Application of PCRTM to Hyperspectral Data

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Outline

- Challenges of modeling hyperspectral data
- Description of PCRTM
- Comparisons of PCRTM with AIRS and NAST-I observations, and other RT models
- Retrieval algorithms related to hyperspectral data
- Applying PCRTM retrieval methodology to NAST-I data
- Summary and conclusions

Challenges dealing with hyperspectral data

- **Modern hyperspectral sensors have thousands of channels**
  - **AIRS: 2378**
  - **CrIS: 1305**
  - **NAST-I: 8632**
  - **IASI: 8461**
- **Commonly used methods for dealing with large amount of channels**
  - **Channel selection**
    - **According to information content (Clive Rodgers)**
    - **Used by IASI, NAST-I, AIRS**
  - **Sub-bands**
    - **Good for chemical species retrievals**
    - **Used by TES**
  - **Superchannels**
    - **Uses smaller number of channels to capture information from measurements**
    - **Optran AIRS**
    - **IASI**
- **Perform radiative transfer calculation in transformed EOF space**
  - **Principal Component base Radiative Transfer Model (PCRTM)**
  - **Used for NAST-I**

Radiative Transfer Equation Infrared Spectral Region

- **Monochromatic Radiance needs to be vertically integrated:**

$$R_\nu = \varepsilon_\nu B_\nu(T_s) t_{s,\nu} + \int_{p_s}^{0} B_\nu(T(p)) \frac{\partial t_\nu(p,\theta_u)}{\partial p} dp$$

$$+(1-\varepsilon_\nu) t_{s,\nu} \int_{0}^{p_s} B_\nu(T(p)) \frac{\partial t_\nu^*(p,\theta_d)}{\partial p} dp + \rho_\nu t_{s,\nu} t_\nu(p_s,\theta_{sun}) F_{0,\nu} \cos\theta_{sun}$$

$$= \varepsilon_{\nu s} t_{\nu,N_{bot}} B_{\nu,s} + \sum_{i=N_{bot}}^{N_{top}} (t_{\nu,i-1} - t_{\nu,i}) B_{\nu,i} + (1-\varepsilon_{\nu s}) t_{\nu,N_{bot}} \sum_{i=N_{top}}^{N_{bot}} (t_{\nu,i}^* - t_{\nu,i-1}^*) B_{\nu,i}$$

$$+\rho_s t_{\nu,N_{bot}} t_{sun}(p_s,\theta_{sun}) F_{0,\nu} \cos\theta_{sun}$$

  - **The first term is the surface emission**
  - **The second term is the upwelling thermal emission**
  - **The third term is the reflected downwelling radiation**
  - **The last term is the reflected solar radiation**

- **Channel radiance is a spectral integral of monochromatic radiances:**

$$R_{\Delta\nu}(\nu) = \frac{\int_{\Delta\nu} \phi(\nu-\nu') R(\nu) d\nu'}{\int_{\Delta\nu} \phi(\nu-\nu') d\nu'}$$

Description of PCRTM

- **PCRTM is not a channel-based RTM**
  - **predicts PC scores (*Y*) instead of channel radiances (*R*)**

$$\vec{Y} = A \times \vec{R}^{mono}$$

$$\frac{\partial Y_i}{\partial X} = \sum_{l=1}^{N_{mono}} a_l \frac{\partial R^{mono}(l)}{\partial X}$$

- **The relationship is derived from the properties of eigenvectors and instrument line shape functions:**

$$\vec{Y} = U^{T} \times \vec{R}^{chan}$$

$$R_i^{chan} = \frac{\sum_{k=1}^{N} \phi_k R_k^{mono}}{\sum_{k=1}^{N} \phi_k}$$

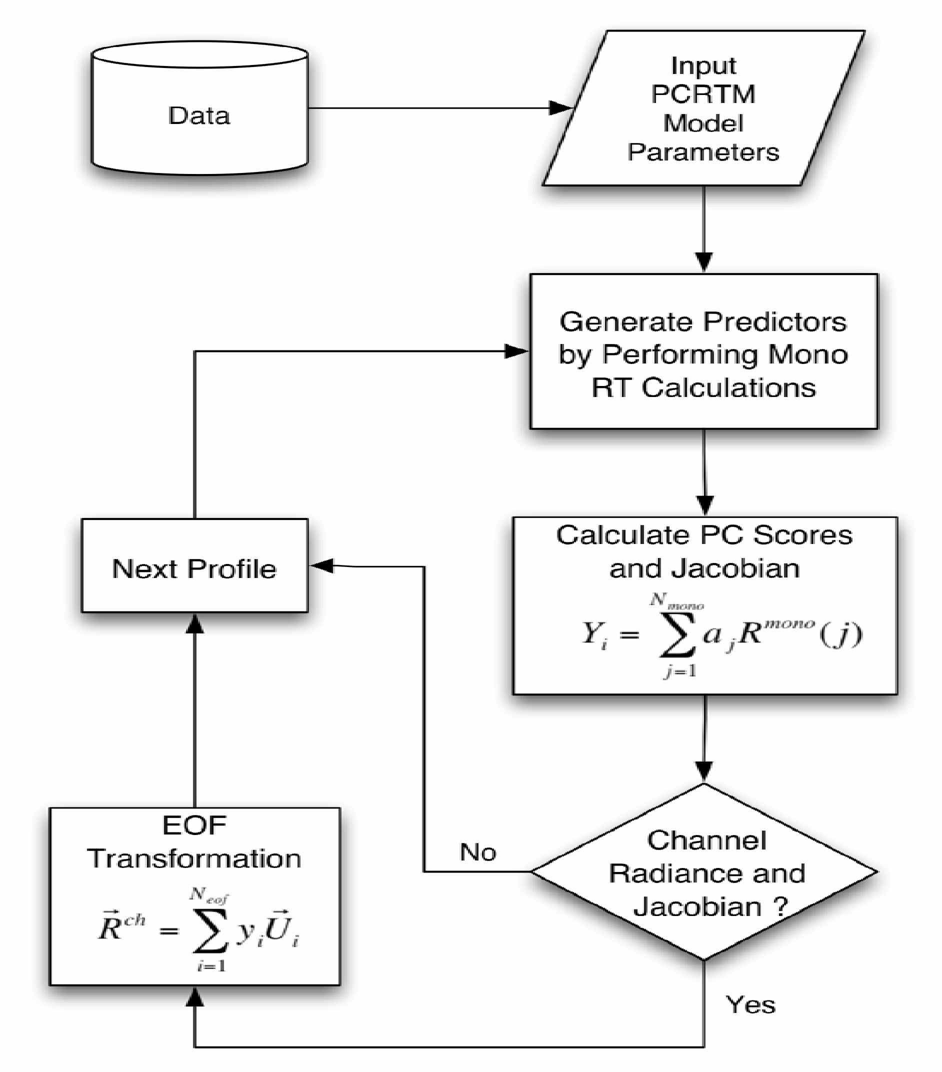
- **Channel radiances (or transmittances) can be obtained by multiplying the PC scores with pre-stored Principal Components (PCs):**

$$\vec{R}^{chan} = U \times \vec{Y} = \sum_{i=1}^{N_{EOF}} y_i \vec{U}_i + \vec{\varepsilon}$$

Description of PCRTM (continued)

- *Y* is a non-linear function of atmospheric state
  - Can be thought as super channels
  - contains essential information about the spectrum
- *U* captures spectral variations from channel to channel
  - Capture details on instrument functions
  - does not change from one spectrum to another
  - No need to include it in inversion process
- *Y* can be predicted from monochromatic radiances directly
  - Linear relationship due to the properties of *U* and ϕ
  - More than an order of magnitude reduction in dimension
- Jacobian can be calculated in EOF domain directly
  - Great advantage to perform retrieval in EOF domain
- RT done monochromatically at very few representative frequencies
  - Easy coupling with multiple scattering models
- Can efficiently deal with any instrument line shape functions
  - e.g ILS with negative side lobes

Forward Model Flowchart



Radiative Transfer Calculation is Simple

- **Radiative Transfer coding is very simple (see example for calculating upwelling radiances):**

$$Initiallize\ R_\nu^{up}:$$

$$R_\nu^{up} = \varepsilon_\nu B_\nu(T_s)$$

$$Do\ l = nBot, nTop, \text{-}1$$

$$\frac{\partial R_\nu^{up}}{\partial \tau_l^0} = [B_\nu(T_l) - R_\nu^{up}]t_{0\to l}\sec(\theta)$$

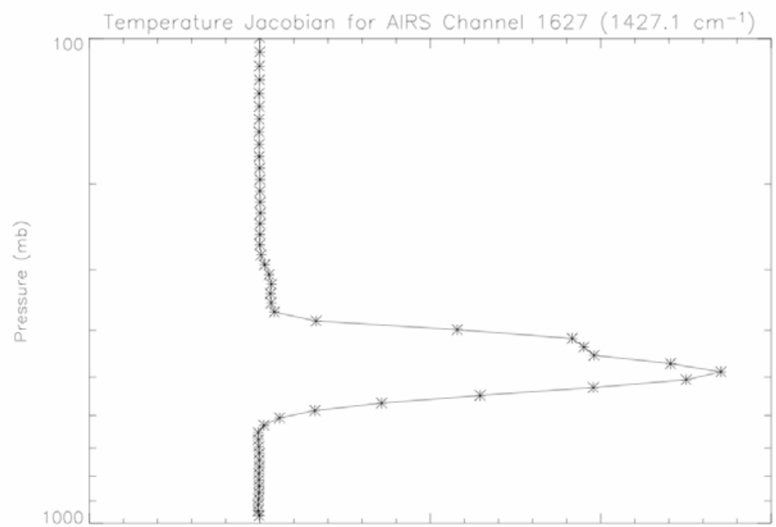
$$\frac{\partial R_\nu^{up}}{\partial T_l} = \frac{\partial R_\nu^{up}}{\partial \tau_l^0}\frac{\partial \tau_l^0}{\partial T_l} + (1 - t_{l\to l})t_{0\to l-1}\frac{\partial B_\nu(T_l)}{\partial T_l}$$

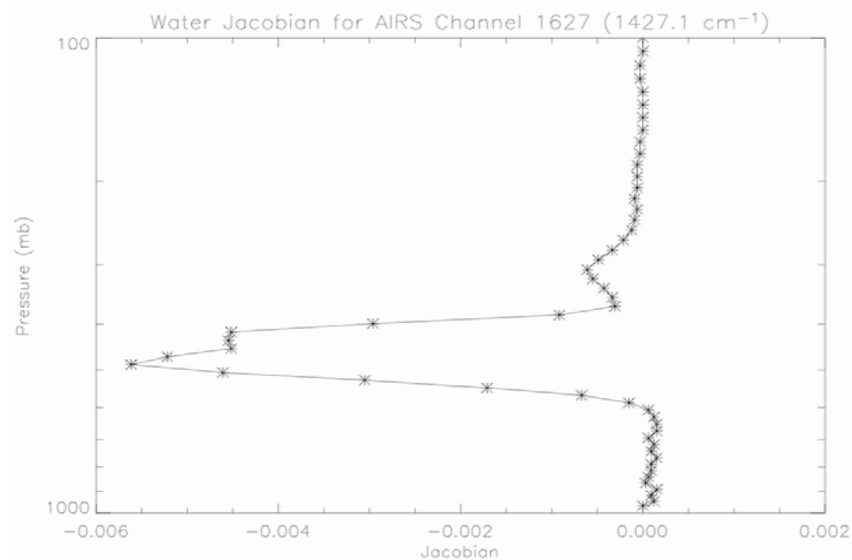
$$\frac{\partial R_\nu^{up}}{\partial H_2O_l} = \frac{\partial R_\nu^{up}}{\partial \tau_l^0}\frac{\partial \tau_l^0}{\partial H_2O_l}$$

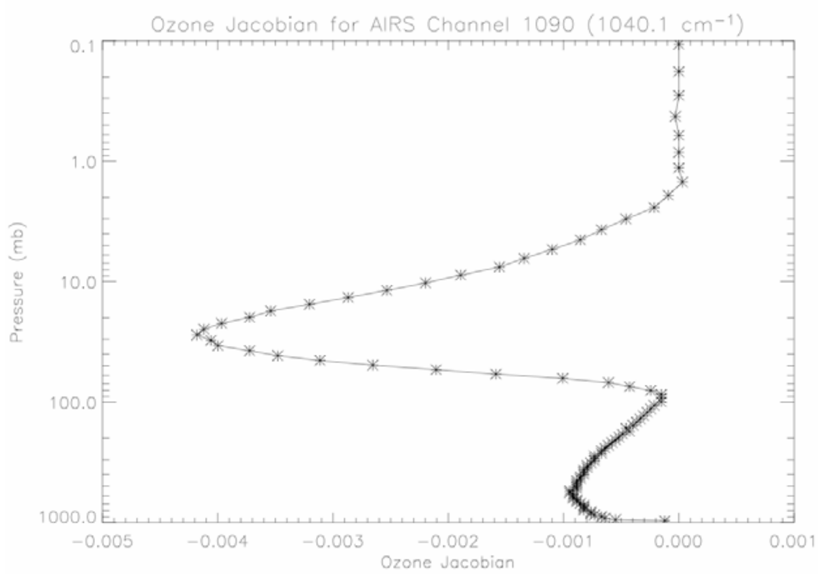
$$R_\nu^{up} = R_\nu^{up}t_{l\to l} + (1 - t_{l\to l})B_\nu(T_l)$$

$$Enddo$$

Examples of PCRTM Jacobian for AIRS Instrument

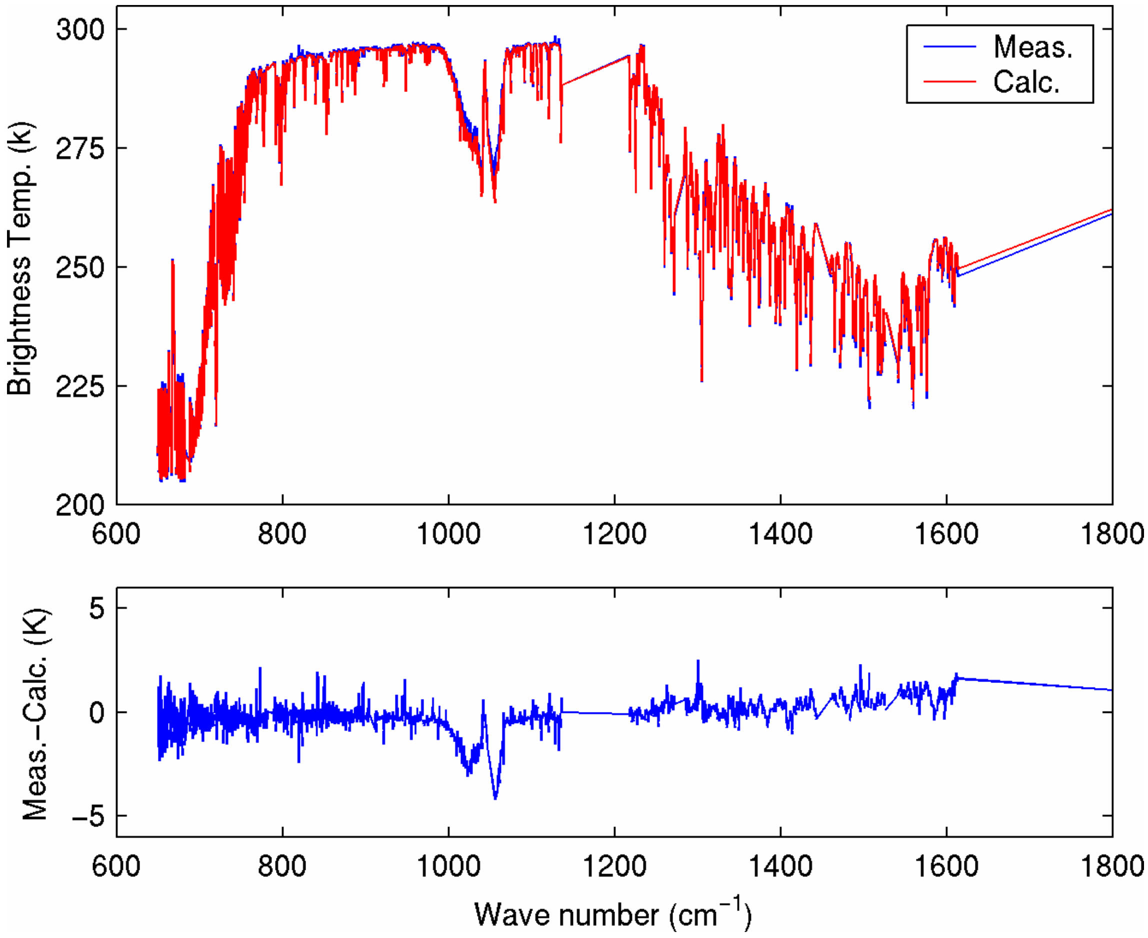






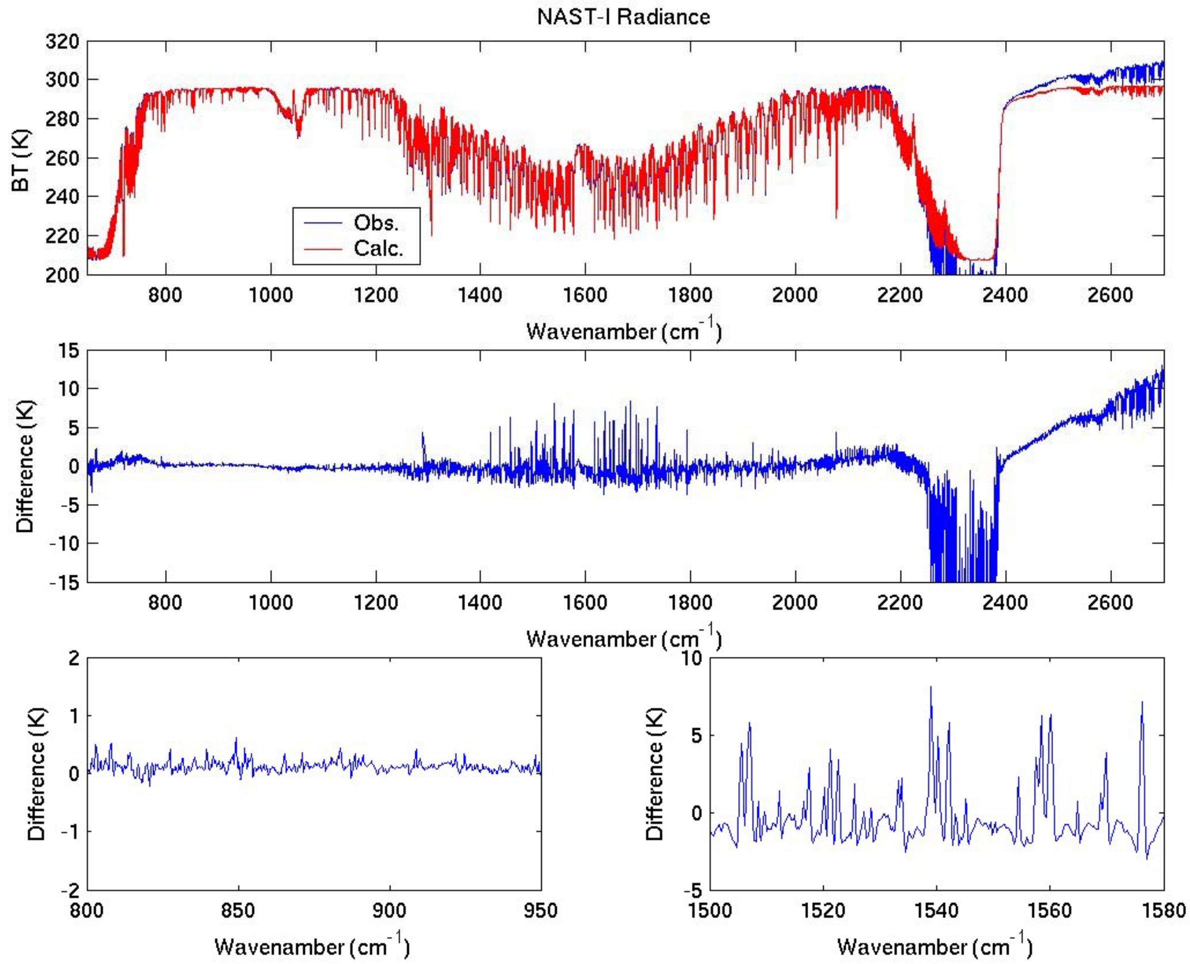
Jacobians for AIRS Instrument

Comparison of Observed AIRS Radiance and PCRTM Calculated Radiance

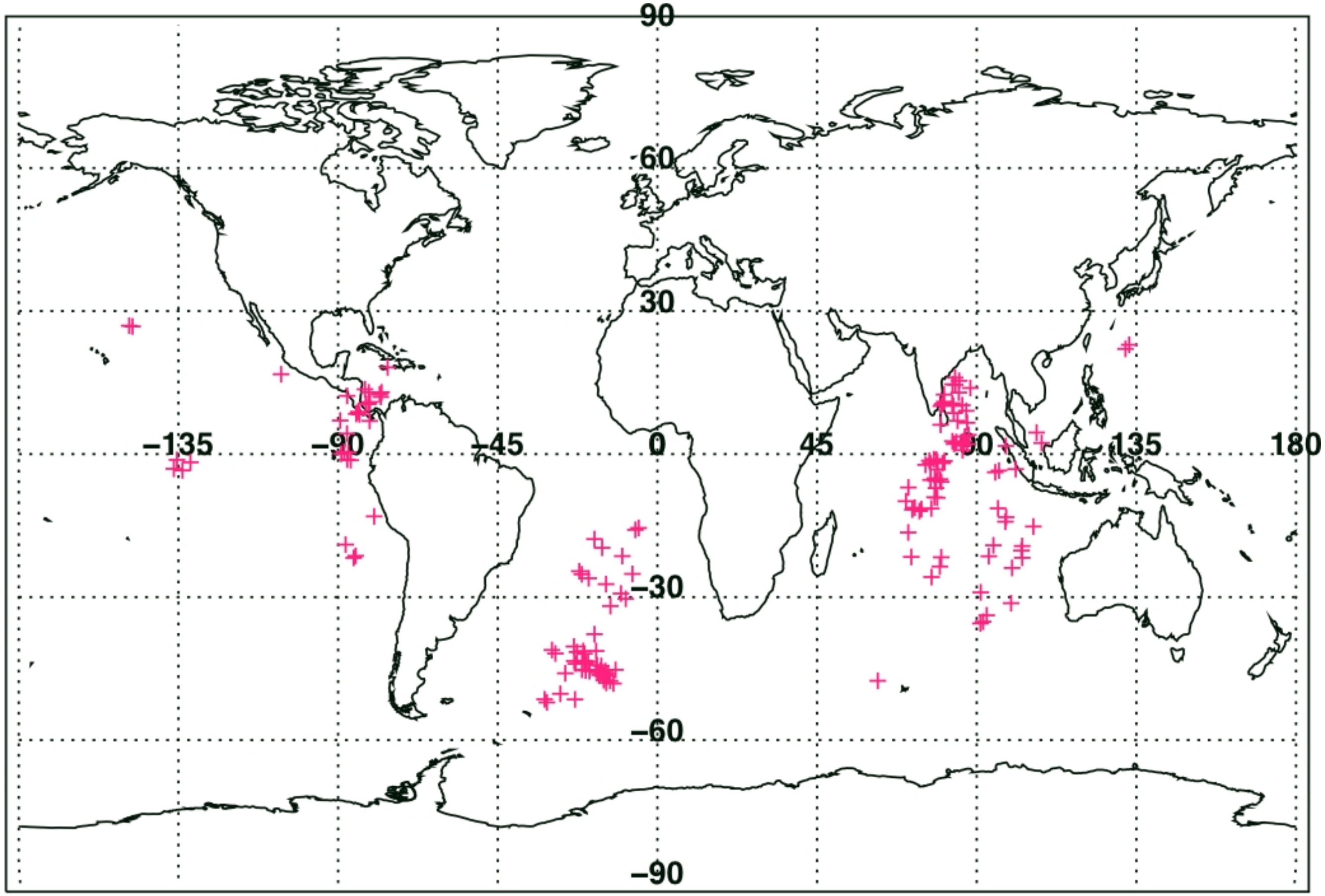


- **Ozone truth is from ECMWF model which may not be accurate**
- **Spikes are due to instrument popping noise which have not been removed**

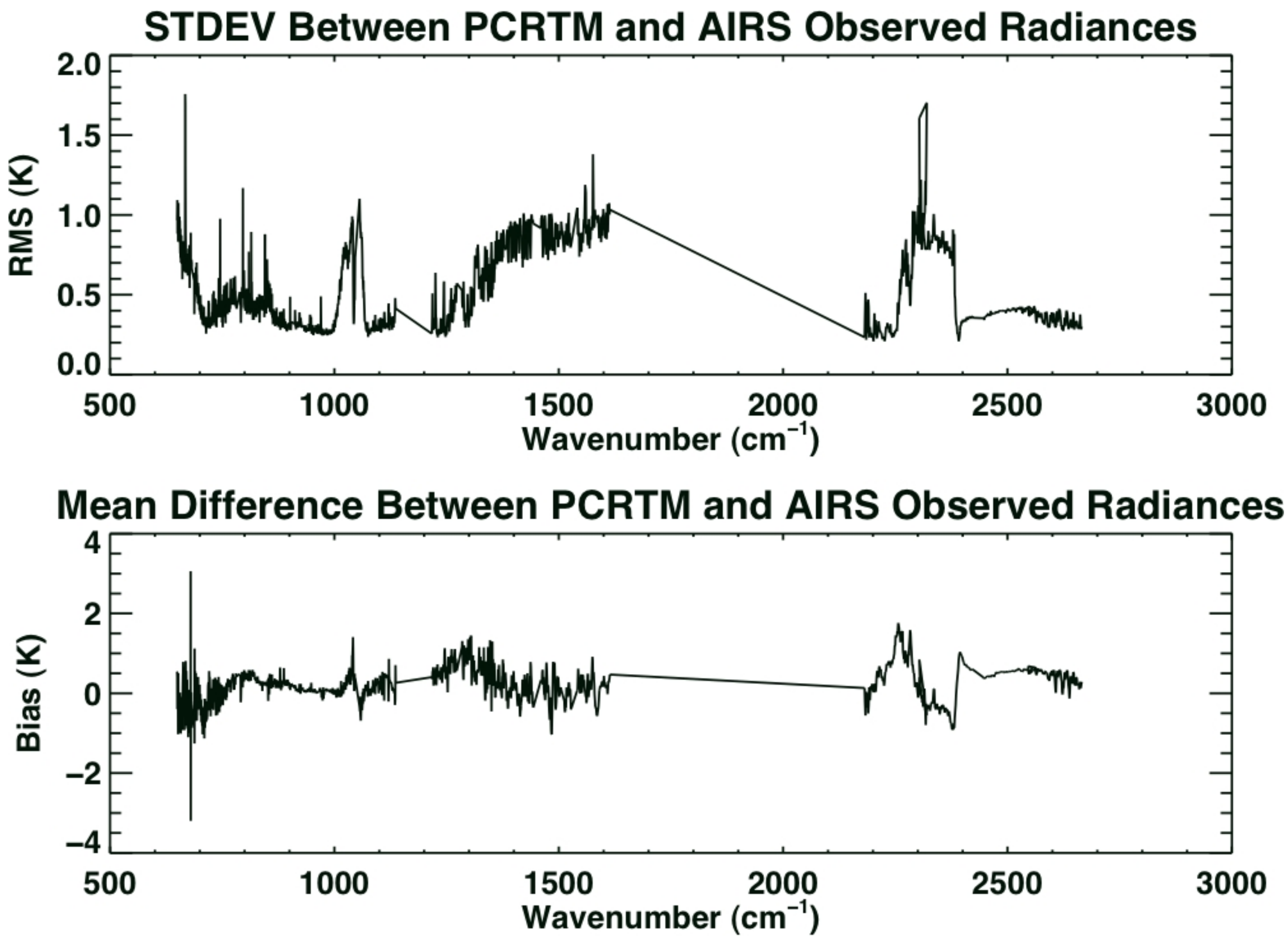
Comparison of NAST-I Observation with PCRTM



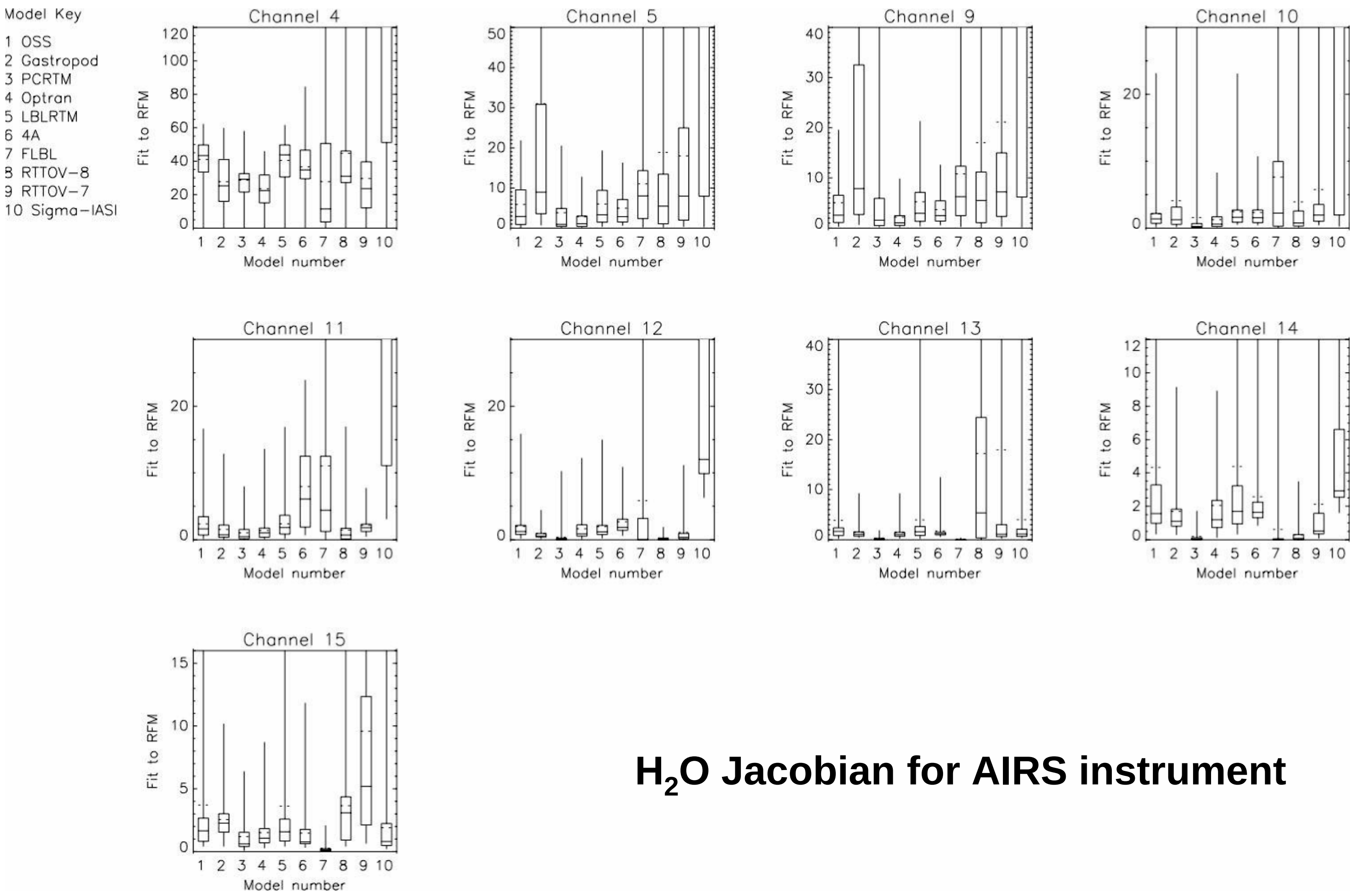
Location of Clear AIRS Observation



Differences between AIRS Observed and PCRTM-Calculated Spectra

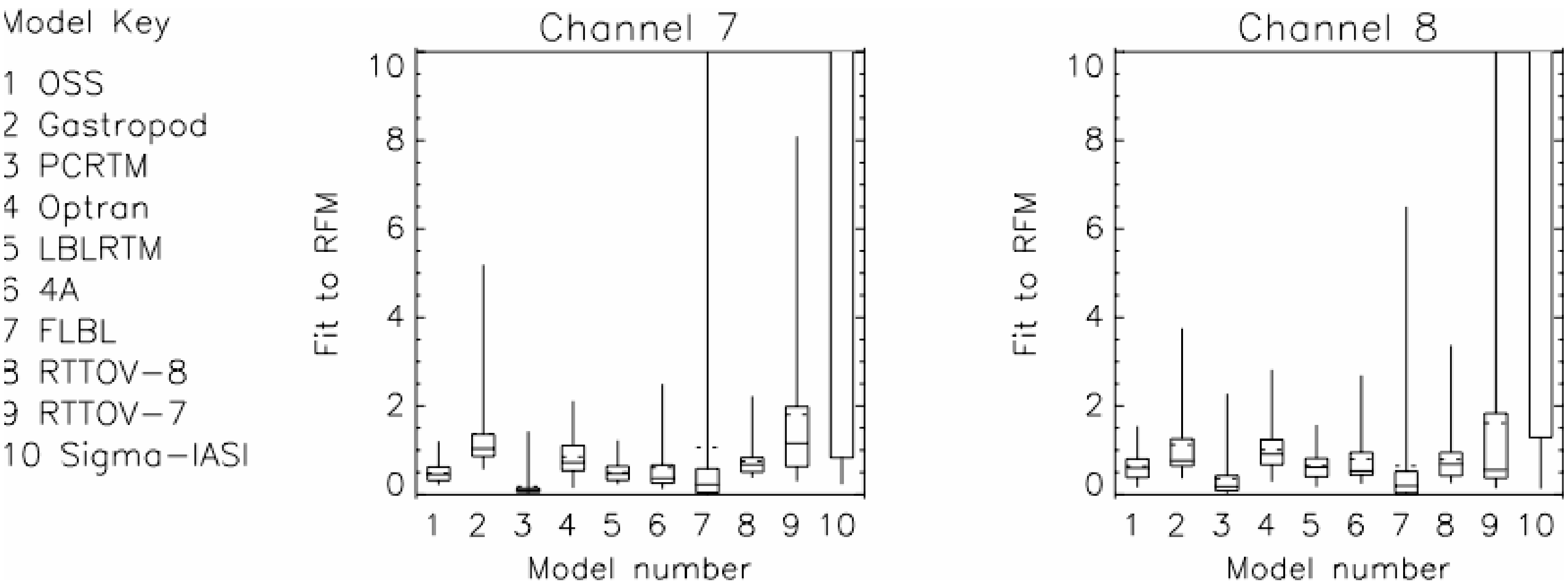


Comparison of PCRTM Jacobian with other forward model (thanks to Roger et al.)



H_2O Jacobian for AIRS instrument

Comparison of PCRTM Jacobian with other forward model (Thanks to Roger et. al.)



Ozone Jacobians for AIRS Instrument

Inversion for atmospheric profile

- Retrieval algorithm based on optimal estimation

$$X_{n+1} - X_a = (K^T S_y^{-1} K + \lambda I + S_a^{-1})^{-1} K^T S_y^{-1} [(y_n - Y_m) + K(X_n - X_a)]$$

  - Levenberg Marquardt method used to handle non-linearity
  - Climatology background and covariance matrix as constraints
  - Either climatology or regression as first guess
- Time consuming to perform physical retrieval using all channels
  - 3 RT model generated for NAST-I (PFAST, OSS, PCRTM)

Retrieval Configuration /Matrix Dimensions	Radiance/Prof
Y	8632
X	100
K	8632x100
S_y^{-1}	8632x8632
S_x	100x100

EOF transformation of Observed Radiances Reduces Inversion Time

$$Y_{PC-R} = {}^{rad}U^T \times Y_{rad}$$
$$^{prof}K_{PC-R} = {}^{rad}U^T \times {}^{prof}K_{rad}$$

- **EOF transformation converts observations (y_{rad}) into PC scores (Y_{PC-R})**
- **Reduce dimension for *K* and S_y^{-1}**
- **Reduce forward model computational time**
- **Reduce matrix multiplication time**
- **PCRTM provides both *Y* and *K* in EOF space directly**
  - **No need to perform EOF transformations of *Y* and *K* at each iteration**
  - **All information from measurements used in inversion**

Retrieval Configuration /Matrix Dimensions	Radiance PC Score/Profile
Y	100
X	100
K	100x100
S_y^{-1}	100x100
S_x	100x100

Use subset of Channels may not be optimal

- **Use subset of channels also reduces computational time**
  - **Reduces dimensions of Y, K, and S_y**
  - **Reduces forward model time**
- **Sub-optimal**
  - **Uses less than 4% of all available channels (300 channels out of 8632)**
  - **More susceptible to noise**
  - **What if the chosen channel has large spectroscopic error?**

Retrieval Configuration /Matrix Dimensions	Selected Radiance/Profile
Y	300
X	100
K	300x100
S_y^{-1}	300x300
S_x	100x100

EOF transformation of state vector reduces inversion time further

$${}^{PC-P}\vec{X} - {}^{PC-P}\vec{X}_a = {}^{Prof}U^T \times {}^{prof}\vec{X}$$

$${}^{PC-P}K_{PC-R} = {}^{Prof}K_{PC-R} \times {}^{Prof}U$$

- **Eigenvectors generated from climatological atmospheric profiles**
- **Regularize the retrieval**
- **Make S_a less singular for highly correlated levels**
- **Minimize vertical level instability in the retrieval**
- **Much smaller matrix dimension for $(K^T S_y^{-1} K + \lambda I + S_a^{-1})^{-1}$**

Retrieval Configuration /Matrix Dimensions	Radiance/Profile PC
Y	100
X	32
K	100x32
S_y^{-1}	100x100
S_x	32x32

Advantages of PCRTM Retrieval Methodology

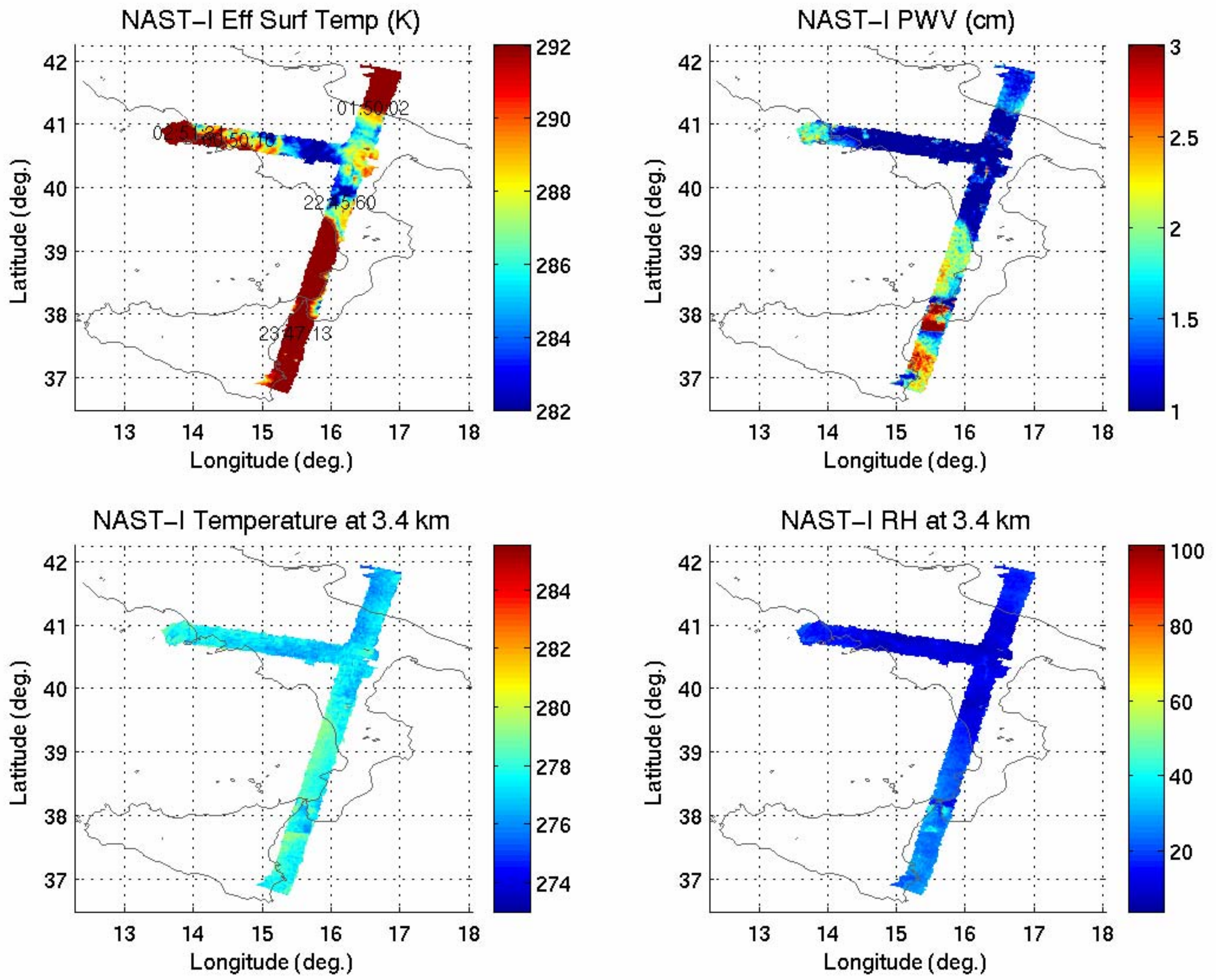
- **All channels included**
  - PC scores contains information from all channels
- **The dimension of S_y is much smaller**
  - Noise correlation included
    - Good to handle interferometer with strong apodization functions
    - Good to include correlated forward model errors
    - Good to include correlated bias correction covariance
- **The dimension of S_x is much smaller**
  - Inversion is faster
  - EOF transformation stabilize state vector inversions
  - Easy to increase state vector size when multiple pixels are used
- **PCRTM provides *K* and *Y* in PC domain directly**
  - No need to convert Jacobian and radiance to PC space at each iteration
  - Big computational saving
- **Fast speed and small matrix sizes are good for**
  - Cloud handling
  - Use spatial and temporal information

Retr. Config/Matrix Dim.	Radiance/Prof	Subset Radiance/Prof	Rad PC/ Prof PC
Y	8632	300	100
X	100	100	32
K	8632x100	300x100	100x32
S_y^{-1}	8632x8632	300x300	100x100
S_x	100x100	100x100	32x32
Time for calc. *K* and *Y*	~2 sec	0.1 sec	0.02 sec

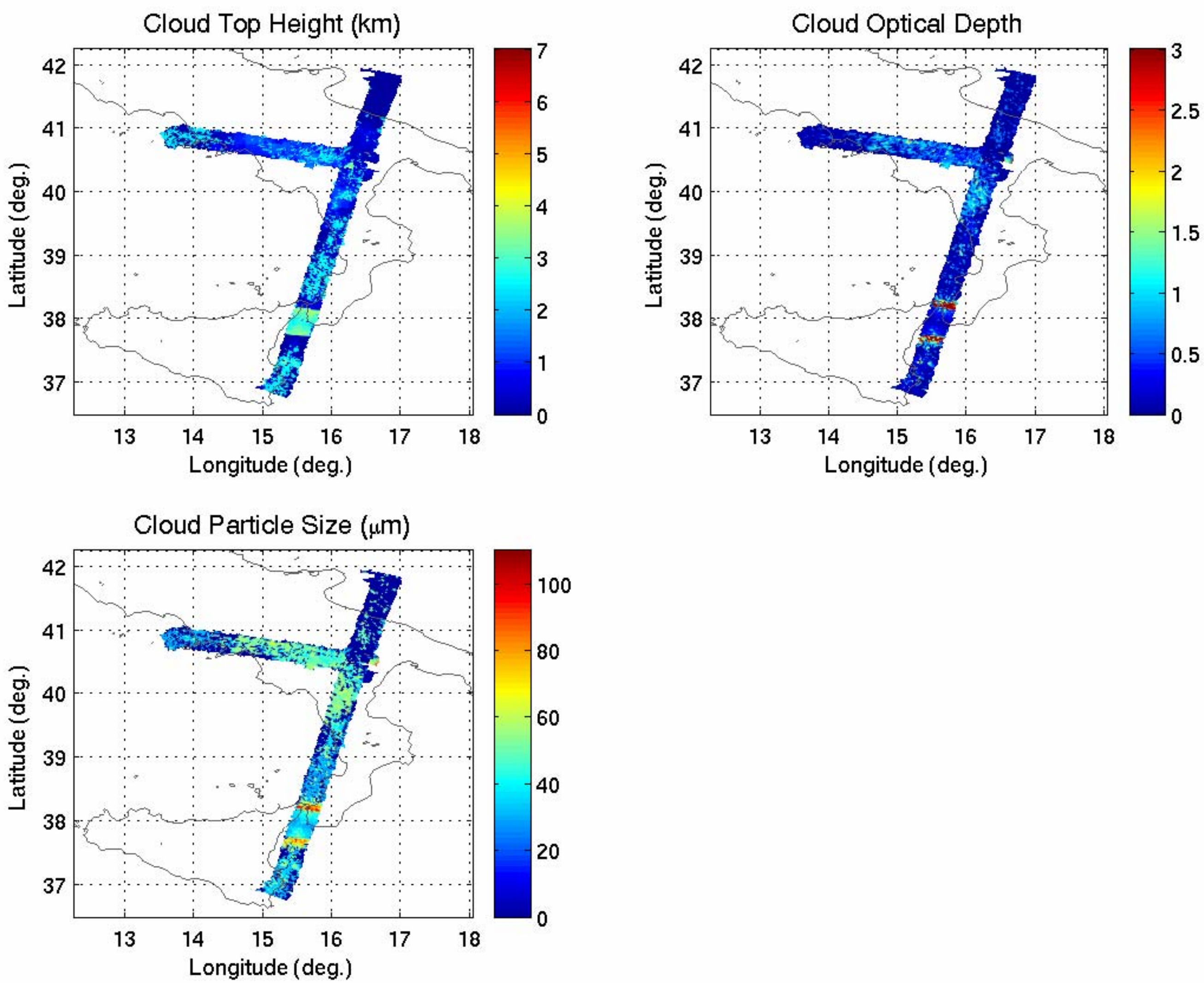
Application of PCRTM to NAST-I Retrieval

- 100 Radiance PC used
- 32 parameters retrieved:
  - 1 surface skin temperature
  - 19 Temperature EOF
  - 8 moisture EOF
  - 4 ozon EOF
- Emissivity fixed
  - Ocean emissivity= measured values from JH database
  - Land emissvity
    - either set to 0.98 (very approximate)
    - or set to regression generated emissivity
- Background covariance generated from NOAA88 database
  - Global variations
- Retrieval starts from global climatology
  - Will try regression first guess later
- Levenberge-Marguardt non-linear inversion with climatology background constraint included
  - Very robust
  - Converges in 3-4 iteration

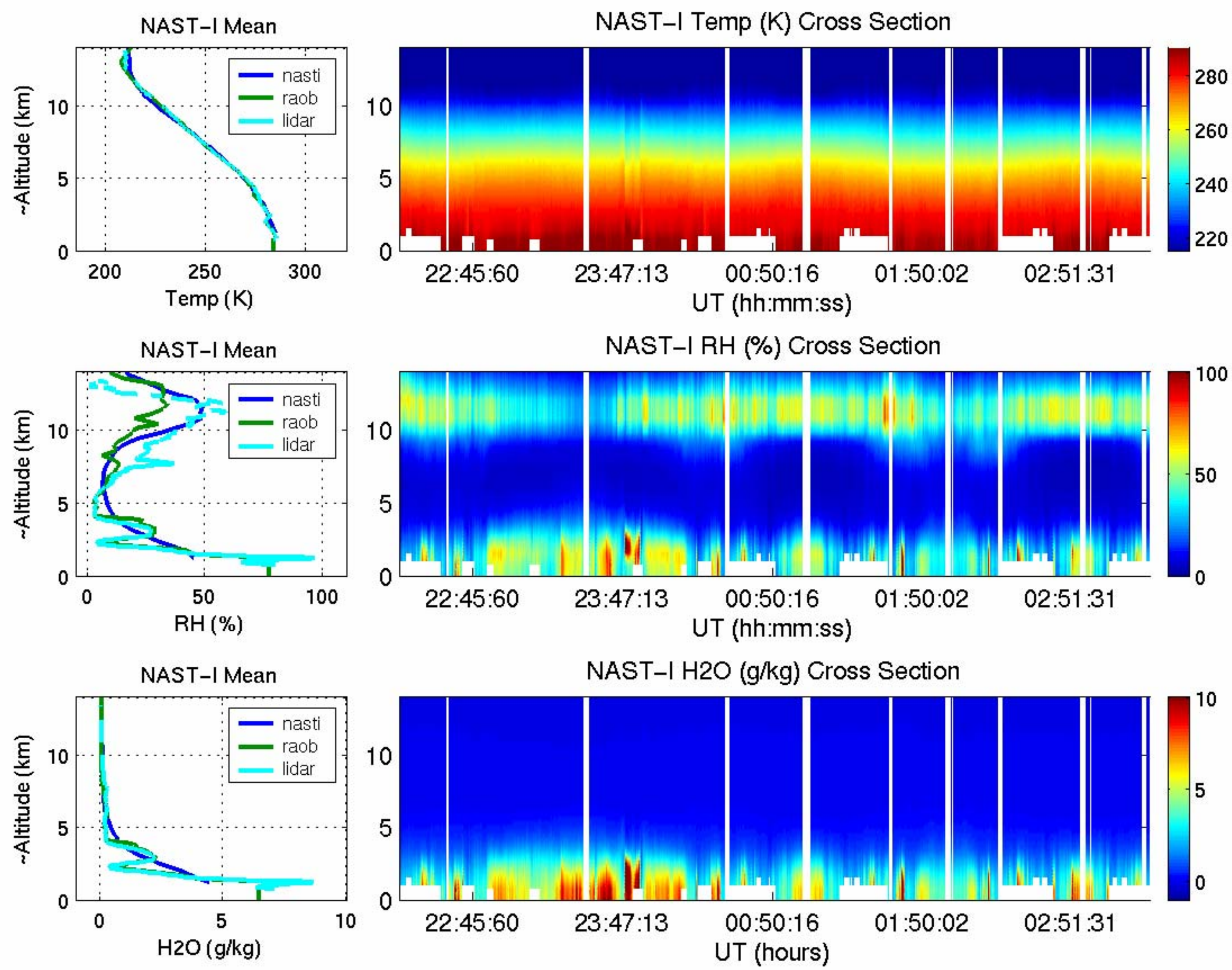
PCRTM Retrieved Ts, PWV, T and RH (09/09/2004)



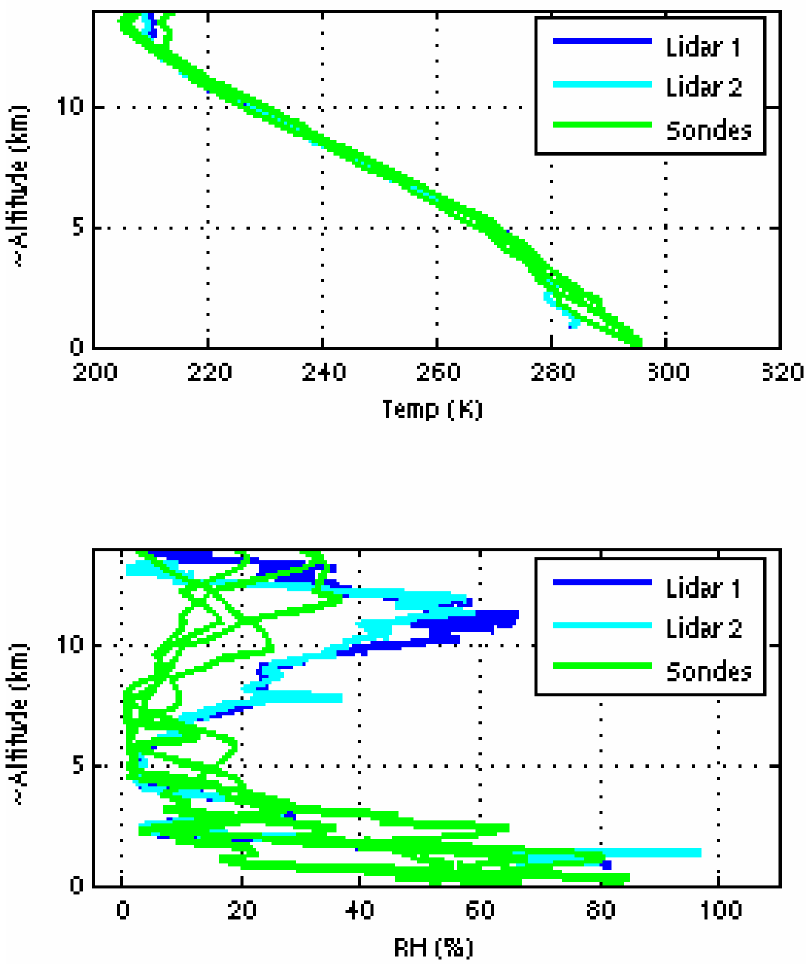
Cloud Properties from NAST-I Standard Regression Retrieval



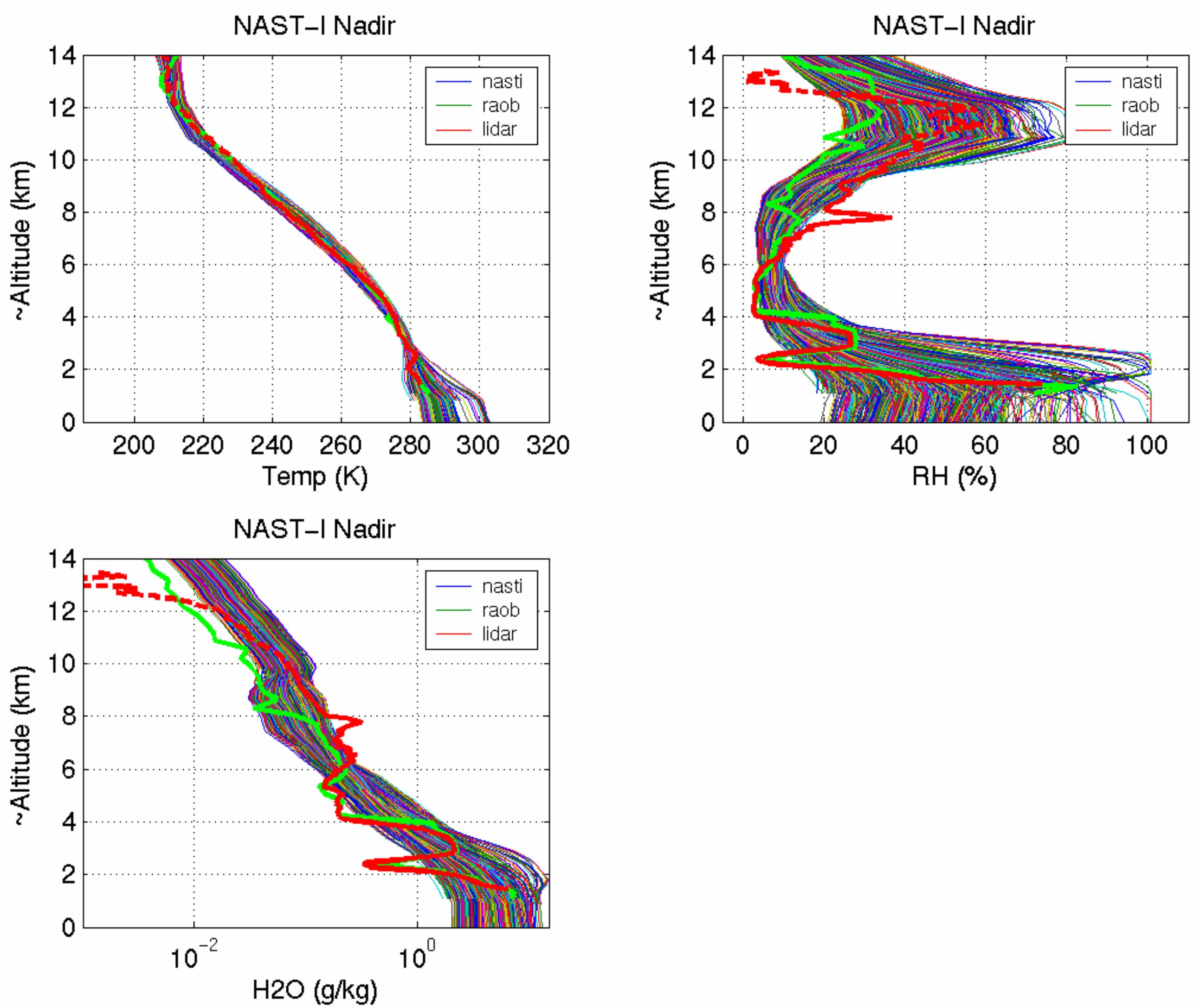
Time Series of Vertical Profiles from PCRTM



Vertical Temperature and RH variations from Radosonde and LIDAR

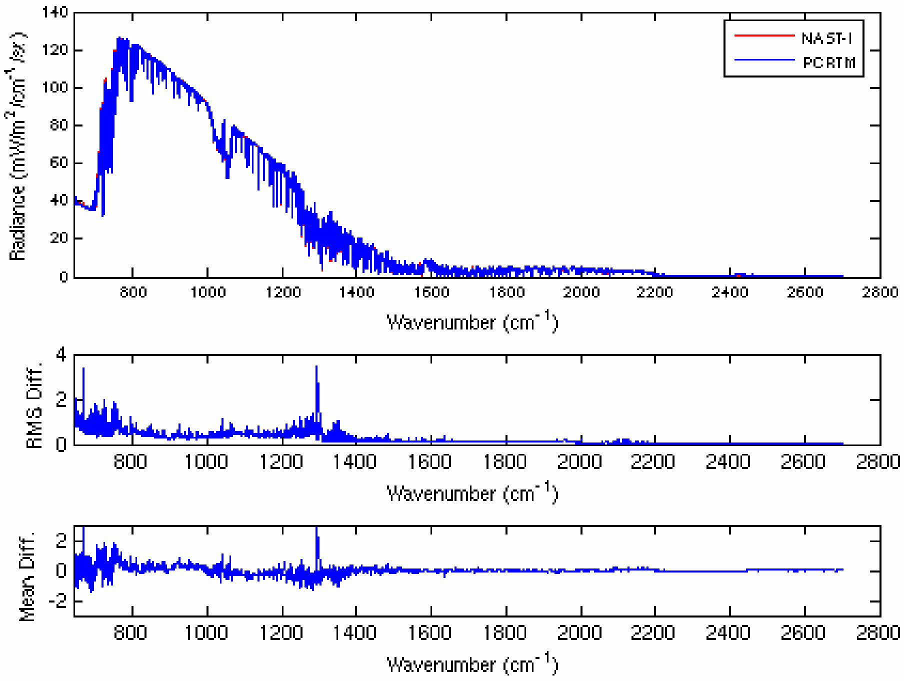


Comparison of PCRTM EOF Retrieved Profiles with Radiosonde and LIDAR



Application of PCRTM EOF retrieval algorithm to EAQUATE NAST-I Data

- **Upper panel: Mean NAST-I and PCRTM radiances**
- **Middle: RMS difference between NAST-I and PCRTM fitting**
- **Bottom: Mean difference between NAST-I and PCRTM**



Summary and Conclusions on PCRTM

- **Physical parameterization**
  - **The radiance variation as a function of T, H_2O, O_3, CH_4, N_2O, CO, T_{skin}, ε, ρ, sec (Θ), P_{obs}…. is captured via monochromatic RT calculations**
    - **PC score predicted by simple a linear model**
  - **The redundant spectral information is captured via EOF representation**
    - **Can deal with any ILS or SFR**
  - **Super channel magnitudes are a linear combination of a few hundred monochromatic radiances**
  - **Channel radiances are a linear combination of EOFs with super channels as weights!**
- **Provides forward model and Jacobians in both spectral and EOF domain**
  - **No need to select sub-set of channels**
  - **Small dimensions, fast speed**
  - **Correlated noise and error sources can be included**
- **A preliminary application of PCRTM to NAST-I data show good results**
  - **Will be tested with more NAST-I datasets**
  - **Further improvements will be made**
    - **CO,CH4 and N2O retrievals**
    - **Surface emissivity retrievals**
    - **Retrieval under cloudy condition**
    - **Characterize forward model errors and include them in retrievals**
- **PCRTM has good potential for hyperspectral remote sensing**
  - **IASI, NWP data assimilation, cloud parameter retrievals**