allows for a more fair comparison of expected performance. For example, AIRS is well characterized. To convert noise to AIRS spectral resolution

$$NEDN'(n) = NEDN(n) * SQRT(FWHM(n)/FWHM_{AIRS})$$

$$FWHM_{AIRS} \sim= \upsilon(n)/1200$$

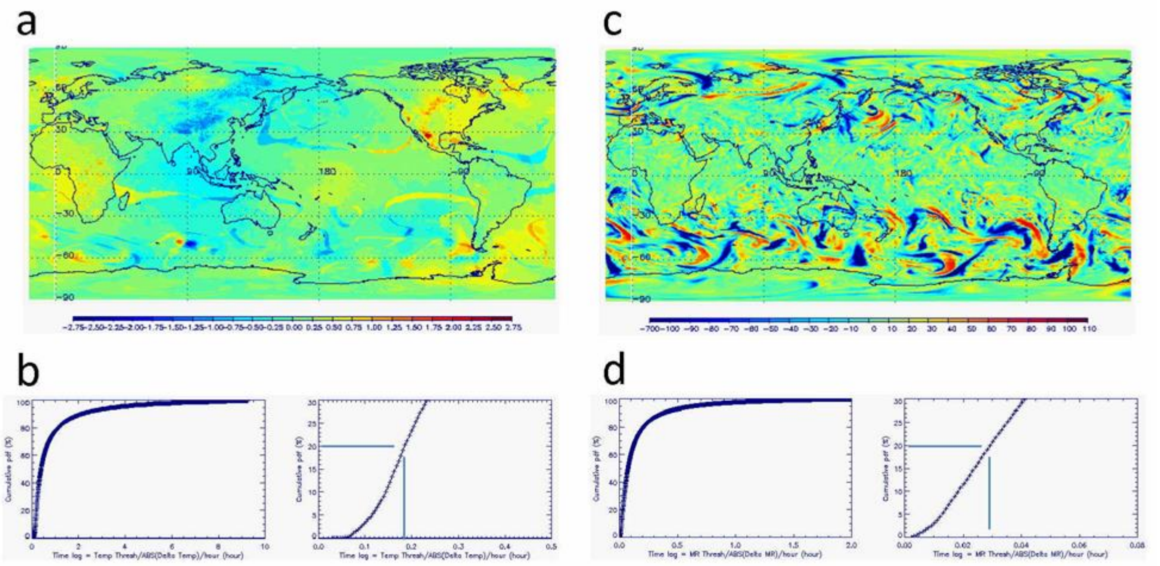
Requirements for NOAA EDR applications (AWIPS, etc.).

- Modern data assimilation and retrieval algorithms exploit both microwave and multi-band infrared measurements.
  - In data assimilation the microwave and infrared are used separately.
  - But for NUCAPS, we spatially co-register the infrared and microwave to meet JPSS EDR requirements within cloudy environments.
- How important is temporal co-registration of microwave for NUCAPS?
  - We have capability to use real data to assess value of microwave
    1. We have run Aqua systems with and without the microwave and compare (next slides).
    2. Aqua continuously drifts up to ~1000 km and +/- 45 minutes from S-NPP
       - NUCAPS can mix and match instruments (e.g., Aqua/AIRS and S-NPP/ATMS) to estimate sensitivity to spatial and temporal co-registration
       - We found (not shown today) that ≈50% of cases each day were within 0.25 deg spatially and that statistically AIRS+ATMS performed as well as AIRS+AMSU
  - We can also use models (e.g., GFS, ECMWF, MERRA-2) to estimate geophysical temporal variability to estimate how long it takes to exceed our requirements.

Quick-look estimate of tolerable temporal offset between microwave and infrared

We used change in ECMWF analysis over 6 hours to estimate when co-location errors will become significant

- 20% of the globe exceeded 0.5 K in ≈12 minutes (0.2 hour)
- 5% moisture in ≈2 minutes (0.03 hour)



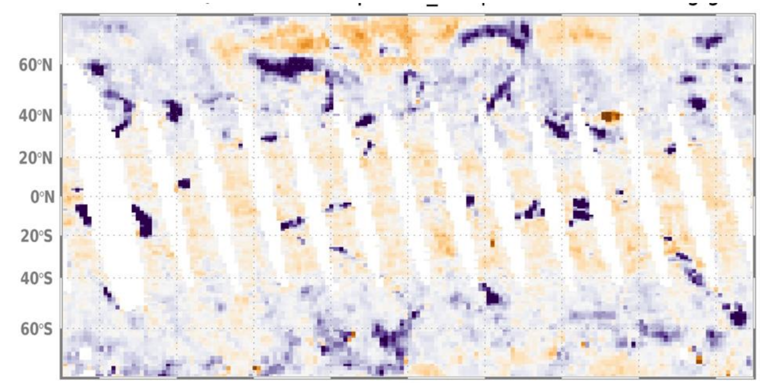
a) ΔT = change in T(850 hPa) in 6 h of ECMWF
b) Percent of cases that exceed 0.5 K versus Δt   Δt = 360•0.5/ΔT

c) Δq = change in q(850 hPa) in 6 h of ECMWF
d) Percent of cases versus Δt that exceed 5%, Δt = 360•5.0/Δq

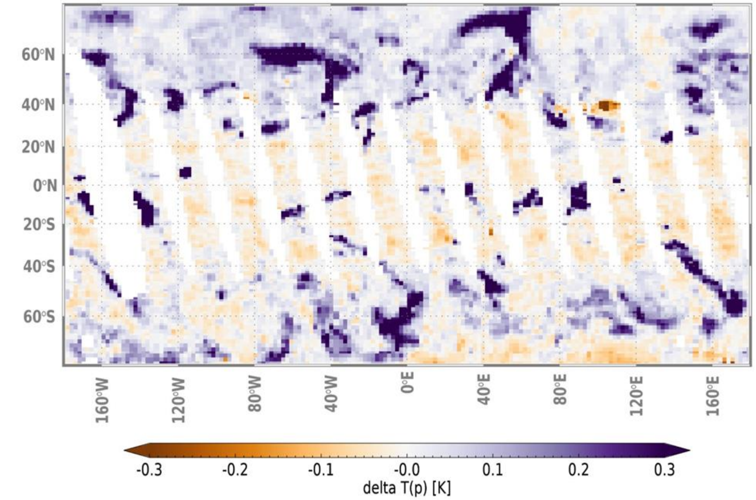
Impact of loss of MW

- At right, the difference of T(500 hPa) is shown for AIRS+AMSU minus AIRS-only for the same focus day.
  - Significant differences are seen near the edges of clouds
  - Strong features in colder scenes (polar)
- Higher noise has more dependence on the microwave.

AIRS+AMSU – AIRS-only T(500 hPa)
T(500 hPa) retrieval w/ normal AIRS noise



AIRS+AMSU – AIRS-only, 4x AIRS noise



How important is the Microwave Sounder to NOAA applications?

- Microwave is most important in cloudy domains where weather is rapidly evolving.
  - Insensitive to non-precipitating clouds
    - can correct or QC cloud contaminated IR radiances
  - Microwave uses a separate well-mixed molecule, oxygen, to improve T(p).
  - Spectroscopy of water is simpler and more linear than infrared.
- The sounder community has demonstrated that spatially co-located microwave and infrared is important for EDR applications.
  - In data assimilation, it is assumed that co-location is not required.
  - Question is: Are the lessons-learned in EDR applications relevant in DA?
- Can EDR applications function without co-located microwave?

  Yes we can.
  - NASA AIRS Science team ***demonstrated that LW and SW bands can be combined to improve retrievals in systems without the microwave.***
    - NOAA NUCAPS team demonstrated that CrIS-only systems perform well.
    - NOAA/TMP5 study demonstrated that CrIS SW-only system degrades more rapidly than CrIS LW-only.
  - However, there is a persistent loss of the most difficult (i.e., useful) scenes.
    - Some of this loss can be mitigated with model information (e.g., GFS, HRRR)
    - Essentially captures the microwave information from all other satellites used in the model.

Some guidelines for new instruments (Slide courtesy of Dave Tobin)

- Slide adapted from Dave Tobin's 2020 presentation at IGARSS Session on Next Generation LEO/GEO MW and IR Sounders
- **I added some additional thoughts (in blue)**

Critical Characteristics for LEO Hyperspectral IR Sounders:

1) Relatively long mission lifetime ← **More important for DA**

2) High on-orbit "up time"

3) Very good radiometric calibration accuracy and stability

4) Very good spectral calibration accuracy and stability

5) Low and stable radiometric noise properties, and

6) Longwave and Midwave spectral coverage. ←

May be more important for DA and we can use existing POR to test concepts. Desire for smaller footprints and shorter refresh times might have advantages in SW-band for some applications.

Some personal thoughts about the future of sounding

- Sounding has a diversity of scientific applications and has a diverse user community.
  - Weather, climate, and composition users have different requirements and needs.
  - Space-assets were primarily designed {and maintained} for weather applications.
- Sounding community in USA has multiple, overlapping funding sources:
  - AIRS project funds instrument calibration, algorithm integration and validation.
  - ROSES TASNPP funds AIRS, S-NPP,JPSS-x science, algorithm development.
  - S-NPP project funds S-NPP/JPSS-x calibration and CrIS forward models (NSR and FSR).
  - NOAA: Supports operational weather applications, CrIS (and IASI) forward models, NUCAPS maintenance for Metop, S-NPP, and JPSS-x w/ reprocessing capability.
- Multi-satellite continuity – we have 19 years of Aqua+JPSS (and potentially 40+ years) that provide new understanding of weather (diurnal scales) and climate (inter-annual scales).
  - We have had ~20 years of well calibrated and extremely stable instruments.
- New satellite concepts will *most likely* complement the program of record (POR) satellites (Aqua, S-NPP, JPSS-x/NOAA-2x, Metop-x, Metop-SG, etc.).
  - New spectral domains to take advantage of new and emerging technology.
  - Smaller footprints or other spatial sampling concepts.
  - Small satellite concepts and new measurement capabilities (GHG monitoring), etc.

Some thoughts on spectral correlations

- As seen in Session #2 – a small correlated error can be handled if it can be modelled in the error covariance matrix.
  - If a correlated error is ignored, it can dramatically degrade the results.
  - Future instruments designs need to have good pixel-to-pixel and band-to-band calibration.
- A big difference between retrievals and data assimilation with the hyperspectral infrared is how we compute spectral correlation
  - DA computes the error covariance empirically.
    - It applies the same matrix to all scenes.
    - It does not partition the errors.
  - In retrievals we can afford to compute a dynamic error covariance matrix.
  - We treat instrument and forward model correlations separately:

$$\delta R \delta R^T = \delta R \delta R^T_{INST} + \delta R \delta R^T_{FM}$$

  - $\delta R \delta R^T_{INST}$ includes all instrument correlations due to electronics, optics, and calibration.
    - For example, the correlation induced by apodization is easily modeled.
  - $\delta R \delta R^T_{FM}$ includes all forward model correlations (spectral transmittance and geophysical correlations).
    - Geophysical correlations can vary from scene to scene.
  - In retrievals we compute $\delta R \delta R^T_{FM}$ as follows:

    $\delta R \delta R^T_{FM} = \text{sum}\{(dR/dX_i)\ (\delta X \delta X^T)_i\ (dR/dX_i)^T\}$

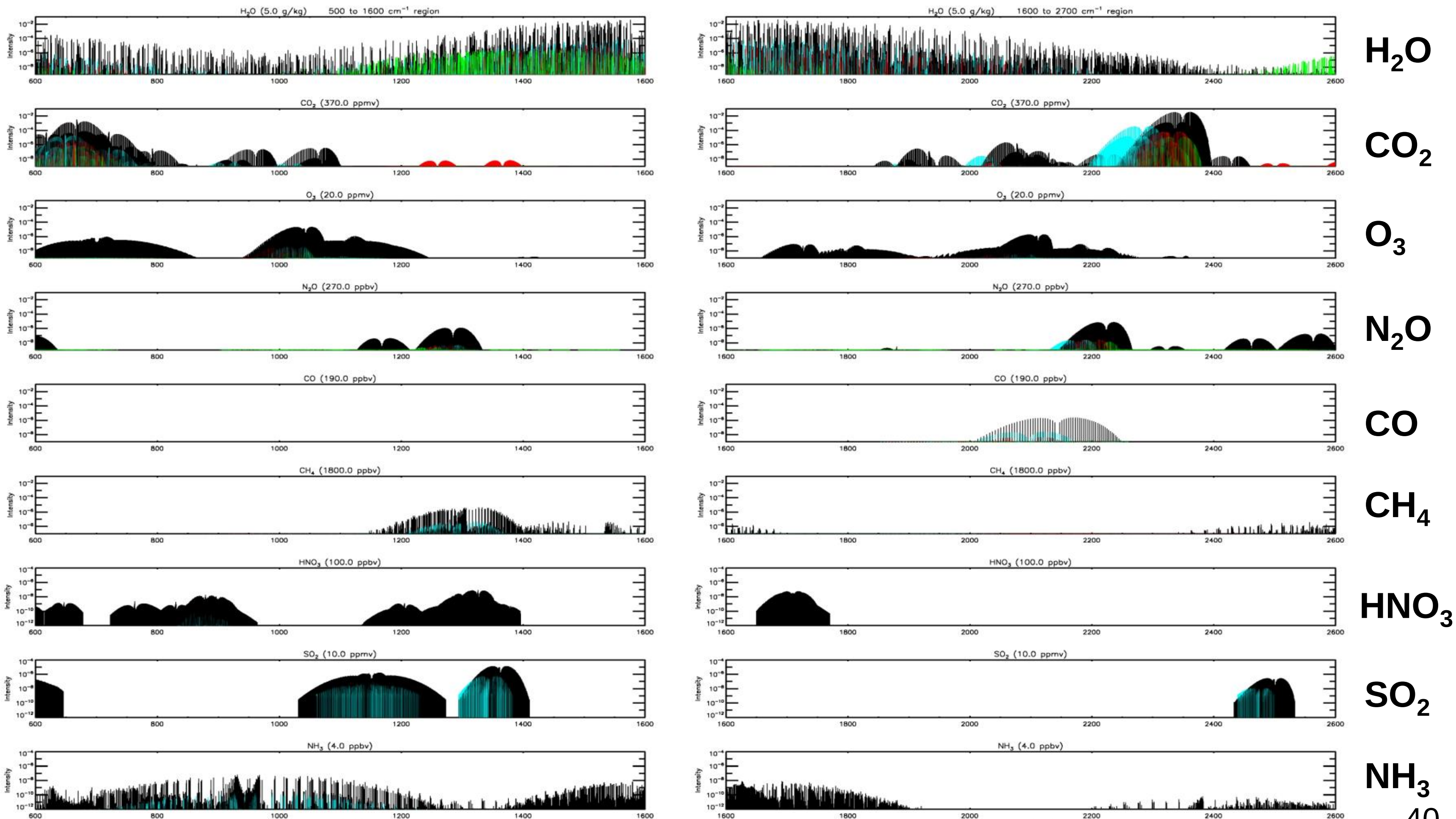
    where X_i = clouds, T_{skin}, T(p), q(p), O_3(p), CO_2(p), NO_2(p), CH_4(p), etc.

    and dR/dX_i can be computed by taking derivatives of the forward model

There is a symmetric of the long-wave side and short-wave side in terms of T(p) and q(p)

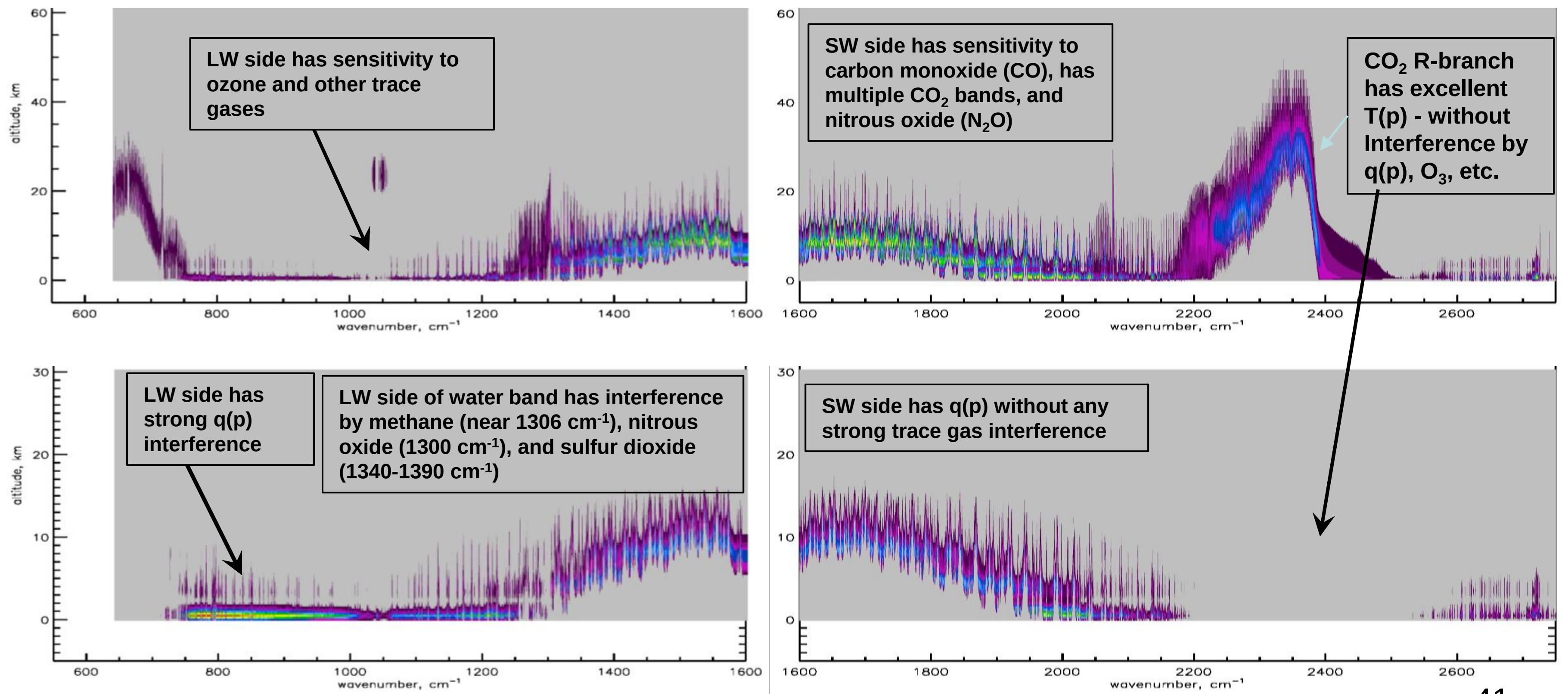
16.7 to 6.25 μm
600 to 1600 cm^{-1}

6.25 to 8.55 μm
1600 to 2600 cm^{-1}



T(p), q(p) sensitivity of LW versus SW regions is very similar

- IASI spectrum (ILS FWHM = 0.5 cm^{-1}) for a mid-latitude case
  - color (i.e., sensitivity) will be dependent on the instruments line shape and band-passes
- Left is 600-1600 cm-1 region, Right is the 1600 to 2700 region
- Top figure: channel sensitivity to T(p) -- that is dR/dT
- Bottom figure: channel sensitivity to q(p) -- that is dR/dlog(q)



My opinion: Future instruments should pick design that optimizes the real needs

- Application specific items are most important:
  - Users care most about latency, calibration, footprint size, boundary layer sensitivity, and product ease of use, availability and longevity.
  - Satellite vendors care most about mass, power, and size.
- Grating vs. interferometer is not important to the user.
  - We know how to handle both.
  - Apodized vs. unapodized is irrelevant, if enough channels are used.
  - Apodized radiances allows more flexibility – simpler forward model and supports use of smaller subsets of channels.
- We are not as dependent on the long-wave anymore.
  - We know how to handle both – but DA community still biased towards long-wave
  - Smaller footprints is probably more important than spectral region.
  - DA experiments (Kevin Garrett, NOAA/STAR) demonstrate that using CrIS SW is not only plausible, it appears to work better than the LW.

Questions?

More information at:
http://goo.gl/twuRtW

~/rs_notes.pdf

- Radiative transfer
- Derivations
- Details about instruments

~/phys640_s04.pdf

- Mathematical methods
- Linear and non-linear Least Squares
- FFT's and Apodization

Backup Slides

Acronyms

- Infrared Instruments
  - AIRS = Atmospheric Infrared Sounder
  - IASI = Infrared Atmospheric Sounding Interferometer
  - CrIS = Cross-track Infrared Sounder
- Microwave Instruments
  - AMSU = Advanced Microwave Sounding Unit
  - HSB = Humidity Sounder Brazil
  - MHS = Microwave Humidity Sensor
  - ATMS = Advanced Technology Microwave Sounder
  - AMSR = Advanced Microwave Scanning Radiometer
- Imaging and Cloud Instruments
  - MODIS = MODerate resolution Imaging Spectroradiometer
  - AVHRR = Advanced Very High Resolution Radiometer
  - VIIRS = Visible/IR Imaging Radiometer Suite
  - ABI = Advanced Baseline Imager
  - CALIPSO = Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations
- Other
  - DA = data assimilation
  - EUMETSAT = EUropean organization for exploitation of METeorological SATellites
  - FOV = field of view
  - FOR = field of regard
  - GOES = Geostationary Environmental Operational Satellite
  - IGOS = Integrated Global Observing System
  - ILS = Instrument Line Shape
  - IPCC = Inter-government Panel on Climate Change
  - JPSS = Joint Polar Satellite System
  - METOP = METeorological Observing Platform
  - NESDIS = National Environmental Satellite, Data, and Information Service
  - NPP = National Polar-orbiting Partnership
  - OCO = Orbiting Carbon Observatory
  - POR = Program of Record (Weather Sat's)