National Environmental Satellite, Data, and Information Service

Introduction to Remote *Sounding* Infrared

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NOAA/NESDIS/STAR

Friday July 10, 2007

JCSDA Summer Colloquium on Data Assimilation

Stevenson, Washington

Sounding Theory Notes for the discussion today is on-line

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ftp site: ftp://ftp.orbit.nesdis.noaa.gov/pub/smcd/spb/cbarnet/

..or.. ftp ftp.orbit.nesdis.noaa.gov, cd pub/smcd/spb/cbarnet

Sounding NOTES, used in teaching UMBC PHYS-741: Remote Sounding and UMBC PHYS-640: Computational Physics (w/section on Least Square Fitting and Instrument Apodization)

~/reference/rs_notes.pdf

~/reference/phys640_s04.pdf

These are *living* notes, or maybe a scrapbook – they are not textbooks.

An excellent text book on the topic of remote sounding is:

Rodgers, C.D. 2000. Inverse methods for atmospheric sounding: Theory and practice. World Scientific Publishing 238 pgs

Acronyms

- Infrared Instruments
  - AIRS = Atmospheric Infrared Sounder
  - IASI = Infrared Atmospheric Sounding Interferometer
  - CrIS = Cross-track Infrared Sounder
  - HES = Hyperspectral Environmental Suite
- 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
  - EUMETSAT = EUropean organization for exploitation of METeorological SATellites
  - FOV/FOR = field of view or regard
  - GOES = Geostationary Environmental Operational Satellite
  - IGCO = International Global Carbon Observation (theme within IGOS)
  - IGOS = Integrated Global Observing System
  - IPCC = Inter-government Panel on Climate Change
  - METOP = METeorological Observing Platform
  - NESDIS = National Environmental Satellite, Data, and Information Service
  - NPOESS = National Polar-orbiting Operational Environmental Satellite System
  - NDE = NPOESS Data Exploitation
  - NPP = NPOESS Preparatory Project
  - OCO = Orbiting Carbon Observatory
  - STAR = office of SaTellite Applications and Research

Topics for this lecture

- Introduction to hyper-spectral infrared instruments
  - Atmospheric Infrared Sounder, AIRS
  - Infrared Atmospheric Sounding Interferometer, IASI
  - Cross-track Infrared Sounder, CrIS
- Examples of infrared products
  - Trade-off between using radiance versus retrieval products.
- Examples of infrared spectra.
  - Information content of infrared hyper-spectral spectrum.
- AIRS science team algorithm
  - Statistical regression
  - Cloud clearing
  - Unconstrained retrievals (least squares fitting)
  - Physical retrieval.

- Side-bar #1 (if time allows) Vertical averaging functions.

- Side-bar #2: (if time allows) Comparison of dispersive and interferometric instruments.
  - Apodization

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

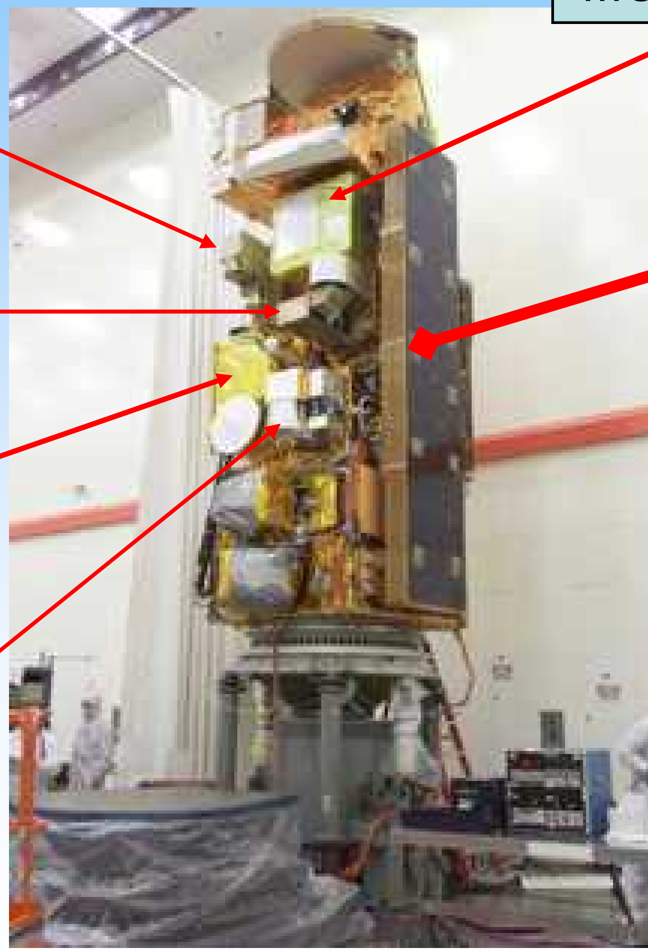
AMSU-A1(3-15

AMSU-A2(1-2)

AIRS

HSB

MODIS



Aqua Acquires 325 Gb of data per day

Delta II 7920

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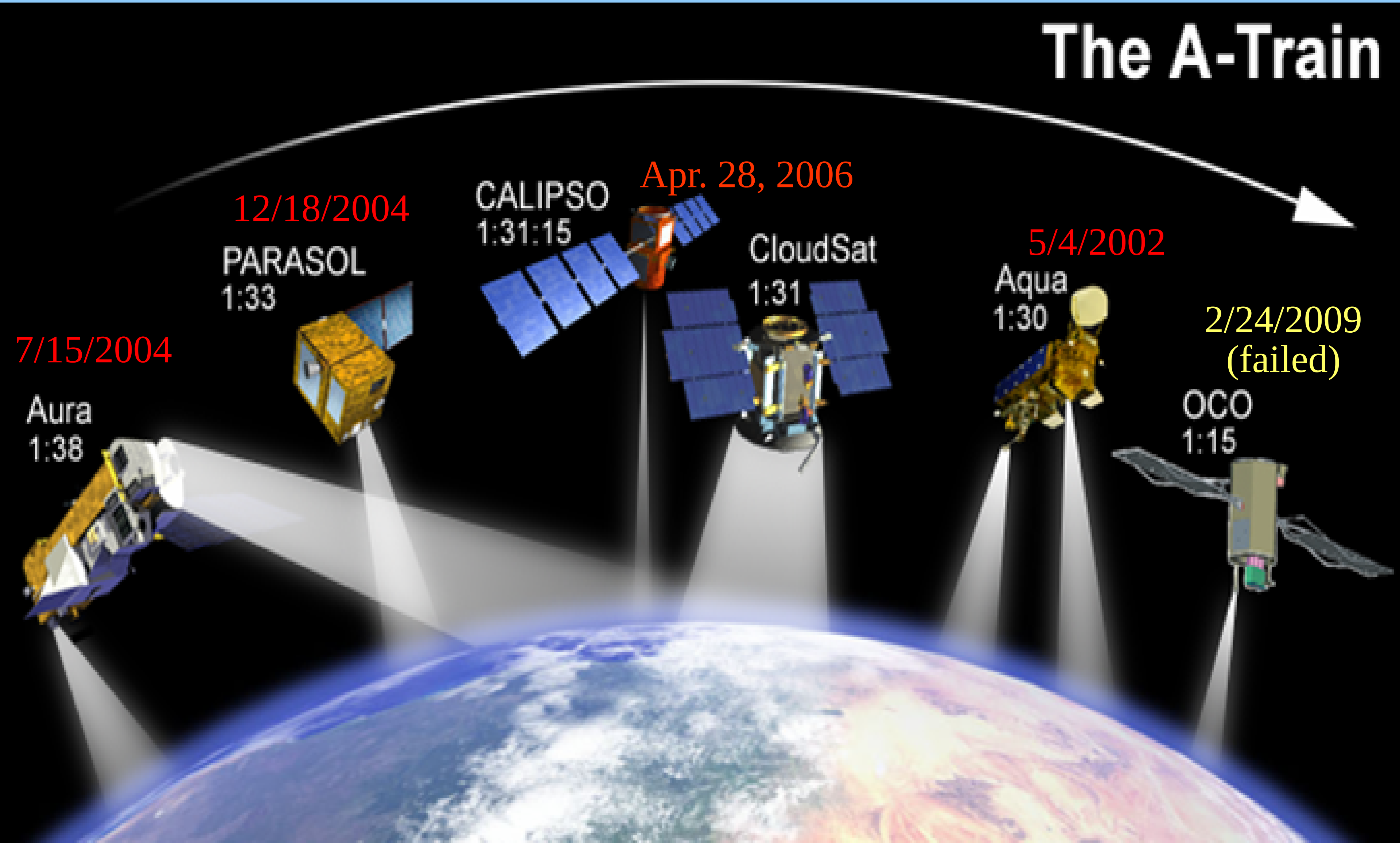
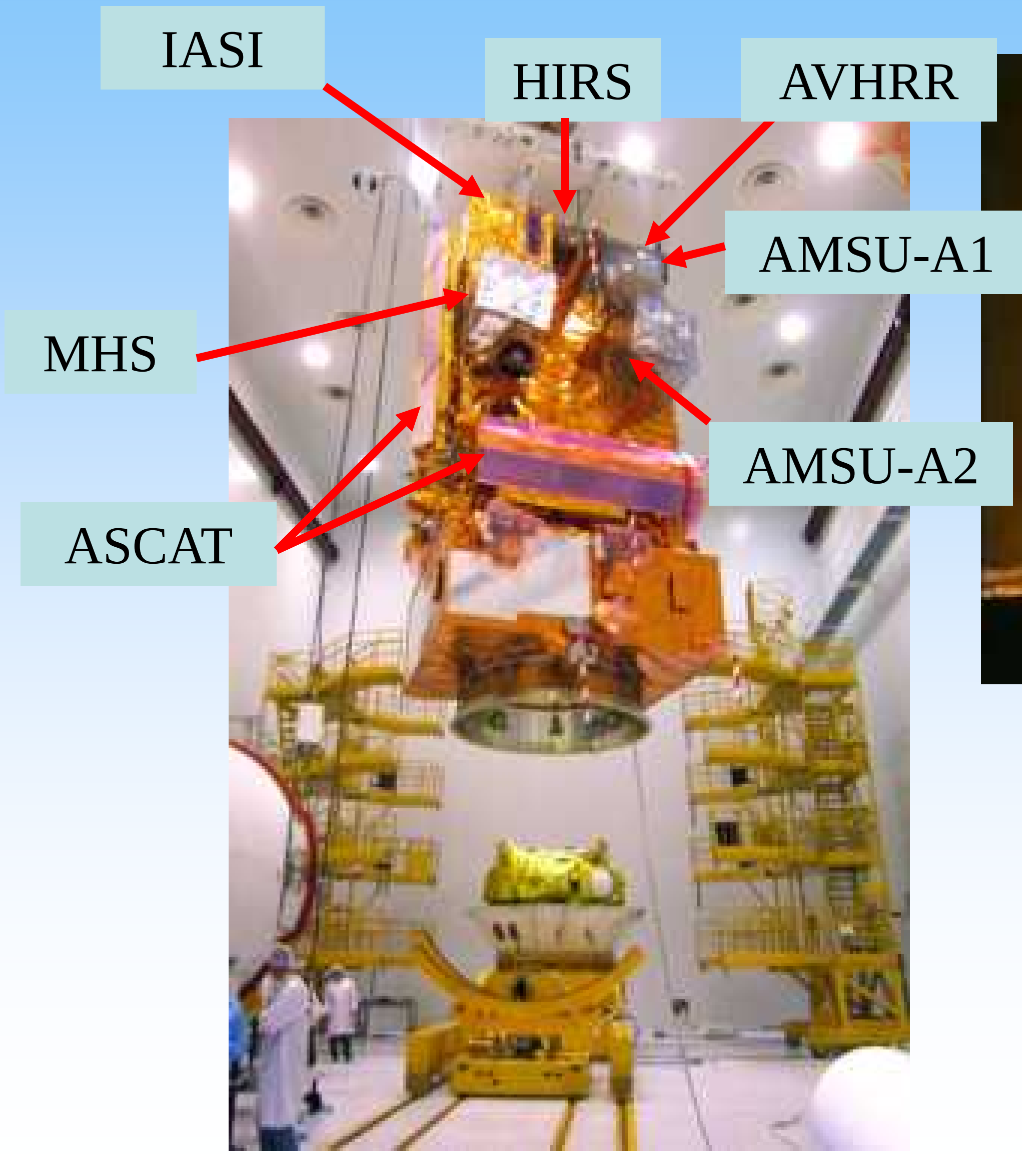
AIRS has a Unique Opportunity to Explore & Test New Algorithms for Future Operational Sounder Missions.



IASI was launched on the MetOp-A Satellite on Oct. 19, 2006

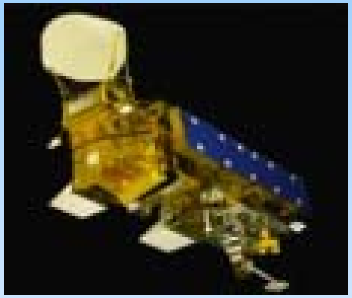


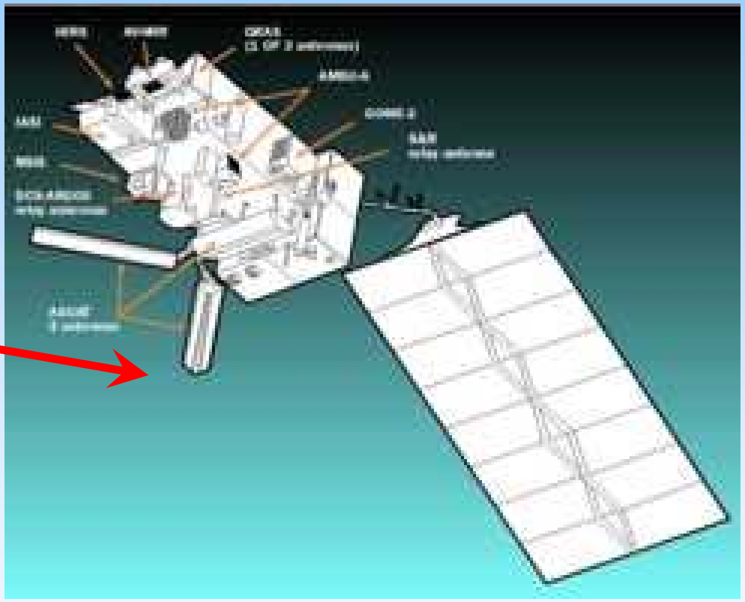
Soyuz 2/Fregat launcher,

Baikonur, Kazakhstan

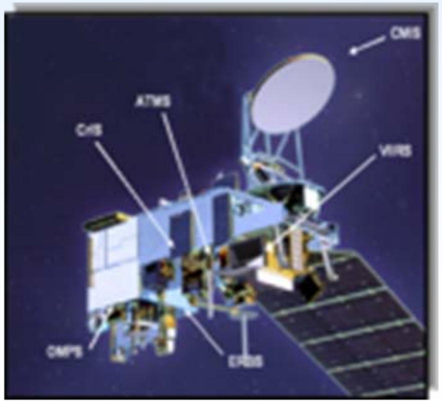
Initial Joint Polar System is a NOAA & EUMETSAT agreement to exchange all data and products.

NASA/Aqua
1:30 pm orbit (May 4, 2002)





NPP & NPOESS
1:30 pm orbit
(2011, 2014, 2020)



EUMETSAT/METOP-A
9:30 am orbit (Oct. 19, 2006, 2012, 2017)

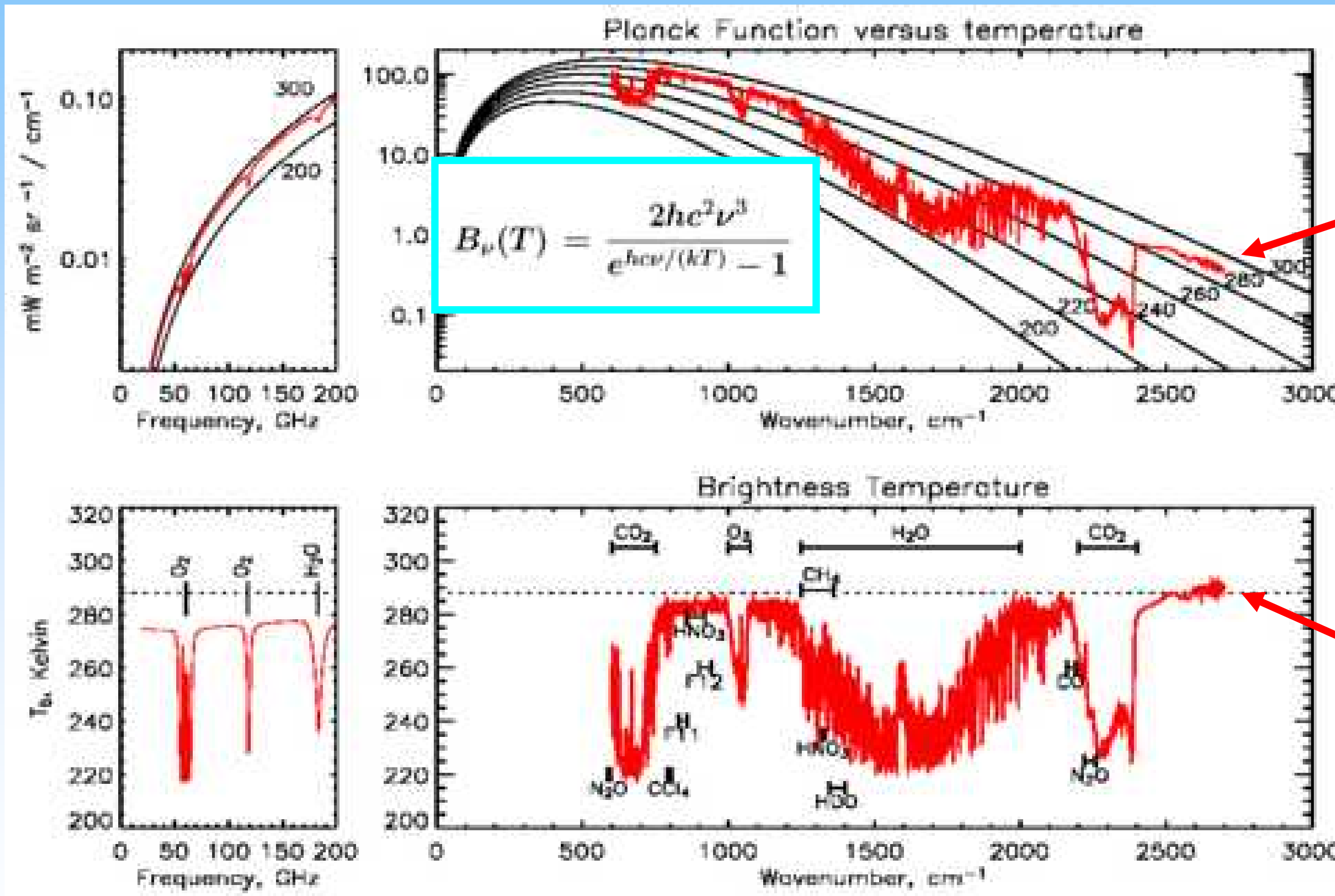
20 years of hyperspectral sounders are already funded for weather applications

In thermal infrared we use wavenumbers to represent channels or frequencies

- Traditionally, in the infrared we specify the channels in units of wavenumbers, or cm^{-1}
  - $\nu \equiv f/c$
    - f = frequency in Hertz (or s^{-1})
    - c = speed of light = 29,979,245,800 cm/s
- Wavenumbers can be thought of as inverse wavelength, for example,
  - $\nu \equiv 10000/\lambda$
    - λ = wavelength in μm (microns)

Instruments measure radiance

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



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.

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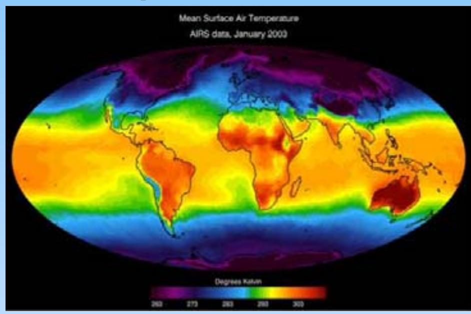
Thermal Sounder "Core" Products (on 45 km footprint, unless indicated)

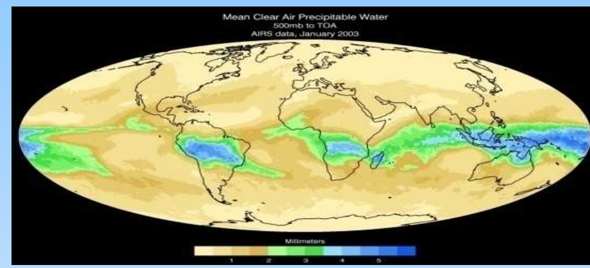
Radiance Products	*RMS Requirement*	*Current Estimate*
AIRS IR Radiance (13.5 km)	3%	< 0.2 %
AIRS VIS/NIR Radiance	20%	10-15%
AMSU Radiance	0.25-1.2 K	1-2 K
HSB Radiance (13.5 km)	1.0-1.2 K	(failed 2/2003)
Geophysical Products	***RMS Requirement***	***Current Estimate***
Cloud Cleared IR Radiances	1.0K	< 1 K
Sea Surface Temperature	0.5 K	0.8 K
Land Surface Temperature	1.0K	TBD
Temperature Profile	1K/1-km layer	1K/1-km
Moisture Profile	15%/2-km layer	15%/2-km
Total Precipitable Water	5%	5%
Fractional Cloud Cover (13.5 km)	5%	TBD
Cloud Top Pressures	0.5 km	TBD
Cloud Top Temperatures	1.0 K	TBD

AIRS Products

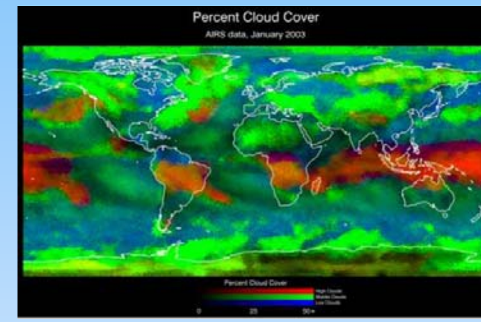
Temperature Profiles



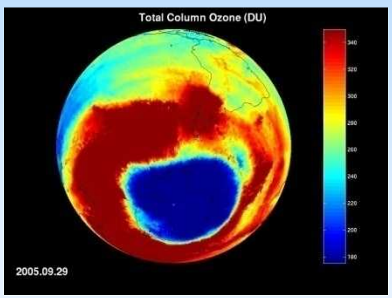
Water Vapor Profiles



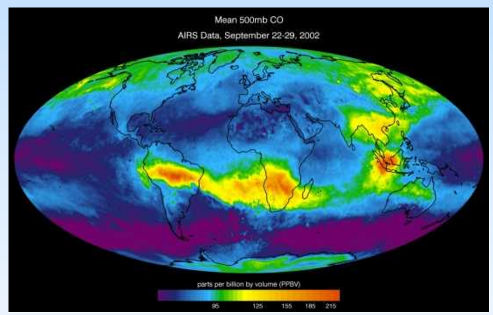
Clouds



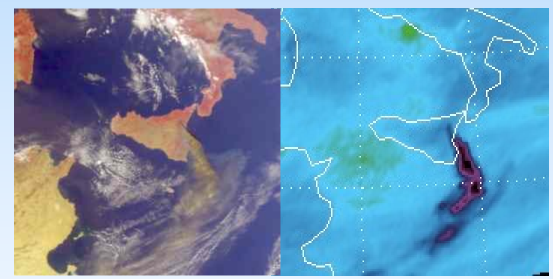
Ozone



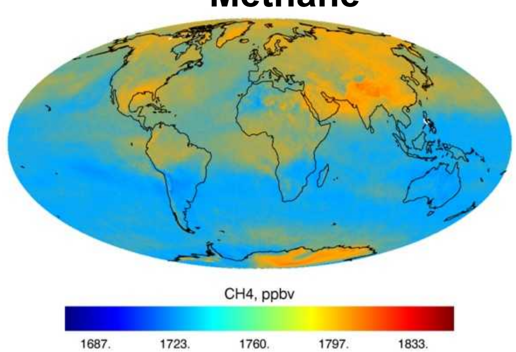
CO



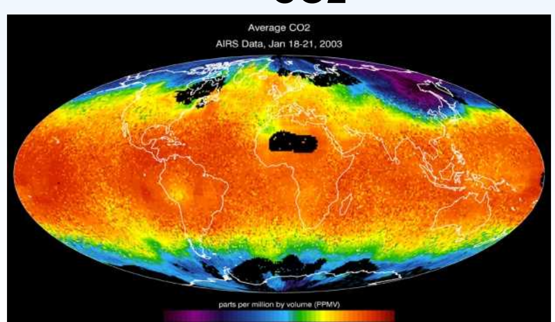
SO2



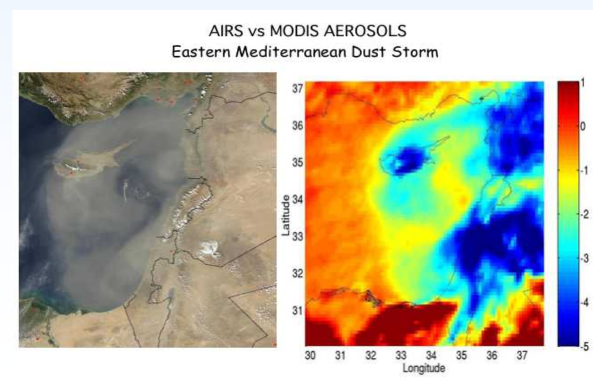
Methane



CO2



Dust

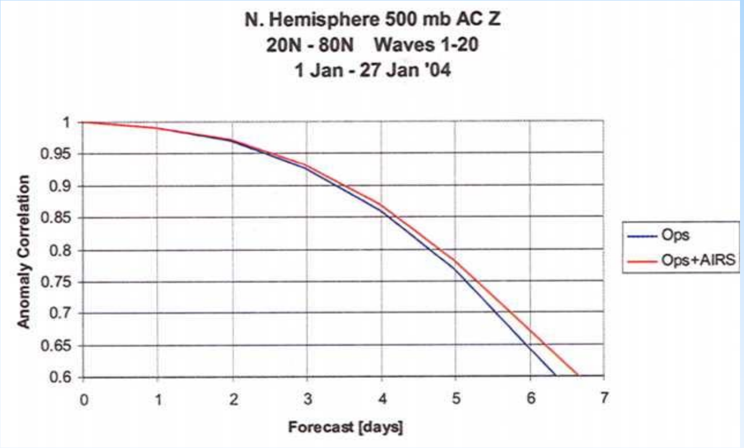


Radiances versus Products

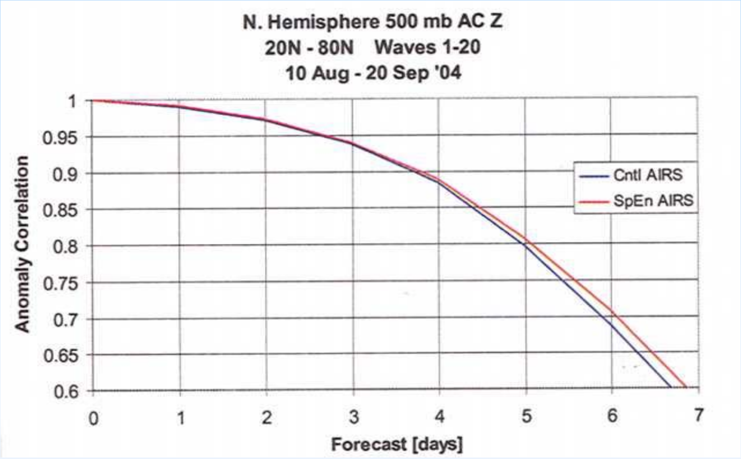
Radiance	Retrieval Products
Product volume is large: In practice, a spectral subset (10%), spatial subset (5%), and clear subset (5%) of the observations is made	Product volume is small: all instrument channels can be used to minimize all parameters (T, q, O_3, CO, CH_4, CO_2, clouds, etc.)
Instrument 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.
Small biases in T(p), q(p), O_3(p),due to model and satellite representation error, have large impact on derived products.	*A-priori* used in retrieval is different than assimilation model; however, vertical kernel information can be used to assimilate product.
Tendency to weight the instrument radiances lower (due to representation error) to stabilize the model. Need correlation lengths to stabilize model horizontally, vertically, and temporally.	Retrieval maximizes the utilization of the radiances, since derived state is on *instrument* sampling "grid" along the line-of-sight.

AIRS Forecast Improvement

Improved Forecast Prediction
1 in 18 AIRS FOV's
(6 hours in 6 Days)
Northern Hemisphere
October 2004 *



Additional Improvement Using
All 18 AIRS FOV's
(11 hours total in 6 Days)
Northern Hemisphere
Preliminary

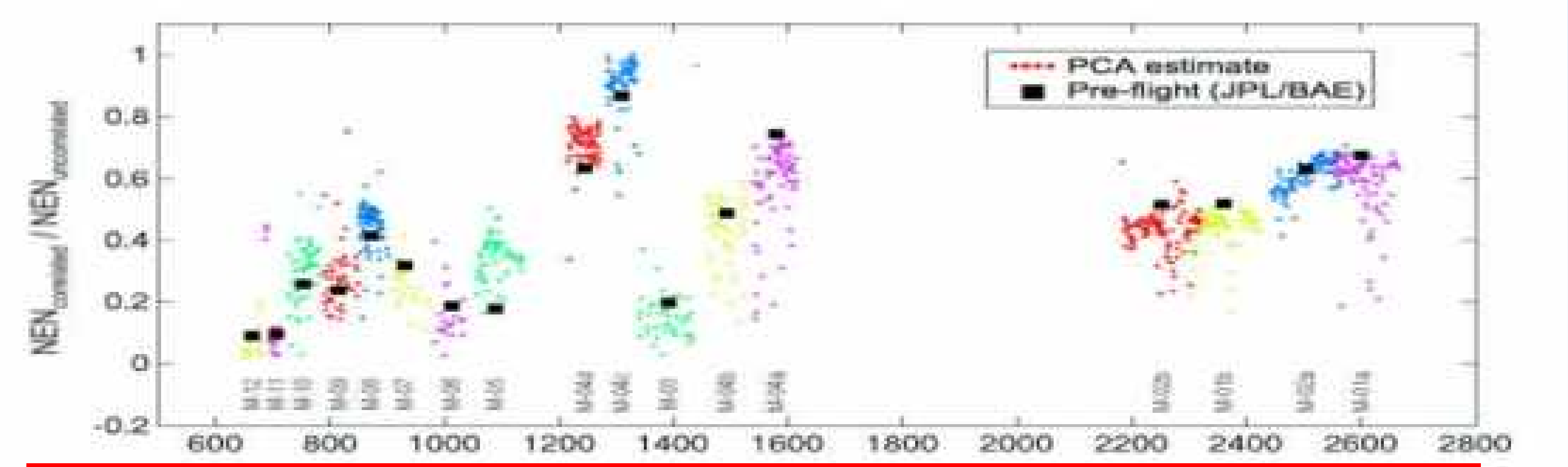


This AIRS instrument has provided a significant increase in forecast improvement in this time range compared to any other single instrument

J. LeMarshall, J. Jung, J. Derber, R. Treadon, S. Lord, M. Goldberg, W. Wolf, H. Liu, J. Joiner, J. Woollen, R. Todling, R. Gelaro "Impact of Atmospheric Infrared Sounder Observations on Weather Forecasts", EOS, Transactions, American Geophysical Union, Vol. 86 No. 11, March 15, 2005

Examples of off-diagonal elements in instrument error coviance.

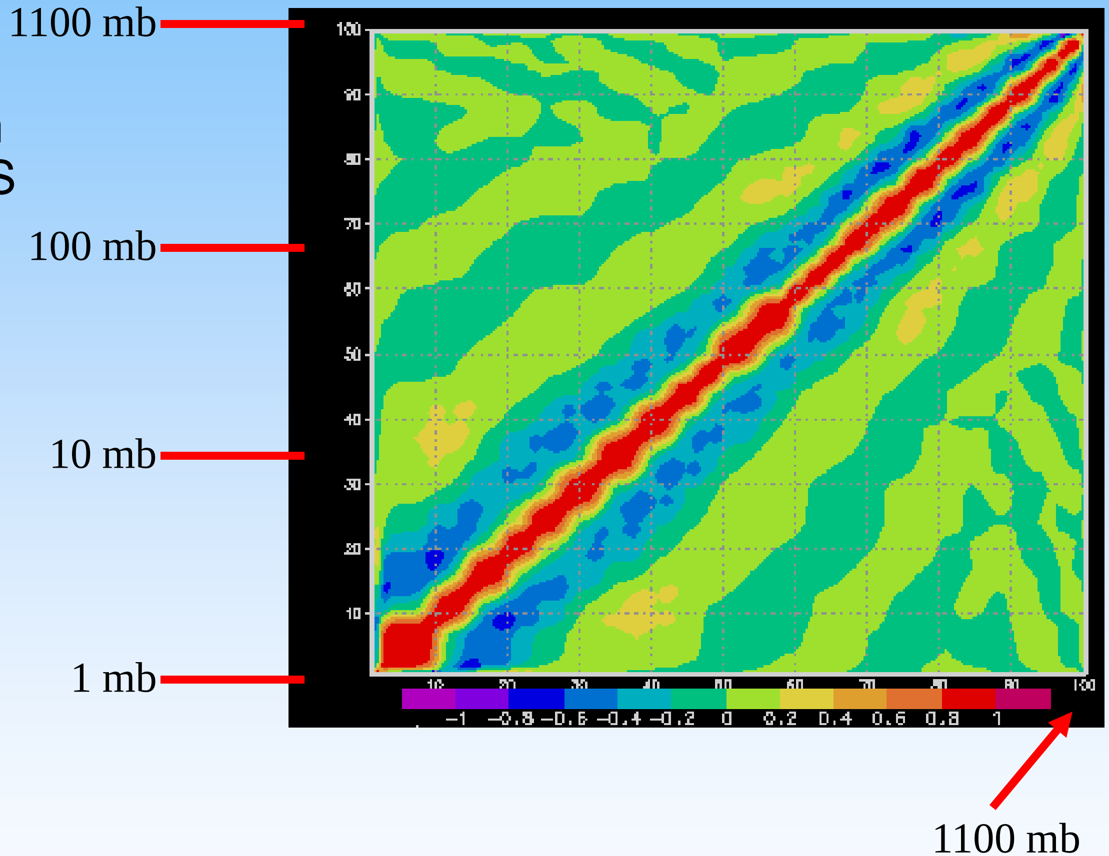
- In any instrument there are optical, electrical, and processing components that can correlate signals.
- In interferometers processing includes as step called apodization to make the instrument spectral characteristics localized (necessary for efficient radiance computations). But, apodization causes a local spectral correlation (a channel is 62% correlated with neighbor (±1 channel), 13% correlated with ±2 channels, 1% correlated with ±3 channels, etc.)
- In dispersive instruments each detector array has spectral correlation due to a common electronics system. For example, in AIRS the spectral correlation is a function of the detector array module:



Therefore, the best use of satellite radiances requires ability to characterize ever detail of the instrument and processing.

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).



Therefore, the use of retrieval products requires knowledge of retrieval "averaging kernels" and/or error *covariance* estimates.

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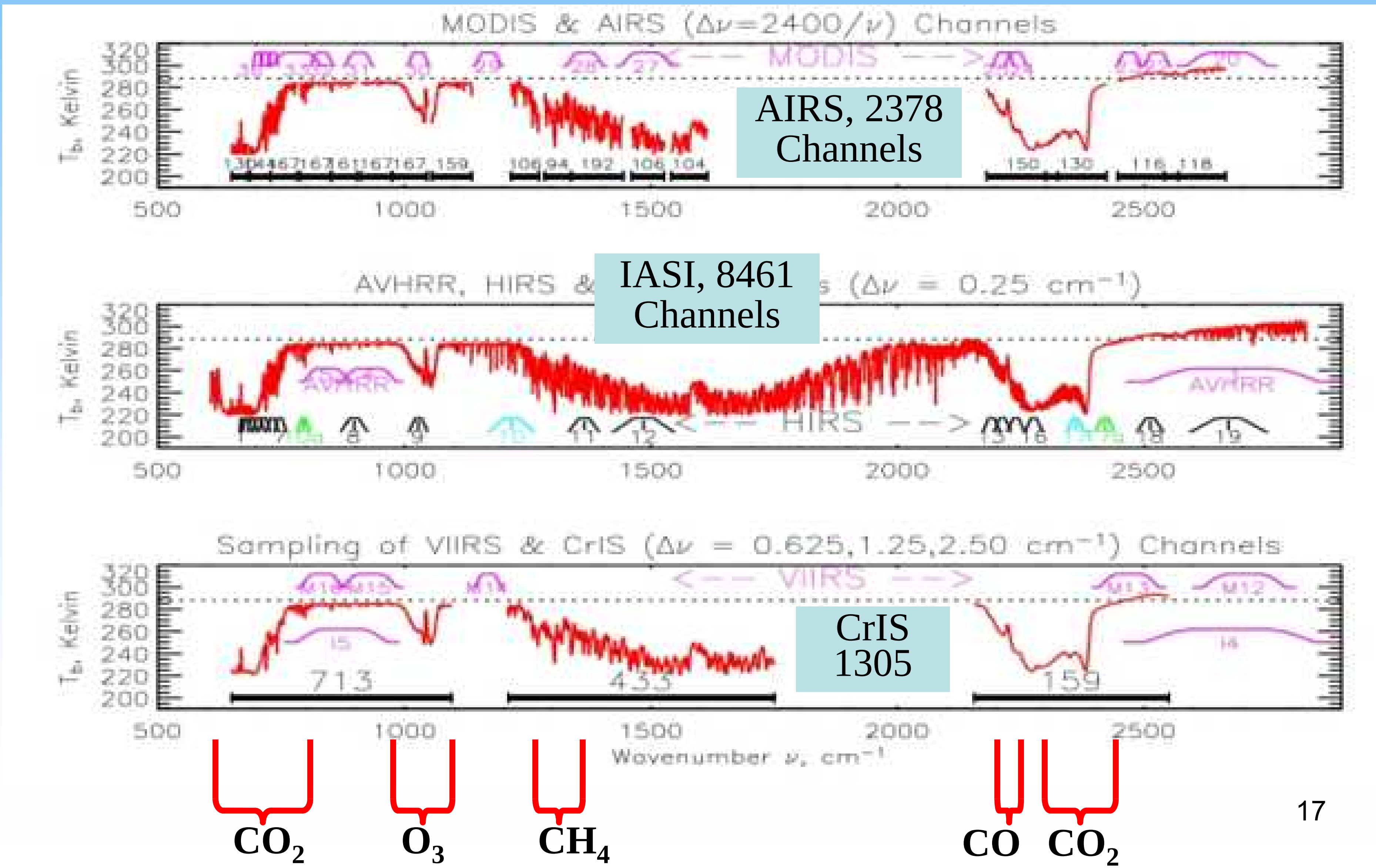
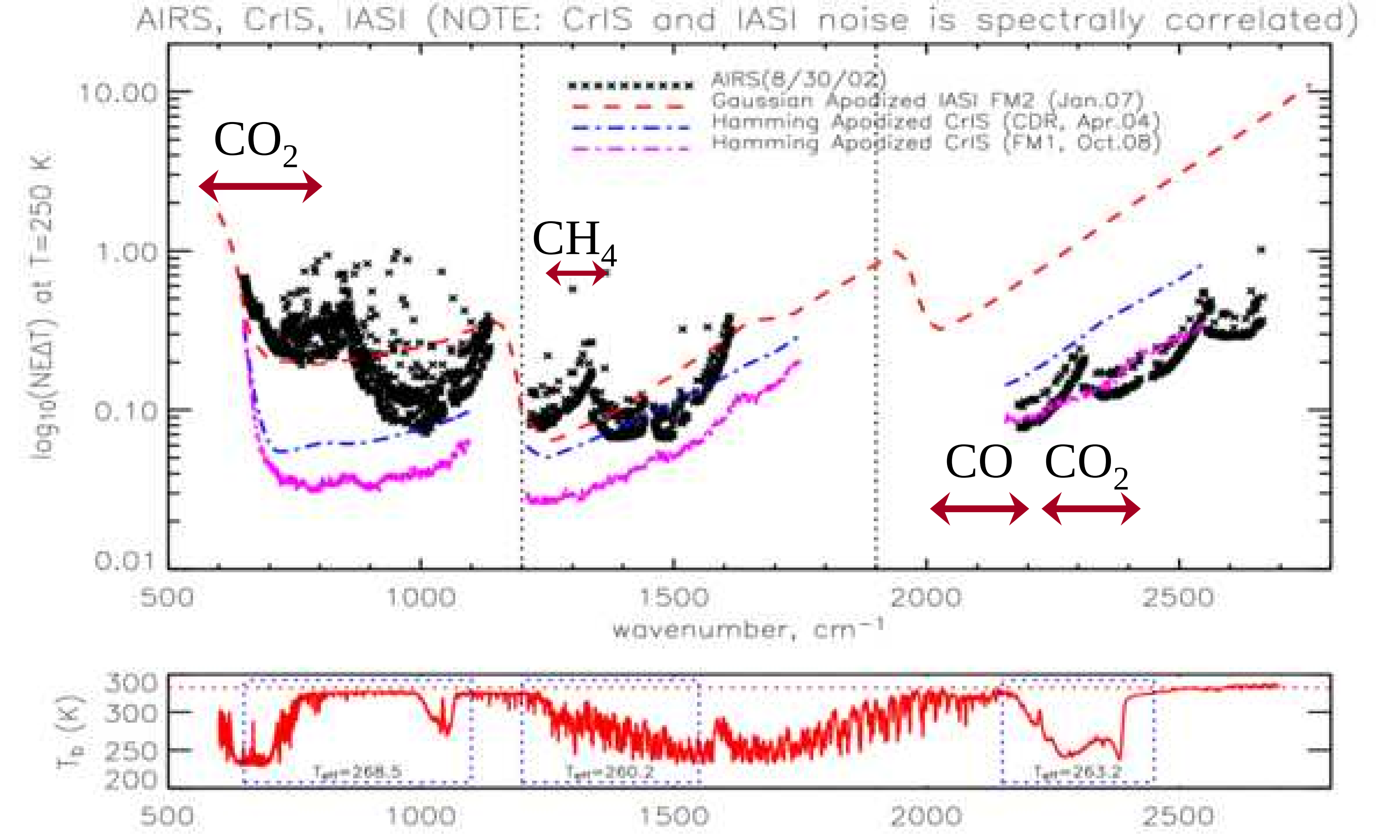
Spectral Coverage of Thermal Sounders (Example BT's for AIRS, IASI, & CrIS)



Instrument Random Noise, NEΔT at 250 K (Interferometers Noise Is Apodized)



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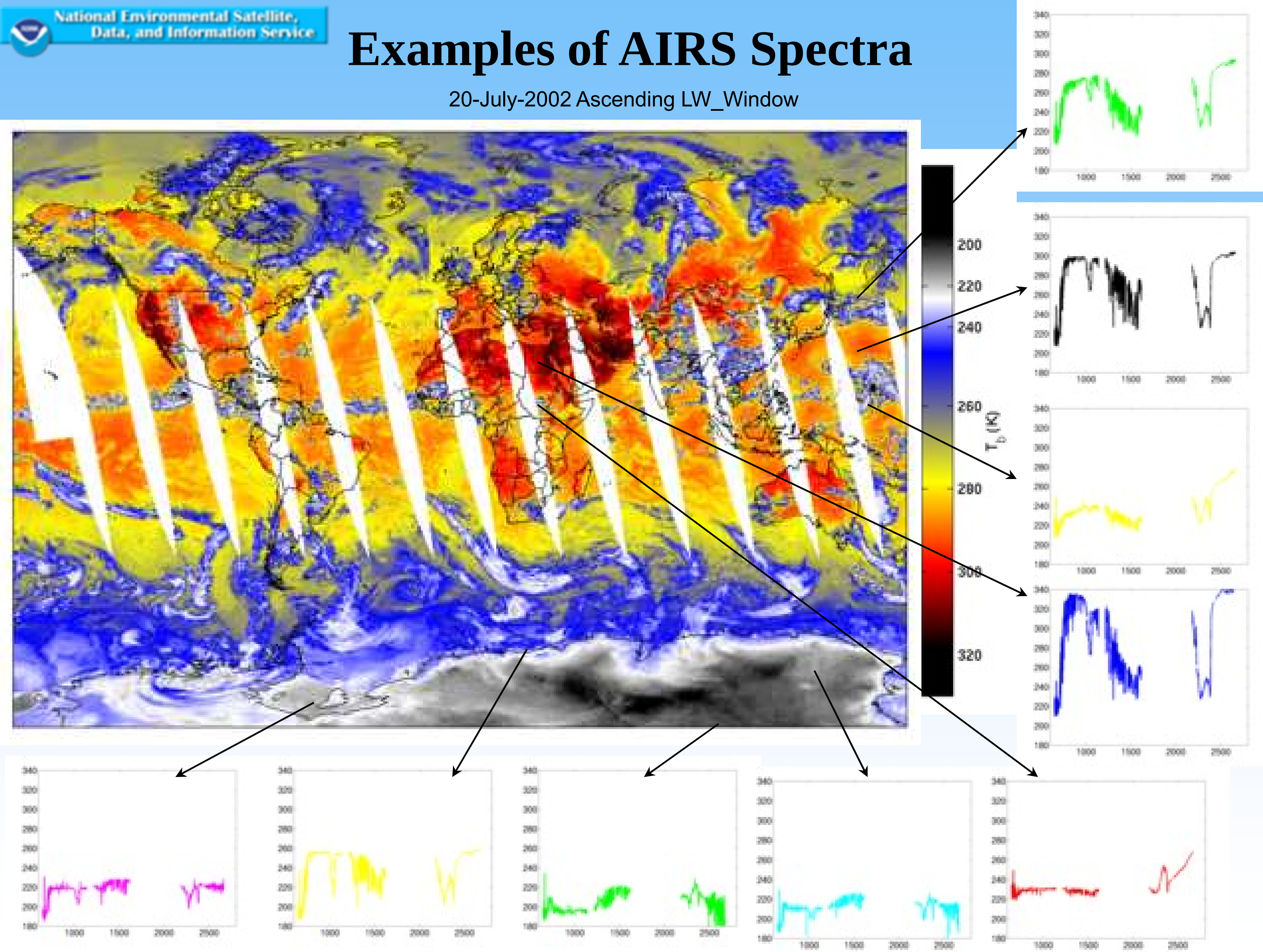
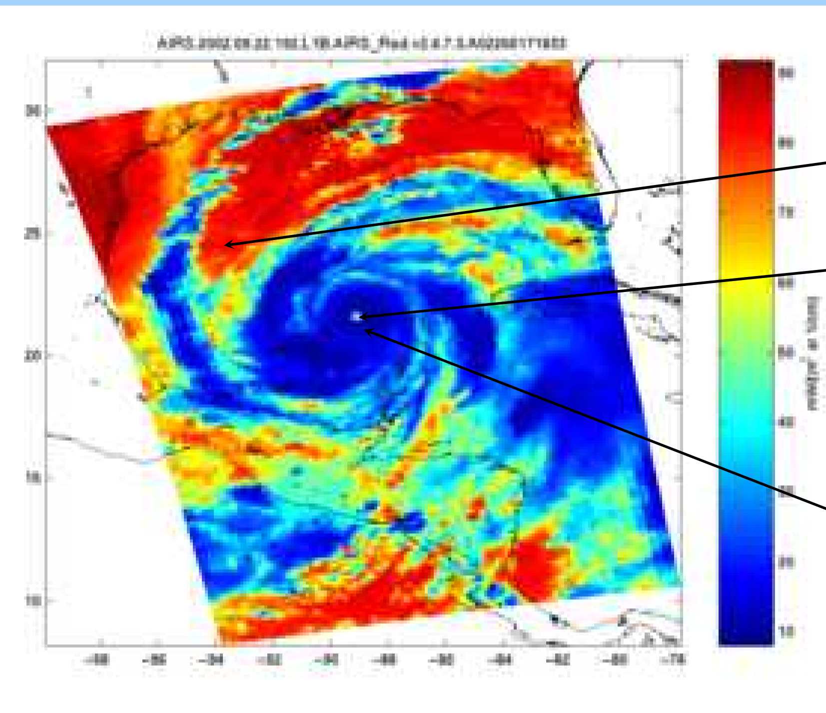
Examples of AIRS Spectra

20-July-2002 Ascending LW_Window

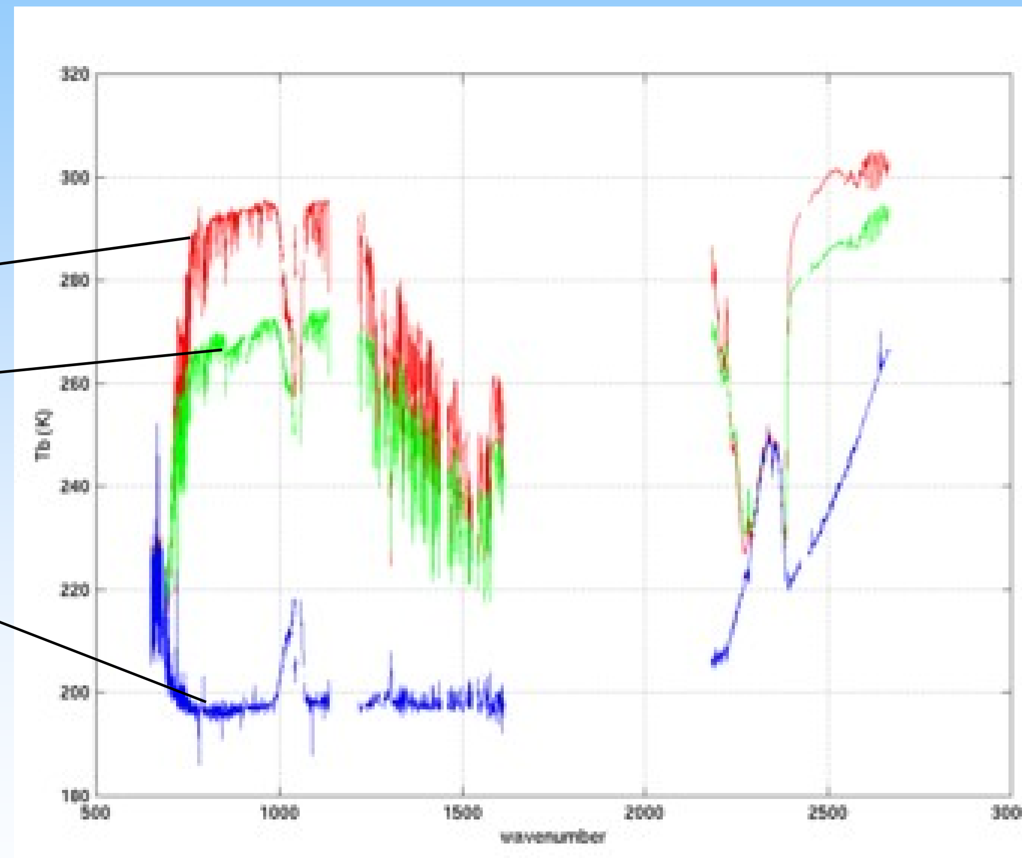


Brightness Temperature Spectra reveal changes in atmosphere from eye to boundary of Tropical Cyclone

~999 cm^{-1} radiances

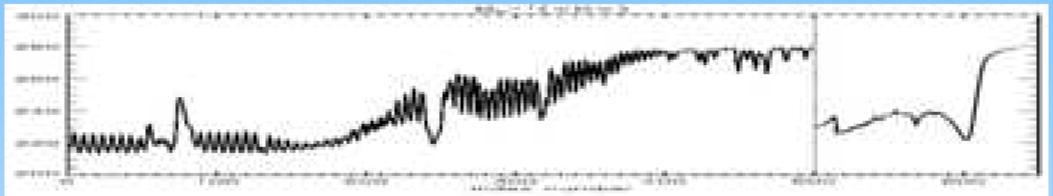


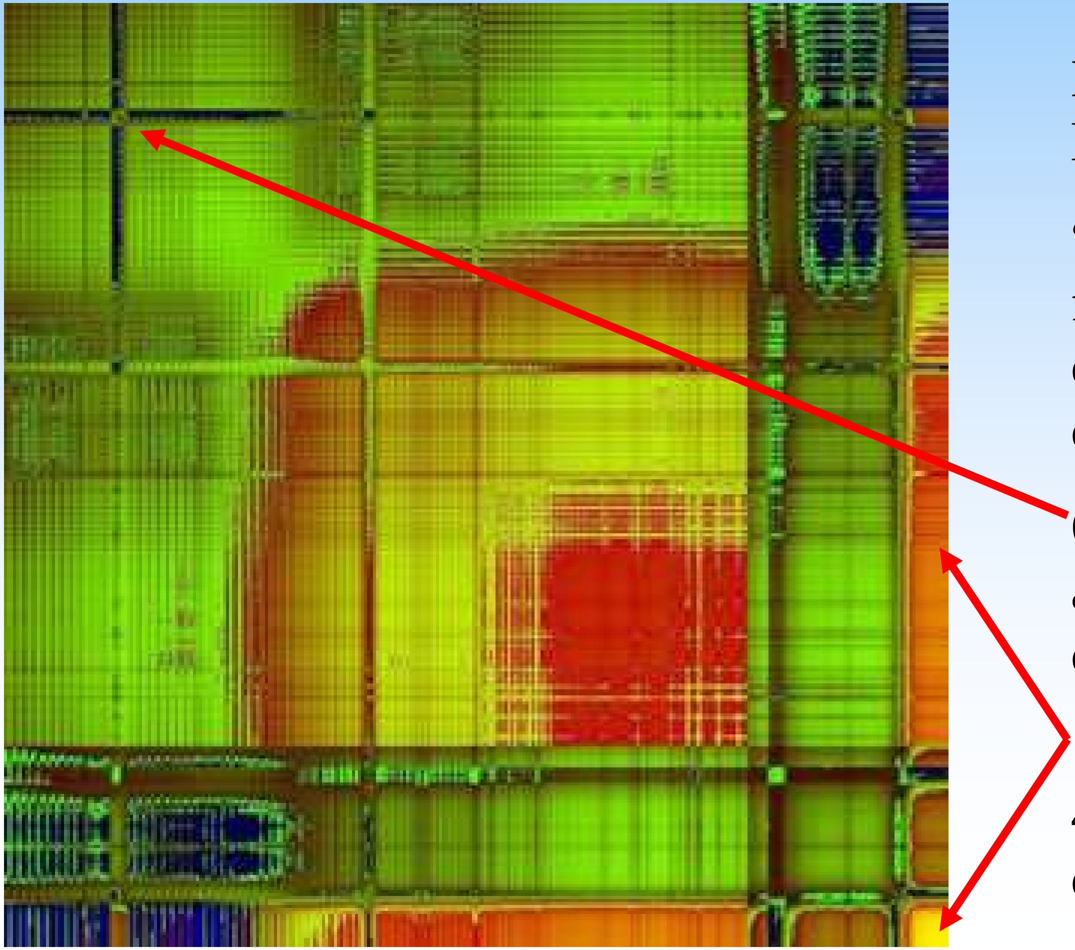
Brightness temperature spectra



AIRS observations of tropical storm Isadore on 22 Sept 2002 @ ~19:12-19:18 UTC

For a large global ensemble we can compute <R> and RR^T





Anticorrelated: BLUE

Positive: Correlation: Green → Yellow → Red

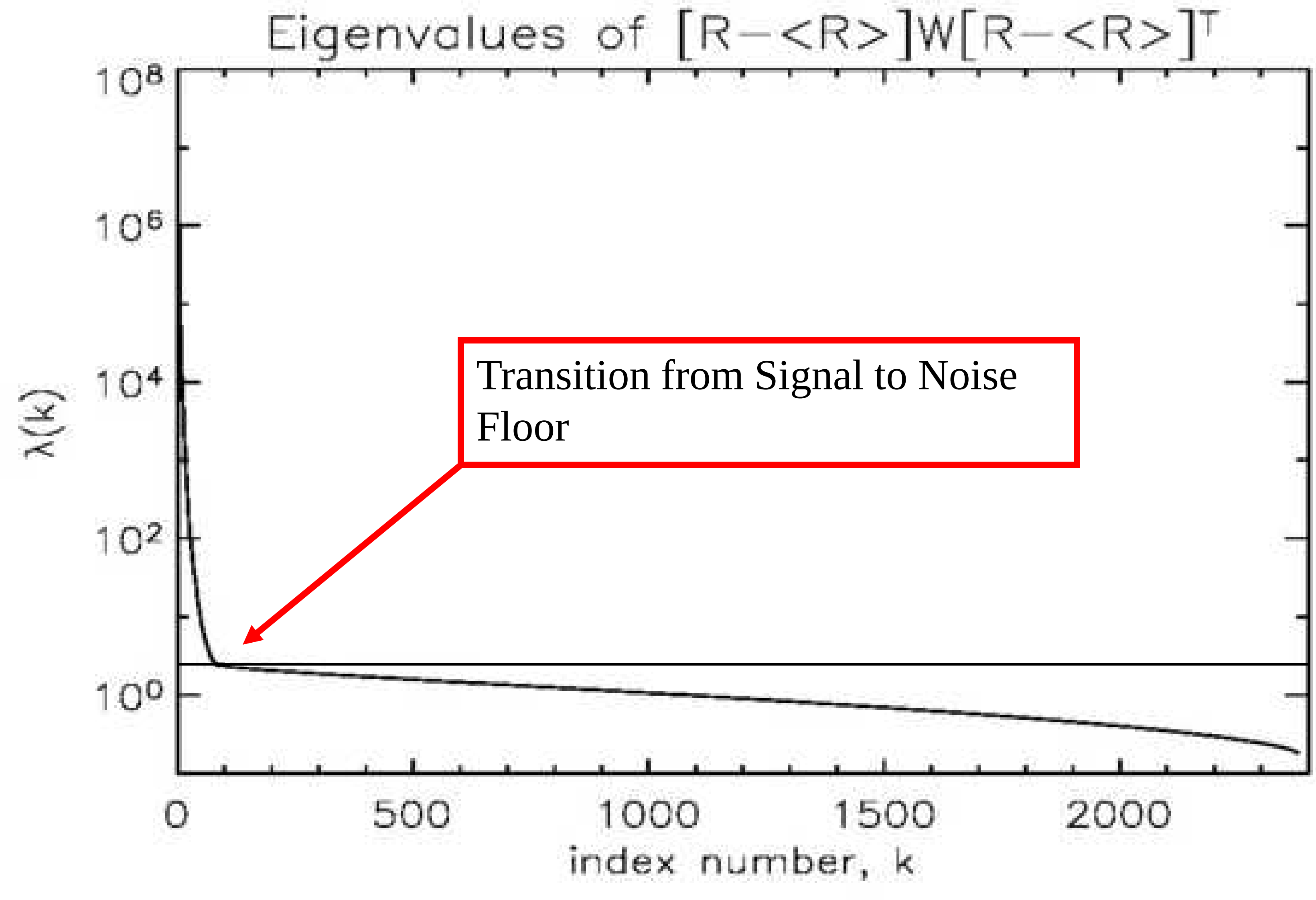
Diagonal is from upper left to lower right in this figure

"Checkerboard" pattern results from wings of lines begin correlated with near neighbor cores of lines.

667 cm^{-1} (stratospheric) is anticorrelated with tropospheric channels.

15 µm band (600-700 cm^{-1}) and 4.3 µm band (2390 cm^{-1}) are correlated (measure same thing)

Information Content of AIRS: Eigenvalues of RR^T



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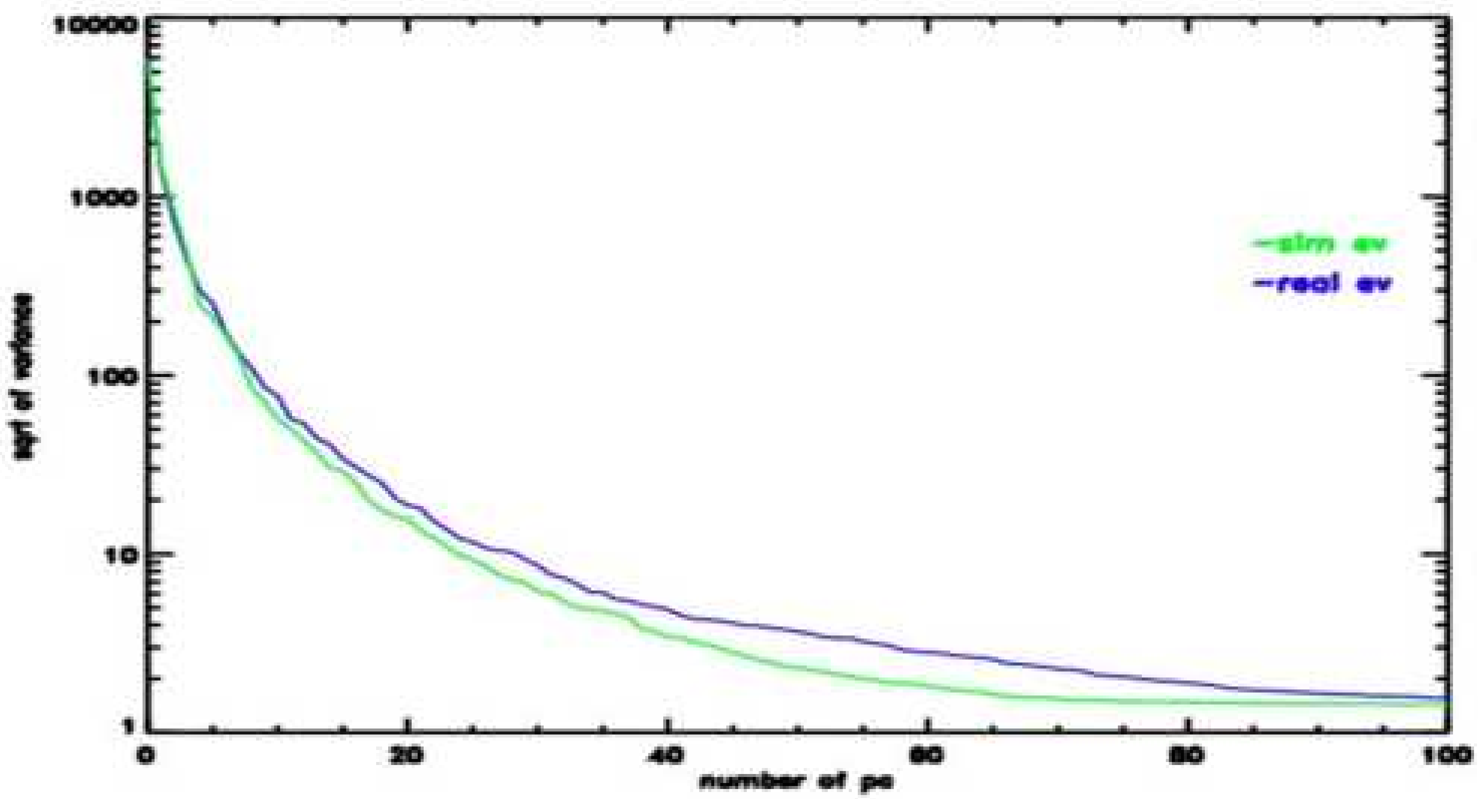
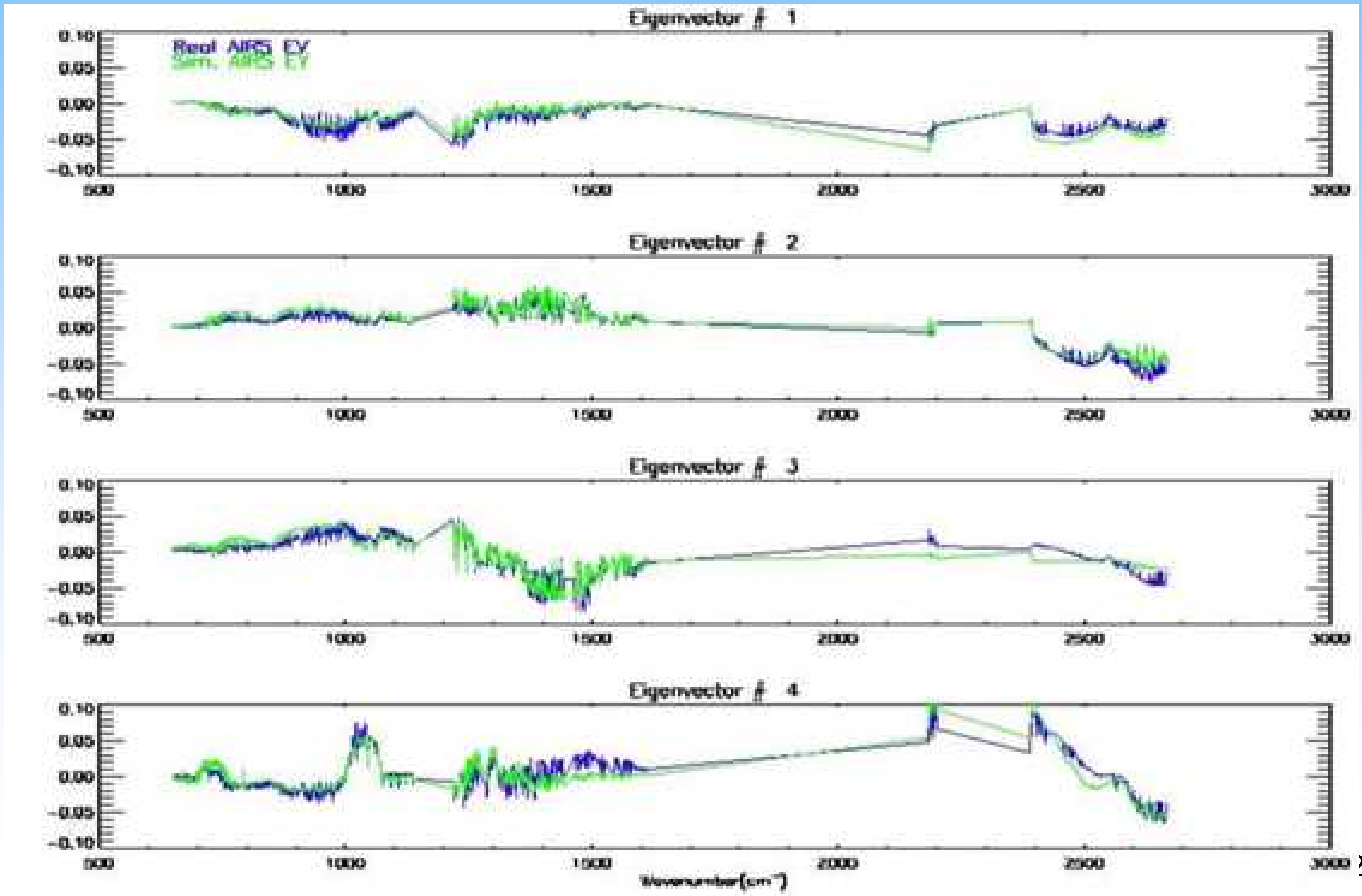
AIRS has roughly 90 pieces of information in 2378 chl's



First 4 Eigenvectors of AIRS Radiances: Real & Simulated



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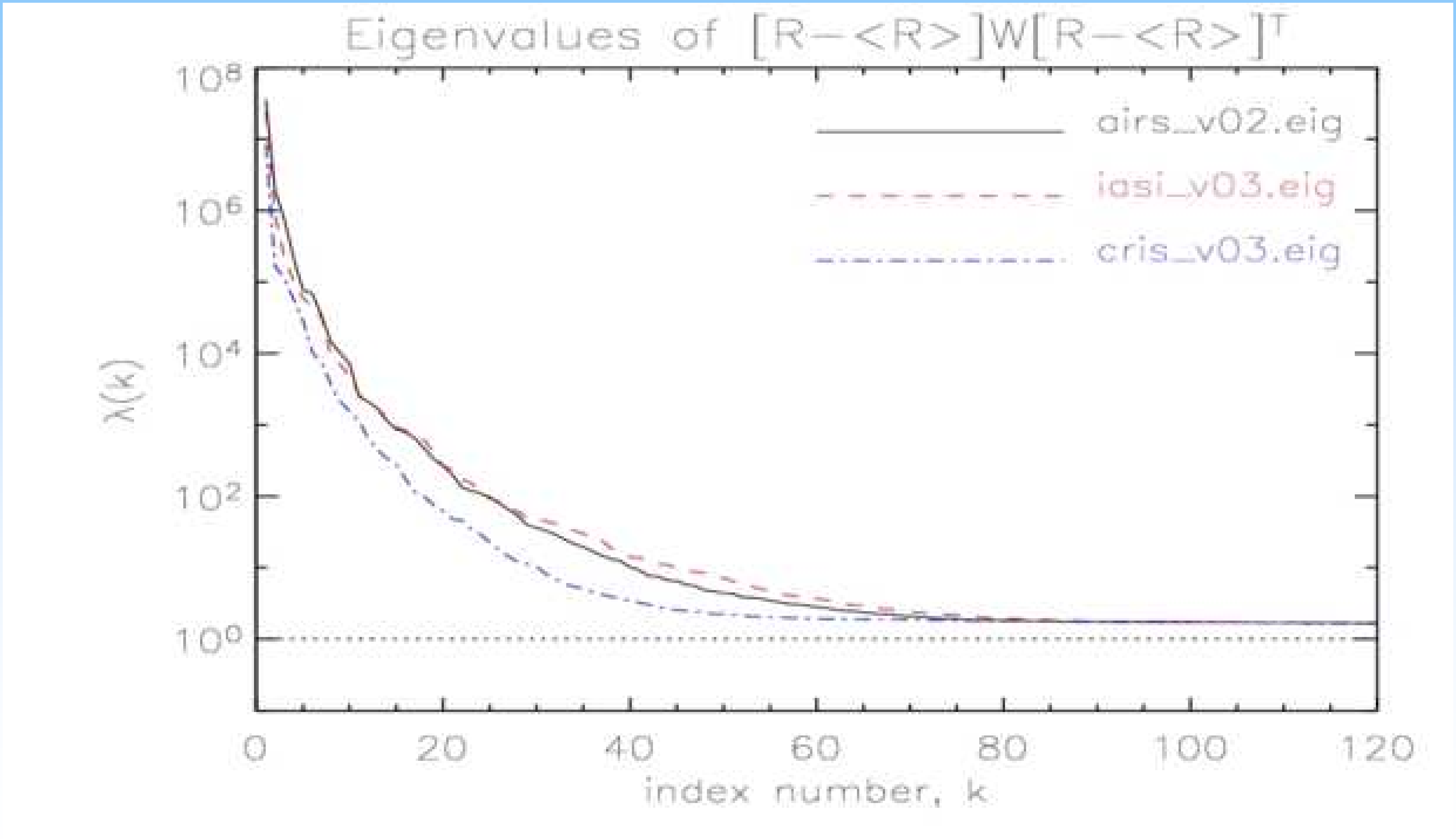
Information content of the AIRS, IASI, and CrIS radiances is approx. the same.



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Constraints and Assumptions for the AIRS Science Team Algorithm

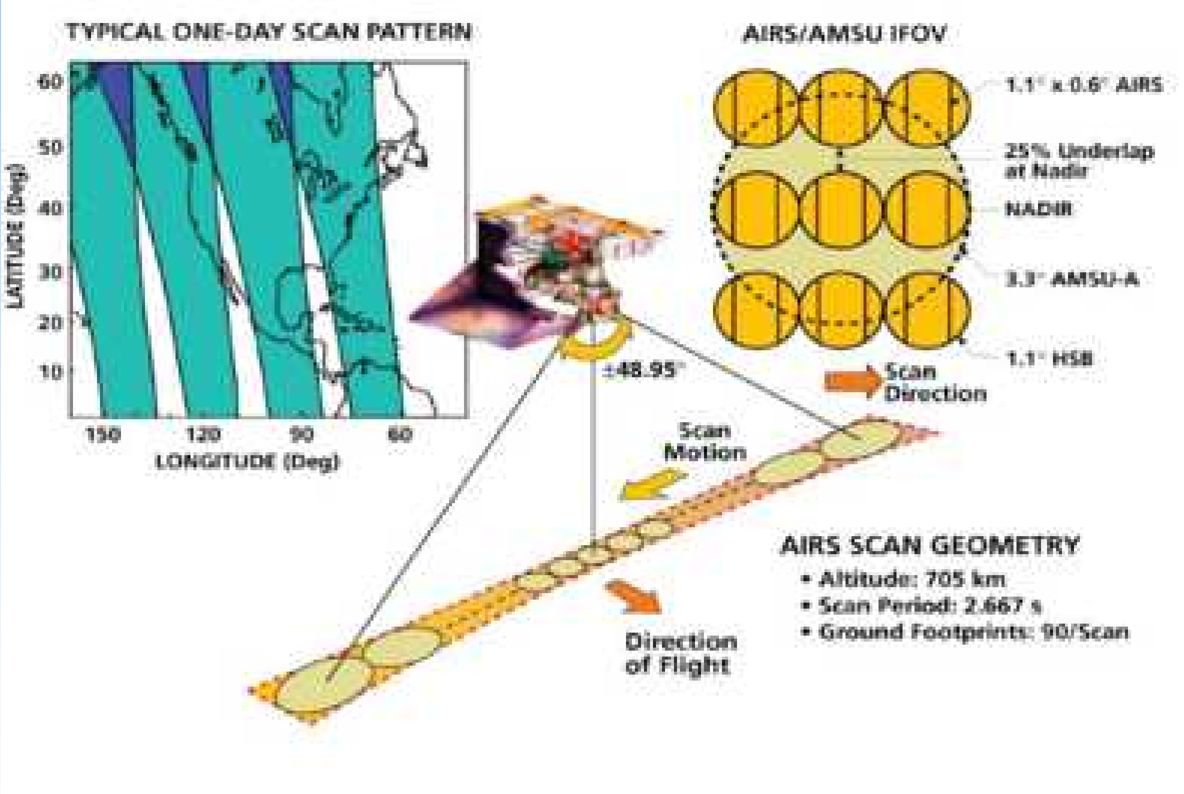
- One Granule of AIRS data (6 minutes or 1350 “golf-balls”) must be able to processed, end-to-end, using ≤ 10 CPU’s (originally 10 SGI 250 MHz CPU’s). That is, one retrieval every 0.266 seconds.
- Only static data files can be used
  - One exception: model surface pressure.
  - Cannot use output from model or other instrument data.
  - Maximize information coming from AIRS radiances.
- Cloud clearing will be used to “correct” for cloud contamination in the radiances.
  - Amplification of Noise, A, is a function of scene $0.33 \le A < \approx 5$
  - Spectral Correlation of Noise is a function of scene
- IR retrievals must be available for all Earth conditions within the assumptions/limitations of cloud clearing.
- Temperature retrievals: “1 K/1-km” was the single “success criteria” for the NASA AIRS mission.

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)
  - Local Angle Correction (LAC) algorithm
- Mitch Goldberg (NOAA)
  - Eigenvector regression operator for T(p), q(p), O3(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) for CO(p), CH4(p), CO2(p), HNO3(p), N2O(p), SO2

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

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

- Assumptions, $R_j = (1-\alpha_j)R_{clr} + \alpha_j R_{cld}$
  - Only variability in AIRS pixels is cloud amount, α_j
    - Reject scenes with excessive surface & moisture variability (in the infrared).
  - Within FOR (9 AIRS scenes) there is variability of cloud amount
    - Reject scenes with uniform cloud amount
- We use the microwave radiances and 9 sets of cloudy infrared radiances to determine a set of 4 parameters and quality indicators to derive 1 set of cloud cleared infrared radiances.
- Roughly 70% of any given day satisfies these assumptions.

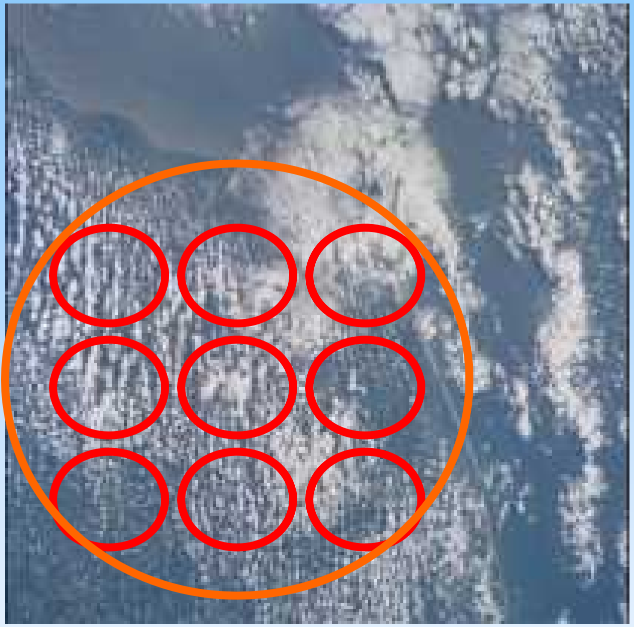


Image Courtesy of Earth Sciences and Image Analysis Laboratory, NASA Johnson Space Center (http://eol.jsc.nasa.gov). STS104-724-50 on right (July 20, 2001). Delaware bay is at top and Ocean City is right-center part of the images.

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

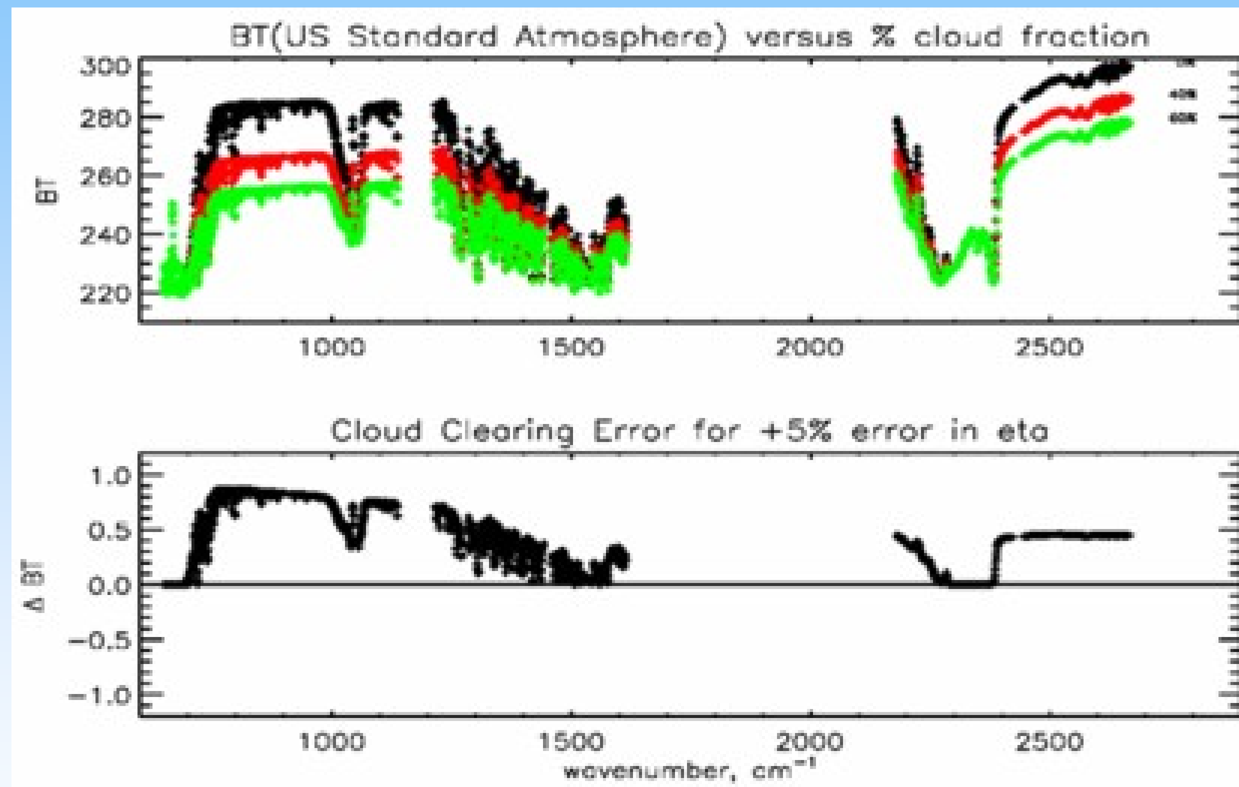
- We use a sub-set (≈ 50 chl's) of computed radiances from the microwave state as a clear estimate, $R_n = R_n(X)$ and 9 sets of cloudy infrared radiances, $R_{n,j}$ to determine a set of 4 parameters, η_j.

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

- Solve this equation with a constraint that $\eta_j \leq$ 4 degrees of freedom (cloud types) per FOR
- A small number of parameters, η_j, can remove cloud contamination from thousands of channels.
  – Does not require a model of clouds and is not sensitive to cloud spectral structure (this is contained in radiances, $R_{n,j}$)
  – Complex cloud systems (multiple level of different cloud types).

Example of cloud clearing correlated error from AIRS Cloudy Spectra

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

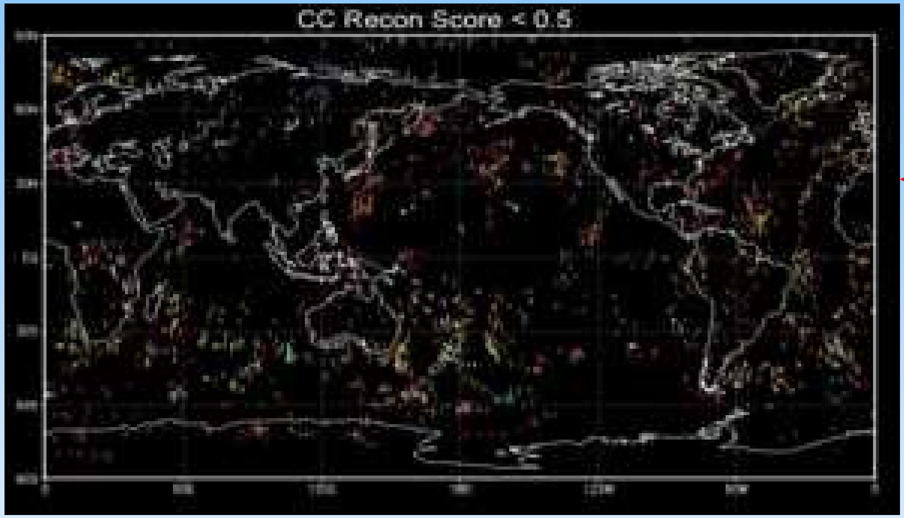


Can use any channels (*i.e.*, avoid window regions, water regions) to determine extrapolation parameters, η_j

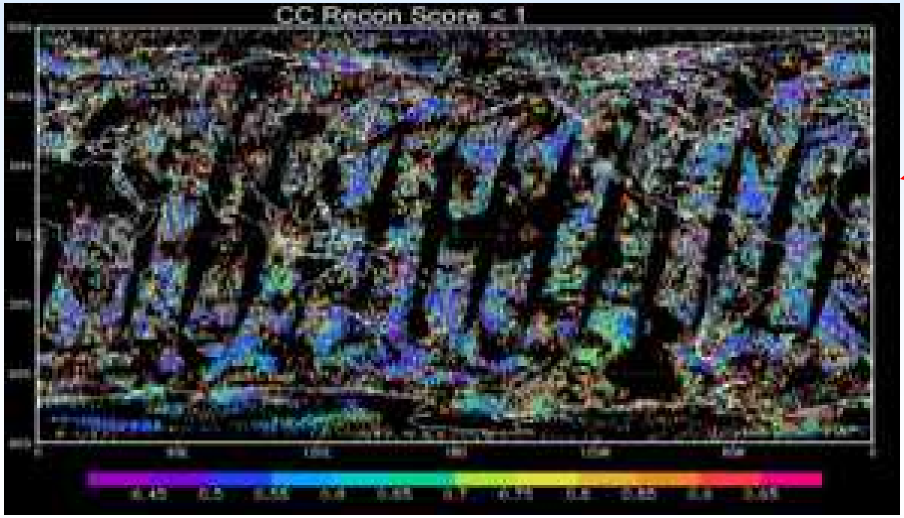
In this 2 FOV example, the cloud clearing parameters, η_j, is equal to $\frac{1}{2}\langle\alpha\rangle/(\alpha_j - \langle\alpha\rangle)$

Note that cloud clearing produces a spectrally correlated error

Cloud clearing dramatically increases the yield of useable products



- *AIRS experience:*
  - Typically, less than 5% of AIRS FOV's (13.5 km) are clear.
  - Typically, less than 2% of AIRS retrieval field of regard's (50 km) are clear.



- Cloud Clearing can increase yield to 50-80%.
- Cloud Clearing reduces radiance product size by 1:9 for AIRS and 1:4 for IASI.

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. The spectral radiance for scene j, $R_{n(m),j}$, can then be represented as principal components, $P_{k,j}$

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

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

- The eigenvectors can be determined using a couple of days of satellite (cloudy) radiances by solving

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

Statistical Regression Retrievals (continued)

- A regression, $A_{i,k}$, between a "truth" state parameter i, $X_{i,j}$, 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, as we will discover in lecture #3, are difficult to come by. We can use models (AIRS Science Team Approach uses ECMWF), radiosondes, etc.
- The equation above is solved by least squares. Since it uses a truncated set of principal components (AIRS Science Team Approach uses 85/1600) the inversion does not need to be regularized.

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.
Application of eigenvector & regression coefficients is VERY fast and for hyper-spectral instruments it is very accurate.	The regression operator does not provide any diagnostics or physical interpretation of the answer it provides.
Since real radiances are used the regression implicitly handles all systematic instrument calibration issues. This is a huge advantage early in a mission.	The regression answer builds in correlations between geophysical parameters. For example, retrieved O_3 in biomass regions might really be a *measurement* of CO with a statistical correlation between CO and O_3.
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 interpretation.

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

$$y_n = K_{n,j} \cdot x_j + \epsilon_n$$

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

$$x_j = K_{j,n}^{-1} \cdot y_n = \left[K_{j,n}^T \cdot K_{n,j}\right]^{-1} \cdot K_{j,n}^T \cdot y_n$$

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

$$\begin{aligned} K_{n,j} \cdot K_{j,n}^{-1} &= I_{n,n} \\ K_{j,n}^T \cdot \left(K_{n,j} \cdot K_{j,n}^{-1}\right) &= K_{j,n}^T \cdot I_{n,n} \\ \left(K_{j,n}^T \cdot K_{n,j}\right) \cdot K_{j,n}^{-1} &= K_{j,n}^T \\ K_{j,n}^{-1} &= \left[K_{j,n}^T \cdot K_{n,j}\right]^{-1} \cdot K_{j,n}^T \end{aligned}$$

Example of LSQ #1 Polynomial

- For example, if the desired fitting equation 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

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

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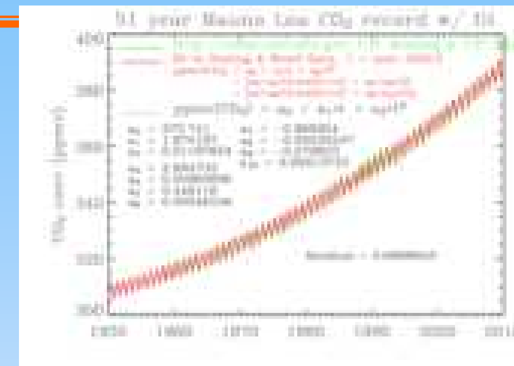
Example of LSQ #2
Polynomial plus sine function



- 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

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

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

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

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

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Unconstrained LSQ retrieval

- For non-linear LSQ (where $K_{n,j}$ may be a function of the state parameters), x_j

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

- And we may want to impose weighting on the observations

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

- The solution can be written in an iterative form

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

- The linear algebra solution is identical to minimization of a cost function

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

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

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

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

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

- Can minimize "null space" error by selecting unique (*i.e.*, non-interacting) geophysical parameters
- Error in product space can be estimated (and propagated)

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

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 (physics *a-priori* spectral information).

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

Covariance of products (*e.g.*, *T(p)*, *q(p)*, $CO_2(t)$) can be used to optimize minimization of this underdetermined problem. Need to decide how much *a-priori* statistics is desired in the product. For climate products one can use a minimum variance approach ($C = \lambda I$) to eliminate inducing correlations. For weather, geophysical correlations (model statistics) are most likely desired.

Derivative of the forward model is required to minimize J.

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

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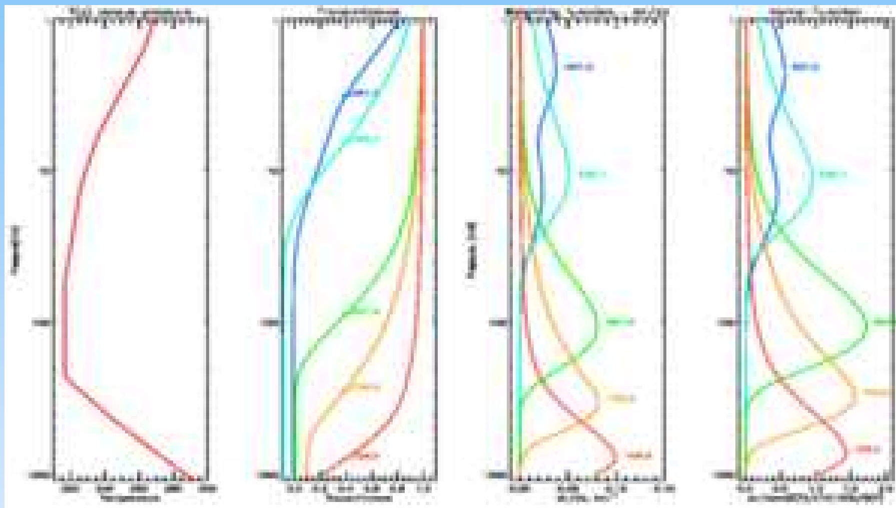
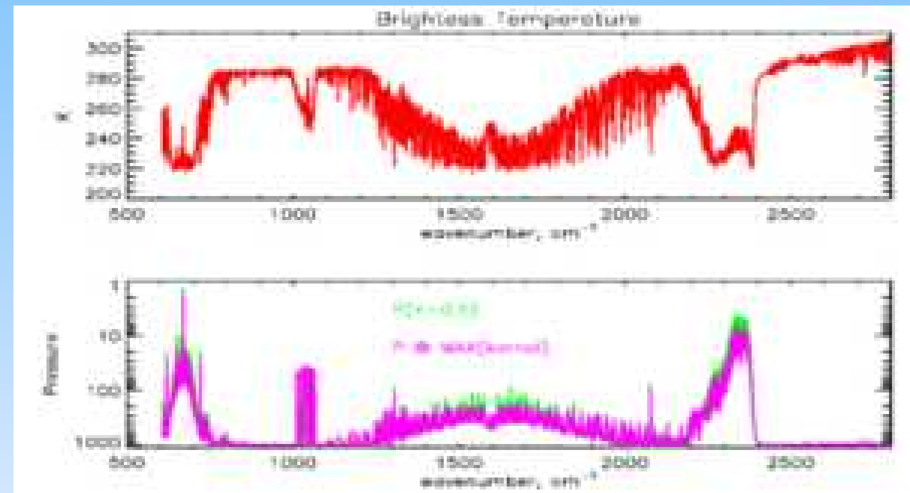
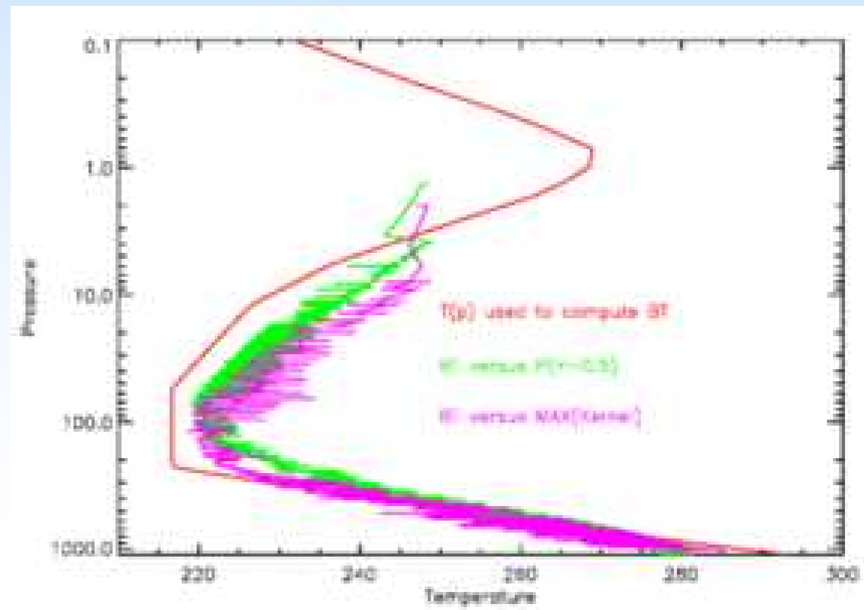
Physics knowledge is what allows interpretation of spectra
(details given radiative transfer talk)

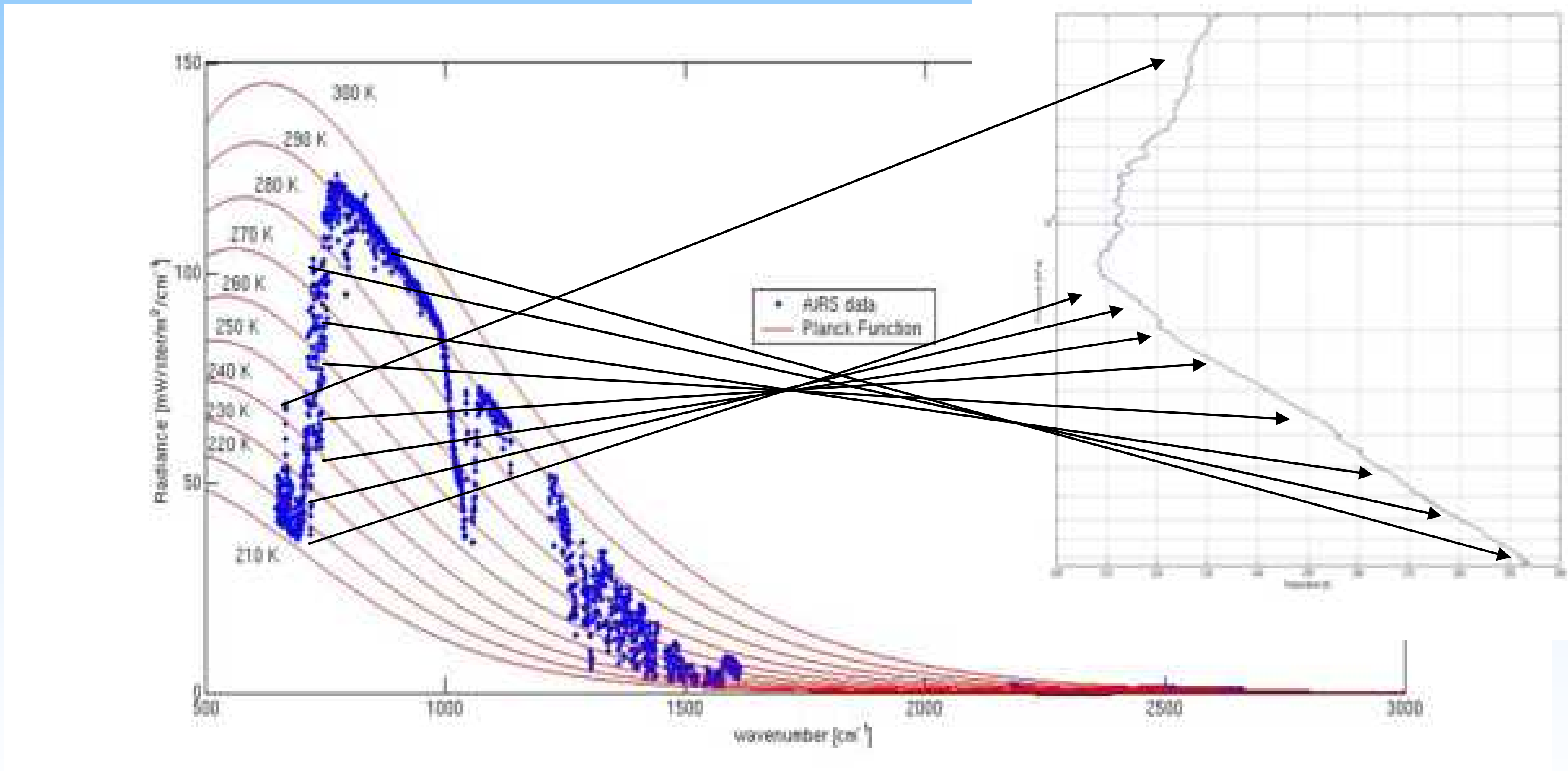




- Given an estimate of the atmospheric state we can compute transmittance.
- Weighting functions, dR/dτ, determine where transmittance changes quickly.
- Kernel functions, K, includes effect of lapse rate on a channels sensitivity.
- If we map measured brightness temperature to altitude of sensitivity we can get a reasonable estimate of the temperature profile directly from the spectrum.

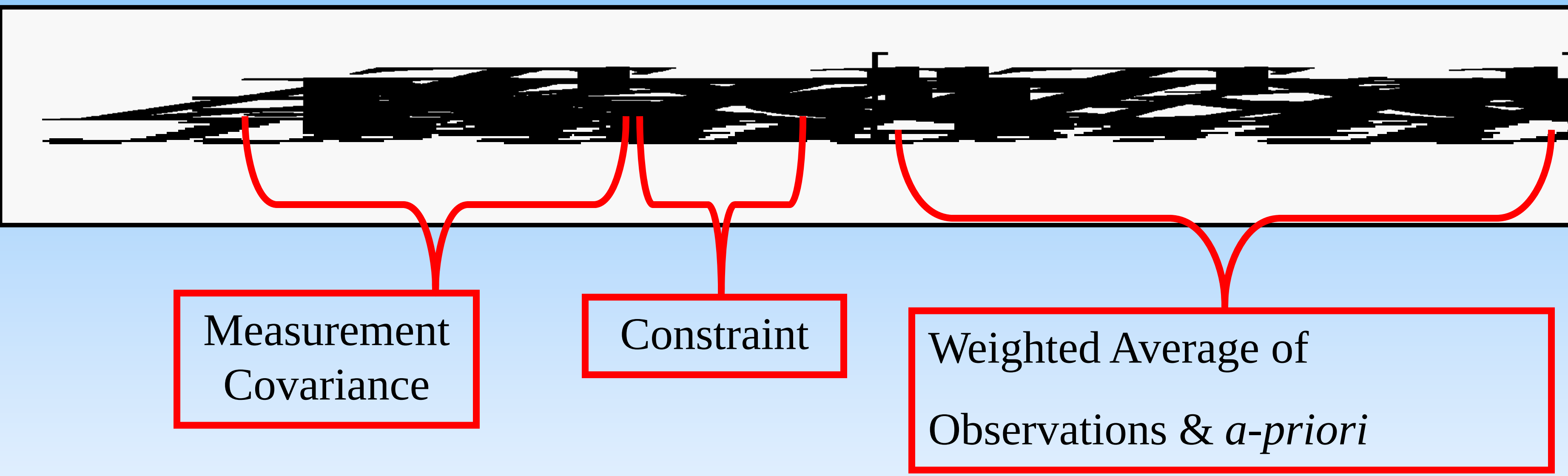


Advantage of high spectral resolution is vertical sampling ..and.. resolution



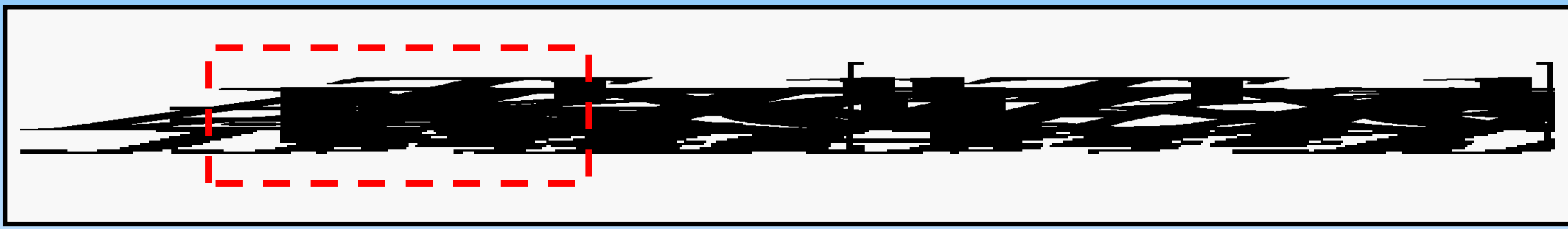
Sampling over rotational bands

The Inverse Solution: Low Resolution Instruments



Traditional methods (Rodgers, Eyre, etc.) had to rely on the statistics of the *a-priori* term (*models, climatologies, etc*) due to lack of information from the measurements (HIRS/MSU had 23 sounding channels). Typically the instrument error is neglected, that is $N^{-1} = I$, in this formulation.

The Inverse Solution: Hyper-spectral Instruments



- **AIRS: 2378 channels**
- **IASI: 8461 channels**

Hyper spectral Instruments measurements have much higher information content:

AIRS *inverse method exploits the high information content of the instrument & a-priori information in the radiative physics without a penalty in execution time.*

Iterative Solution to the Cost Function has many forms

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

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

- 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 obs-calc's to converge to a regularized solution. Form used in our algorithm:

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

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The cost function minimizes differences between observations and computed radiances

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

- Linear minimization of cost function is equivalent 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.

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

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

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.

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

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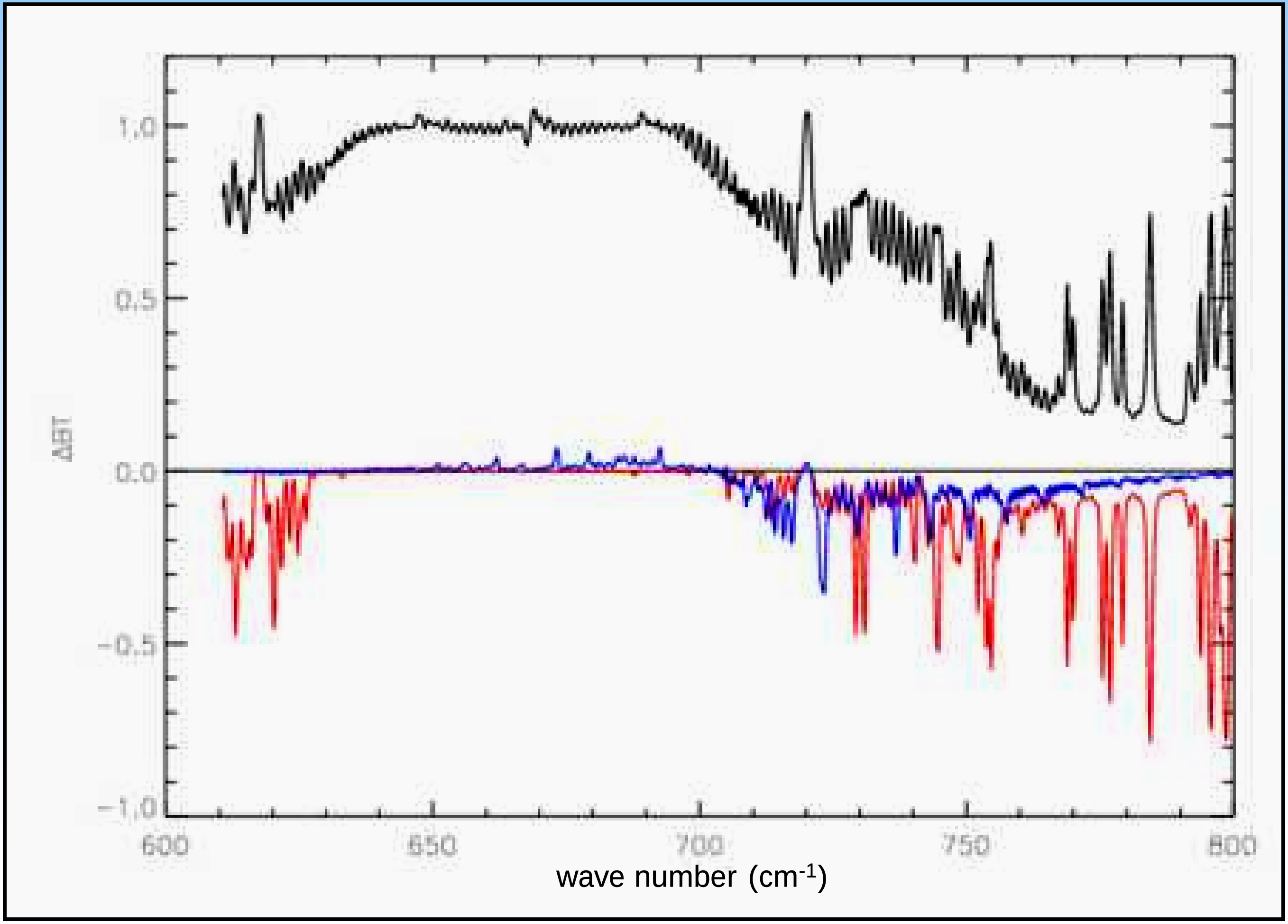
Sensitivity Analysis for Temperature Retrieval in 15 µm Band



1K temperature perturbation

10 % water perturbation

10 % ozone perturbation

Step 1: *Temperature* Solution

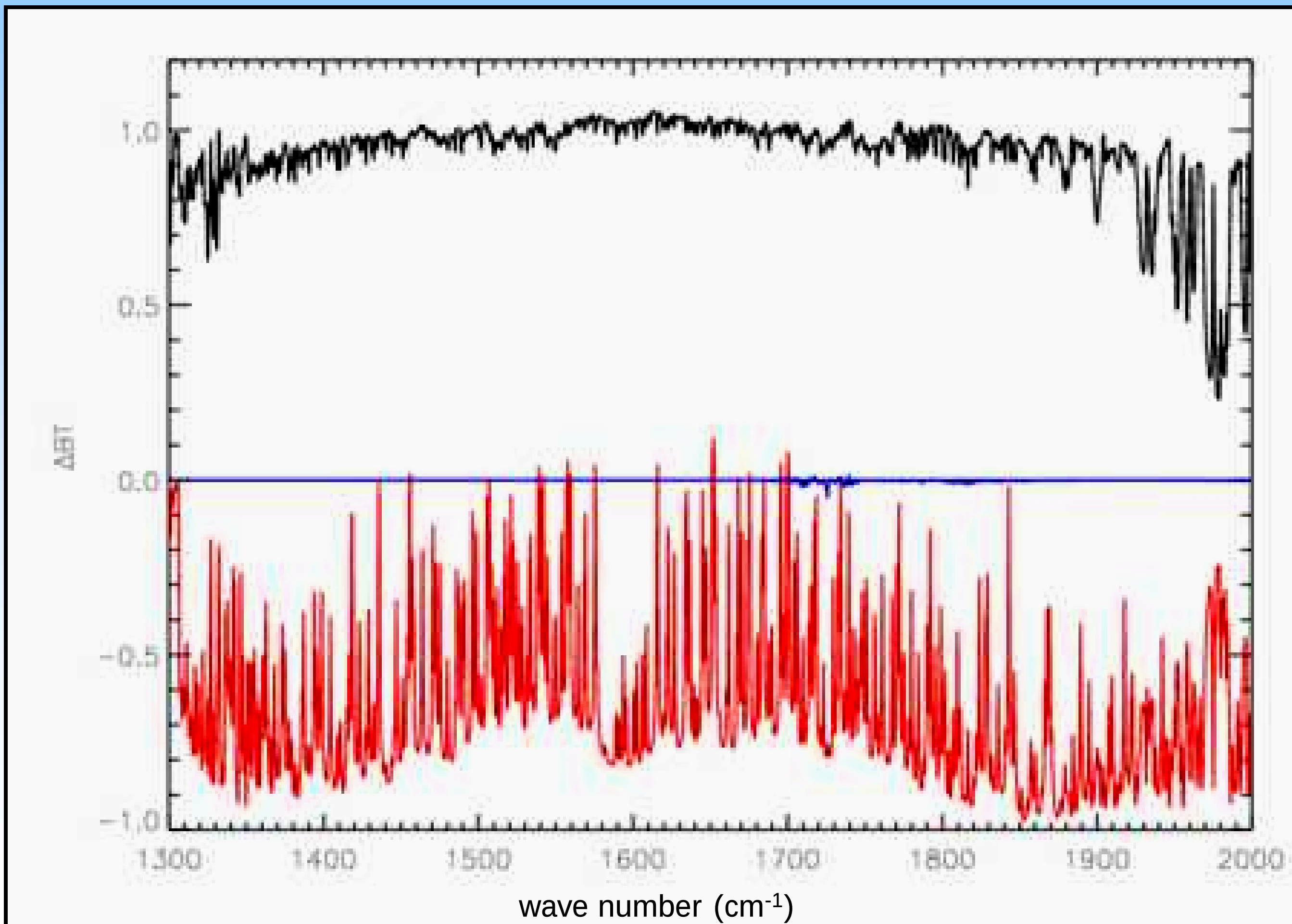
$$R_n^{obs} - R_n(\vec{X}) \approx K_{n,i}^{1} \cdot \Delta\vec{T}_i + e_n$$

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

[illegible]

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

Sensitivity analysis for water vapor retrieval in 6.7 µm band



1K temperature perturbation

10 % water perturbation

10 % ozone perturbation

Step 2: *Water vapor* solution

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

$$e_n = K_{n,i}^1 \cdot \delta\vec{T}_i + K_{n,i}^3 \cdot \delta\vec{O}_{3_i} + K_{n,i}^4 \cdot \delta\vec{CO}_i + \ldots + \varepsilon_n$$

[illegible]

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

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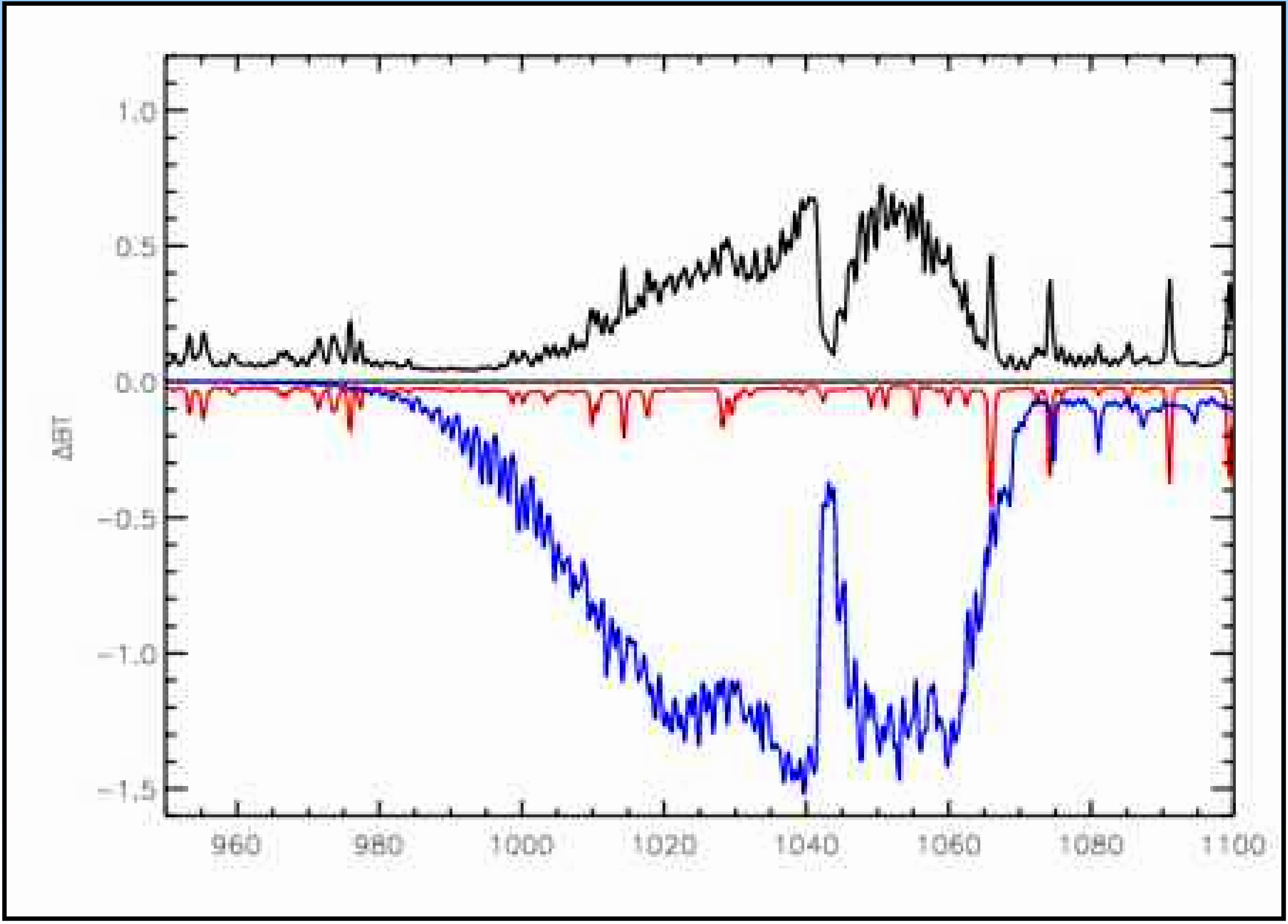
Sensitivity analysis for ozone retrieval in 9.6 µm band



1K temperature perturbation

10% water perturbation

10% ozone perturbation

Step 3: *Ozone* solution

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

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

[illegible]

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

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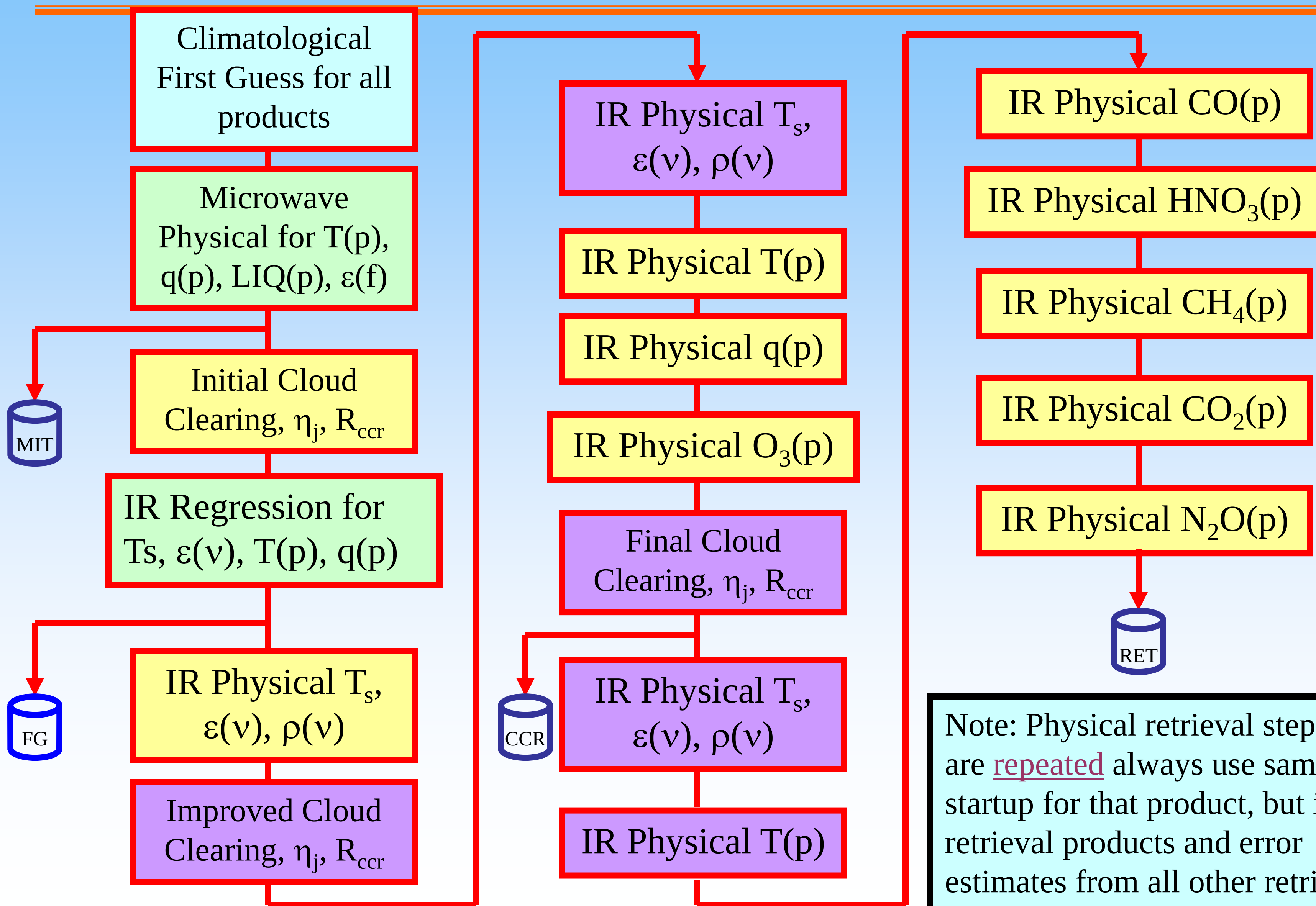
Simplified Flow Diagram of AIRS Science Team Algorithm



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

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1DVAR versus AIRS Science Team Method

1DVAR	AIRS Science Team Approach
Solve all parameters simultaneously	Solve each state variable (*e.g.*, T(p)), separately.
Error covariance includes only instrument model.	Error covariance is computed for all *relevant* state variables that are held fixed in a given step. Retrieval error covariance is propagated between steps.
Each parameter is derived from all channels used (*e.g.*, can derive T(p) from CO_2, H_2O, O_3, CO, … lines).	Each parameter is derived from the best channels for that parameter (*e.g.*, derive T(p) from CO_2 lines, q(p) from H_2O lines, etc.)
A-priori must be rather close to solution, since state variable interactions can de-stabilize the solution.	*A-priori* can be simple for hyperspectral.
Regularization must include *a-priori* statistics to allow mathematics to separate the variables and stabilize the solution.	Regularization can be reduced (smoothing terms) and does not require *a-priori* statistics for most geophysical regimes.
This method has large state matrices (all parameters) and covariance matrices (all channels used). Inversion of these large matrices is computationally expensive.	State matrices are small (largest is 25 T(p) parameters) and covariance matrices of the channels subsets are quite small. Very fast algorithm. Encourages using more channels.
Has never been done simultaneously with clouds, emissivity(ν), SW reflectivity, surface T, T(p), q(p), O_3(p), CO(p), CH_4(p), CO_2(p), HNO_3(p), N_2O(p)	*In-situ* validation and satellite inter-comparisons indicate that this method is robust and stable.

Some Final Thoughts on Remote Sounding Approaches

- Simultaneous (1DVAR) versus sequential steps 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
  - Use of geophysical covariance to regularize the under-determined problem.
- 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 22.2 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 may explore some simultaneous retrievals (T(p)/emissivity, etc.) to improve the products.

Sidebar: Vertical Averaging Functions

Using the inversion equation to derive Vertical Averaging Functions

- Our retrieval equation can be written as

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

$$K_{n,j} \equiv \frac{\partial R_n\left(\vec{X}^{i-1}\right)}{\partial X_j}\Big|_{X^{i-1}}$$

- Note that this equation is really a weighting average of the state determined via radiances and the *a-priori*.
  - The radiance covariance can be written as $K^T N^{-1} K$, in geophysical units, and
  - The product covariance is given by $[K^T N^{-1} K + C^{-1}]^{-1}$

We can derive the averaging function from our minimization equation

- As we approach a solution, we can linearize the retrieval about a state that approaches the "truth"

$$R_n^{obs} \simeq R_n(\hat{X}) + \epsilon$$

$$X_j^i = X_j^A + \left[\hat{K}_{j,n}^T \cdot N_{n,n}^{-1} \cdot \hat{K}_{n,j} + C_{j,j}^{-1}\right]^{-1} \cdot \hat{K}_{j,n}^T \cdot N_{n,n}^{-1} \cdot \left[\epsilon + \hat{K}_{n,j} \cdot \left(\hat{X} - X_j^A\right)\right]$$

$$\hat{K}_{n,j} \equiv \frac{\partial R_n\left(\vec{X}\right)}{\partial X_j}\Big|_{\hat{X}} \simeq K_{n,j}$$

- And simplify by replacing the region highlighted in green above with the variable G

$$X_j^i - X_j^A = G_{j,n} \cdot \left[\epsilon_n + K_{n,j} \cdot \left(\hat{X} - X_j^A\right)\right]$$
$$= A_{j,j} \cdot \left(\hat{X}_j - X_j^A\right) + G_{j,n} \cdot \epsilon$$

zero

Computing the averaging function

- The vertical averaging function is the amount of the derived state that came from the radiances

$$A_{j,j} \equiv G_{j,n} \cdot K_{n,j}$$
$$A_{j,j} \equiv \left[K_{j,n}^{T} \cdot N_{n,n}^{-1} \cdot K_{n,j} + C_{j,j}^{-1}\right]^{-1} \cdot K_{j,n}^{T} \cdot N_{n,n}^{-1} \cdot K_{n,j}$$

- And I-A is the amount that came from the prior

$$I_{j,j} - A_{j,j} = \underbrace{\left[K_{j,n}^{T} \cdot N_{n,n}^{-1} \cdot K_{n,j} + C_{j,j}^{-1}\right]^{-1}}_{\text{Retrieval covariance}} \cdot \underbrace{C_{j,j}^{-1}}_{\text{Inverse of } a\text{-priori covariance}}$$

Retrieval covariance

Inverse of *a-priori* covariance

Value of the vertical averaging function?

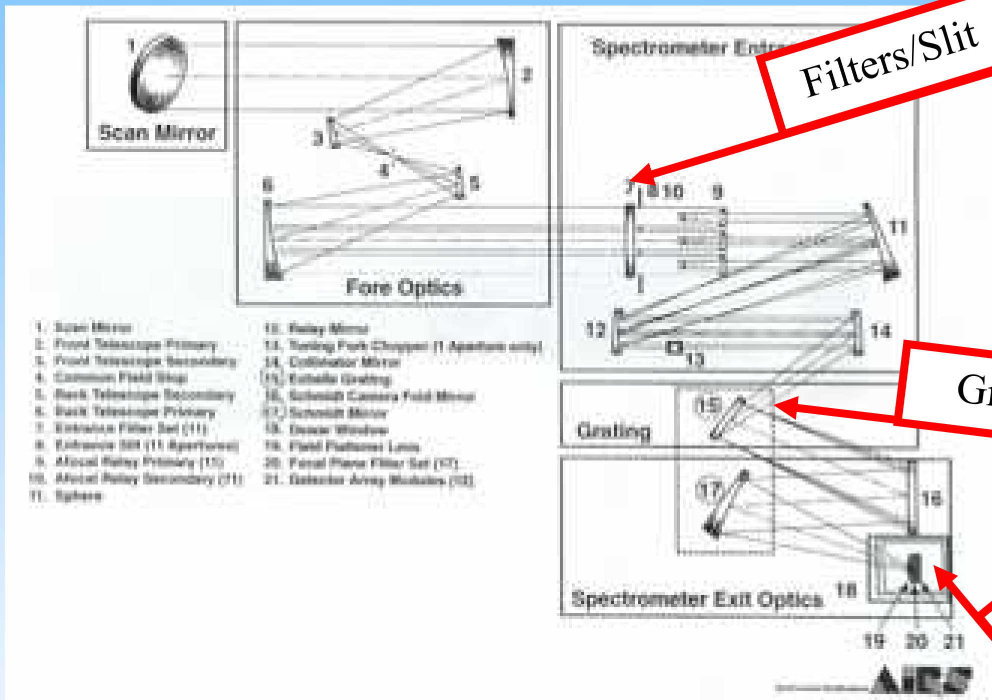
- A is the retrieval weighting of the channel kernel functions (think of a retrieval operator as an integrator of data)
- When comparing correlative measurements (such as high vertical resolution sondes or profiles acquired by aircraft) the validation measurements
  - Must have similar vertical smoothing and
  - Should be "degraded" by the fraction of the prior that entered the solution (*i.e.*, in regimes were we don't have 100% information content)
  - In essence, the "truth" data is run through the retrieval filter (averaging function) to produce a profile that is directly comparable to the product derived from the instrument radiances.
- When using retrieval products the A matrix
  - Describes the vertical correlation between parameters
  - Tells you how much to believe the product and where to believe the product.
  - *A-priori* assumptions can be removed from the solution if we are in a linear domain.
  - Given the error covariance of the *a-priori*, $C_{j,j}$, the averaging function can be used to derive the propagated error covariance of the retrieval.

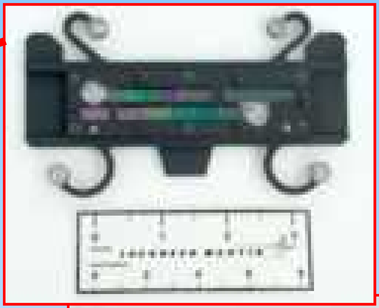
Sidebar:

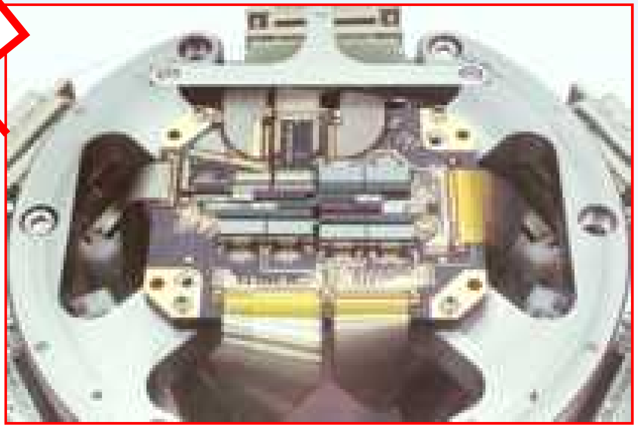
Comparison of Dispersive and Interferometric Instruments

(10 Slides)

AIRS Optical Diagram





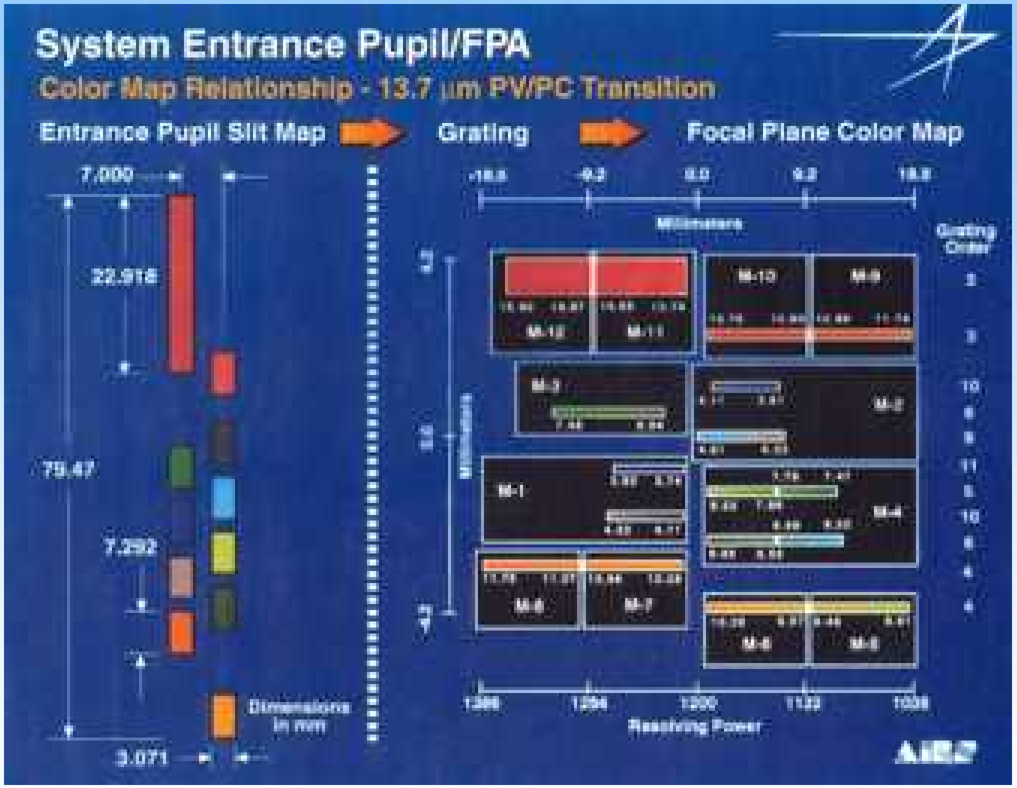


Only moving parts on AIRS are

1. Scan mirror
2. Sterling Cooler Pistons (mechanical cooler required to cool & control focal plane at 58K)

AIRS Instrument (continued)

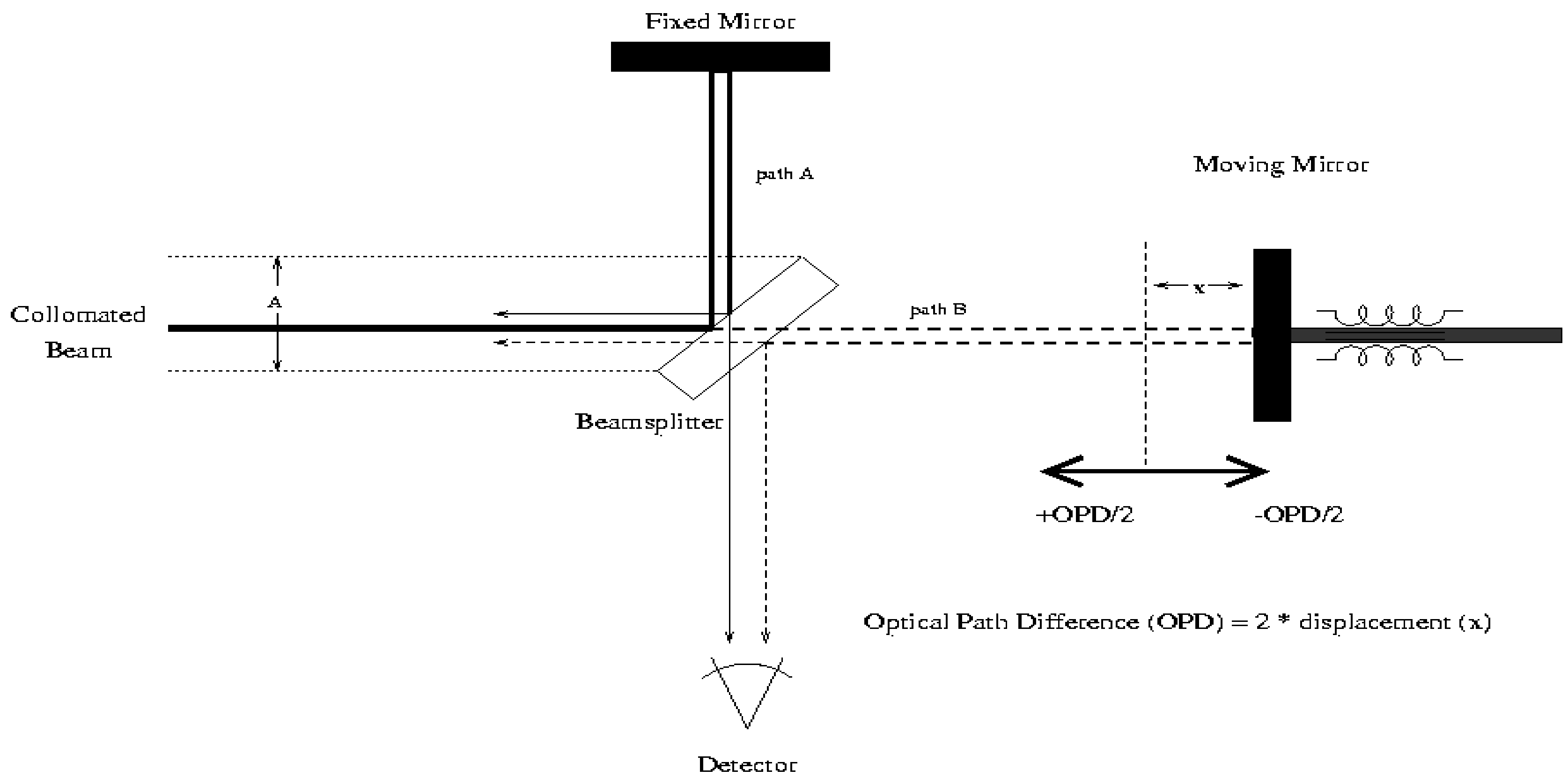
- Entrance Slits, with interference filters to select grating order and to remove stray light, are used to map spectral regions onto focal plane linear arrays.
- Optical design is “pupil imaging” to eliminate spatial sensitivity within a FOV
- Resolving Power is inversely related to slit width R_{AIRS}=1200



NOTE: Each detector is ≅ 50 μm

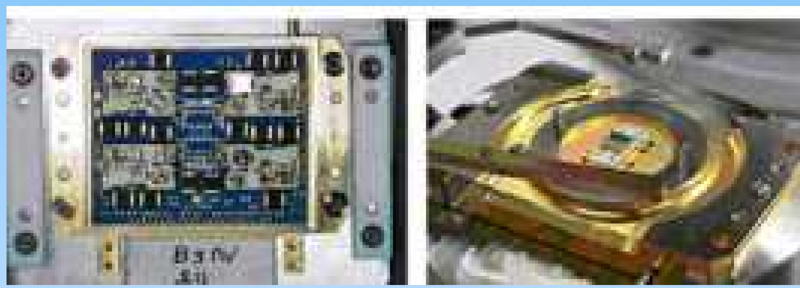
$R = (FL/W)*\tan(\theta) = 227/3*\tan(85^o)$

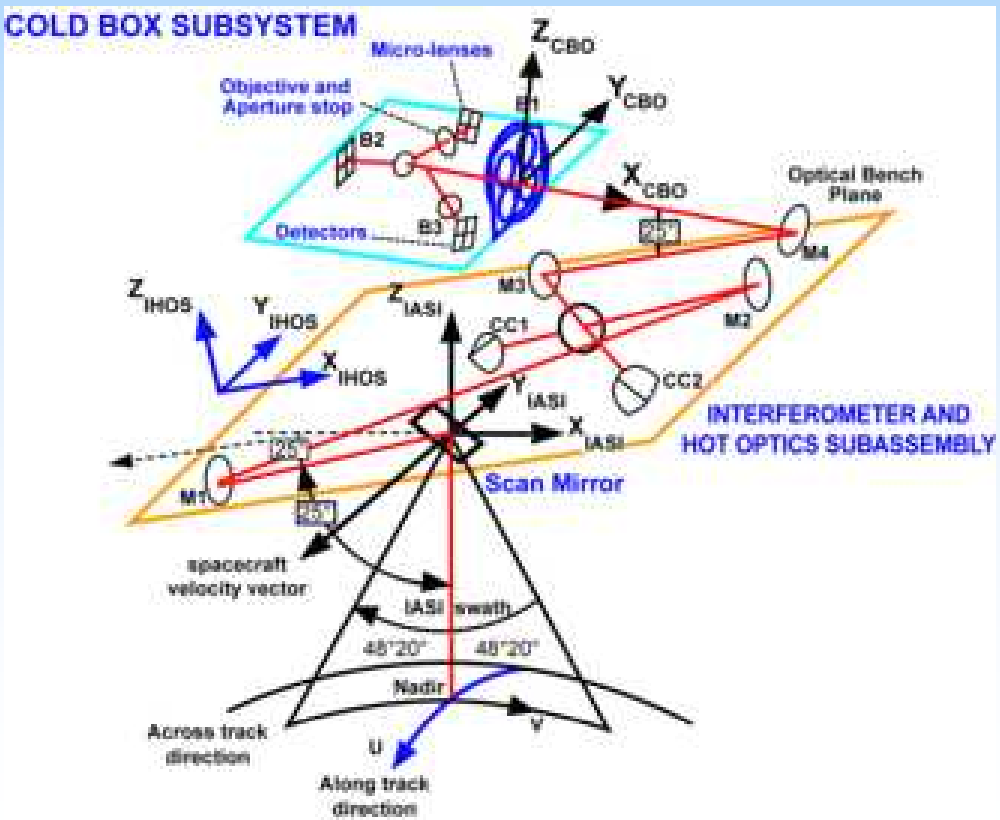
Illustration of a Simplified Michelson Interferometer



NOTE: The IASI design is much more complex. Mirrors are corner cubes (2 reflections, but very easy/stable to align). Twelve detectors are employed to improve signal-to-noise (3 bands/spectra) and sample 4 FOV's simultaneously.

IASI Optical Diagram





IASI has 4 FOV's measured simultaneously

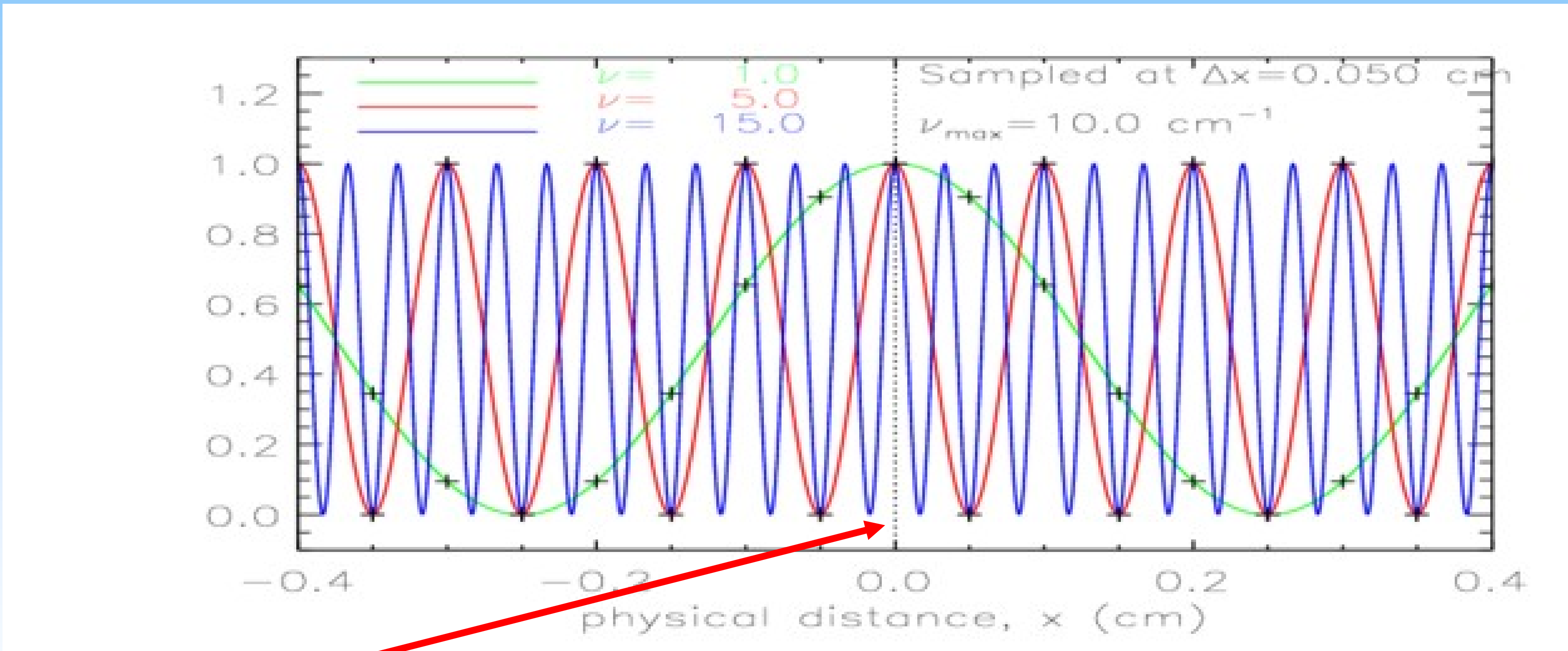
Corner cubes are used to maintain alignment in space environment.

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

Moving parts in IASI:

1. Scan mirror
2. Corner Cube (CC1)

Interferometer Measures the Cosine Transform of Radiance



- At x=0, a large contribution from all frequencies occurs. The “center burst” is equal to the total radiance within a spectral band.
- At x <> 0, the detector measures the sum of all frequencies in the pass-band. Constructive and destructive interference occurs as a function of OPD .

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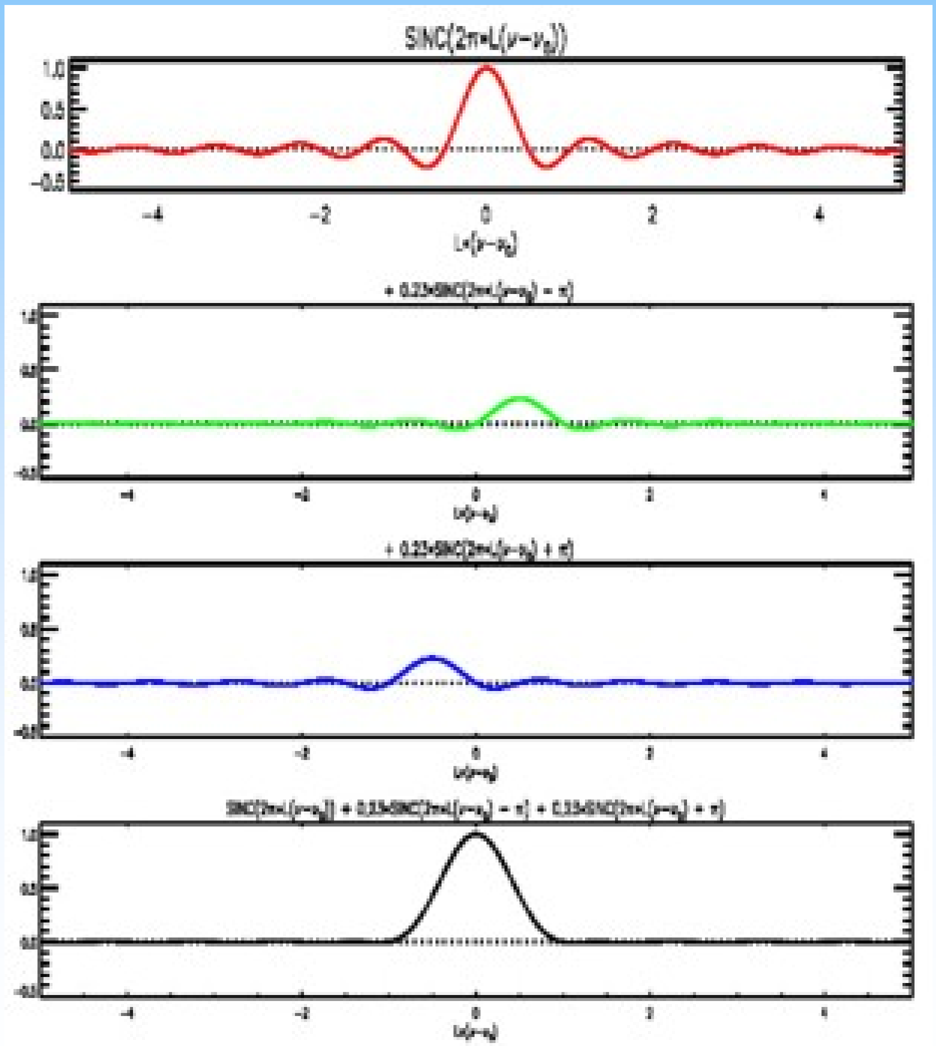
What is Apodization
(literal translation is "remove the foot")

- An apodization function is a multiplied by interferogram.
  - Most interferometers have some amount of "self-apodization" due to change in throughput as the mirror moves.
  - If the apodization function does not have zeroes, then the process is reversible.
- This is equivalent to a running mean in the spectral domain.
- Hamming's apodization function is a 3-pt weighted running mean.
- Apodization is a trade-off between side-lobes and the width (or area) of the central lobe



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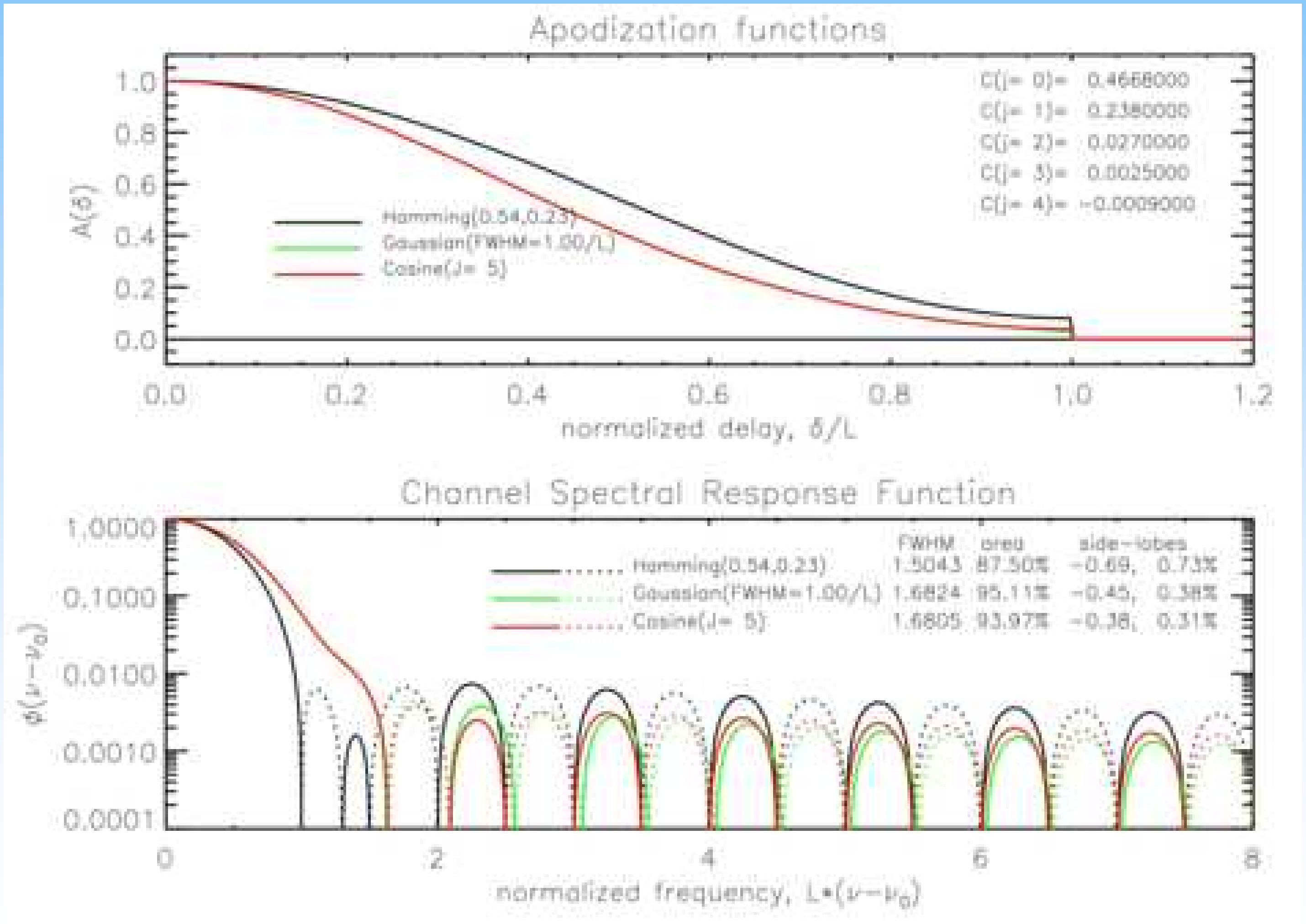
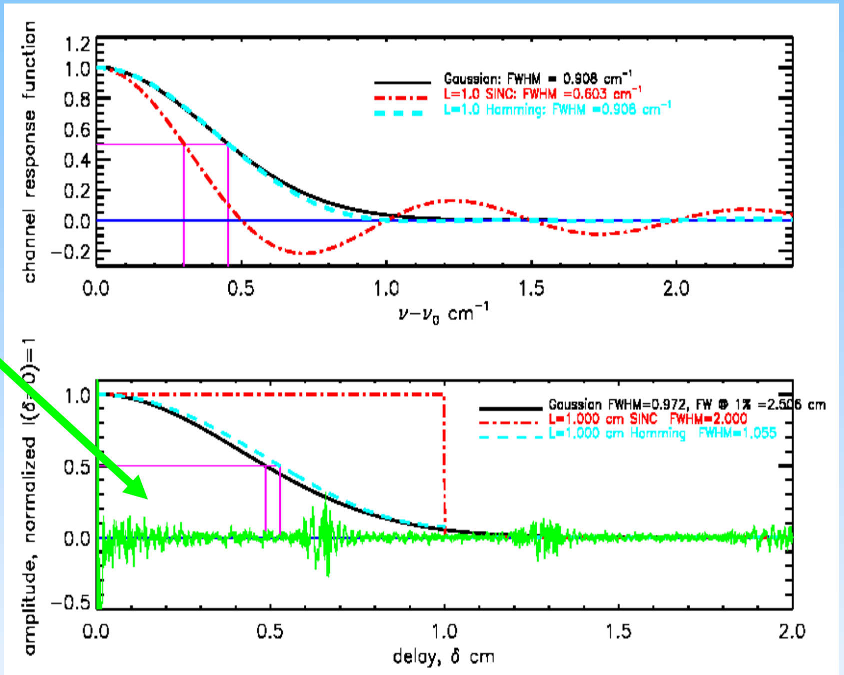
IASI Apodization Function is a Truncated Gaussian



NOTE: Gaussian Apodization DOES NOT Change the Information Content of Radiances

Apodization Alters the ILS and Spectally Correlates the Noise.

- Interferometers measure interferograms (green curve) signal as a function of optical delay, δ
- Performing a inverse cosine transform will yield the spectrum.
- Un-apodized transforms (red) have a SINC(x)=SIN(x)/x instrument line shape (ILS).
- AIRS has a Gaussian ILS (black)
- Apodization can produce a ILS that is localized and has small (< 1%) side lobes. But the tradeoff is that the central lobe is wider and the signal is spectrally correlated between neighboring channels



	Gaussian	Hamming	Blackman
FWHM / FWHM(SINC)	1.682	1.5043	1.905
Random Noise reduction	1.735	1.586	1.812
Maximum Side-Lobe	0.45%	0.73%	0.12%
% of signal in central Lobe	95.1%	87.5%	99.8%

Channel Spacing	Gaussia n	Hamming	Blackman
±1	70.74%	62.5%	75.5%
±3	25.0%	13.3%	31.6%
±4	4.43%	-	6.57%
±5	0.38%	-	0.53%
±6	0.025%	-	-

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Dispersive versus Interferometer

Dispersive optics are solid state, grating is analogous to a solid state interferometer"	Interferometer requires moving mirror that is stable over integration time (150 milli-sec for IASI & CrIS).
Linear arrays w/ read out integrated circuits make a large number of detectors feasible and very fast to read out. Large number of detectors and read out circuits requires cooling.	Multiplex (Fellgett's) Advantage: all f's measured by one detector (sampled in interferogram domain). Each time sample measures entire spectrum, therefore, each wavelength sampled N times.
Detector operates in a more linear domain because only small region of the spectrum is measures (*i.e.*, there is no "center burst").	Throughput (Jacquinot's) Advantage: does not require a slit & optics less complicated. One half of the light entering instrument strikes detector.
Frequencies are determined by geometry, therefore, instrument must be held constant in temperature. Small remnant frequency drift must be handled in radiative transfer.	Connes Advantage: Mirror distance (determines frequency of channels) can be measured with a reference laser that has a known frequency and is stable – therefore, a standard set of frequencies can be maintained.
Instrument design for multiple FOV's is too complex; however, low noise means fast integration time and having all FOV's measured by the same instrument can be considered an advantage.	Multiple FOV's can be measured simultaneously. Sampling and resolution is determined by optical path and therefore, FOV's must be
Gratings are constant resolving power, therefore, both sampling and resolution change with frequency, $\Delta\nu = R/\nu$	Continuous spectrum at constant resolution that is Nyquist sampled, $\Delta\nu \cong 0.9/L$

Which approach is most suitable for the space environment?

- All optics must be stable to vibration during integration time
  - AIRS has no moving optical components except the scan mirror (common to all scanning instruments).
  - IASI has corner cube mirror that moves 2 cm in 145 milli-seconds.
  - CrIS has “porch swing” mirror that moves 0.8 cm in 145 milli-seconds.
- Interferometers for Earth applications are passively cooled.
  - Detector responsivity is a non-linear function of temperature and small drifts will make it difficult to calibrate.
- Small drift in reference laser (laser diodes used are sensitive to temperature) makes long-term frequency calibration difficult.
- Interferogram has a large dynamic range and detector response is non-linear, therefore, the interferometer calibration is more complicated.
- Detectors are more sensitive to emissions from optics and spectrometer body and makes calibration more difficult due to phase shifts between scene and instrument.
- Calibration for cold-scenes is difficult, both due to non-linearity issues, and corrections for phase shift (instrument emission begins to dominate).