



Fast and Accurate Radiative Transfer Model Development in Support of CLARREO Studies

X. Liu¹, H. Li², W. Wu², Z. Jin², ¹S. Kato¹, C. Lukashin¹,
D. Feldman³, X. Huang⁴, P. Yang⁵

1. NASA Langley Research Center
2. SSAI
3. Lawrence Berkeley National Lab
4. University of Michigan
5. Texas A & M



Presentation outline

- Motivations
- Approach: Principal Component-based Radiative Transfer Model (PCRTM)
- Examples of PCRTM Applications
- Summary and Conclusions



Motivations

- Radiative Transfer (RT) model is a key component in satellite remote sensing
 - $y = F(x, \nu, \theta, \dots)$
 - Observation System Simulation Experiment (OSSE)
 - End-to-end sensor performance simulations or sensitivity studies
 - Retrieval and data assimilations
- Line-by-line RT model is too slow
 - Over a million RT needed to cover infrared spectral region
- Traditional Channel-based RT models deal with one channel at a time
 - Modern sensors have thousands of channels and 0.1-1 million spectra per day
 - Only 4-10% of data are used in satellite data assimilations
 - Too slow for climate OSSE
- **It is essential to have a RT model**
 - Accurate and fast
 - Works in all spectral regions
 - Includes accurate physics
 - Takes advantage of spectral correlations
 - Can handle cloud and aerosols
- PCRTM (Principal Component-based Radiative Transfer model) was developed to satisfy the need listed above

Examples hyperspectral sensors:

- AIRS 2378 x 1 x 1
- CrIS 1305 x 3 x 3
- NAST-I 8632 x 1 x 1
- IASI 8461 x 2 x 2
- FIRST ~1500x10 (or more)
- CLARREO thousands



Approach

- Explore spectral correlation in hyperspectral data
 - No need to calculate spectrum one channel at a time
 - Compress spectra into compact form using PCA, wavelet, Fourier Series etc
 - Reduce dimension of the data
- PCA is a good approach for compressing spectra and capture information
 - Only the first ~50-100 leading eigenvectors are used for optimal fingerprinting
 - Leading EOFs captures all essential information of thousands of channels
 - PCA has been used to reduce instrument noise and to compress spectra
- PCRTM parameterization is physical-based fast model

$$y_i = \vec{R}^{ch} \times U_i = \sum_{j=1}^{N_{mono}} \phi_j R_j^{mono} \vec{U}_i = \sum_{j=1}^{N_{mono}} A_j R_j^{mono}$$

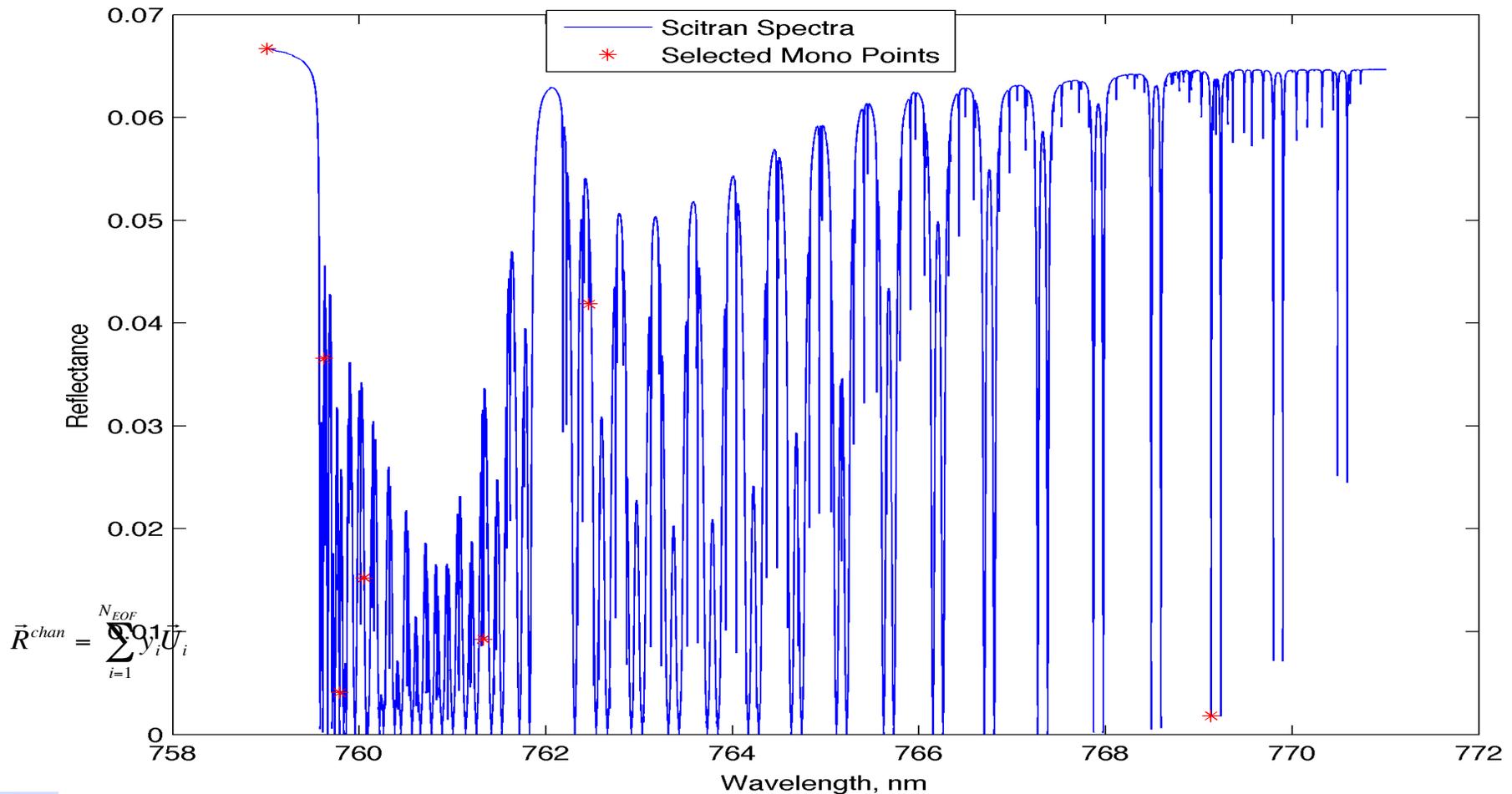
$$\vec{R}^{ch} = \sum_{i=1}^{N_{EOF}} y_i \vec{U}_i + \vec{\varepsilon}$$

- Radiative transfer done monochromatically at very few frequencies
- Very accurate relative to line-by-line (LBL) RT model (< 0.05K or 0.05%)
- 3-4 orders of magnitude faster than LBL RT models
- A factor of 2-100 times faster than channel-based RT models
- Provides Jacobian or radiative kernel needed for retrievals and climate studies
- Includes accurate cloud RT



PCRTM is Physical and Fast

- Example of O₂ A-band
 - 12000 monochromatic RT LBL calculations needed to cover 759-771 nm spectral region
- PCRTM reduces monochromatic RT calculation to 7
 - 1700 times faster than LBL
 - Been trained for OCO (~0.04 nm) and SCIAMACHY (~0.2 nm) spectral resolutions





Computational Speed up in Solar Spectral Region

- PCRTM reduces MODTRAN RT calculation by a factor of 28-928 depending on spectral resolution and MODTRAN accuracy chosen
 - PCRTM can handle ice and water clouds
 - Aerosols
 - Various trace gases
 - Land and ocean surfaces
 - Multiple scattering calculation uses 4-32 streams
- It takes 1 day to simulate 1 years of all sky SCIAMACHY spectra using PCRTM with 30 CPUs
- It will take more than 2 years for the MODTRAN to do the same

0.3 μm -2.0 μm	PCRTM RT	MODTRAN RT	speed up
Ocean 1 cm^{-1}	956	259029	270
Land 1 cm^{-1}	1339	259029	193
Ocean 4nm	279	259029	928
Land 4nm	354	259029	731
Oc/ld 10 nm	109	3079	28



Computational Speed in IR Spectral Region

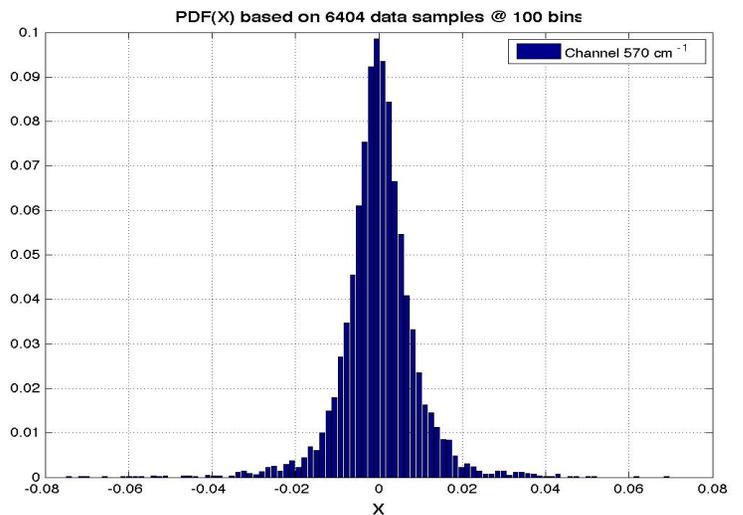
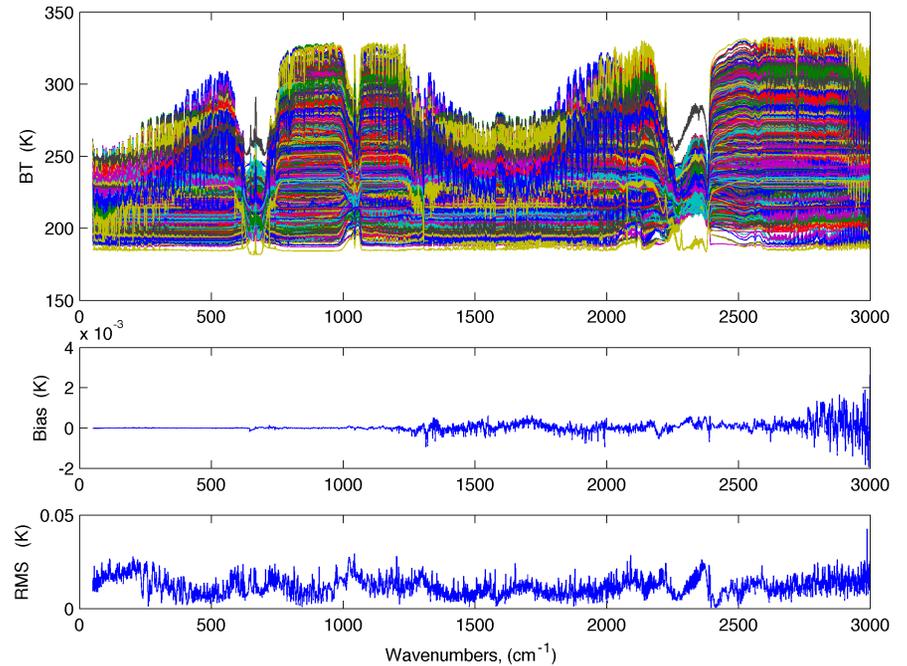
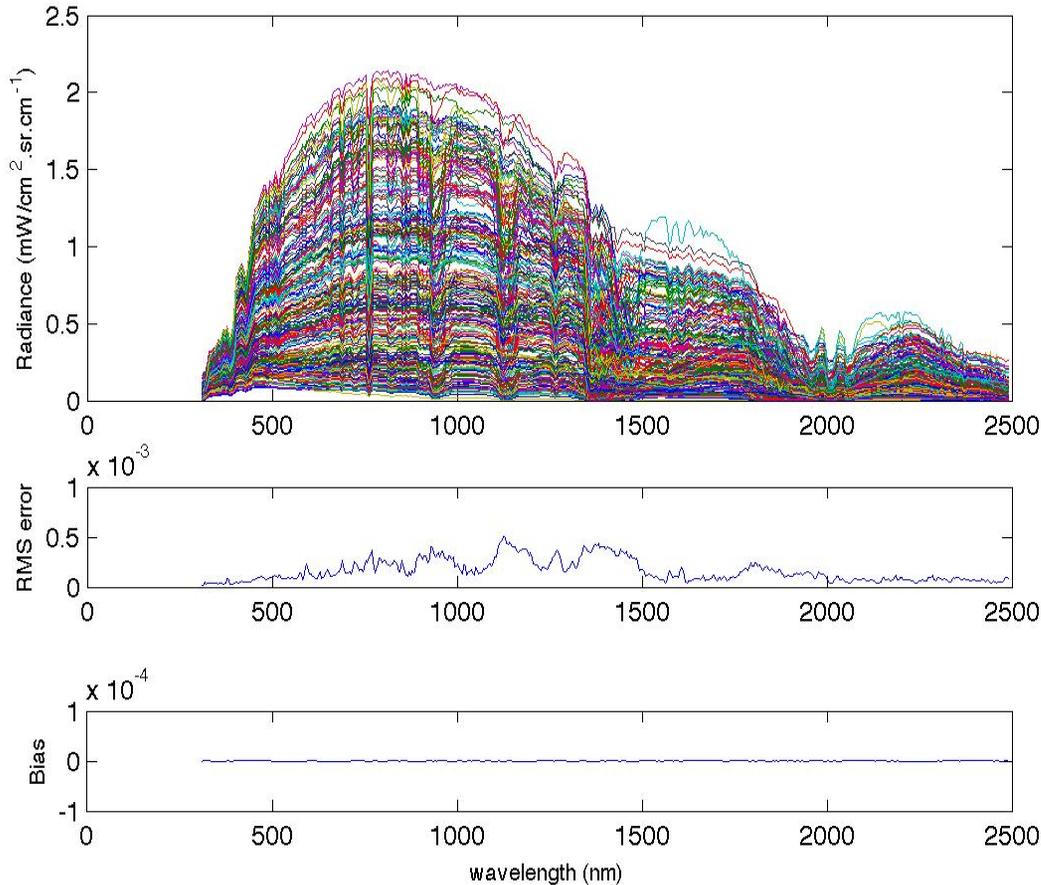
Sensor	Channel Number	PC score (seconds)	PC score + radiance	PC score + PC Jacobian
CLARREO, 0.1 cm ⁻¹	19901	0.014 s	0.022 s	0.052 s
CLARREO, 0.5 cm ⁻¹	5421	0.011 s	0.013 s	0.039 s
CLARREO, 1.0 cm ⁻¹	2711	0.0096 s	0.012 s	0.036 s
IASI, 0.25 cm ⁻¹	8461	0.011 s	0.012 s	0.044 s
AIRS, 0.5-2.5 cm ⁻¹	2378	0.0060 s	0.0074 s	0.031 s
CrIS, 0.625-2.5 cm ⁻¹	1317	0.0050 s	0.0060 s	0.021 s
NAST-I, 0.25 cm ⁻¹	8632	0.010 s	0.013 s	0.045 s
S-HIS, 0.5 cm ⁻¹	4316	0.008 s	0.008 s	0.038 s
CrIS, 0.625 cm ⁻¹	2211	0.009 s	0.009 s	0.033 s

- Milliseconds to fraction of seconds in IR
- CrIS, CrIS-full-res, IASI, NAST-I and S-HIS have multiple databases corresponding to different instrument lineshape function
- Spectral coverage (50-3000 cm⁻¹)
- Multilayer, multiple scattering clouds included
- 15 variable trace gases
- It provide radiative kernel/ Jacobian with minimum additional computations.



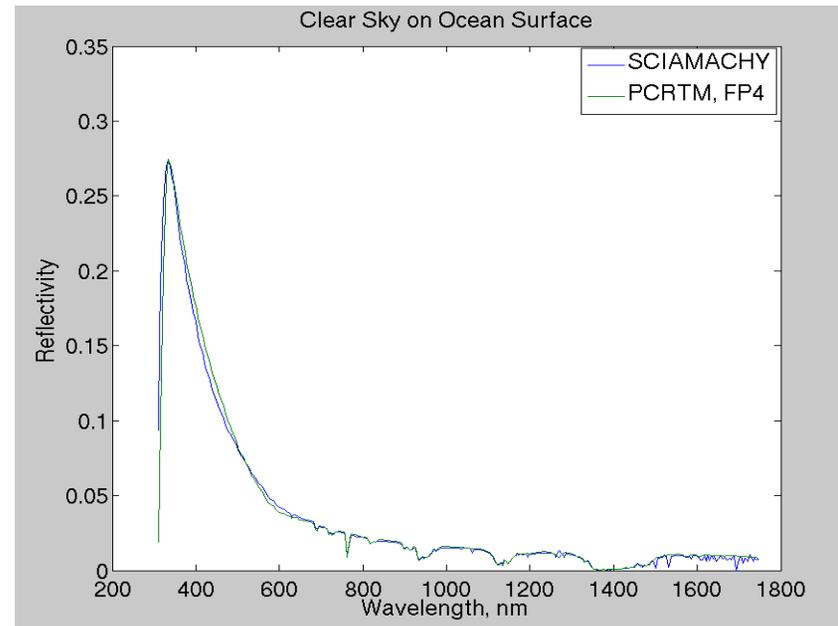
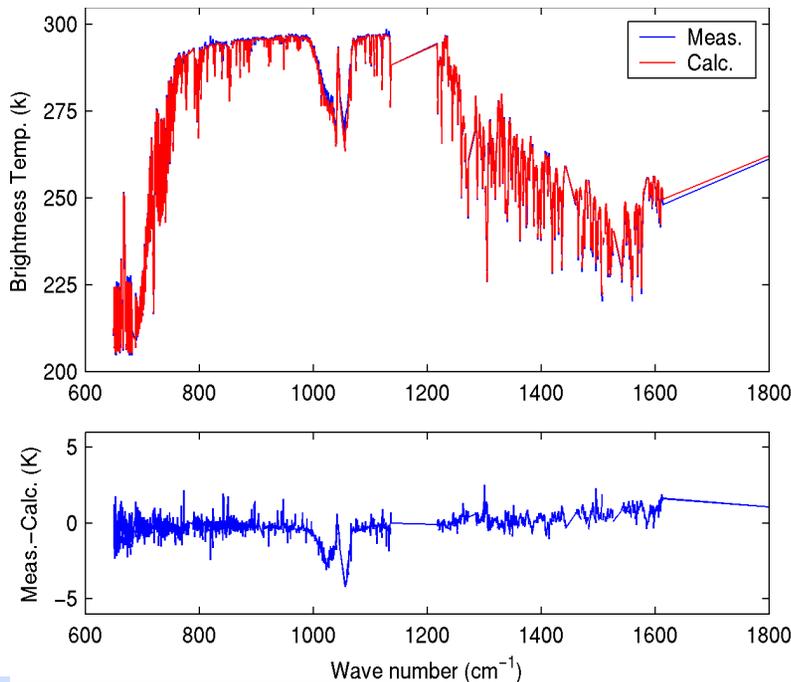
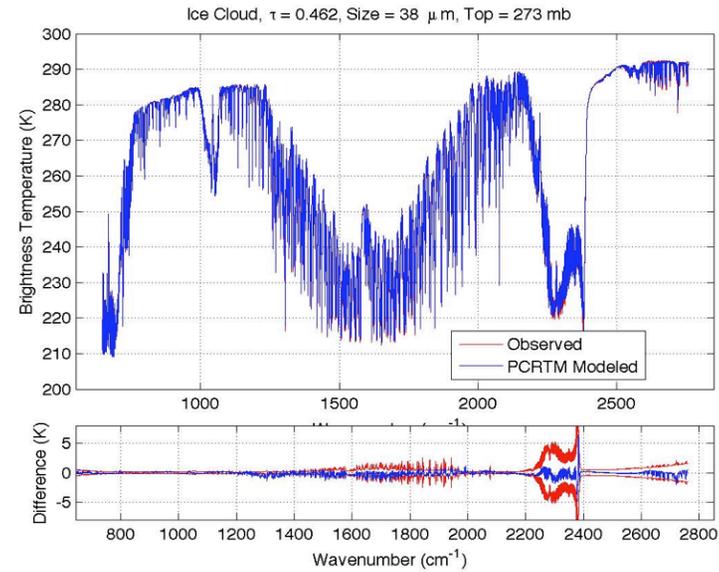
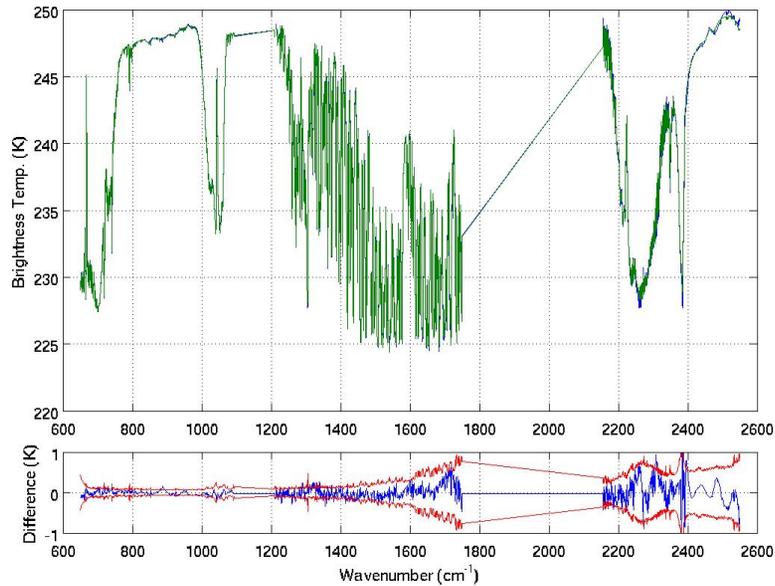
Accuracy of PCRTM is very good relative to reference RT models

- Bias error relative to LBL is typically less than 0.002 K
- The PDF of errors at different frequencies are Gaussian distribution
- RMS error < 0.03K for IR and < 5×10^{-4} mW/cm²/sr/cm⁻¹ for solar (< ~0.02%)





PCRTM has been validated using CrIS, IASI, AIRS, NAST-I, and SCIAMACHY real data



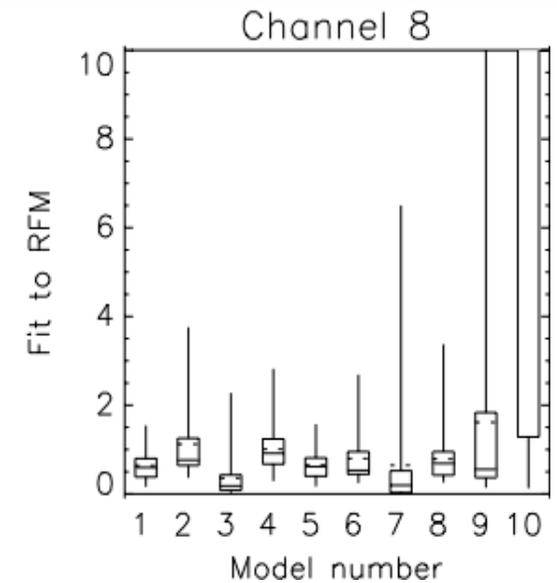
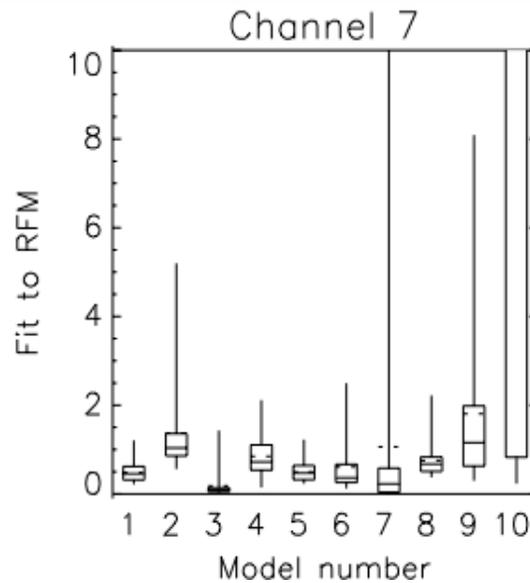


Example of Jacobian and Radiative Kernel from PCRTM

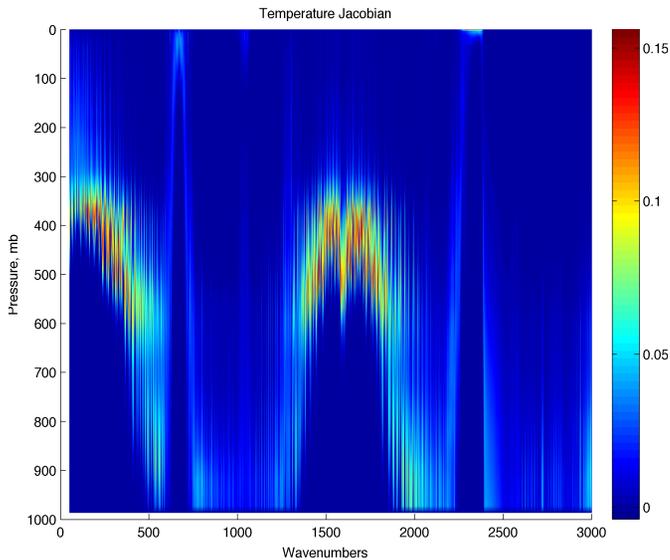
- Comparison of ozone Jacobian from different models (*Saunders et al. JGR, 2006*)

Model Key

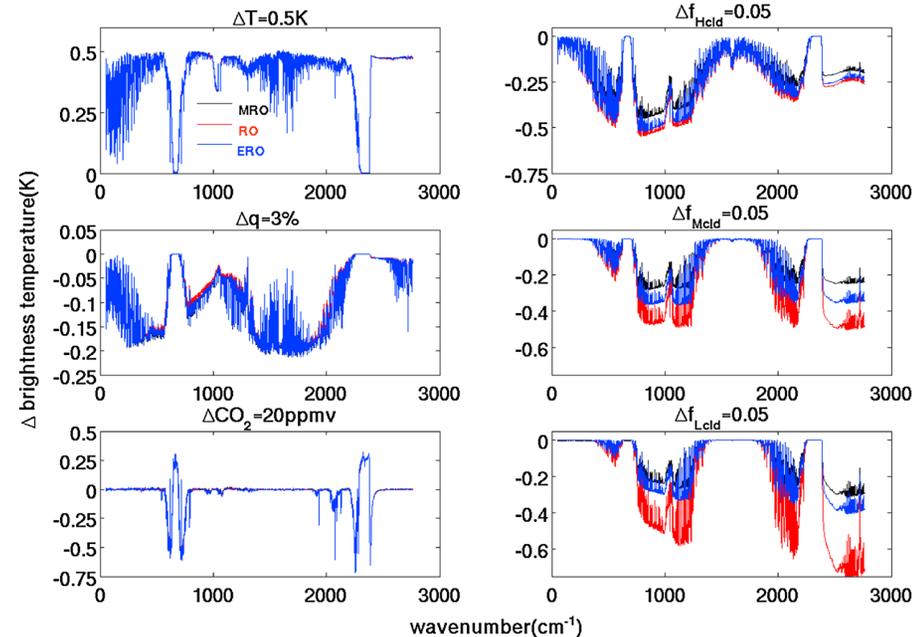
1	OSS
2	Gastropod
3	PCRTM
4	Optran
5	LBLRTM
6	4A
7	FLBL
8	RTTOV-8
9	RTTOV-7
10	Sigma-IASI



Temperature Jacobian calculated from PCRTM

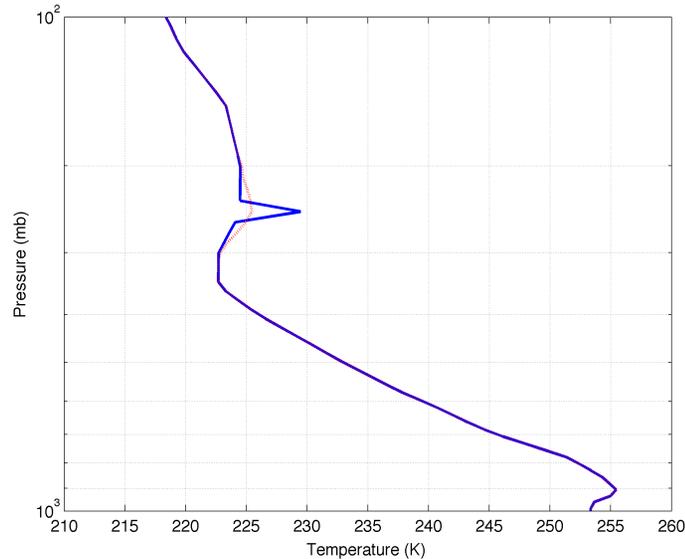


Spectral fingerprints derived from perturbing the 12-hourly GFDL model output using PCRTM model





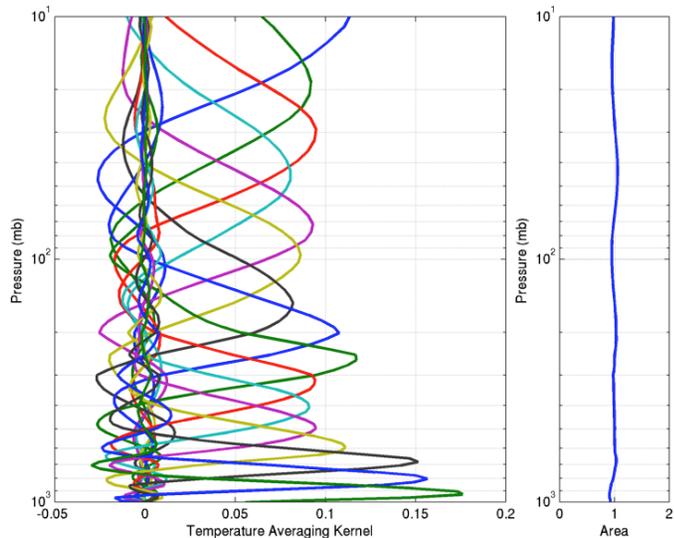
CLARREO Information Content Analysis (methodology)



$$A_x = \frac{\partial x_n}{\partial x} = (K^T S_y^{-1} K + S_a^{-1})^{-1} K^T S_y^{-1} K$$

$$H_x = -\frac{1}{2} \sum_i \ln |I - A_x|, \quad d_x = \text{tr}(A_x)$$

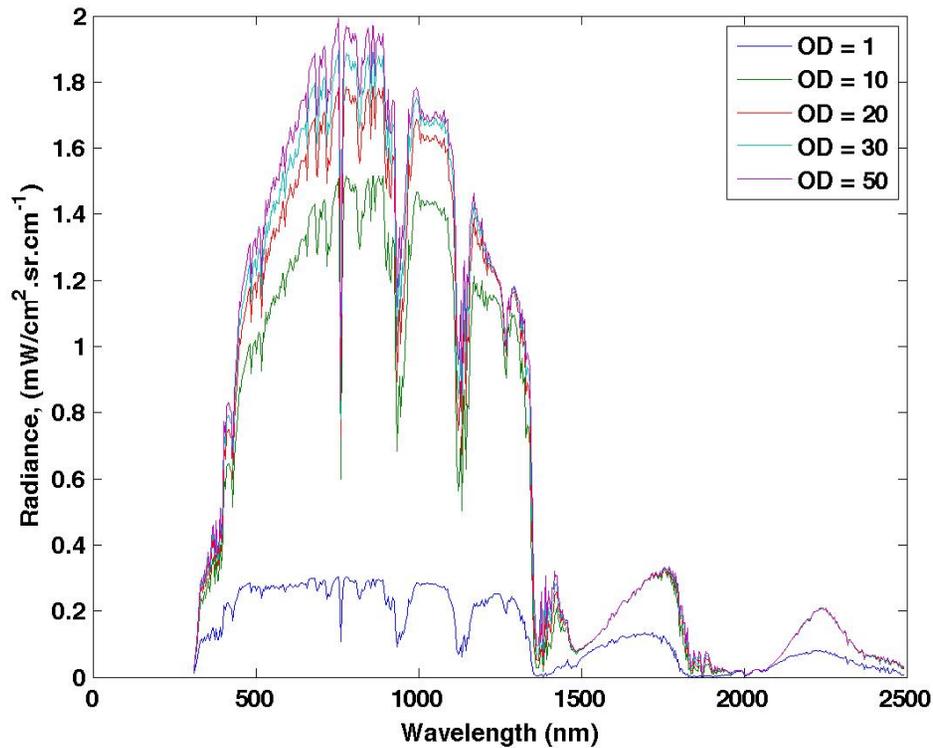
- Averaging kernel provide information on retrieval system
 - Location and magnitude of the peaks relate to information at a particular height
 - Width of the peaks relate to vertical resolution
 - Integrated area of the averaging kernel provides relative contribution from a priori and measurements
 - Trace of A_x provides degree of freedom
- Averaging kernel is profile dependent
 - Generate CLARREO spectra with hundreds of atmospheric profiles
 - Probability Density Function (PDF) or mean of the A_x For different instrument configurations (K)
 - Different noise (S_y)
 - Different spectral resolution (K)
 - Different band coverage (K)
 - With and without Far IR band (K)



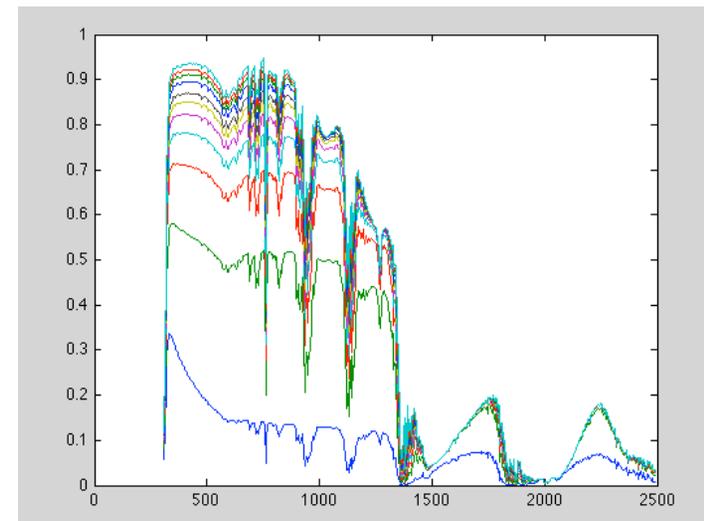
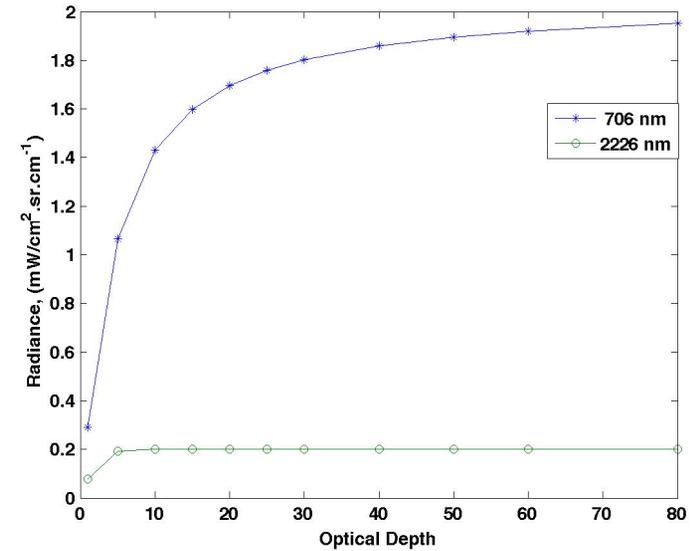


Ice cloud dependency on cloud optical depth

Note different sensitivity of near IR vs visible spectral regions



TOA radiance



TOA reflectance

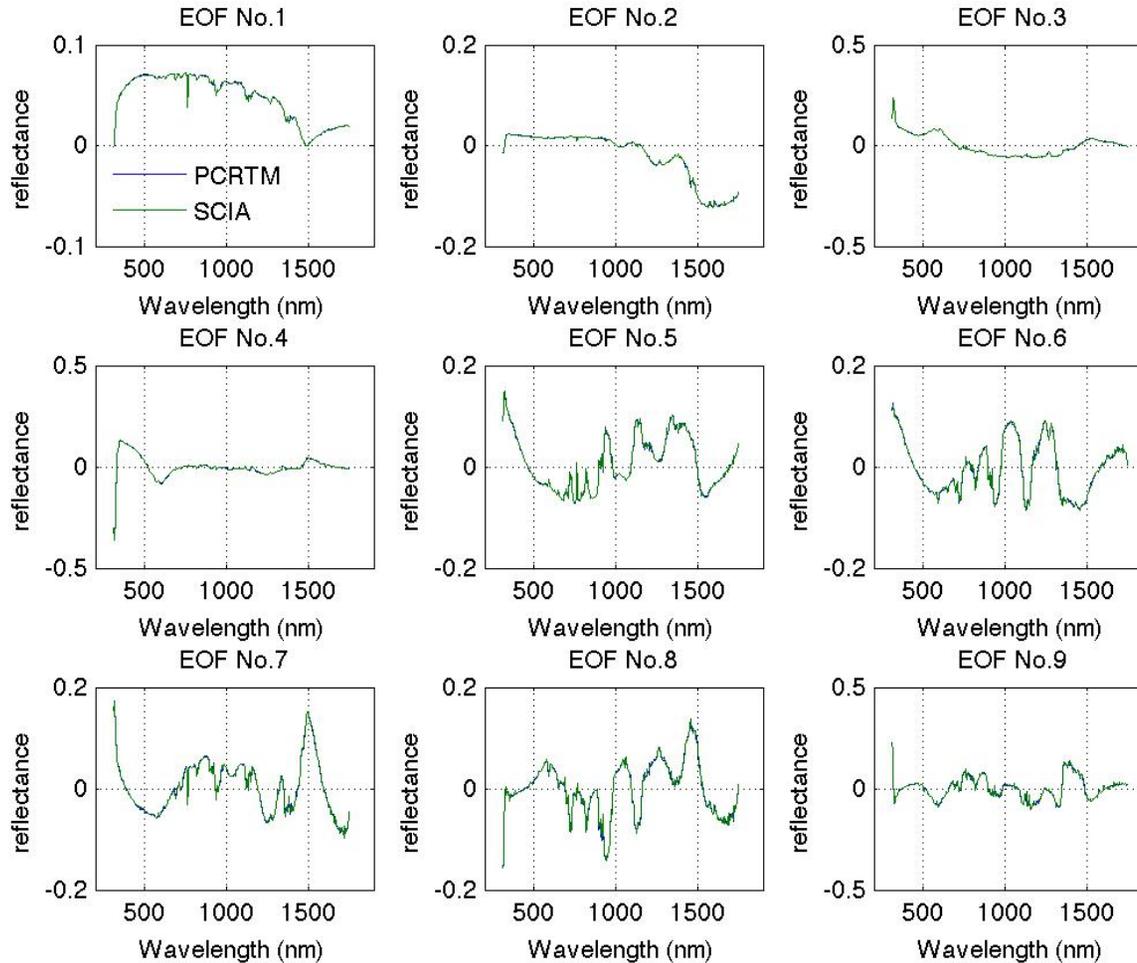


Intersection PCA analysis of observed and simulated SCIAMACHY reflectance spectra

- One year of SCIAMACHY observed reflectance spectra
- One year of PCRTM simulated reflectance spectra
 - 214769 ocean spectra, 56019 land spectra
 - CERES and MODIS products are used as PCRTM inputs
- PCA analysis done for land and ocean separately
 - EOF obtained from PCRTM simulated spectra
 - EOF obtained from real SCIAMACHY spectra
 - Perform intersection PCA analysis
 - Very high correlations between the two transformed eigenvectors

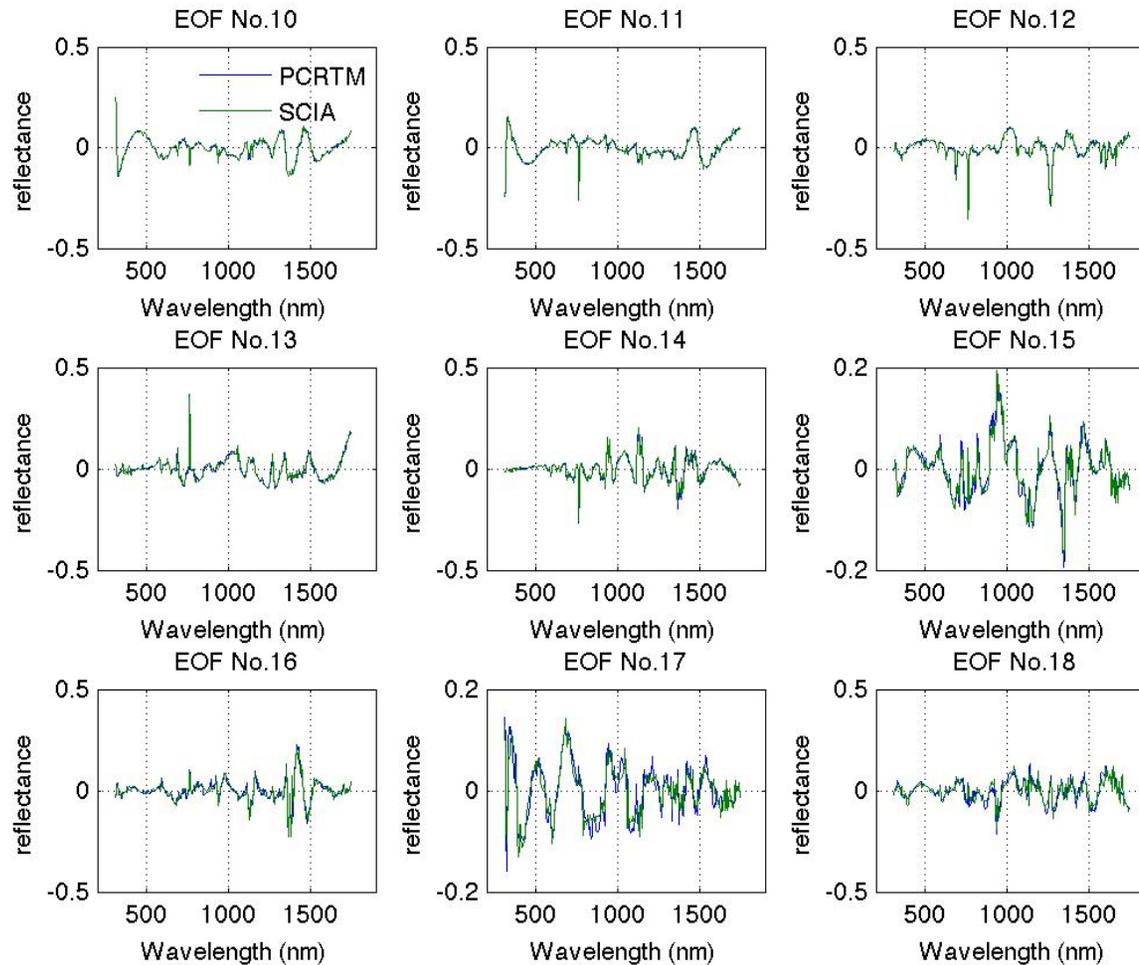


Intersection EOFs from both SCIAMACHY and PCRTM Over Ocean



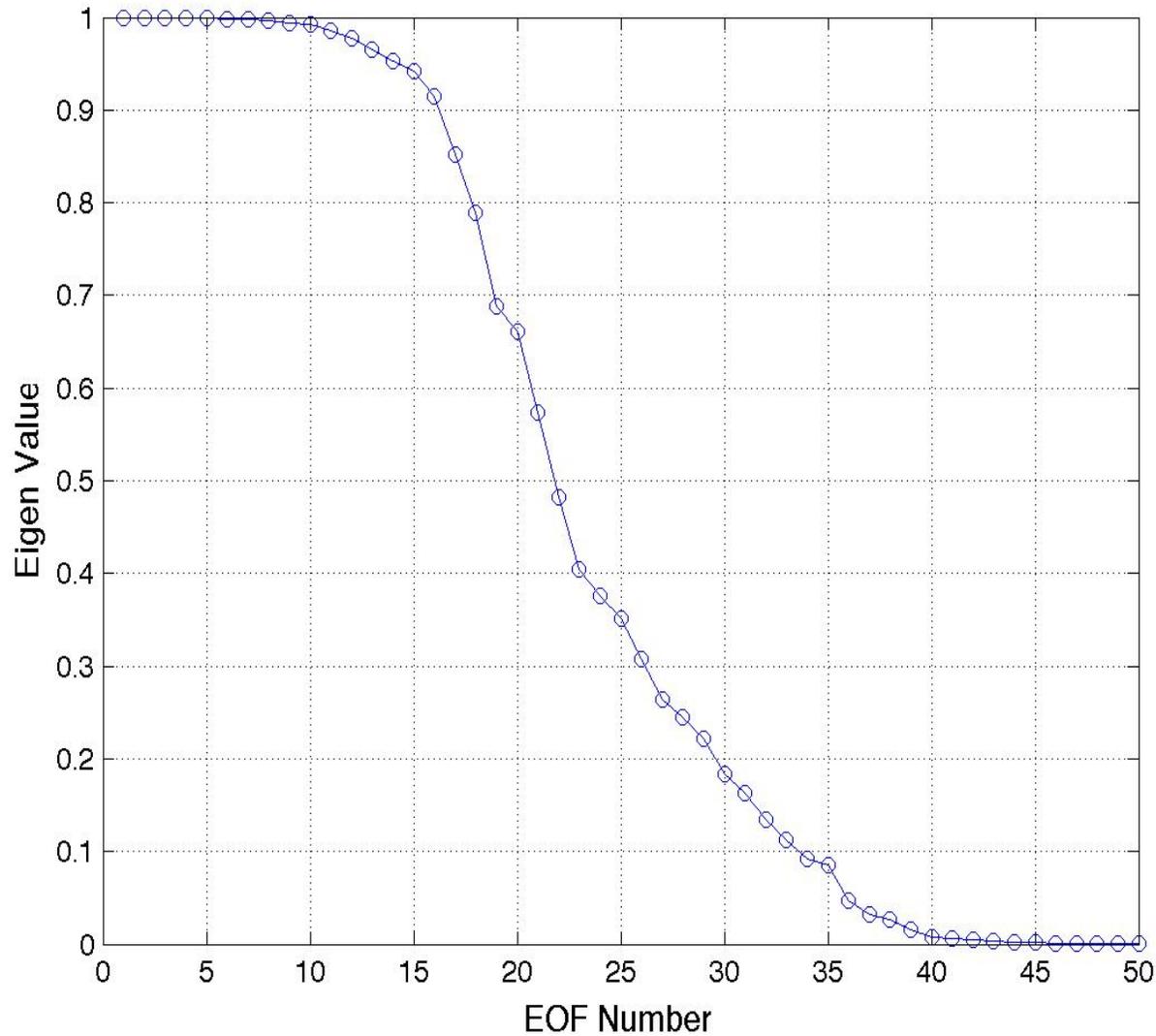


Intersection EOFs from both SCIAMACHY and PCRTM Over Ocean



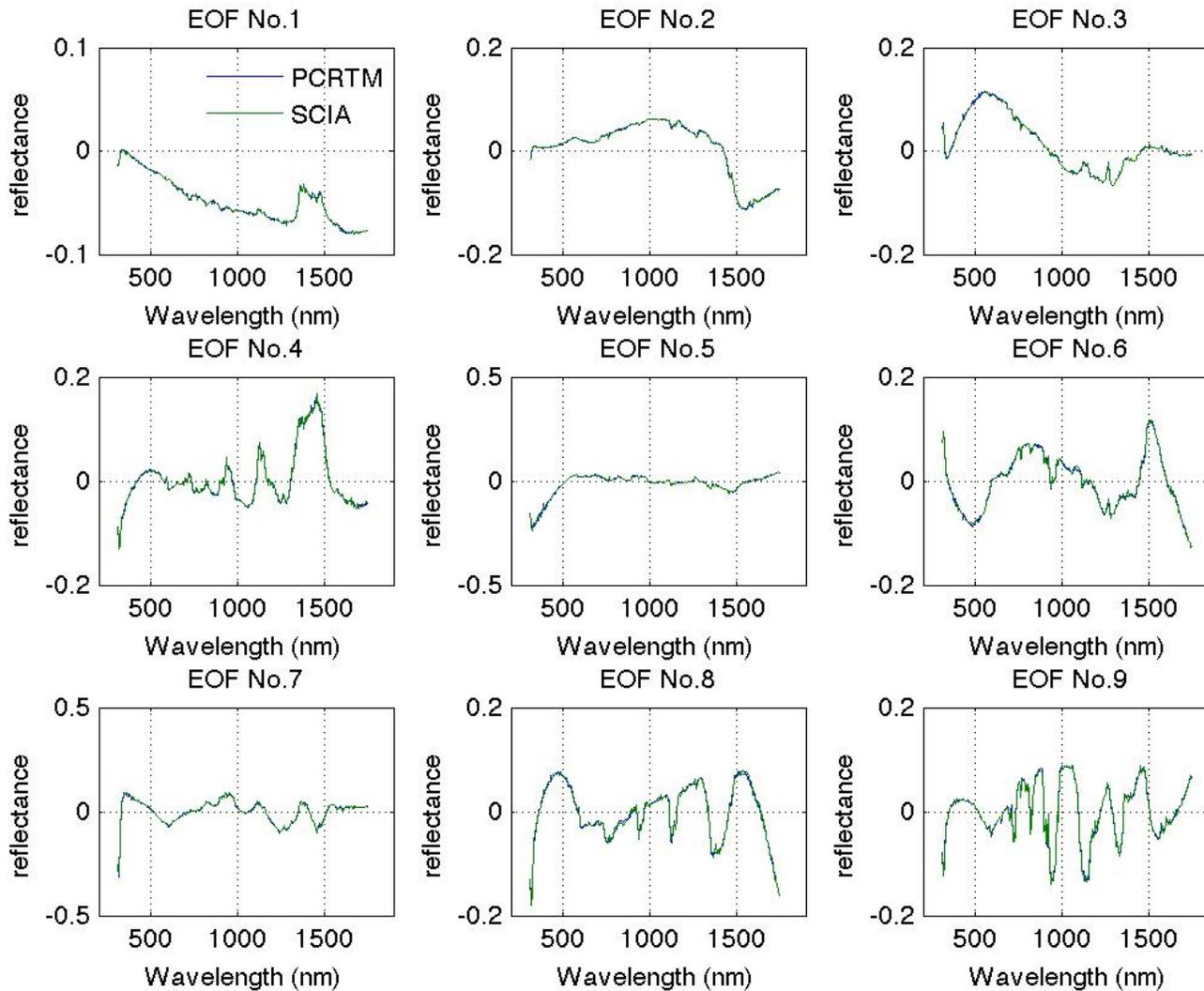


Eigenvalues from intersection PCA analysis Over Ocean



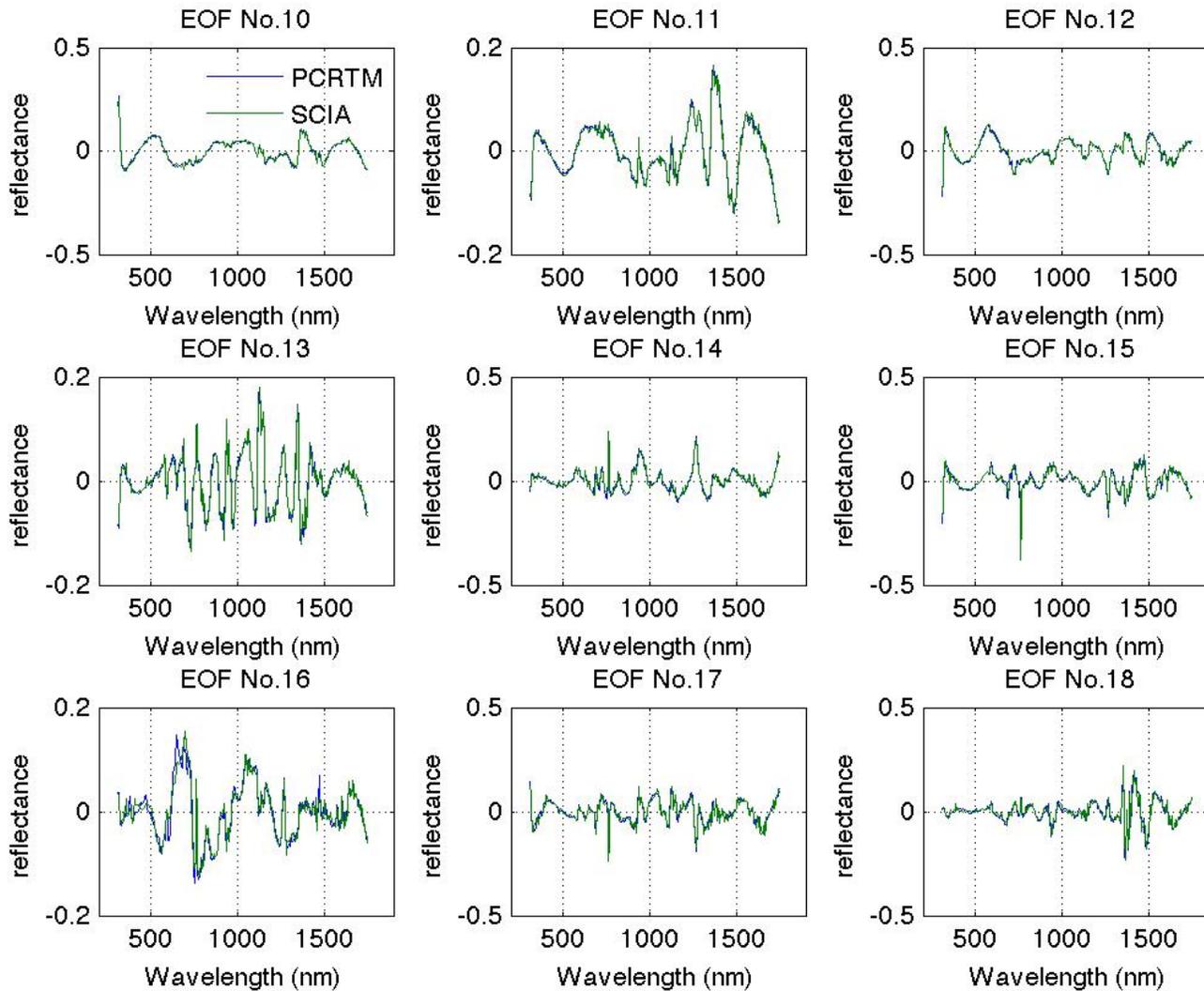


Intersection EOFs from both SCIAMACHY and PCRTM Over Land



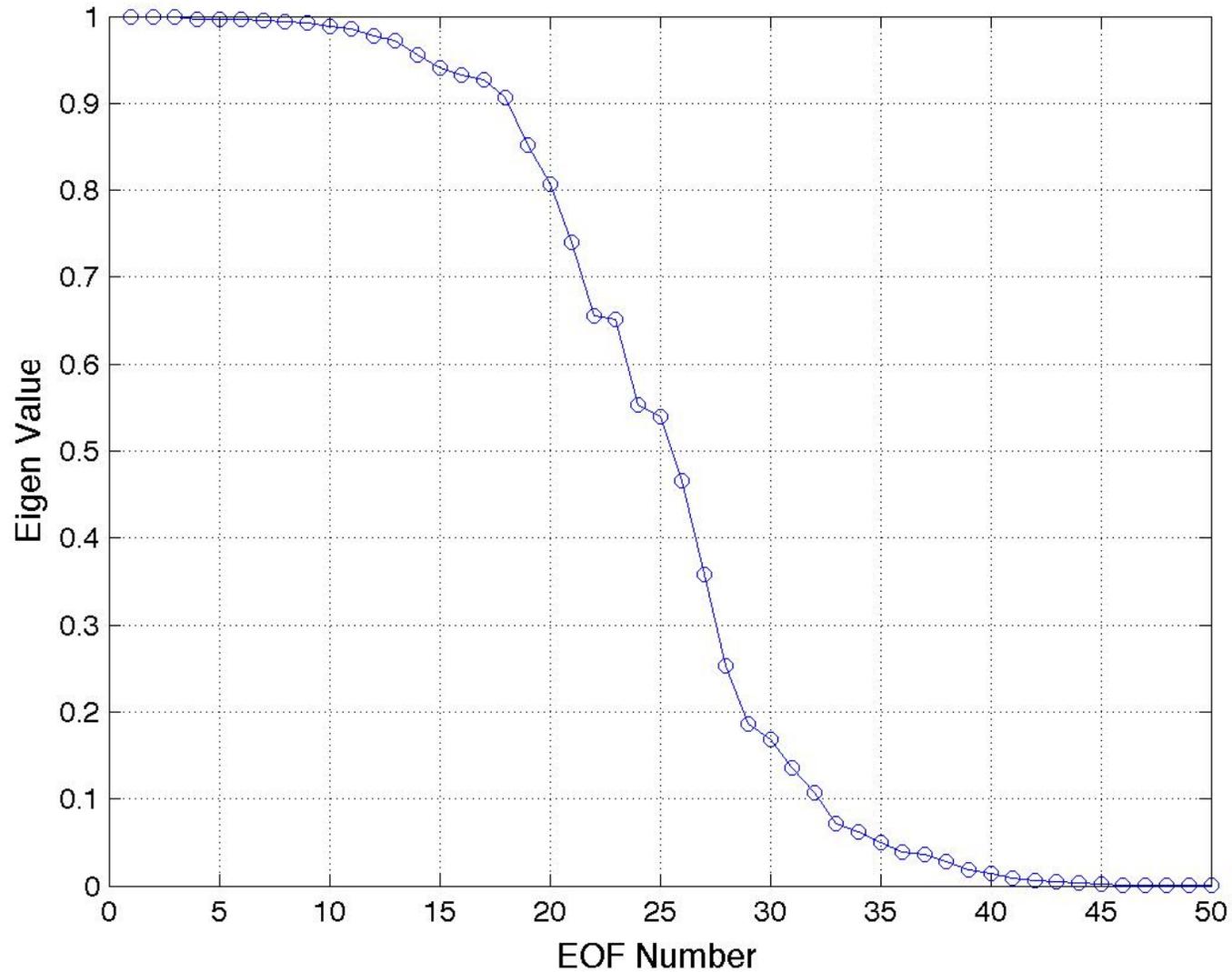


Intersection EOFs from both SCIAMACHY and PCRTM Over Land



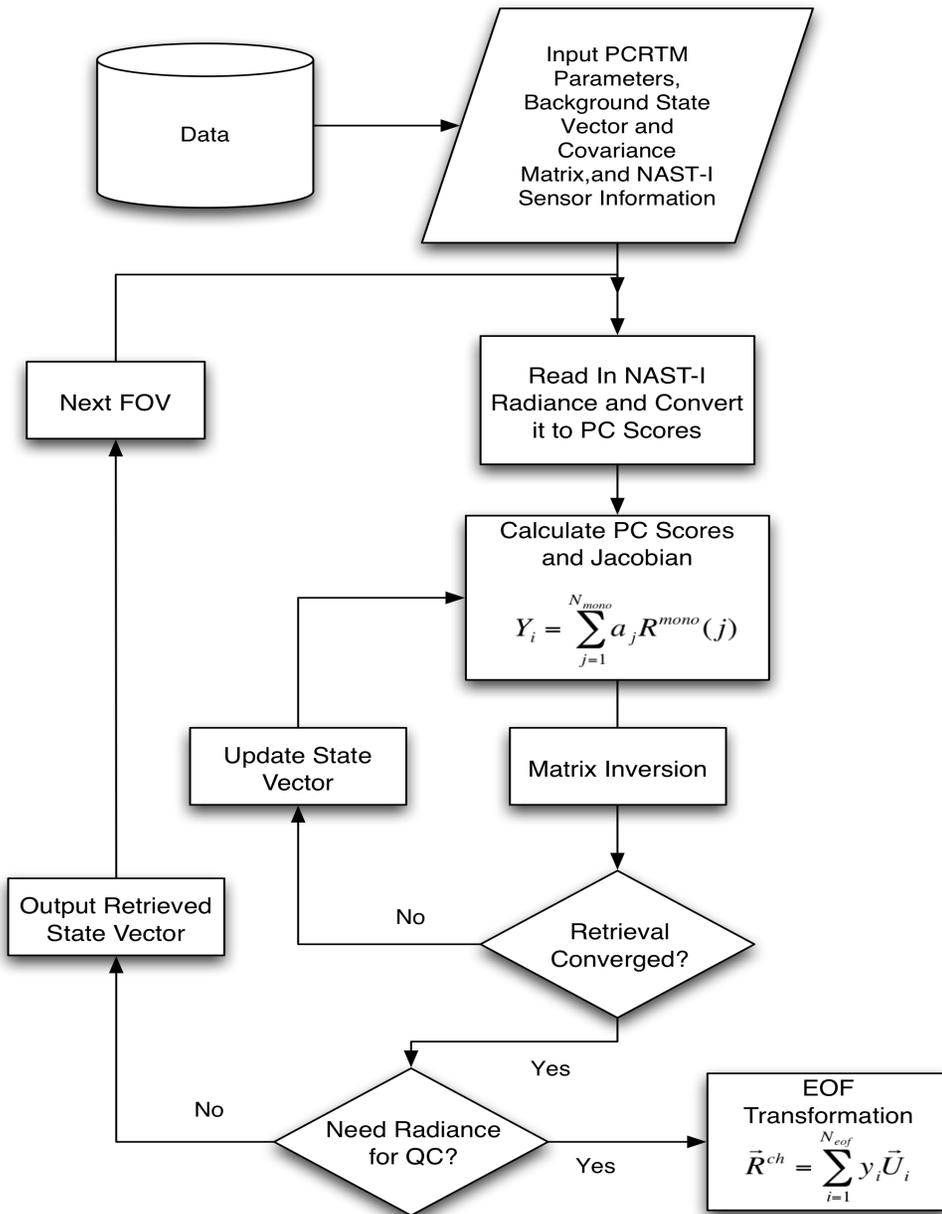


Eigenvalues from intersection PCA analysis Over Land





A brief description of the PCRTM Optimal Estimation Retrieval Algorithm



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

PCRTM models PC scores directly

- Small matrix and vector dimensions
- All 8000 channels from IASI and NAST-I used

Both y and x vectors are in EOF domain

- Small matrix and vector dimensions
- 100 super channels instead of thousands of channels
- Simply minimizing cost function
- Channel-to-channel correlated noise handled

All parameters retrieved simultaneously

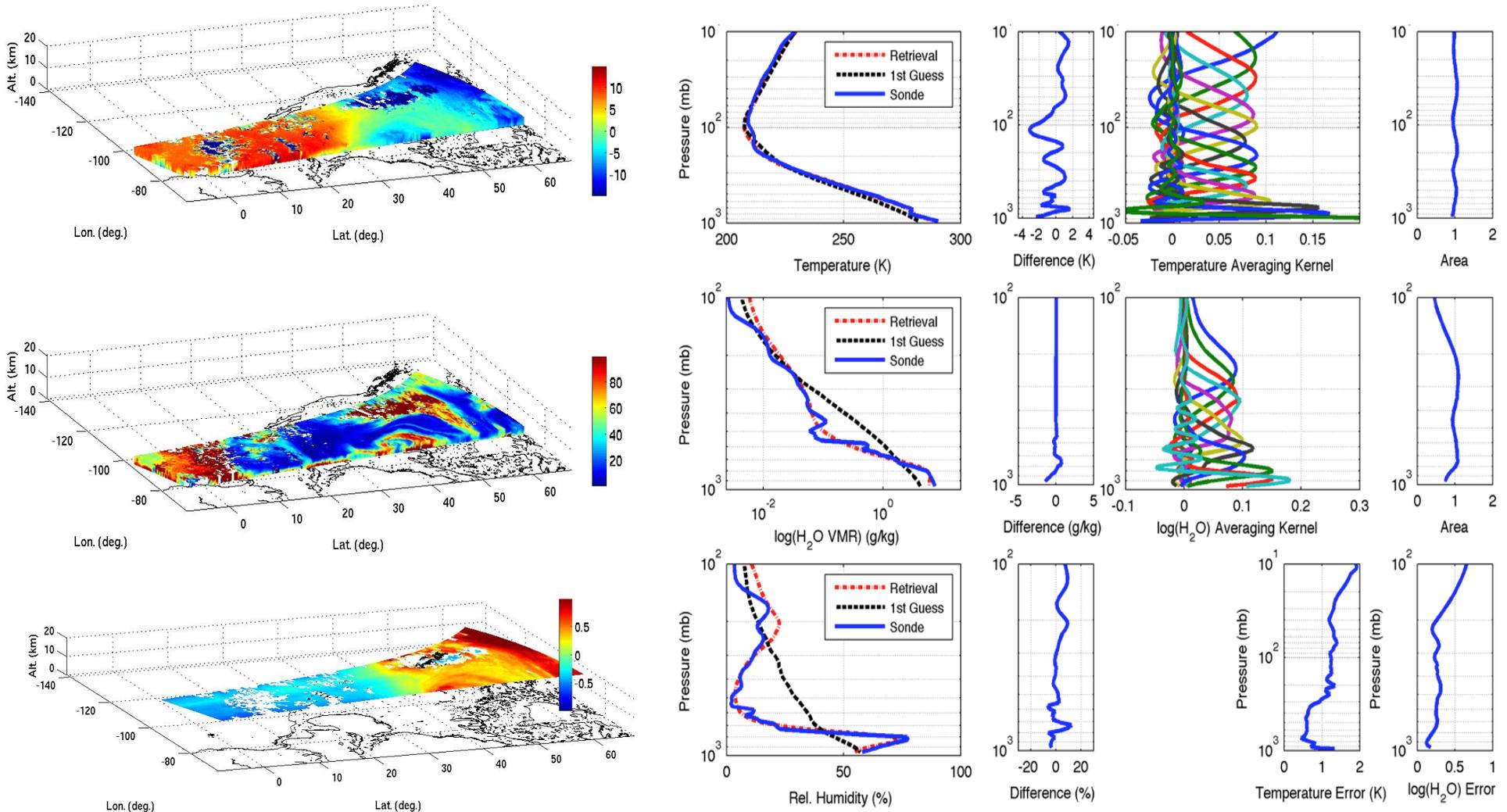
- No need to estimate errors of non-retrieved parameters
- Temperature
- Water
- Trace gases (CO₂, CO, CH₄, O₃, N₂O)
- Surface temperature and emissivities
- Cloud optical depth/size/phase/height

Retr. Config/ Matrix Dimension	Radiance/ Profile	Subset Radiance/ Profile	Radiance PC/ Profile PC
Y	~8400	300	100
X	100	100	41
K	8400x100	300x100	100x41
S_y^{-1}	8400x8400	300x300	100x100
S_x	100x100	100x100	41x41



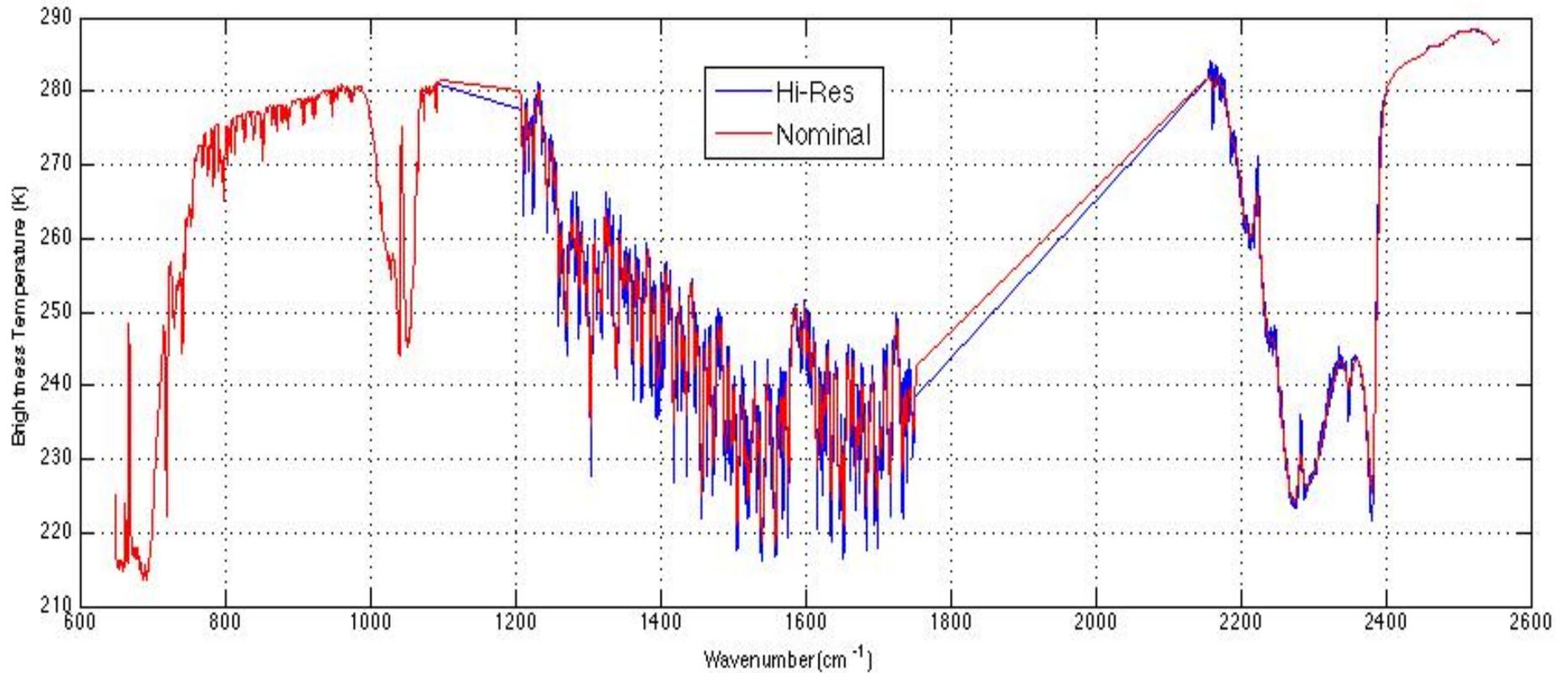
Comparison of PCRTM retrieval with radiosondes

- Temperature, moisture, and ozone cross-sections
- Plots are deviation from the mean
- Fine water vapor structures captured by the retrieval system
- A very cloudy sky condition





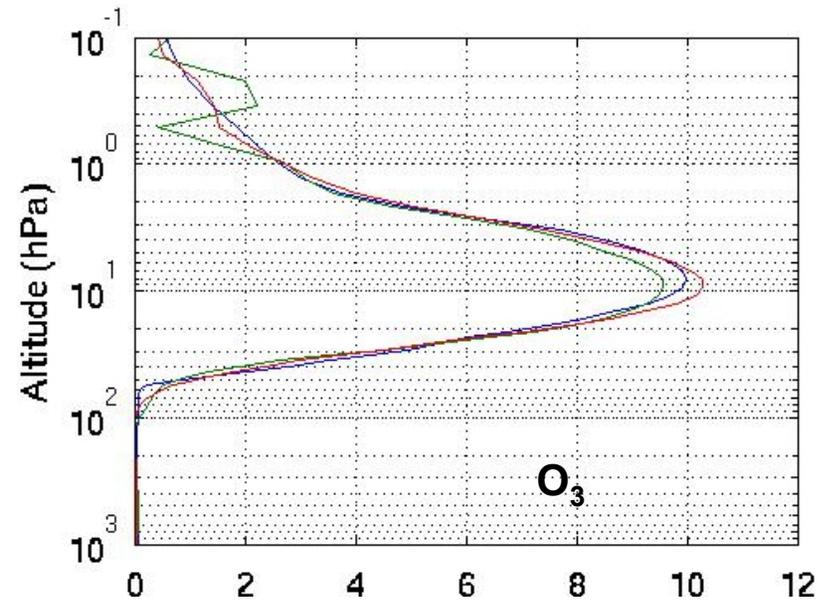
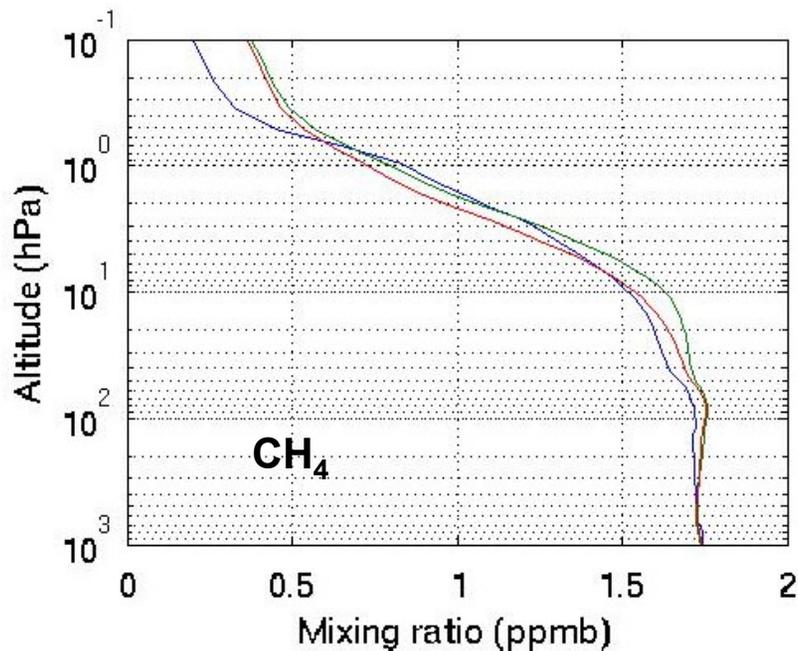
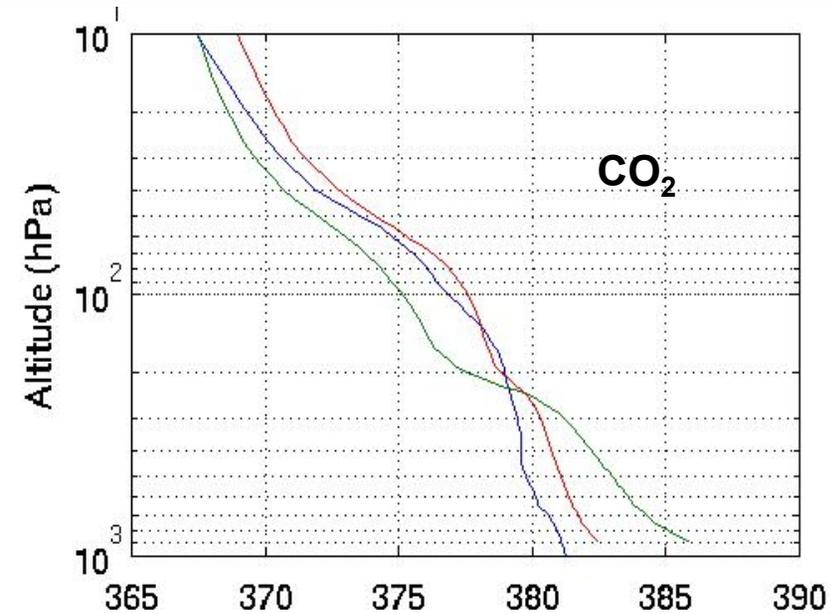
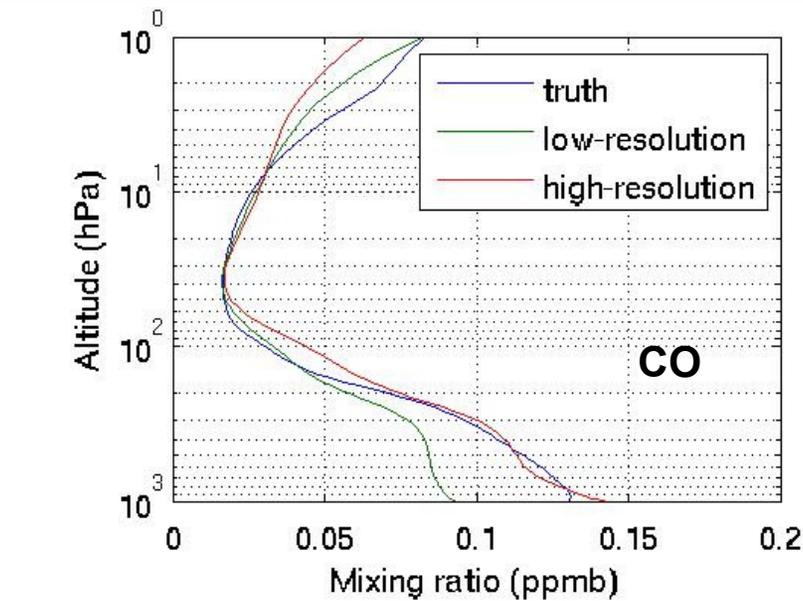
Recent Application of PCRTM to S-NPP CrIS data



	CrIS (LW)	CrIS (MW)	CrIS (SW)
Nominal Res	0.625 cm ⁻¹	1.25 cm ⁻¹	2.5 cm ⁻¹
High Res.	0.625 cm ⁻¹	0.625cm ⁻¹	0.625cm ⁻¹



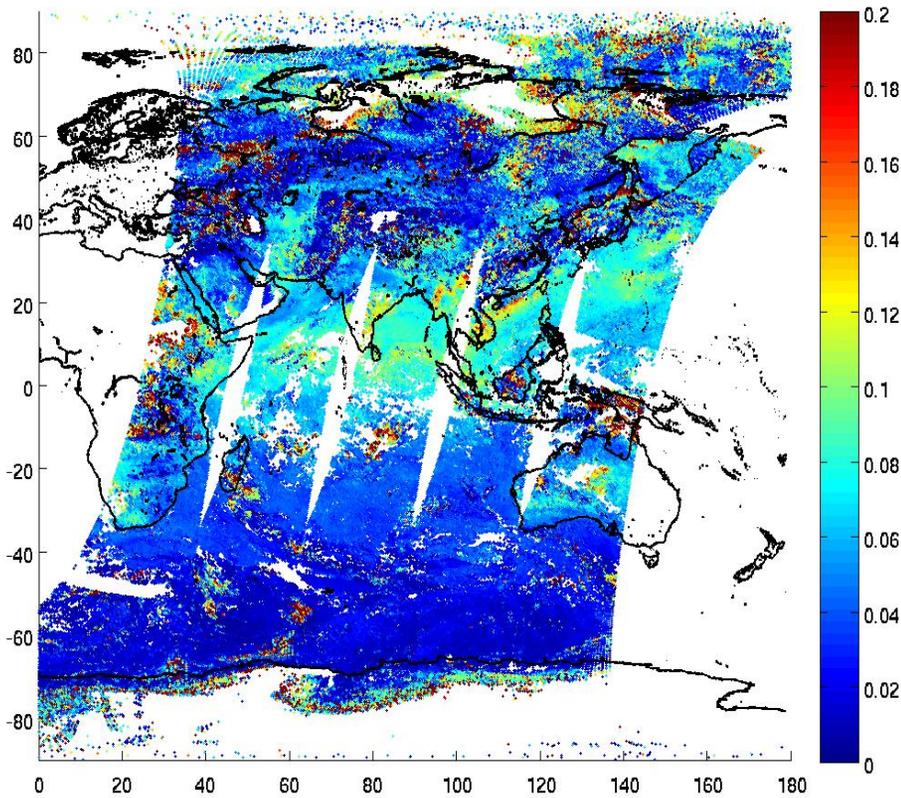
Trace gas retrievals from CrIS with different spectral resolutions (from simulation studies)



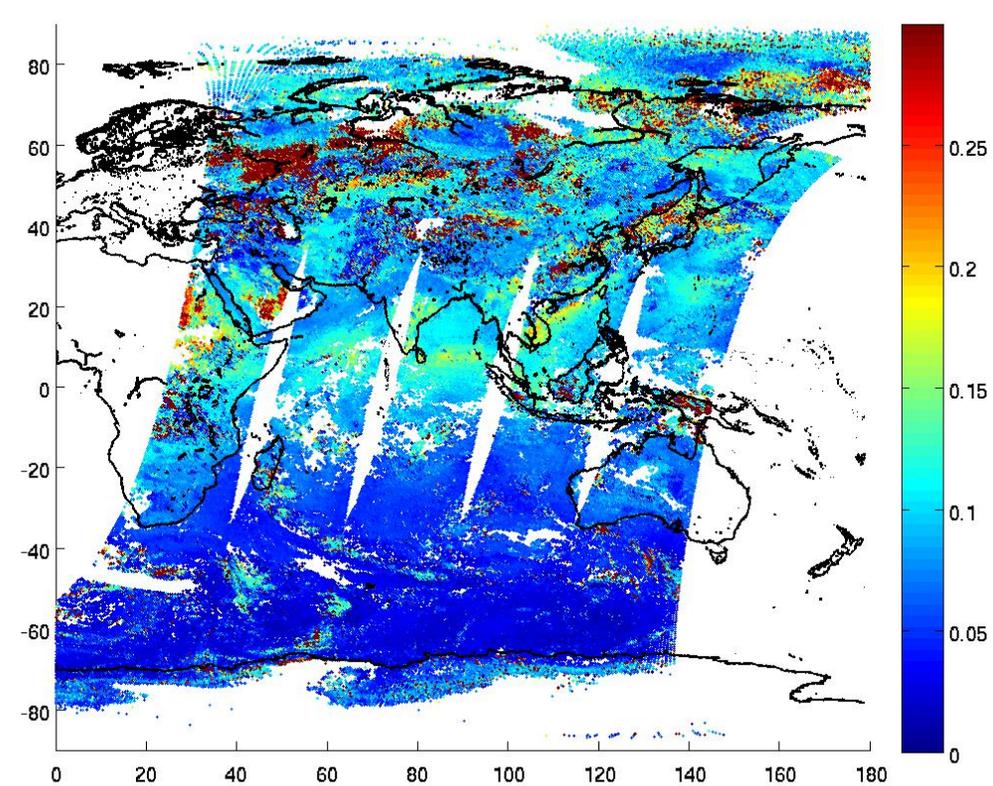


CO retrieved from full-resolution CrIS data

From nominal resolution CrIS



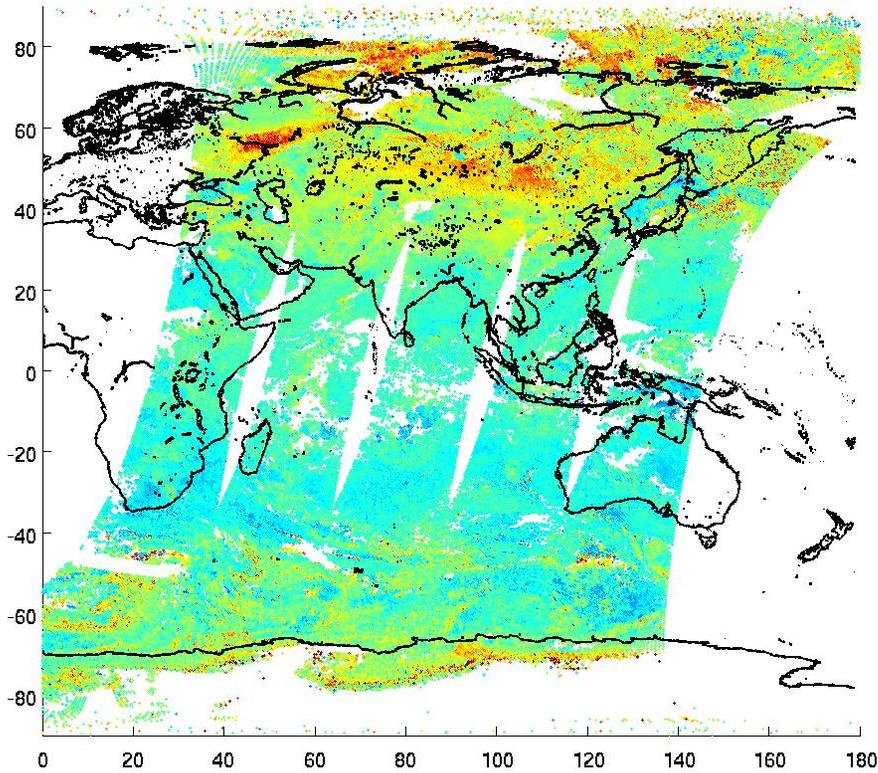
From high resolution CrIS



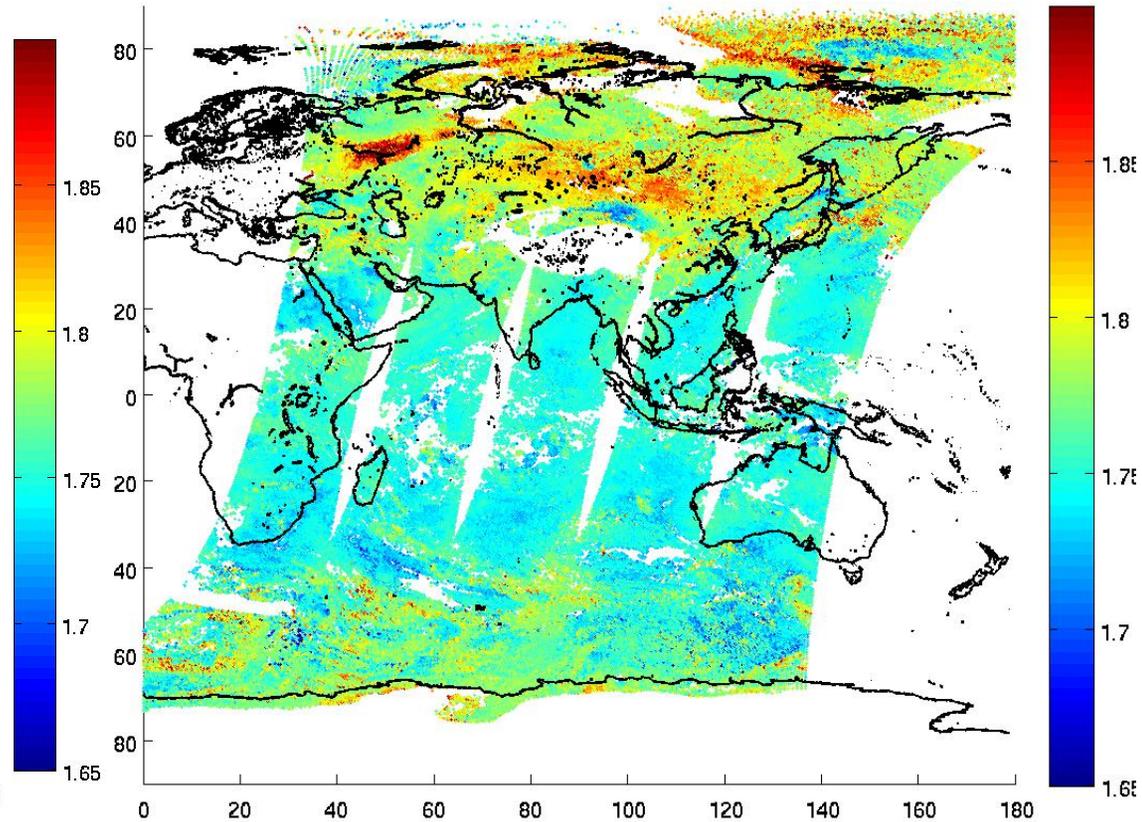


Tropospheric CH₄ (500 mb) from CrIS

From nominal resolution CrIS

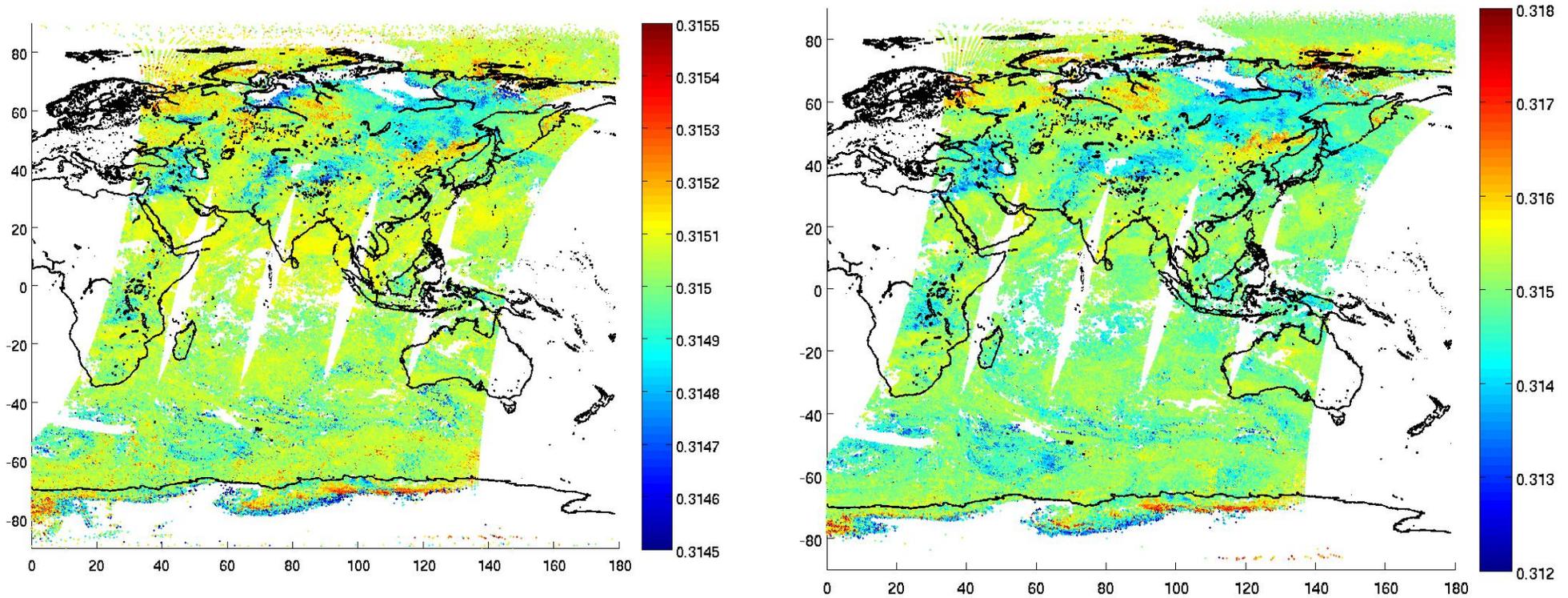


From high resolution CrIS



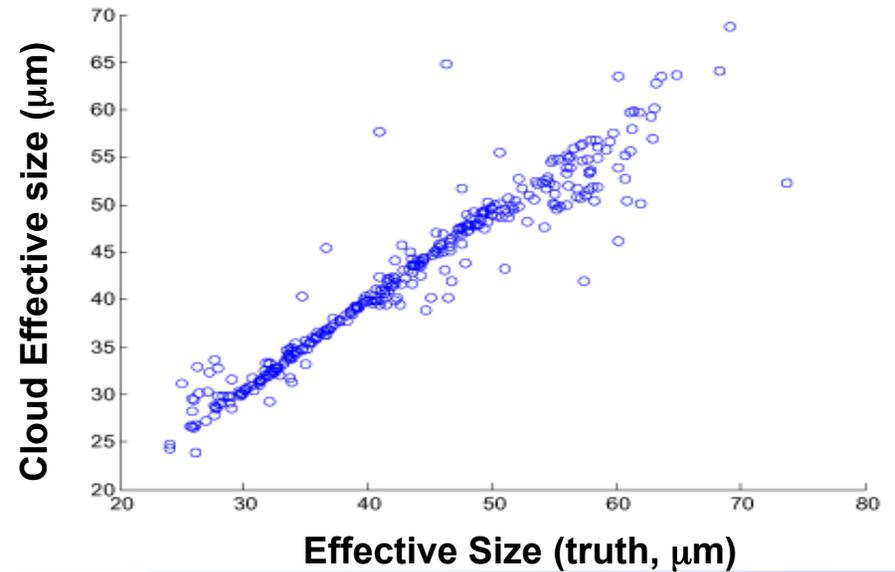
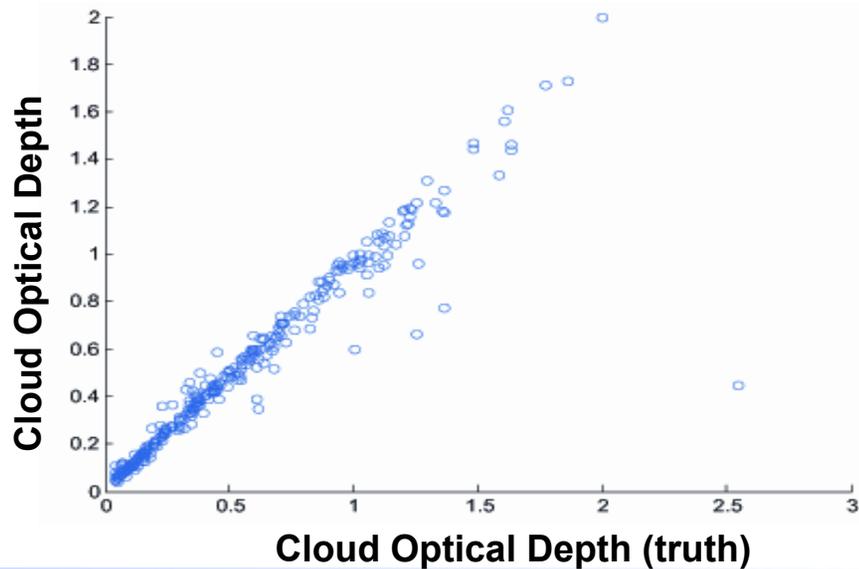
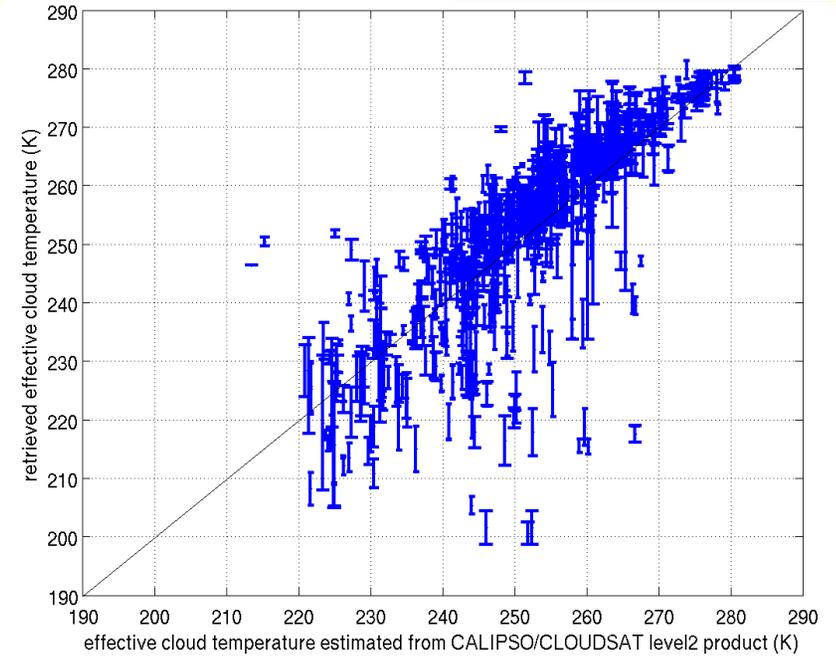
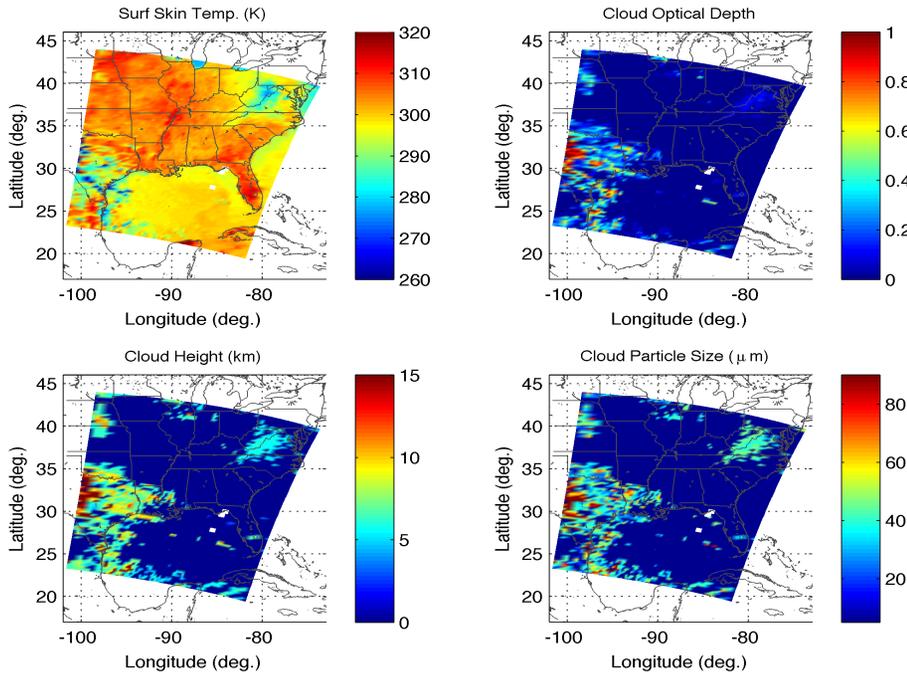


N2O at 500 mb Retrieved from CrIS





Example of retrieved cloud properties



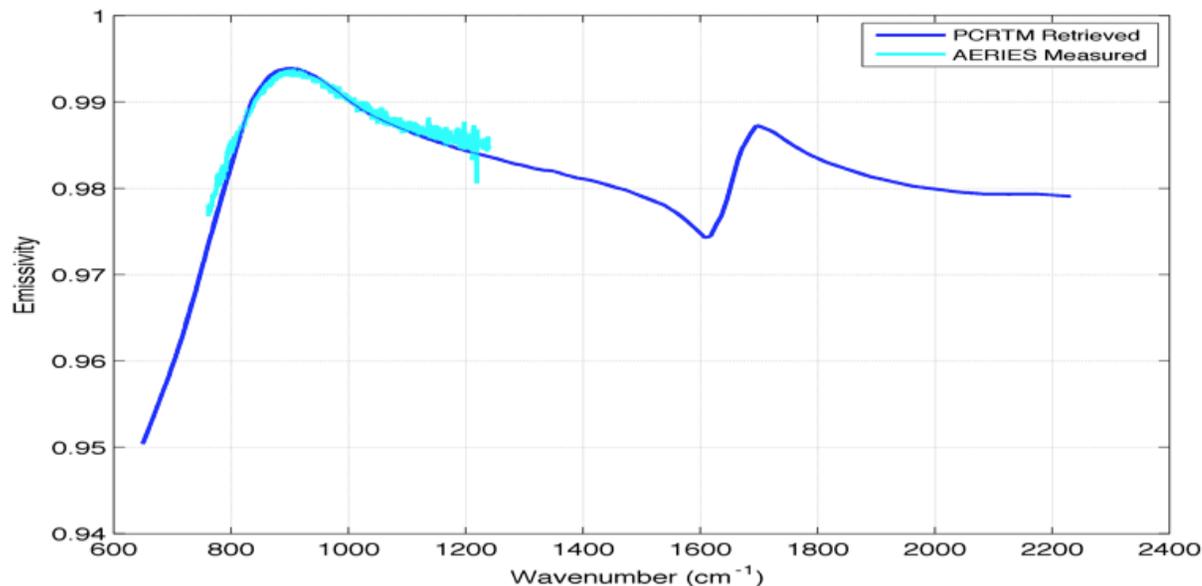


Example of retrieved surface temperature and emissivity and comparison with field validation data

Comparison of PCRTM retrieved surface skin temperature with ARIES measured T_{skin}

Date	Location	Surface Pressure (hPa)	ARIES Measured skin temperature (K)	IASI-retrieved surface skin temperature (K)
19 April 2007	ARM CART site	972.0	284.7	284.8
29 April 2007	Gulf of Mexico	1021.7	297.8	297.6
30 April 2007	Gulf of Mexico	1017.5	298.6	298.1
4 May 2007	Gulf of Mexico	1009.9	297.4	297.1

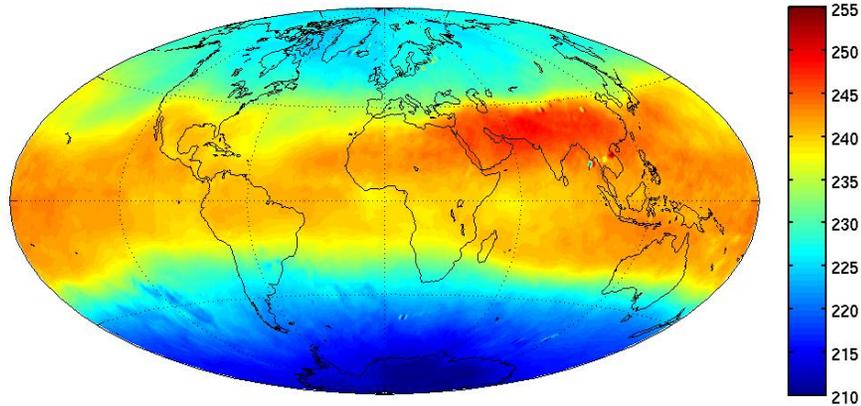
Comparison of retrieved ocean emissivity with ARIES aircraft measurements



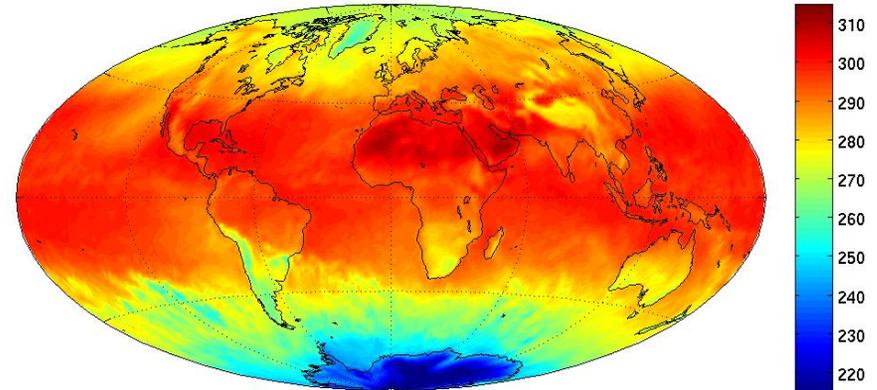


Example of retrieved global distribution of climate related properties retrieved using the PCRTM algorithm

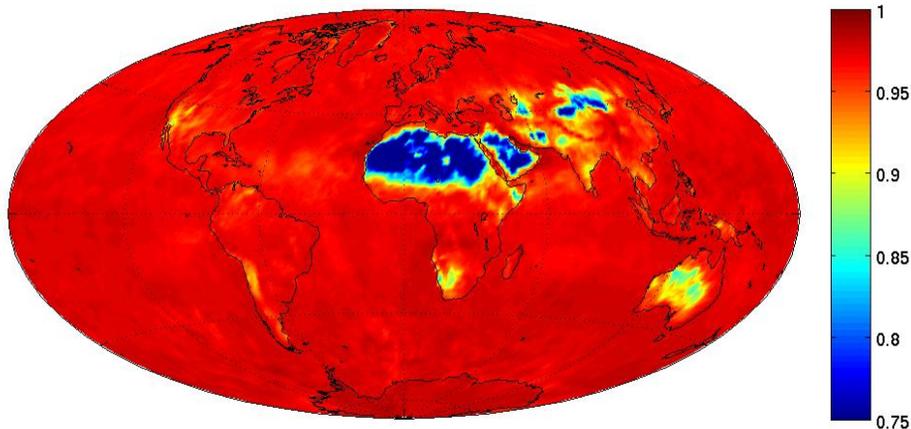
Atmospheric temperature at 9 km for July 2009



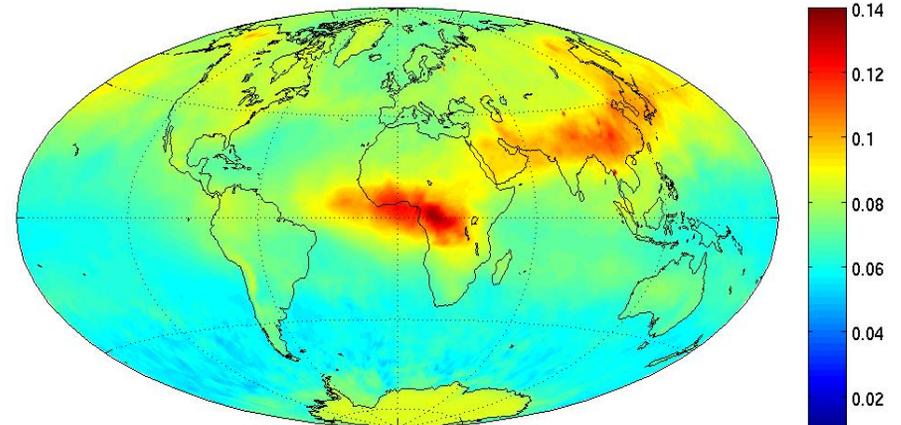
Surface skin temperature for July 2009



Surface emissivity for July 2009



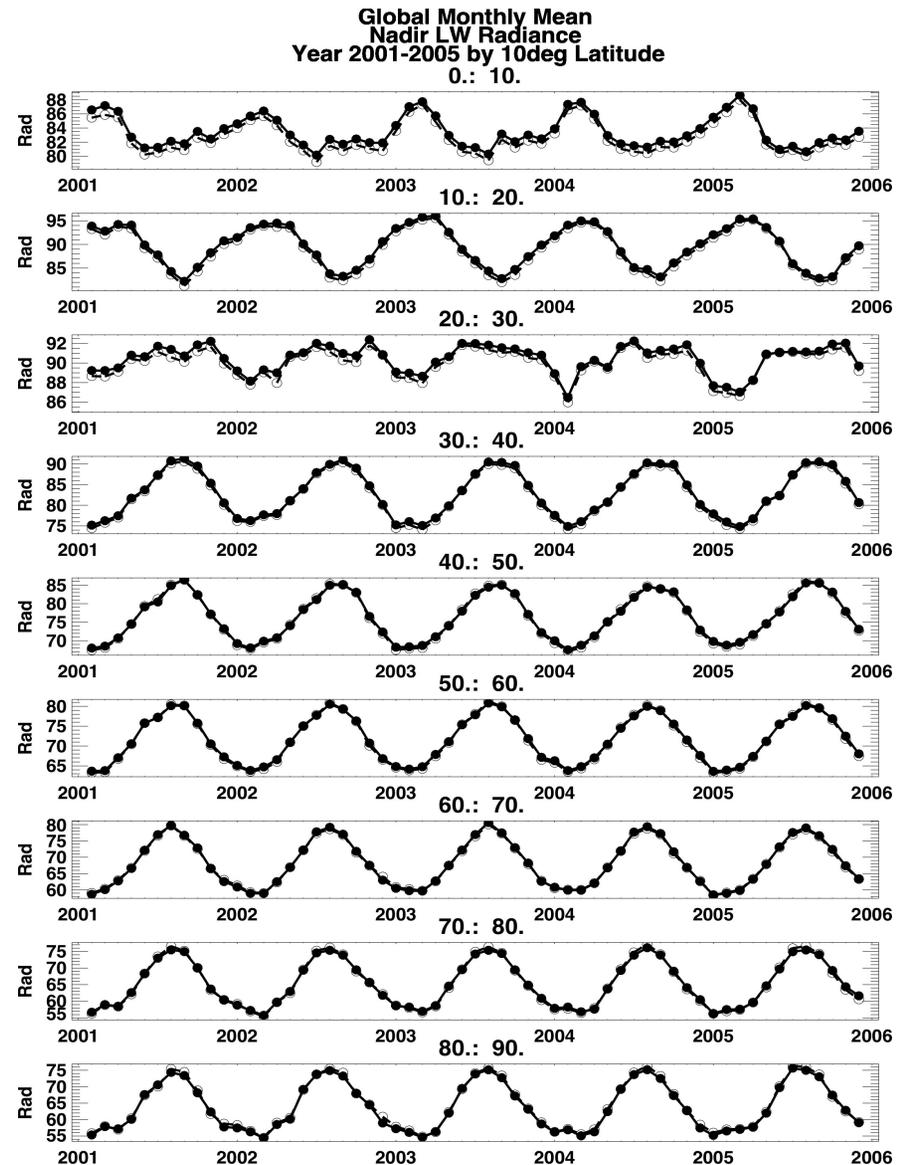
Atmospheric carbon monoxide mixing ratio for July 2009





Applying PCRTM to calculate the OLR and comparison with CERES observations

- Work done by Fred Rose and Seiji Kato at NASA Langley
- PCRTM used to calculate cloudy radiance from 50 cm^{-1} to 2800 cm^{-1} using MODIS/CERES cloud fields and model atmospheres
- PCRTM OLRs are compared with CERES observations
- Orders of magnitude faster than Modtran
- Good agreement for 6 years of record





Summary and conclusions



- Forward model is a key component in analyzing hyperspectral data
 - End-to-end sensor trade studies
 - Realistic global long term data simulations and OSSE experiment
 - Geophysical properties retrievals and data assimilations
- CLARREO PCRTM has been developed
 - Covers spectral range from 0.31 μm to 200 μm
 - With more than 10 variable trace gases
 - Multiple scattering clouds included
 - Physical and accurate
 - Very fast relative to LBL and traditional fast RT models
 - Been applied to numerous hyperspectral sensors: AIRS, IASI, CrIS, NAST-I, SCIAMACHY
 - Algorithm developed to retrieve temperature, water, trace gas profiles, cloud and surface properties from numerous satellite sensors
- Thanks for the collaborations and feedback from CLARREO SDT members
 - LaRC, UC Berkeley/LBNL Umich, UW, HU, UMBC,UM, Imperial College of London
- Future work
 - Continue supporting CLARREO SDT
 - Improve speed in solar spectral region using fast multiple scattering schemes
 - Explore information from both IR and solar spectral regions using simulated CLARREO spectra with consistent cloud and surface properties using PCA...