Latest Development in Radiative Transfer Models and Retrieval Algorithms Using Principal Components

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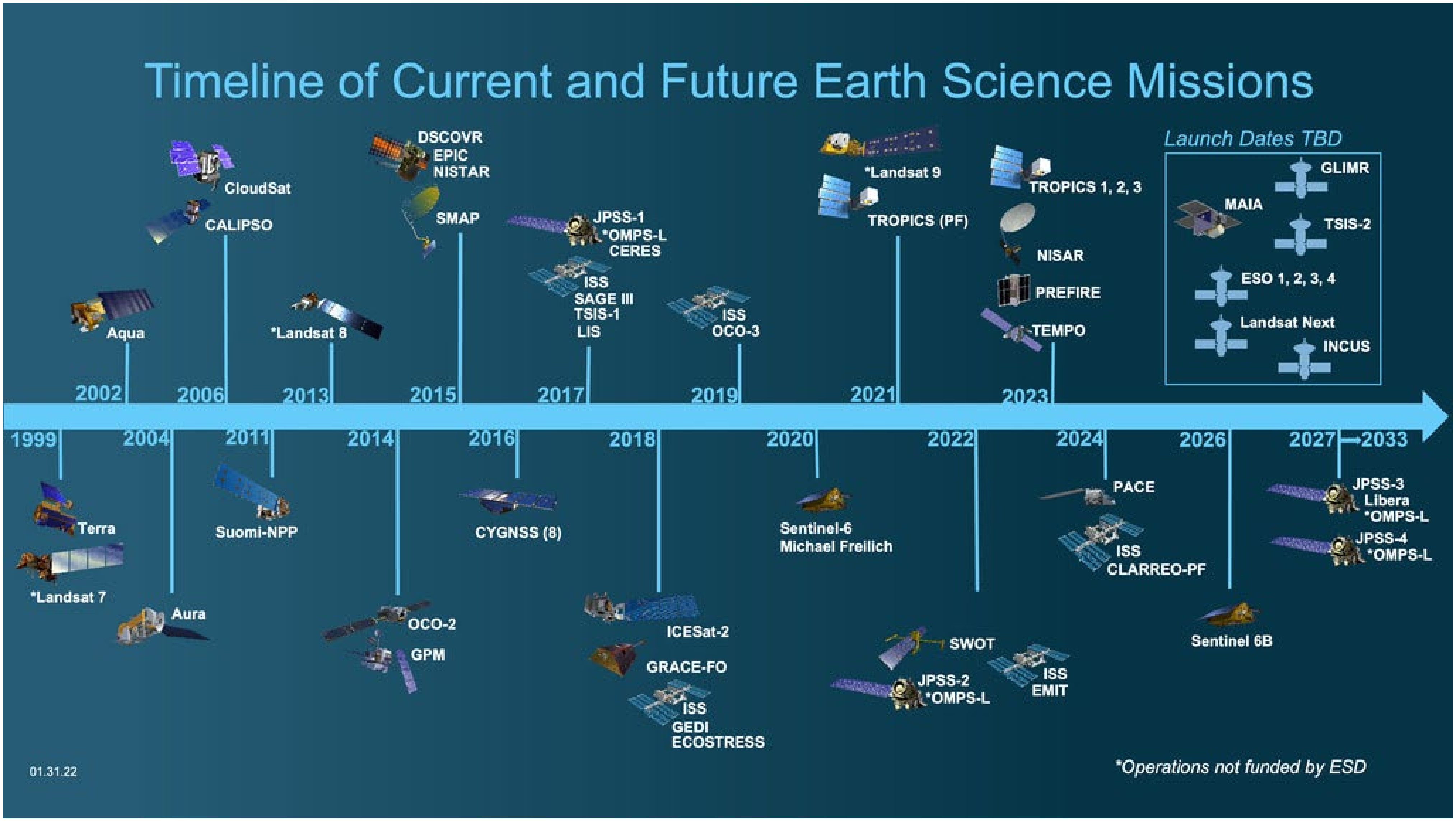
Outline

- Introduction to satellite remote sensing
- Challenges of radiative transfer modeling for hyperspectral remote sensing
- Description of PCRTM
- Applications of PCRTM
  - High-fidelity simulator and end-to-end performance simulations
  - Forward model for L2 and L3 retrieval algorithms
  - Satellite calibration and intercalibrations
  - Generating high-quality training data for AI-based forward and inverse models
- Inversion Algorithms for Satellite Remote Sensing
- Summary and Conclusion



Timeline of Current and Future Earth Science Missions
Launch Dates TBD
GLIMR
MAIA
TSIS-2
ESO 1, 2, 3, 4
Landsat Next
INCUS
CloudSat
CALIPSO
Aqua
*Landsat 8
DSCOVR
EPIC
NISTAR
SMAP
JPSS-1
*OMPS-L
CERES
ISS
SAGE III
TSIS-1
LIS
ISS
OCO-3
*Landsat 9
TROPICS (PF)
TROPICS 1, 2, 3
NISAR
PREFIRE
TEMPO
2002
2006
2013
2015
2017
2019
2021
2023
1999
2004
2011
2014
2016
2018
2020
2022
2024
2026
2027→2033
Terra
*Landsat 7
Aura
Suomi-NPP
OCO-2
GPM
CYGNSS (8)
ICESat-2
GRACE-FO
ISS
GEDI
ECOSTRESS
Sentinel-6
Michael Freilich
SWOT
JPSS-2
*OMPS-L
ISS
EMIT
PACE
ISS
CLARREO-PF
Sentinel 6B
JPSS-3
Libera
*OMPS-L
JPSS-4
*OMPS-L
01.31.22
*Operations not funded by ESD

Challenges for Performing Radiative Transfer (RT) Calculations

- Line-by-line radiative transfer calculations through atmosphere is very time consuming
  - Multi-scattering calculation is very time-consuming (Rayleigh, aerosol, and clouds)
  - Need to properly resolve the atmospheric gas absorption lines (limited by Doppler Width)
    - More than 2 million monochromatic RT calculations for IR (3-20 μm)
    - More than 2 million monochromatic RT calculations for VSWIR (0.25-2.5 μm)
    - ~70 thousand monochromatic RT calculations for TEMPO (0.29-0.49 μm, 0.54-0.74 μm)
- Convolving monochromatic radiances with Sensor Response Function (SRF) is also time consuming
  - Traditional fast RT models usually perform RT calculation at channel frequency grid (e.g correlated-K, CRTM, RTTOV etc…)
  - Still too many RT calculations for high spectral resolution remote sensors such as TEMPO
  - The Beer's Law is no longer valid after convolving with SRF:
  - It's difficult to handle inhomogeneous path and multiple gases
- Principal Component-based Radiative Transfer Model (PCRTM) accelerates RT calculations in two ways
  - Explore the spectral correlations by Principal Component Analysis (PCA)
  - Perform RT calculations at fewer monochromatic frequencies than the number of spectral channels

Overview of Different Fast RT Models

Model Type	Characteristics	Notes
Band Model	Simple parameterization Fast	Limited accuracy Not accurate for multiple gases
Neural net	Simple Fast	Jacobian calculations? Non-physical parameterization
Correlated k Distributions (CKD)	Monochromatic (g-v mapping) Level to level k correlation is approximate Overlapping gases treatment is approximate	Not perfect for inhomogeneous path and overlapping gases
Exponential Sum Fitting Transmissions (ESFT)	Monochromatic (select few k terms or v points) Level to level k correlation is approximate (methods exist to handle it) Overlapping gases treatment is approximate	have been extended to handle inhomogeneous path and overlapping gase (Armbrushter & Fisher 1996, Tjemkes & Schmetz 1997)
RTTOV ,SARTA, CRTM….	Polychromatic Smart way to treat overlapping gases Teat inhomogeneous path	Effective layer optical depth depends on layer above it
Optimal Spectral Sampling (OSS)	Monochromatic Parameterization is physical Accurate	Very good treatment of inhomogeneous path and overlapping gases
PCRTM	Fast and Accurate Physical Parameterization Requires minimum monochromatic RT calculations	Not a channel-based RTM EOF used to compress and store info Same set of predictors used for all PC scores (or superchannels)

PCRTM is a Physical-based Fast Radiative Transfer Model

- Calculates channel radiances (or transmittances) by linearly combine a set of pre-stored EOF:

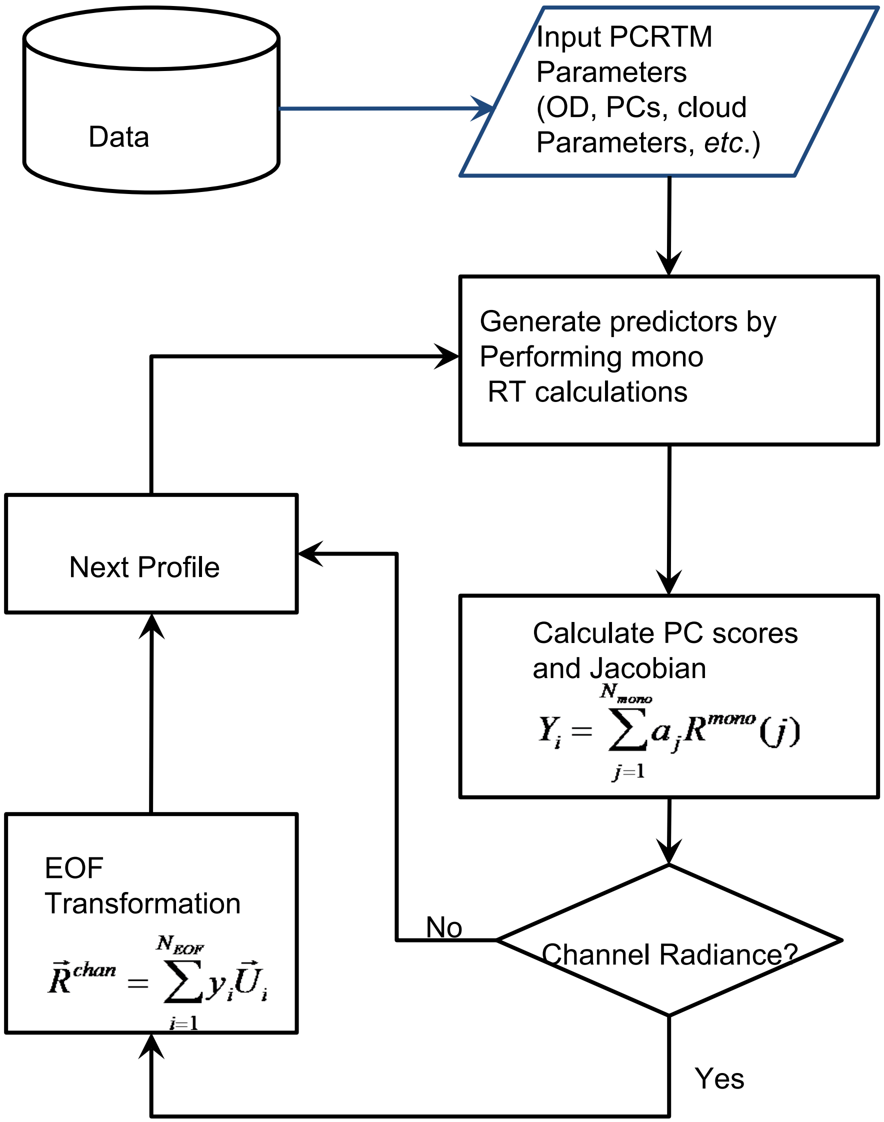
$$\vec{R}^{ch} = \sum_{i=1}^{N_{EOF}} c_i \vec{U}_i + \vec{\varepsilon} = \sum_{i=1}^{N_{EOF}} \left(\sum_{j=1}^{N_{mono}} a_j R_j^{mono} \right) \vec{U}_i + \vec{\varepsilon}$$

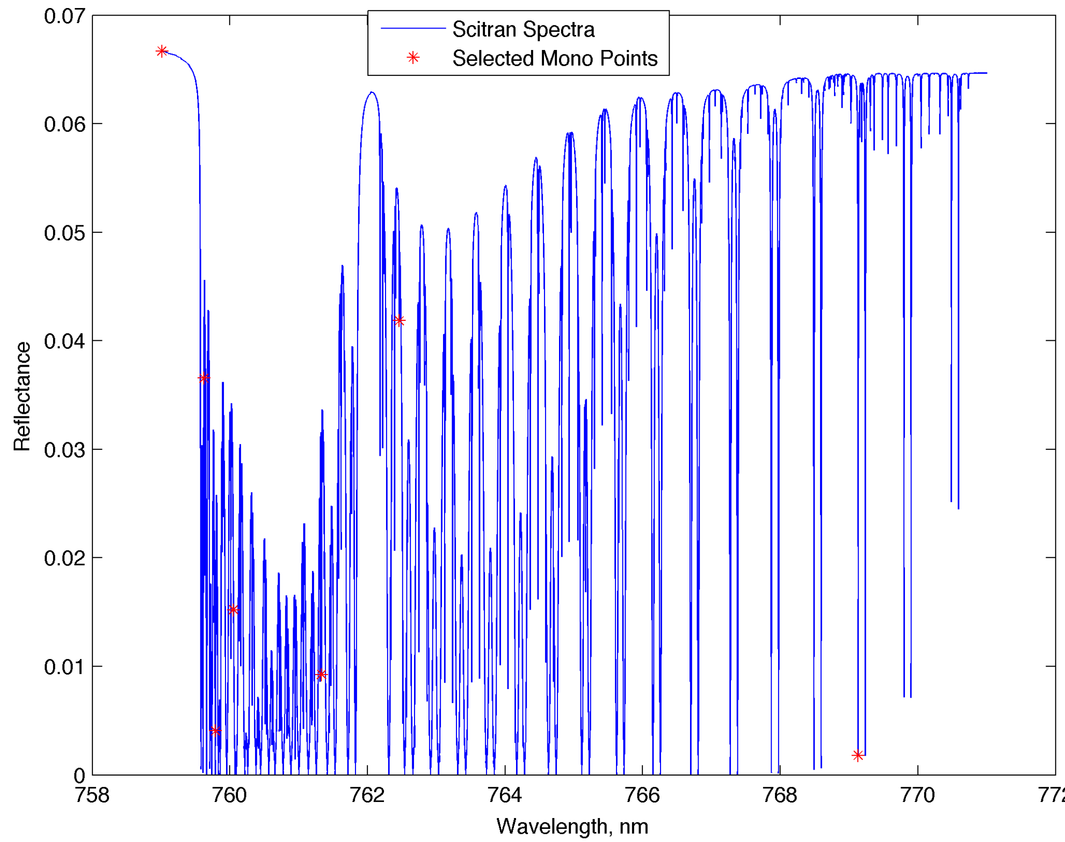
- Coefficient C_i are predicted from a few monochromatic radiances
  - The relationship is derived from the properties of eigenvectors and SRF
- Treats the whole spectra as a whole
  - No need to perform redundant RT calculations
  - RT calculations are performed monochromatically with a number much smaller than the number of spectral channels
  - A factor of 2-100 times faster than channel-based RT models
- Therefore, the PCRTM is physical-based RTM
  - Accuracy relative to LBL can be adjusted by increasing/decreasing the number of monochromatic RT calculations
  - Provide radiative derivatives of radiance or reflectance with respect to atmospheric and surface variables

NAST-I Spectral Band	Number of Channels	No. of RT Calc. for All NAST Channels	Predictors per Channel
PCRTM	8632	310-900	0.04-0.1
PFAST	8632	8632	~40
OSS	8632	22316	2.59

How does PCRTM work?

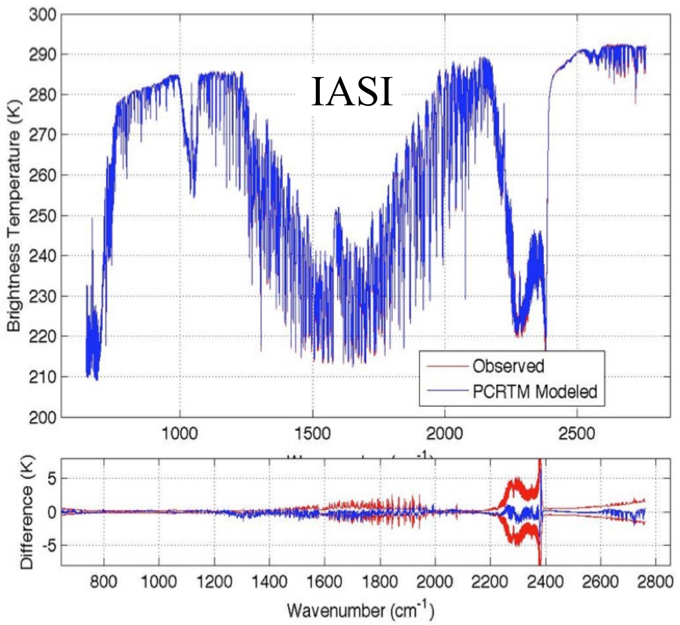
Flow diagram of the PCRTM forward model

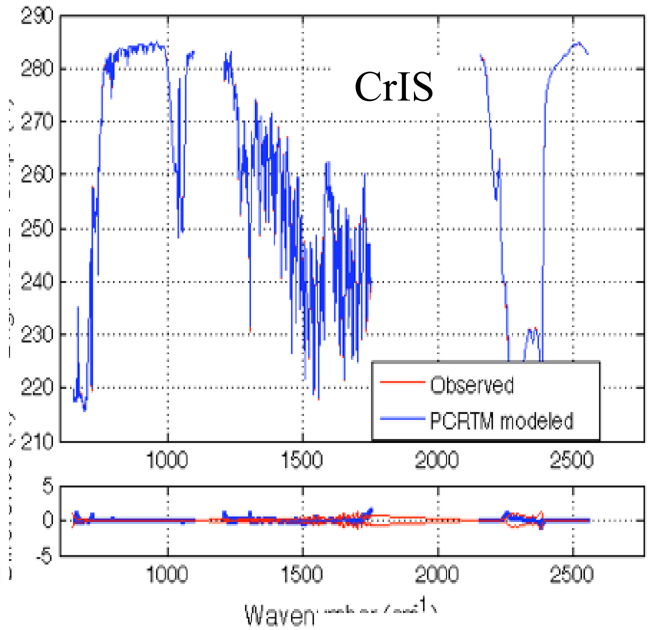


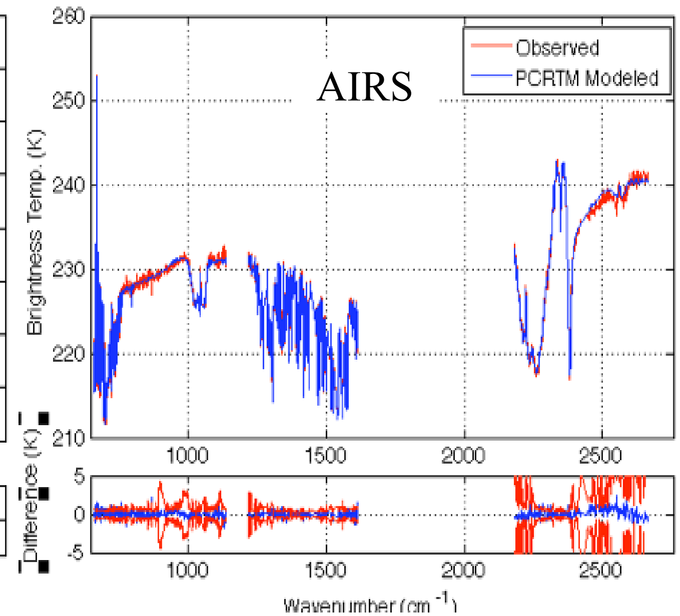


- O_2 A-band (12000 mono RT calculations using LBL)
- Only 7 Mono frequencies are essential when modeling at the OCO and SCIAMACHY spectral resolution

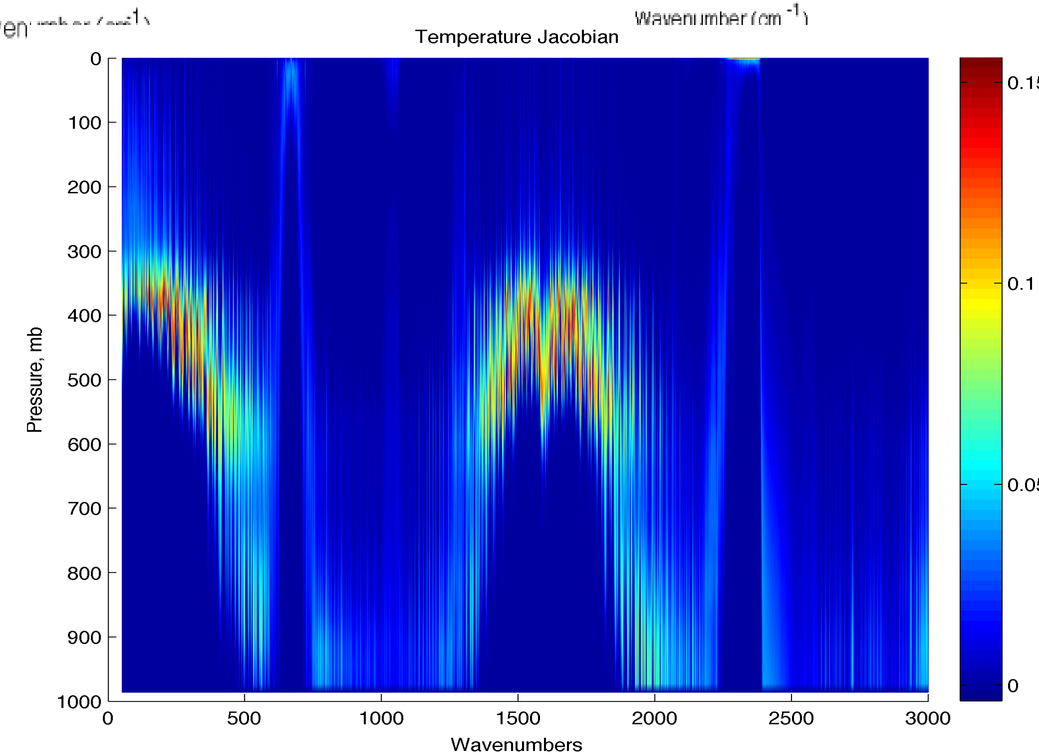
Demonstration of Speed and Accuracy of PCRTM for IR sounders





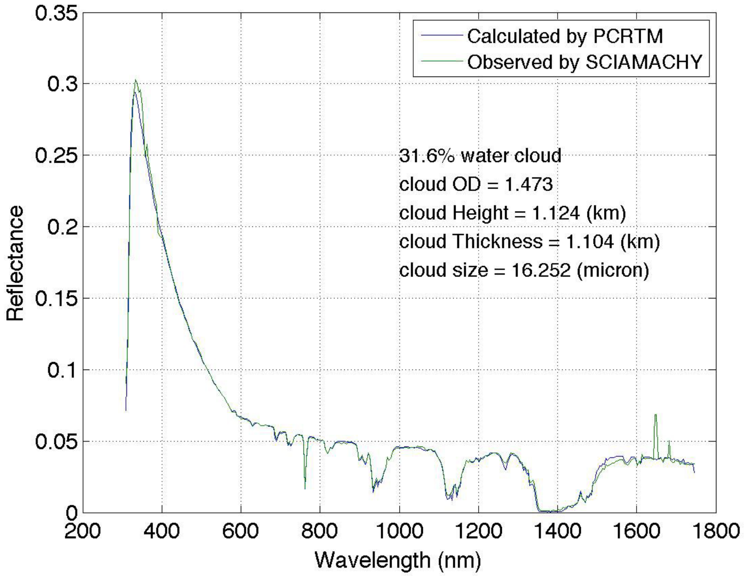


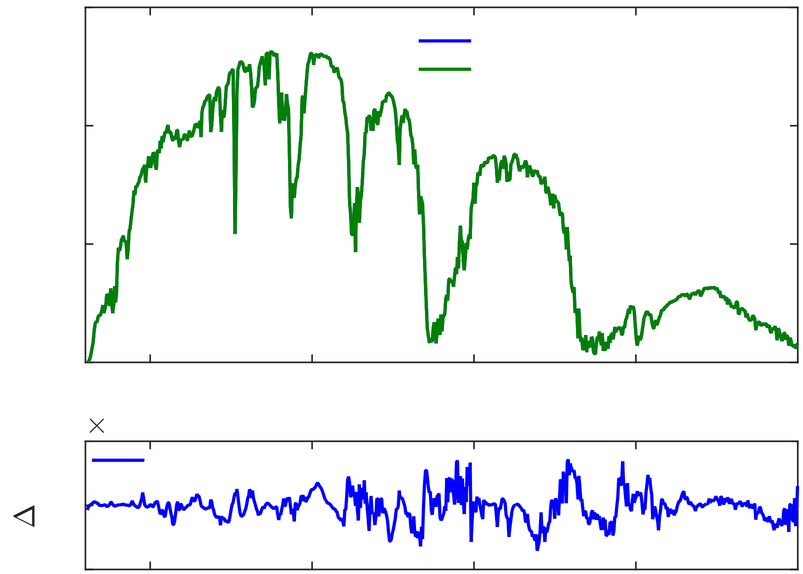
Sensor	Channel Number	PC score (seconds)
CLARREO, 0.1 cm^{-1}	19901	0.014 s
CLARREO, 0.5 cm^{-1}	5421	0.011 s
CLARREO, 1.0 cm^{-1}	2711	0.0096 s
IASI, 0.25 cm^{-1}	8461	0.011 s
AIRS, 0.5-2.5 cm^{-1}	2378	0.0060 s
CrIS,0.625-2.5 cm^{-1}	1317	0.0050 s
NAST-I, 0.25 cm^{-1}	8632	0.010 s
S-HIS, 0.5 cm^{-1}	4316	0.008 s
CrIS, 0.625 cm^{-1}	2211	0.009 s



PCRTM Reduces RT Calculations by 3-4 Oders of Magnitude Relative to Correlated- Method for CPF-type Spectrometer

SCIAMACHY





PCRTM	*nmo*	*nch*	*npc*	*nsmo*	*Speed-up*
Land (8 nm)	259,029	546	220	262	988
Ocean (8 nm)	259,029	546	267	240	1079

Number of radiative transfer calculations for PCRTM are reduced by 3 orders of magnitude relative to modtran for spectral range from 300 nm to 2500 nm

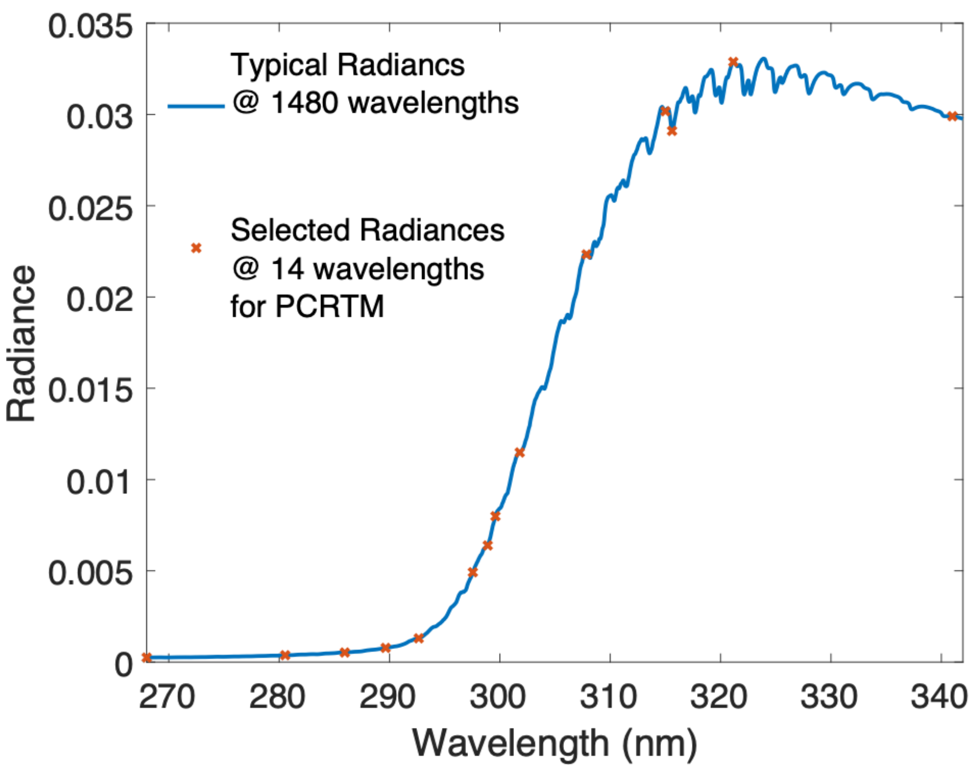
PCRTM	M1	M2	Speedup to Regular PCRTM-SOLAR	Speedup to MODTRAN 5
Land 8 nm	263	49	5	5286
Ocean 8 nm	241	23	10	11,262

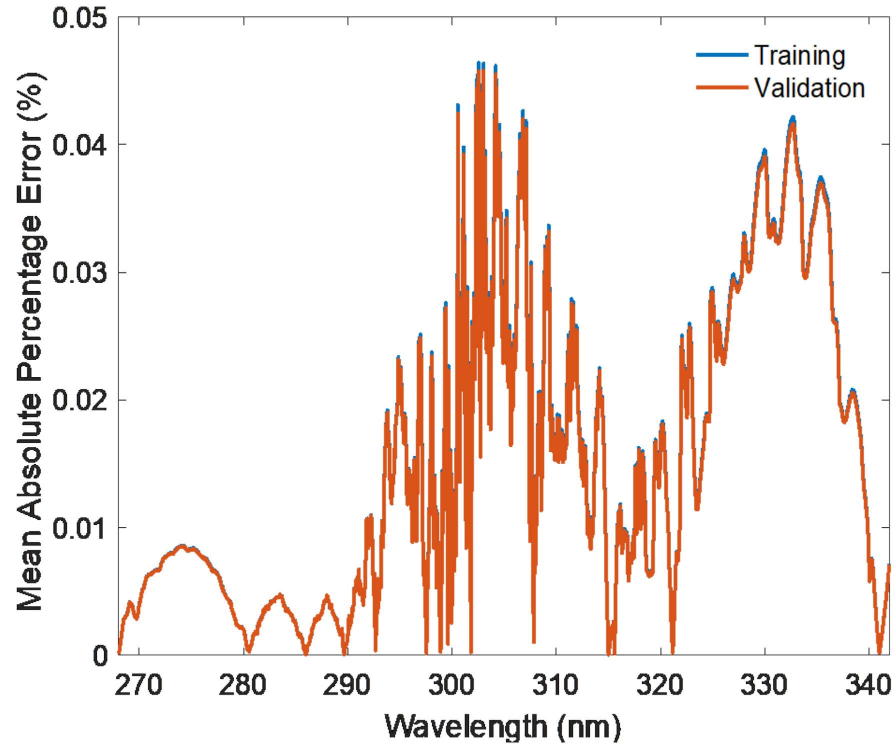
Hybrid Stream method further speed up PCRTM-SOLAR by another factor of 5-10 relative to 32-stream PCRTM

(Xu.Liu-1@nasa.gov)

Example of Selected Wavelength Locations and RMS Errors for TEMPO/OMI Ozone Spectral Regions

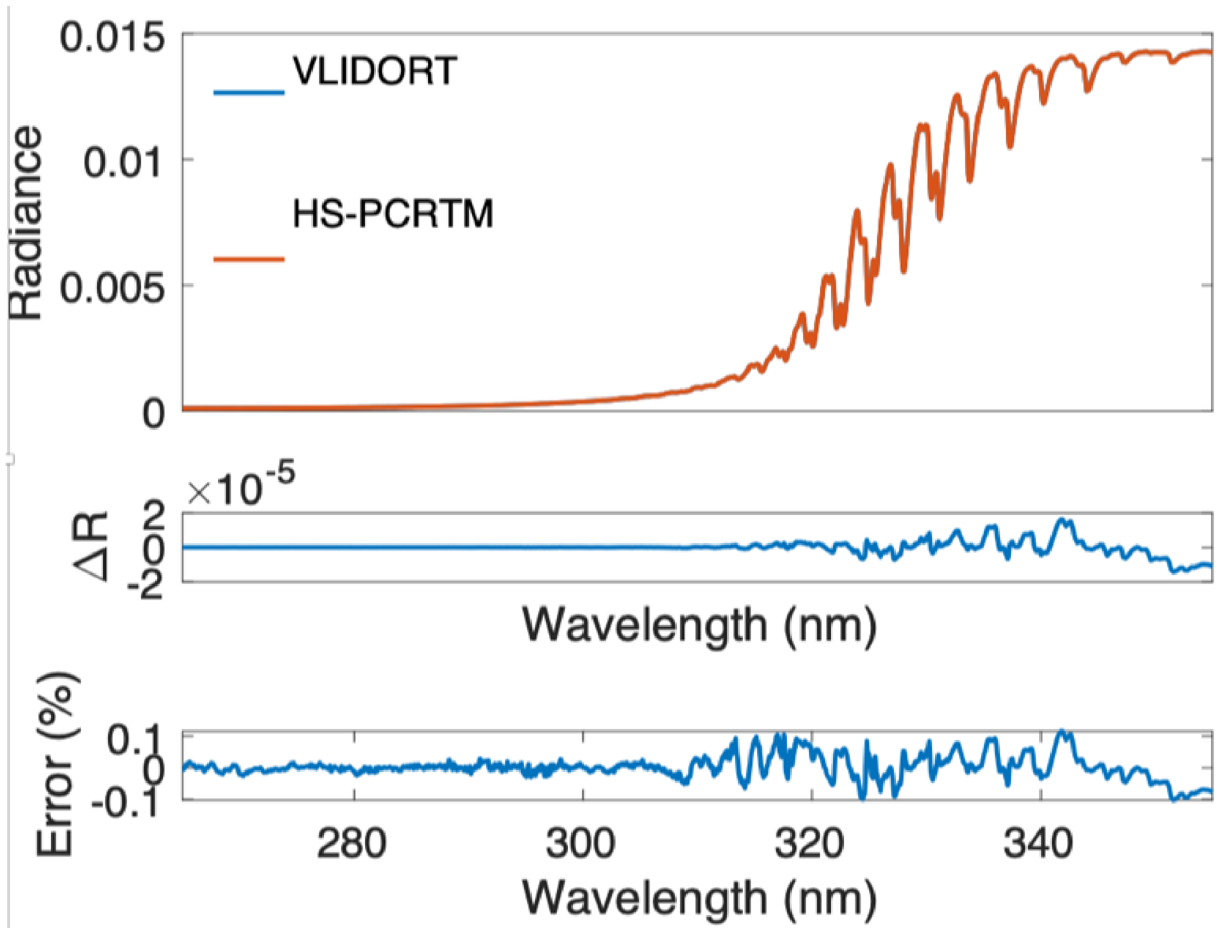
- 2 Orders of magnitude speed up in the OMI Ozone spectral region for a high-spectral resolution (0.05 nm) PCRTM
- Redundant RT calculations are avoided in PCRTM approach
- Can further reduce the number RT calculations at TEMPO or OMI spectral resolutions





Example of HS-PCRTM Accuracy Relative to VLIDORT for TEMPO/OMI Ozone Spectral Region

- The Hybrid Stream PCRTM (HS-PCRTM) can further reduce the computational time
  - Perform 2-stream monochromatic RT calculations at original PCRTM selected frequencies
  - Perform higher streams RT calculations at even less monochromatic frequencies
  - The accuracy is not comprised (see example below)



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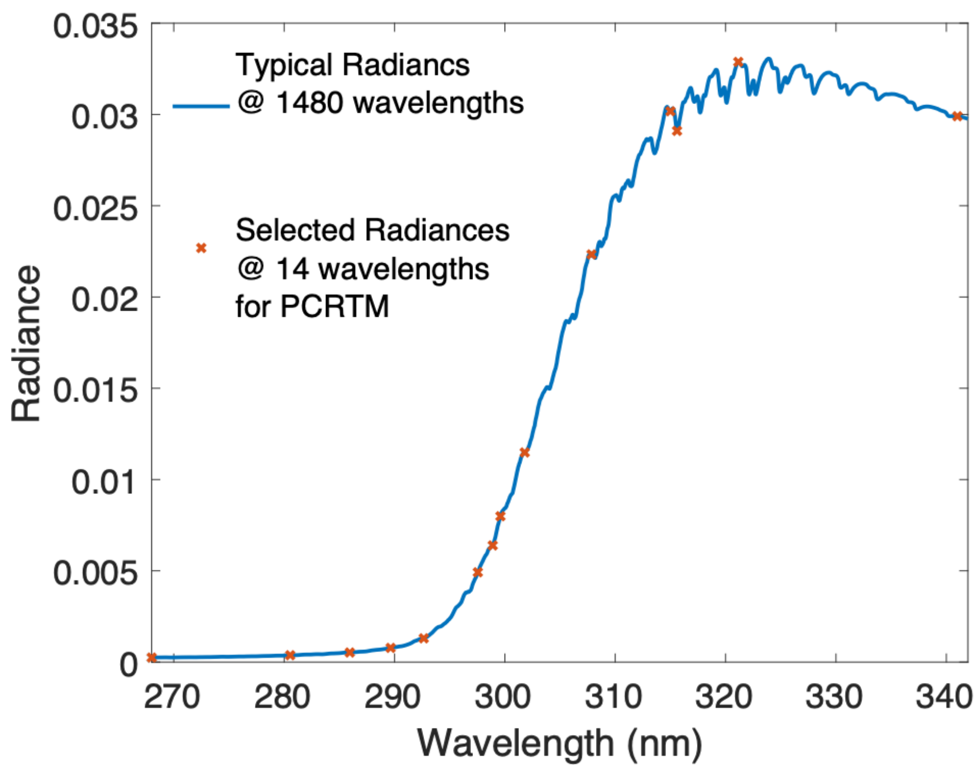

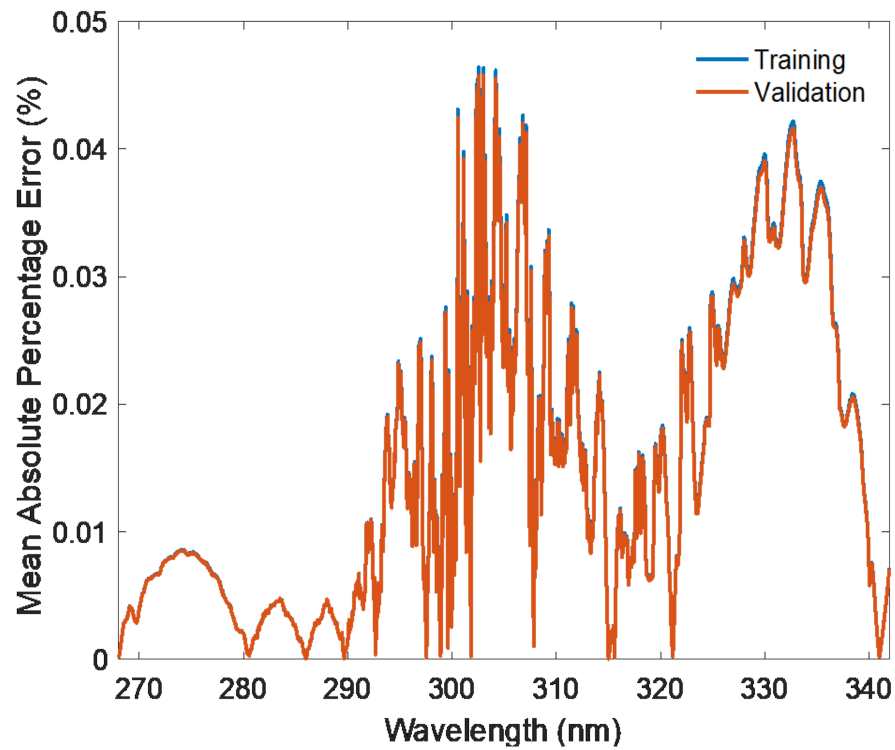

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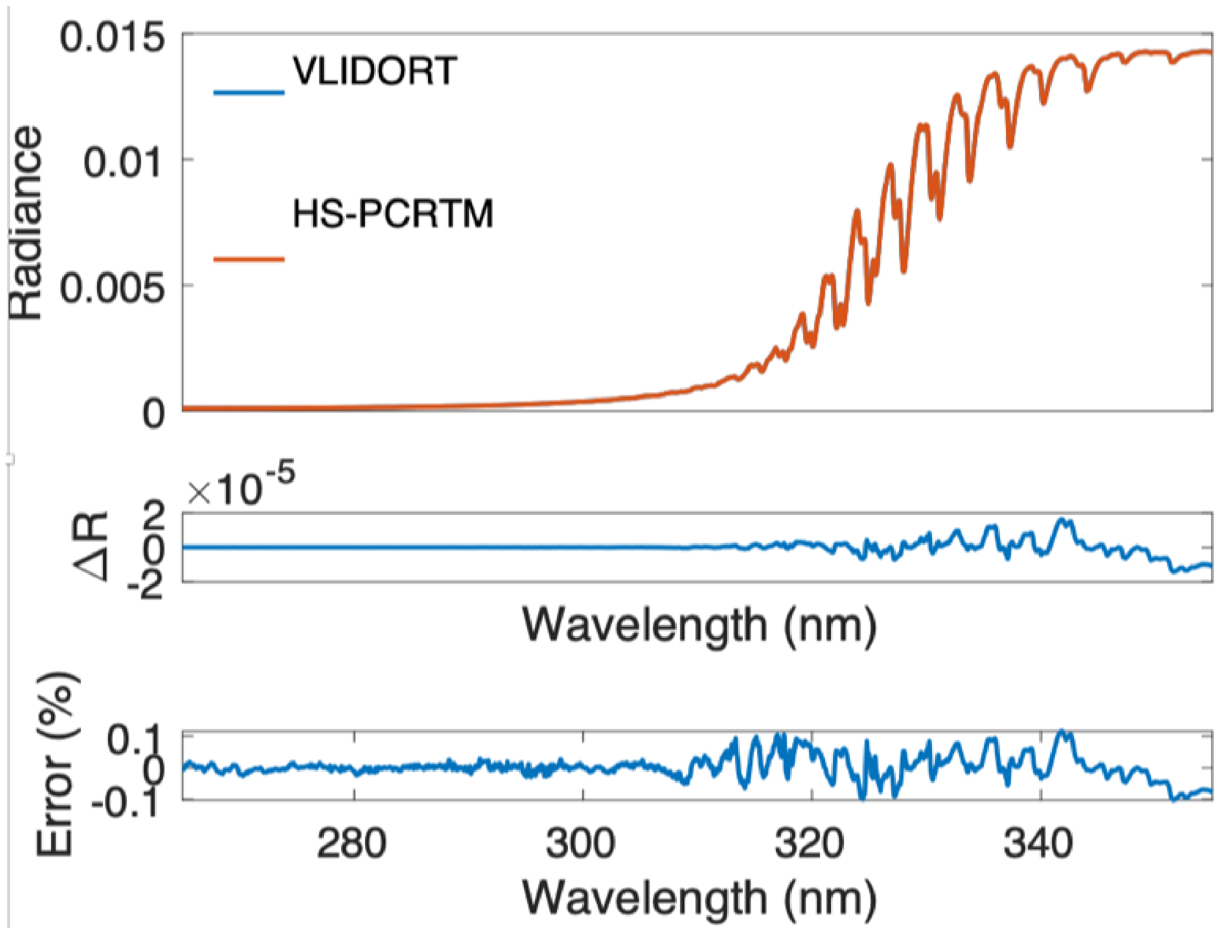
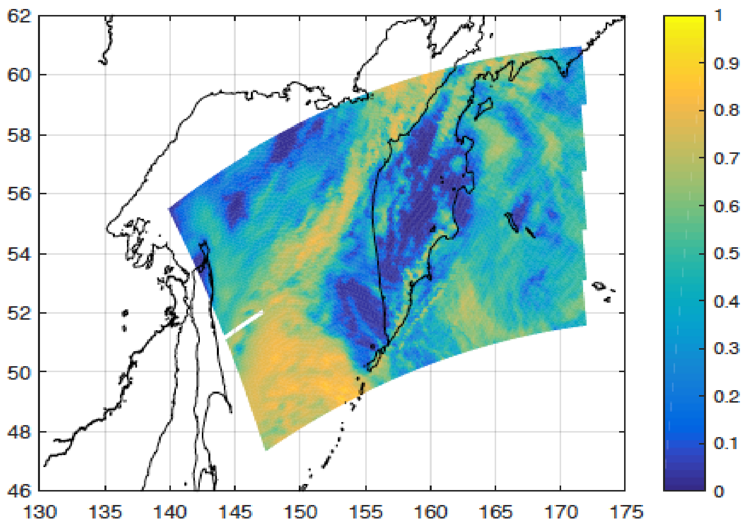
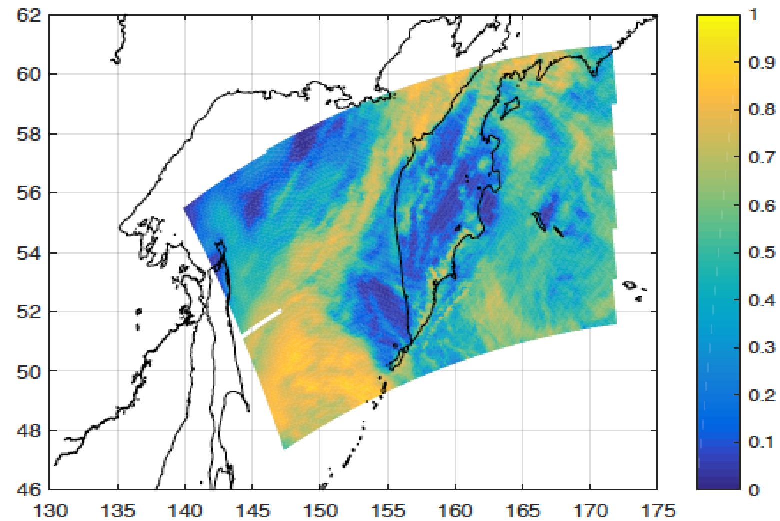


PCRTM for Reflected Solar Region

PCRTM Simulated Reflectance @646 nm using MODIS L2 data

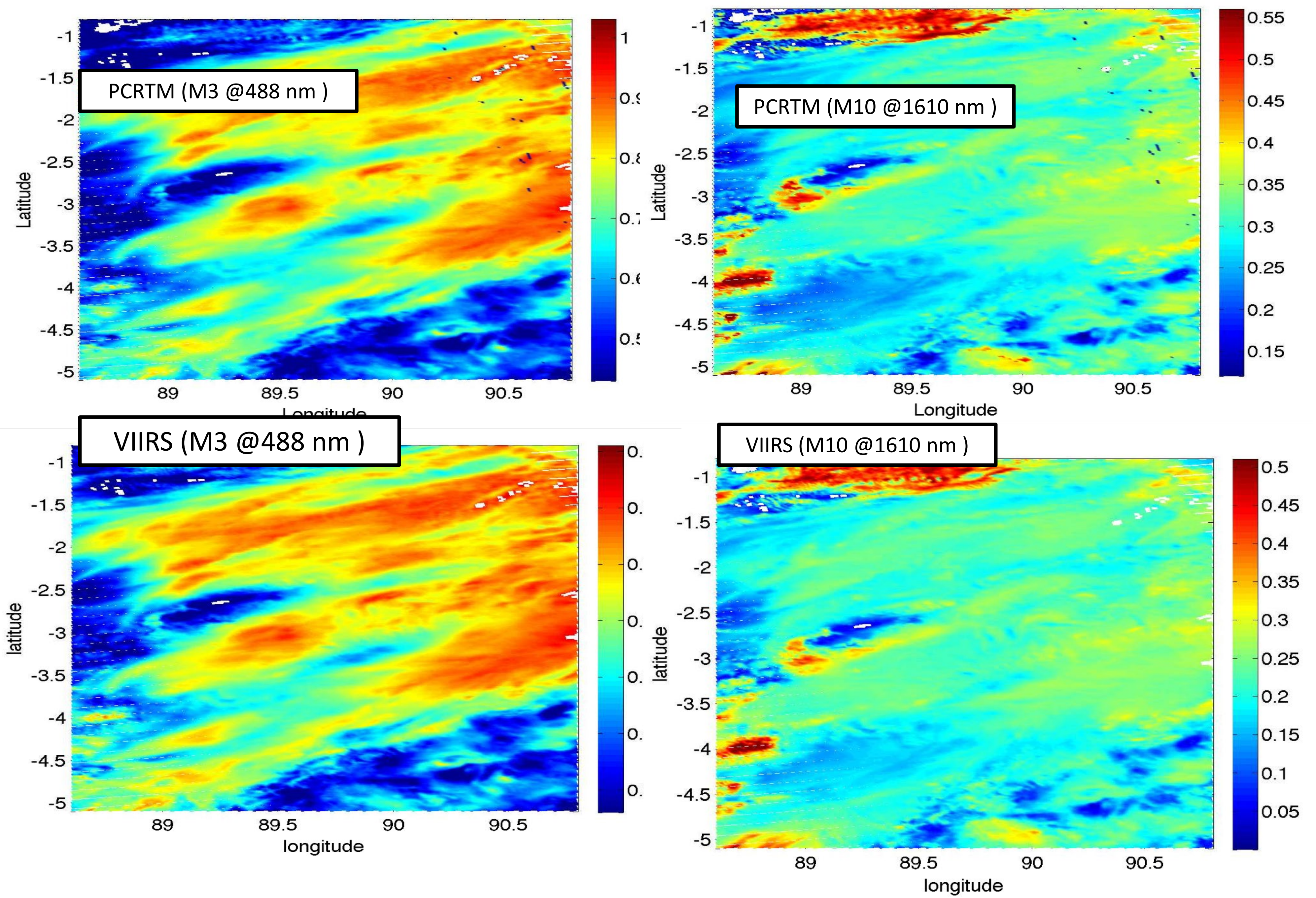


MODIS L1 Observed Reflectance @646 nm

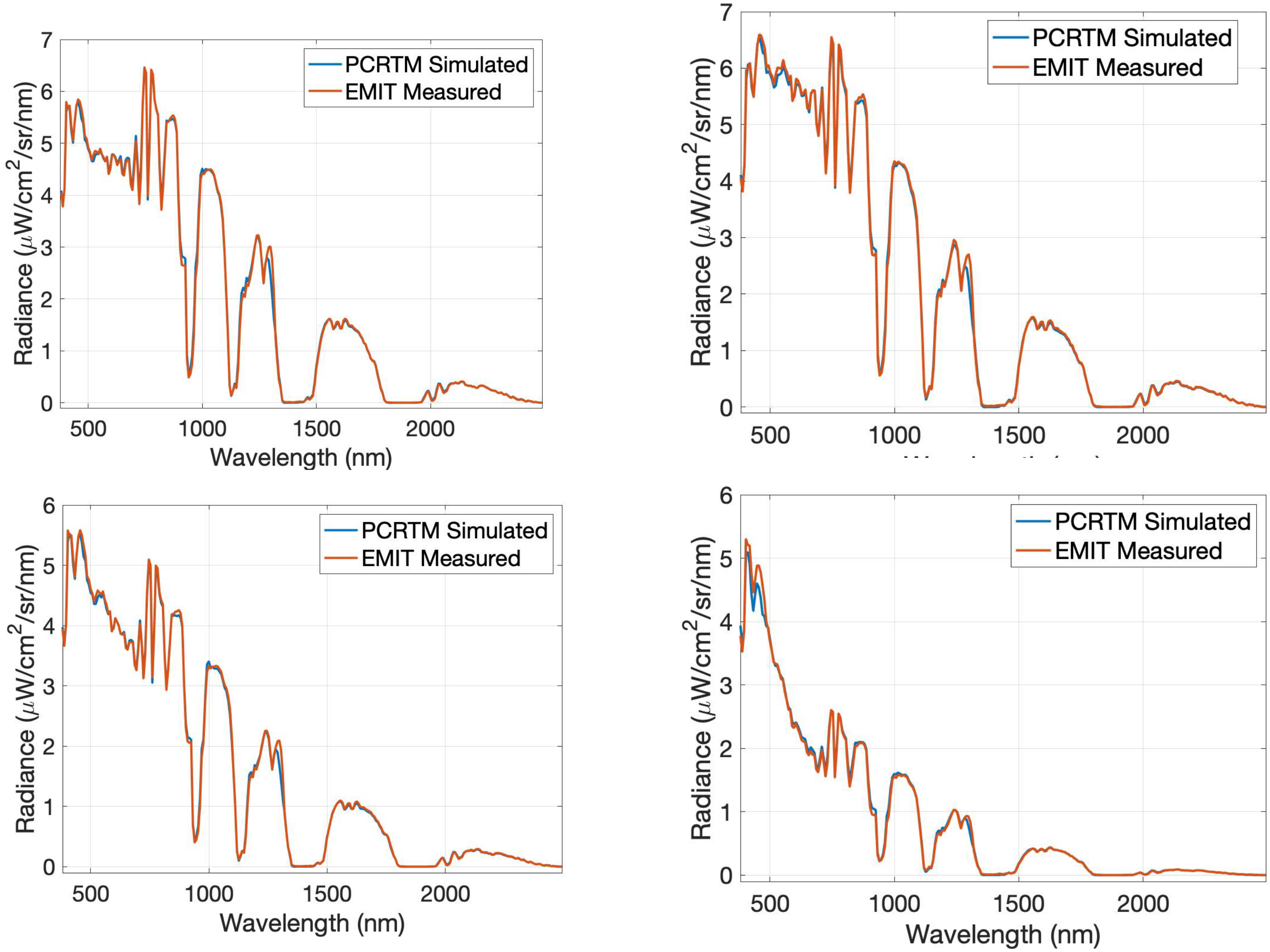


- PCRTM calculated reflectances agree well with those observed by SCHIAMACHY and MODIS
- PCRTM is 3-4 orders of magnitude faster than MODTRAN
- A Climate OSSE, which will take MODTRAN 10 years to run on one CPU, can be accomplished with PCRTM in 10-20 hours using one CPU
- MODTRAN-based PCRTM has been developed for CALRREO, CPF, EMIT, and SCHIAMACHY
- VLIDORT-based PCRTM (which accounts for polarization) has been developed for OMI/TEMPO O_3 spectral region and being developed for EMIT and SBG
- PCRTM has been extensively used by CLARREO and CPF for various studies (spectral fingerprinting, spectral band expansion, angular mismatch error correction for satellite inter-cal etc.

High Fidelity CPF Simulator Validated Using VIIRS Observations

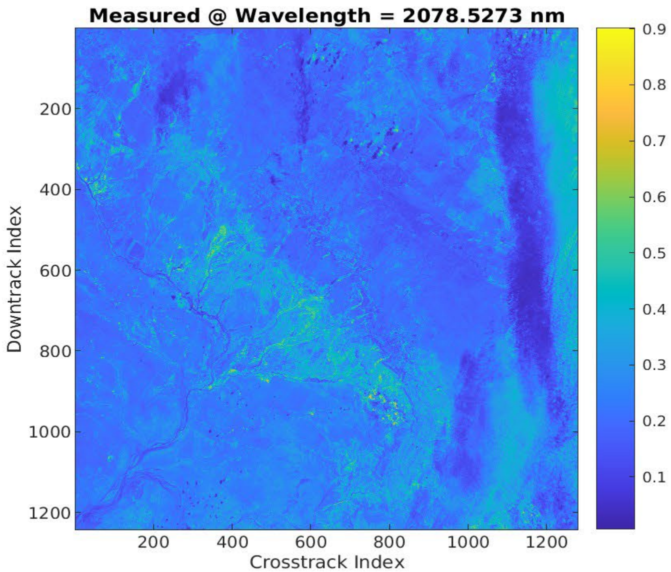


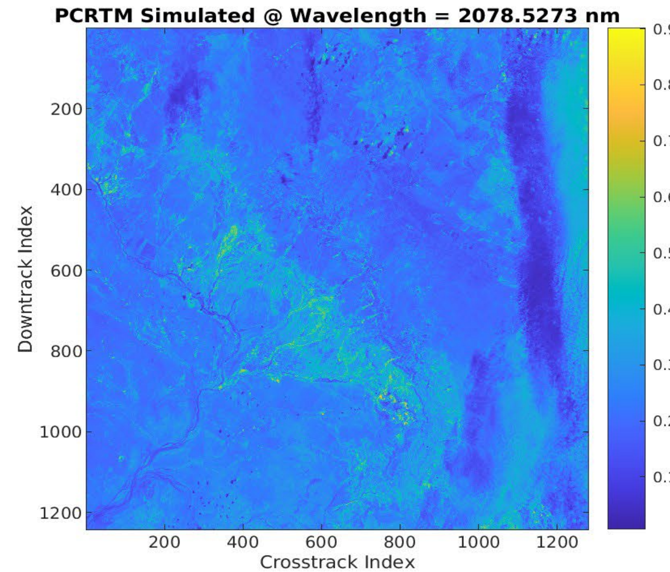
Examples of PCRTM simulated and EMIT observed spectra



PCRTM simulated spectra agree all well with EMIT observation at different wavelengths and 1.6 million pixels

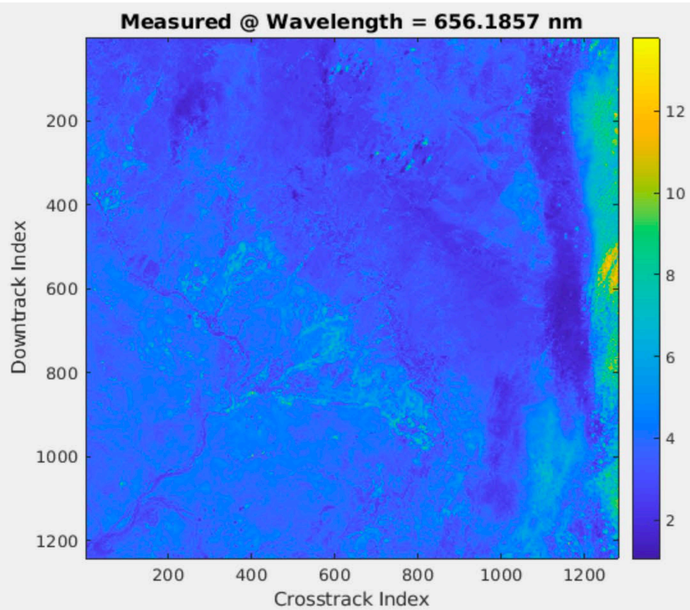
EMIT observed radiance at 2078.5 nm

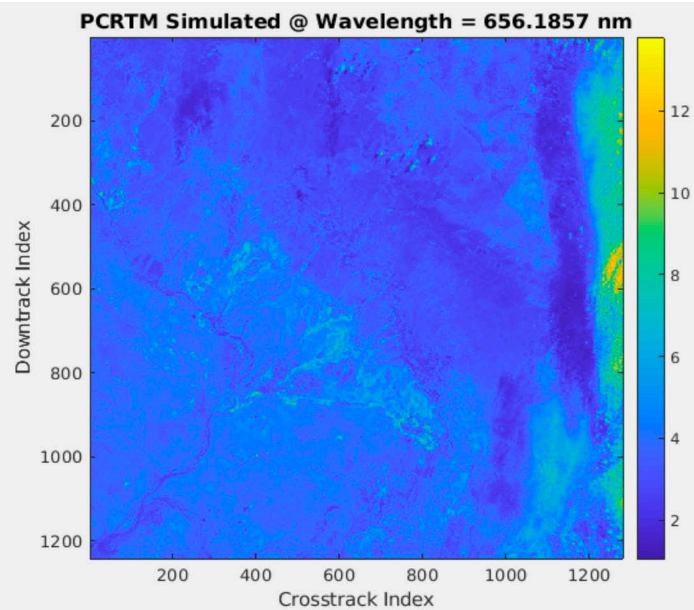




PCRTM simulated radiance at 2078.5 nm using EM L2 product as input

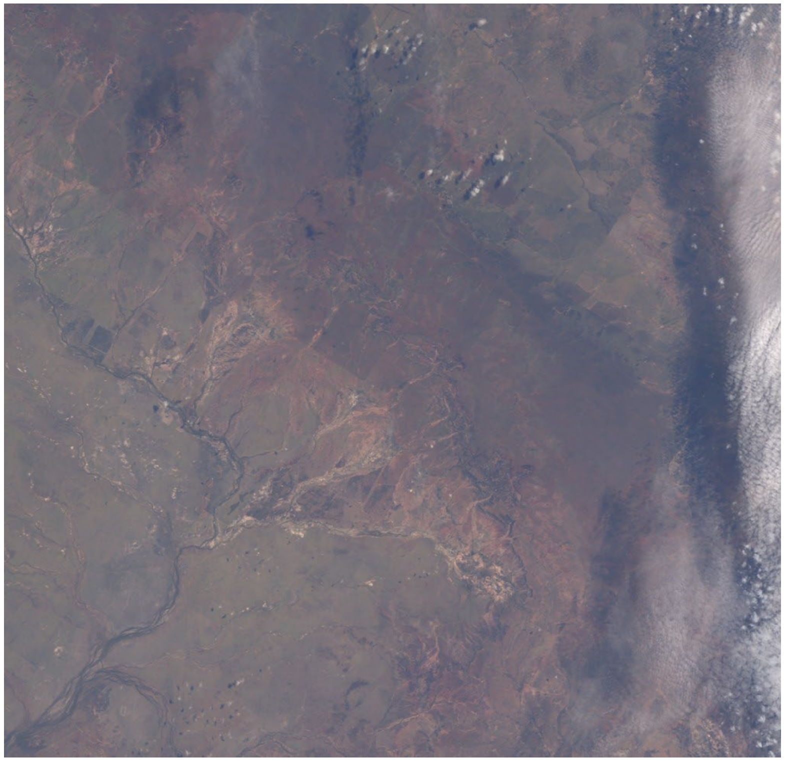
EMIT observed radiance at 656.2 nm



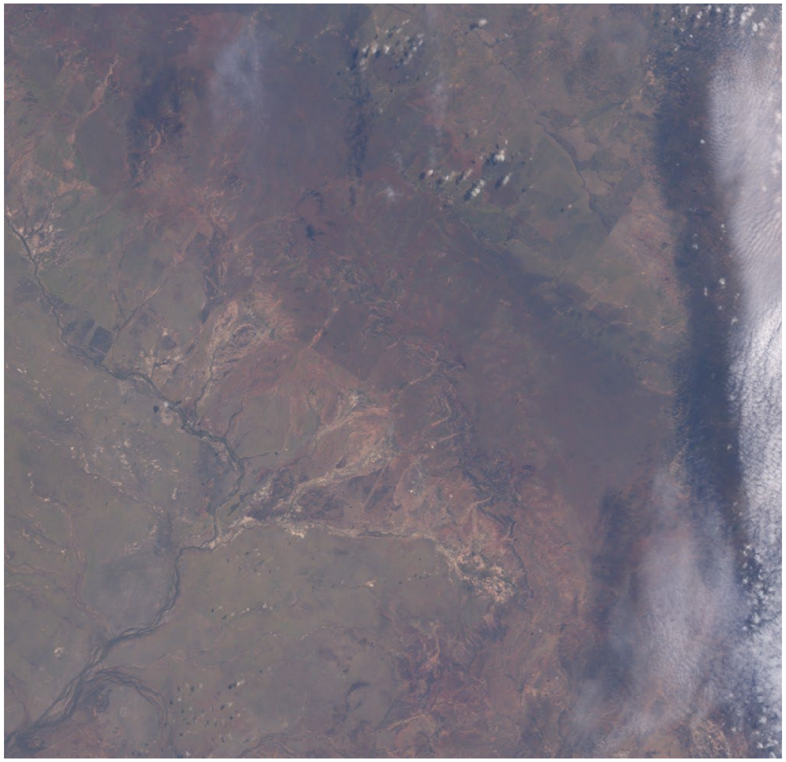


PCRTM simulated radiance at 656.2 nm using EM L2 product as input

PCRTM Simulated RGB image and spectra agree well with EMIT L1 observations (indicating high EMIT L2 product quality)



EMIT RBG Image



PCRTM Calculated EMIT RBG Image

Overview of different retrieval algorithms for inverting hyperspectral IR sounder data (1)

- Iterative physical retrieval algorithms based on fitting ”cloud-cleared” radiance
  - ➢ Only clear sky radiative transfer model (RTM) needed
  - ➢ Uses Cloud-Clearing (CC) method to remove the cloud spectral features from the radiance spectra
    - o Needs good a priori
    - o Scarifies spatial resolution
    - o Radiometric closure with CC radiance
  - ➢ Examples of CC algorithms
    - o NUCAPS (NOAA Unique Combined Atmospheric Processing System)
    - o CLIMCAPS (Community Long-Term Infrared Microwave Combined Atmospheric Product System)
    - o AIRS V7 (AIRS V7 Level-2 algorithm)
- Iterative physical retrieval algorithm based on fitting all-sky radiance
  - ➢ All-sky RTM needed
  - ➢ 9-times higher area spatial resolution relative to CC method
  - ➢ Radiometric closure with all-sky observed radiances
  - ➢ Examples of cloudy algorithms
    - o SiFSAP ((Single Field-of-view Sounder Atmospheric Product): fit all spectral channels + 22 ATMS spectral channels
    - o JOSFRA (Joint Single Footprint Retrieval Algorithm): fit selected channels

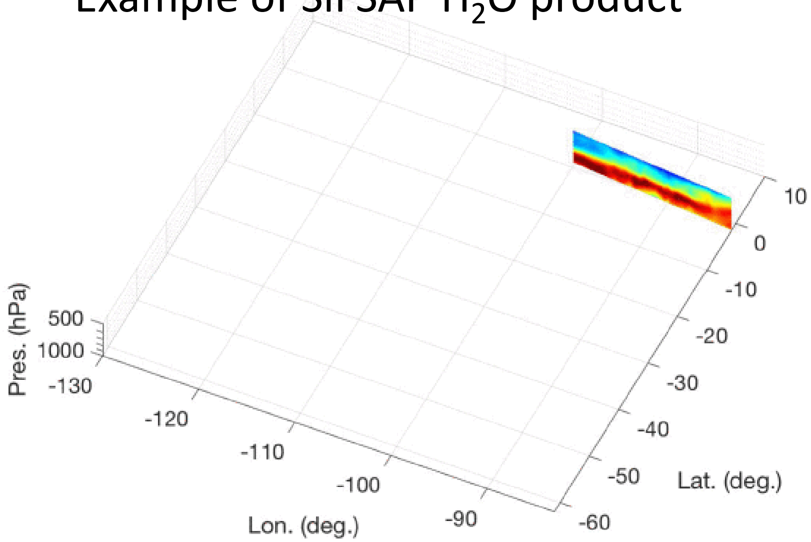
Overview of different retrieval algorithms for inverting hyperspectral IR sounder data (2)

- Statistical based retrieval algorithm based on all-sky radiances
  - Much faster than iterative physical retrieval algorithms
  - Using stratification/classification/AI to reduce non-linearity
  - PCA is used for dimension reduction
  - Performance highly depends on the quality of training data
  - No radiometric closure to the observed radiances
  - Trained based on RTM simulated radiance
    - Dual-regression algorithm with PCRTM-based de-aliasing (Bill Smith)
  - Trained using collocated ECMWF T/Q/O3:
    - IASI operational Level-2 retrieval algorithm: PWLR (Piece-Wise Linear Regression)
    - MIT Lincoln Laboratory Stochastic Cloud Clearing/Neural Network algorithm (SCCNN)
- Spectral fingerprinting method based on physical retrieval algorithm (***new!***)
  - As fast as statistical retrieval algorithm
  - Accurate retrieval with performance equivalent to a physical algorithm
  - Radiometric closure with the observed all-sky radiance
  - ClimFiSP (Climate Fingerprinting Sounder Product)
    - Machine-learning linear inversion based on SiFSAP physical retrievals
    - Consistent radiative kernels used for different satellite sensors
    - Can generate products using single-FOV or spatial-temporally averaged radiances
    - Suitable for real-time and long-term climate applications

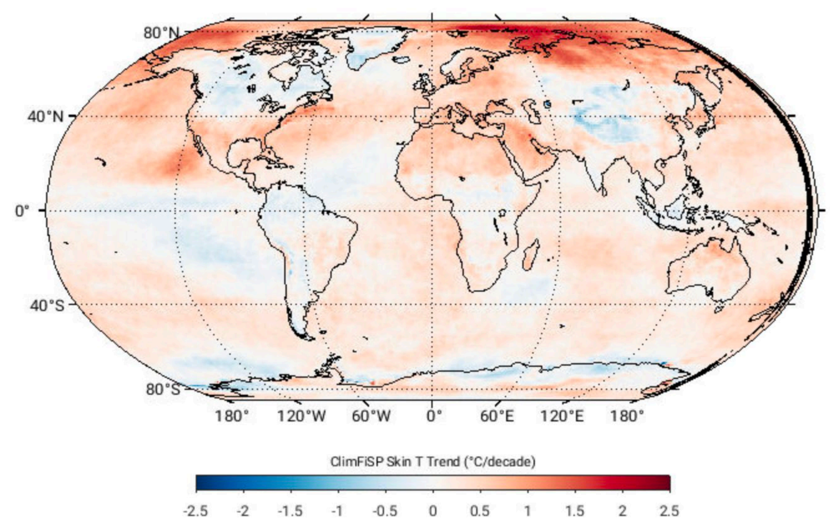
Two PCRTM-based Inversion Algorithms

- L2 products: Single Field-of-view Sounder Atmospheric Product (SiFSAP)
  - 3-times higher spatial resolution
  - Uses all spectral channel
  - All sky algorithm-retrieves cloud explicitly
  - Retrieve temperature, clouds, trace gases, and surface properties simultaneously
- L3 Products: Climate Fingerprinting Sounder Products (ClimFiSP)
  - Works on spatiotemporally averaged radiance spectra
  - Use consistent radiative kernels for all three satellite sensors
  - Ensure radiometric closures
  - Generates high-quality climate product from multiple satellite data (20 years AIRS, SNPP CrIS, and NOAA20 CrIS)
- Both products will be available at NASA GES DISC for public access
- The PCRTM based algorithm has been extended to solar spectral region

Example of SiFSAP H_2O product

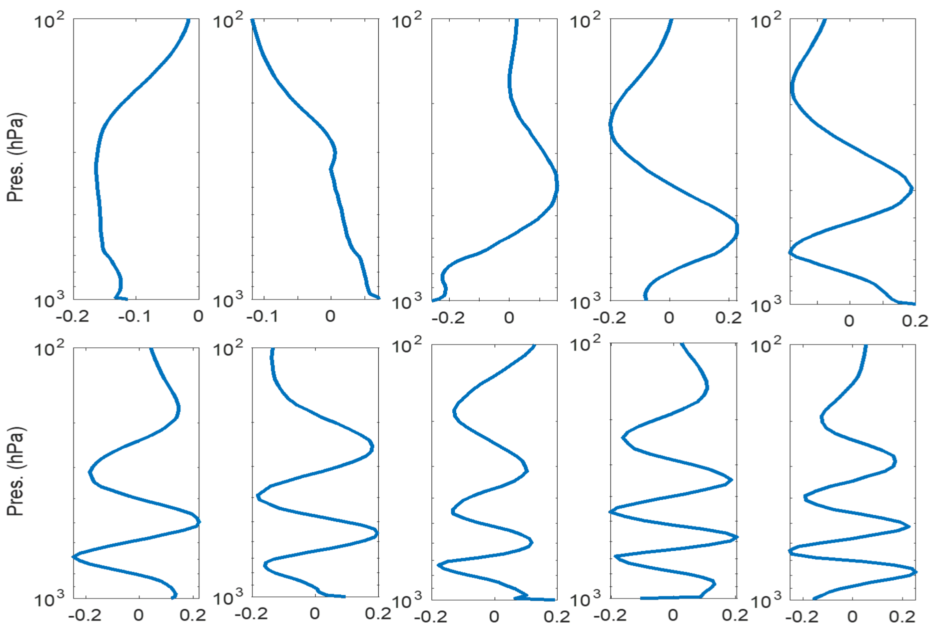


Example of ClimFiSP derived global surface temperature trend



Compression of both Hyperspectral Observations and Retrieved Parameters

Example of PCs representing H2O vertical profiles

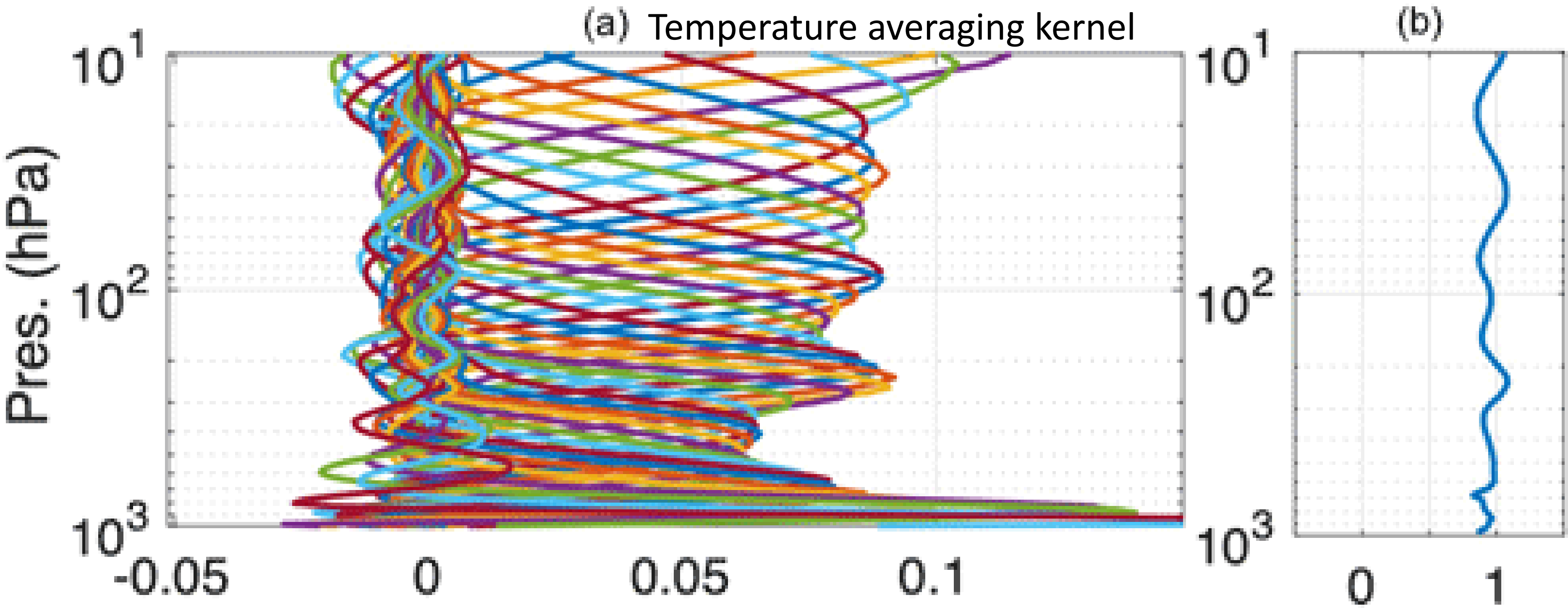


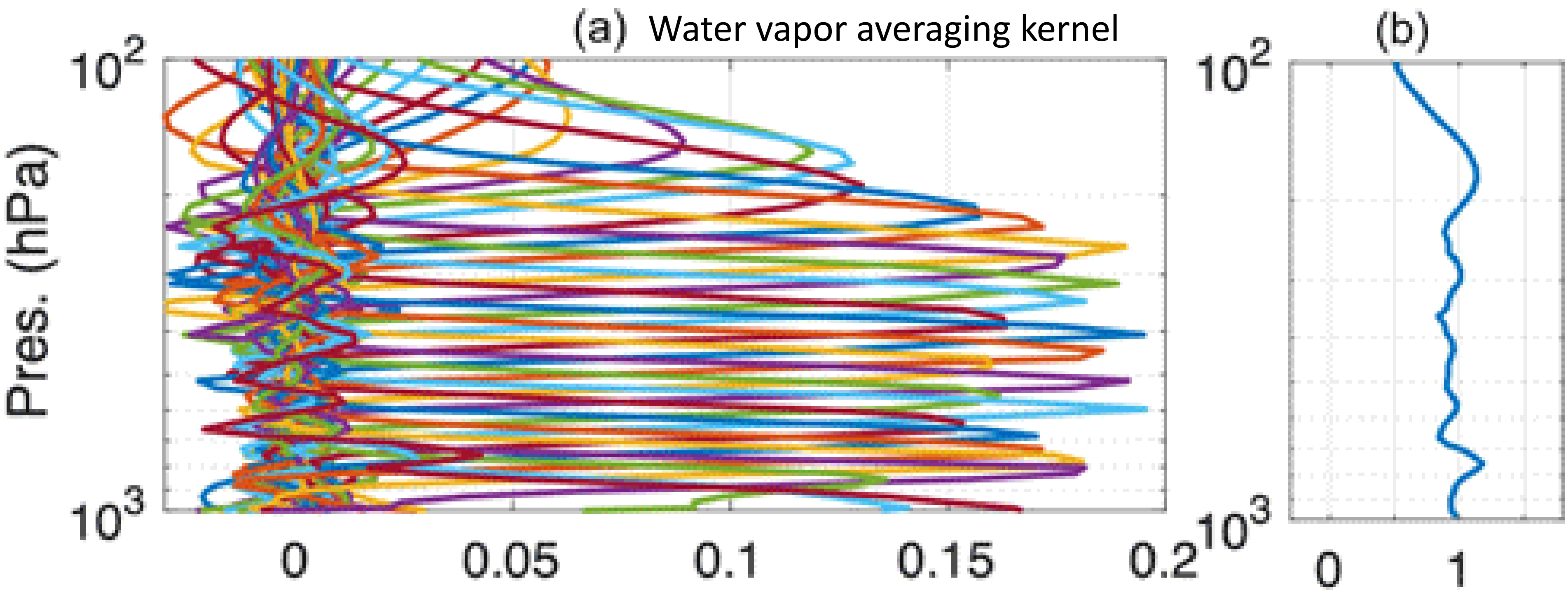
Reducing AIRS, CrIS, and IASI dimensions

Satellite Sensors	Original Dim	PC-compressed Dim
CrIS	2211	124
AIRS	2378	120
IASI	8461	190

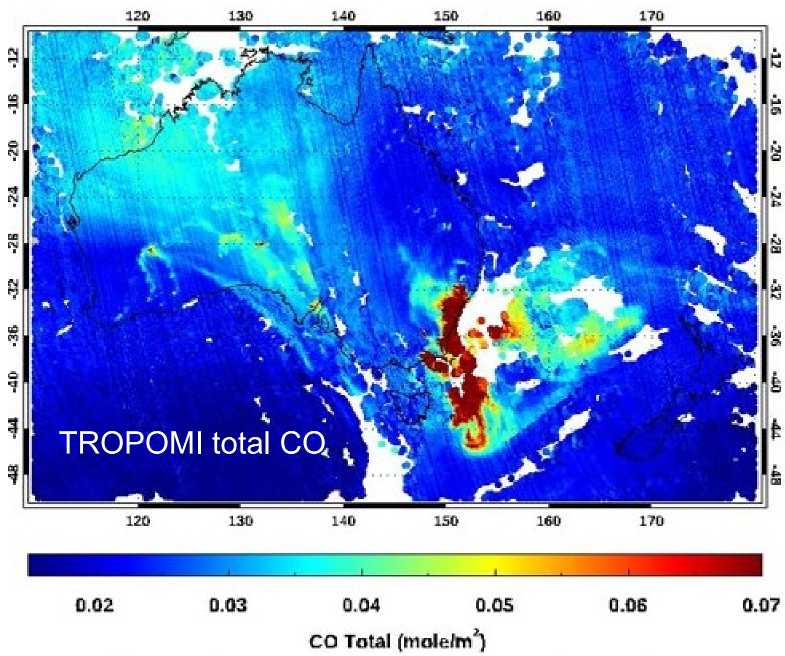
Reducing atmospheric temperature, water vapor, and trace gas profile dimensions and surface emissivity dimensions using PCA

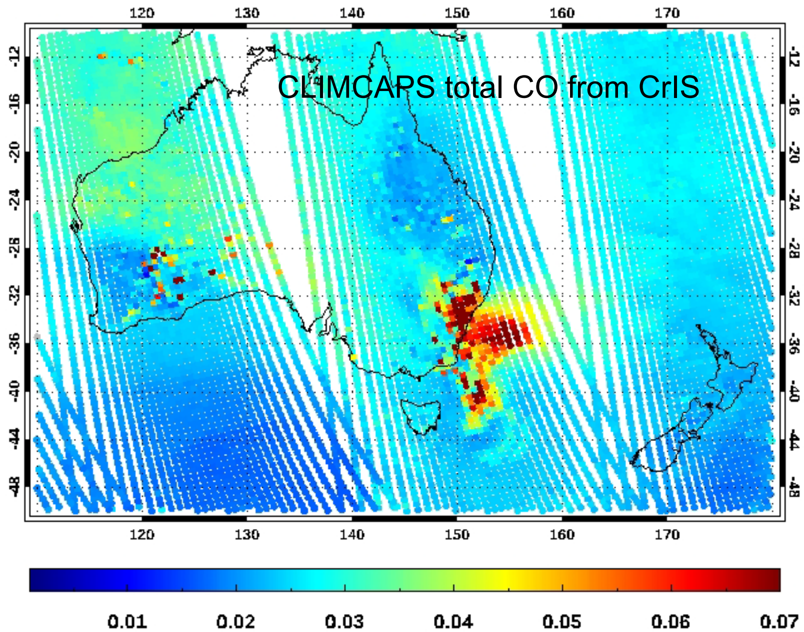
Geophysical Parameters	Original Dimension	PC-compressed Dimension
Temperature	101	20
H2O	101	15
CO2	101	1
O3	101	10
CO	101	4
CH4	101	2
N2O	101	2
IR Surface Emissivity	Hundreds - thousands	8
MW Surface Emissivity	15-22	5

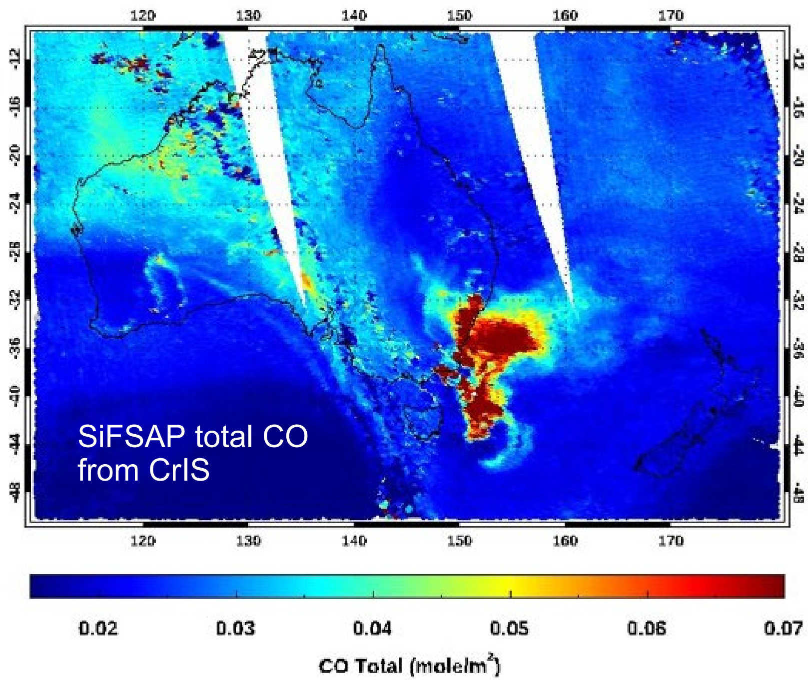

(a) Temperature averaging kernel
(b)
Pres. (hPa)
10^1
10^2
10^3
-0.05
0
0.05
0.1
1


(a) Water vapor averaging kernel
(b)
Pres. (hPa)
10^2
10^3
0
0.05
0.1
0.15
0.2
1

High Spatial Resolution SiFSAP CO from CrIS and comparison with TROPOMI for Australia Fires on December 30, 2019







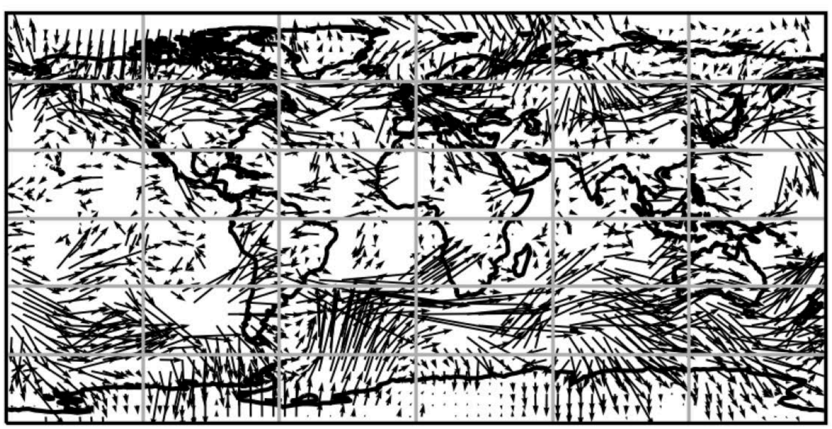
- Both TROPOMI (4 km resolution) and SiFSAP (14 km) capture fine CO plume spatial distributions
- CLIMCAPS cannot capture the fine CO features
  - Low resolution retrieval (45 km)
  - Less coherent CO due to errors in cloud clearing
- SiFSAP is less affected by the fire particular (dust) emission relative to TROPOMI
  - SiFSAP retrieves effective cloud optical depth to compensate for fire particular contributions
  - TROPOMI has many non-successful retrievals due to clouds and fire dust emissions

Example of 3-D Atmospheric Wind Vectors Derived from SNPP/CrIS and NOAA20/CrIS SiFSAP (Univ. Arizona)

SIFSAP (July 7, 2020)

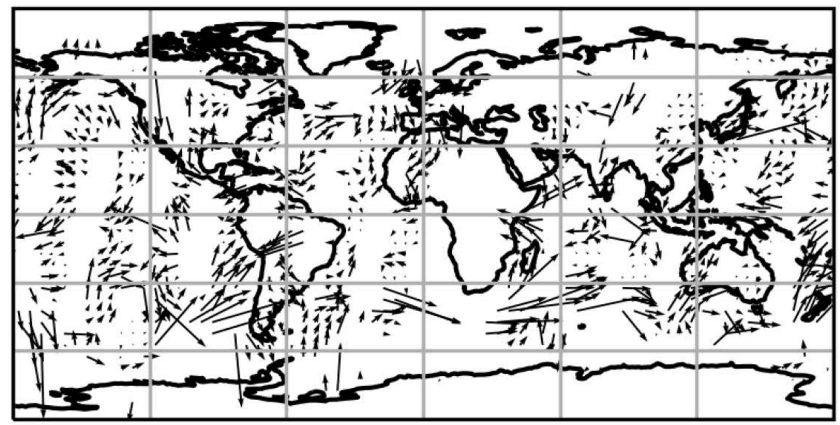
RMSVD = 6.1 m/s 850 hPa Δs = 0.77 m/s

RMSVD = 5.87 m/s 500 hPa Δs = -0.91 m/s

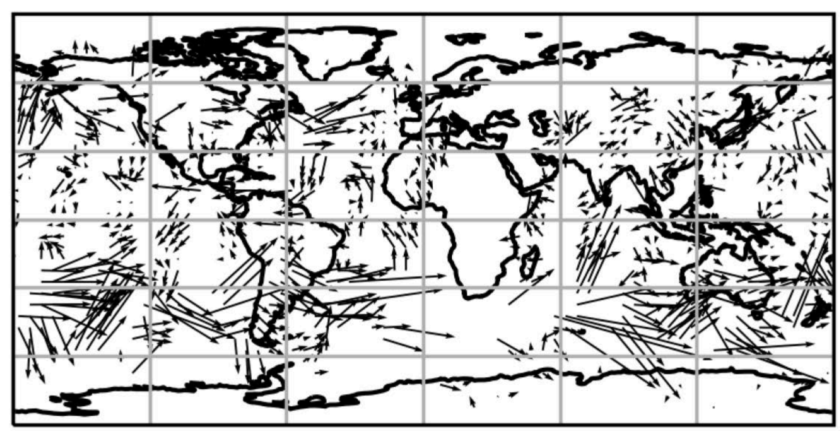


CLIMCAPS (July 7 2020)

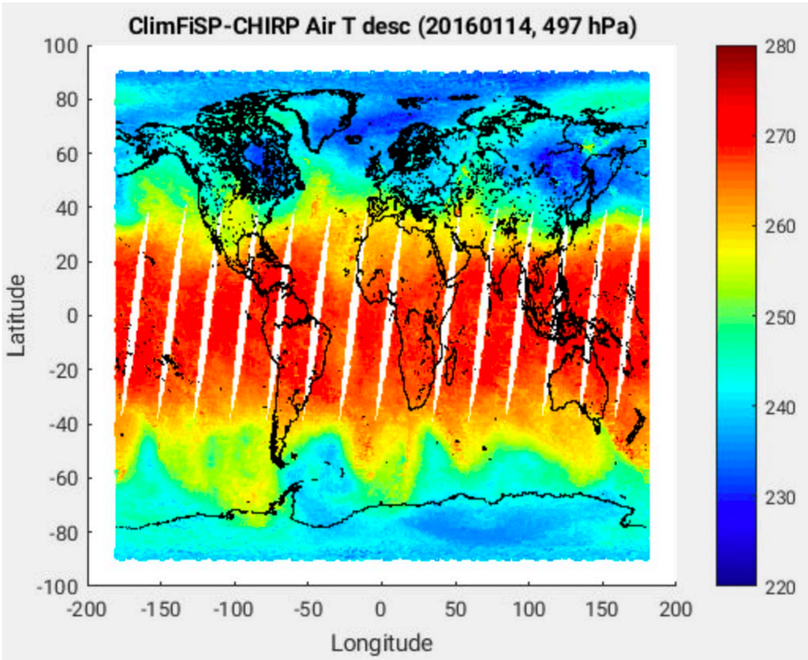
RMSVD = 5.72 m/s 850 hPa Δs = -2.18 m/s

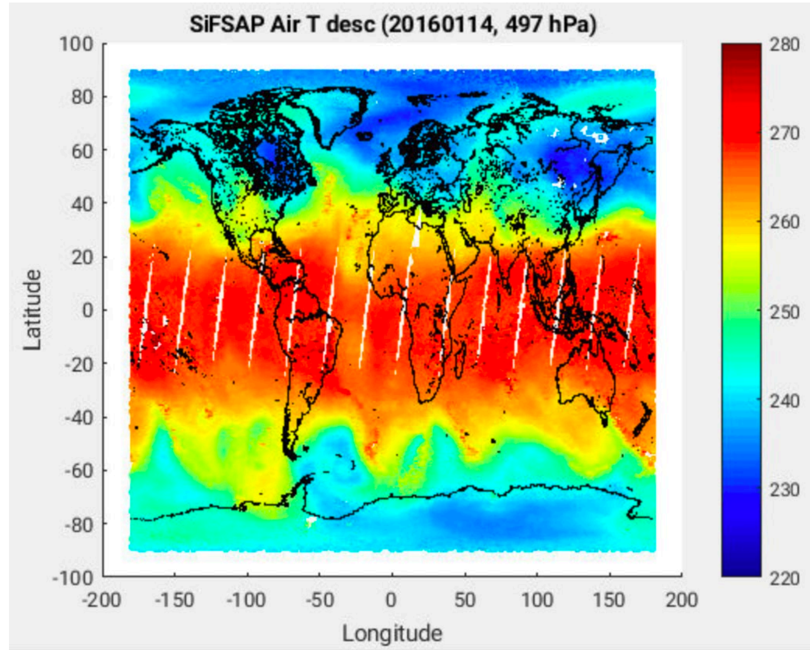


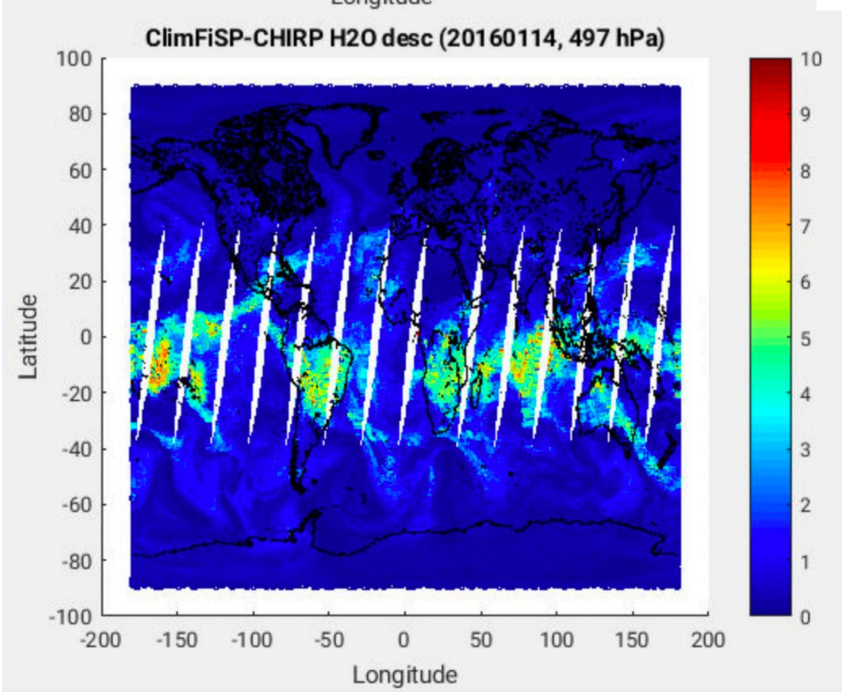
RMSVD = 5.99 m/s 500 hPa Δs = -2.09 m/s

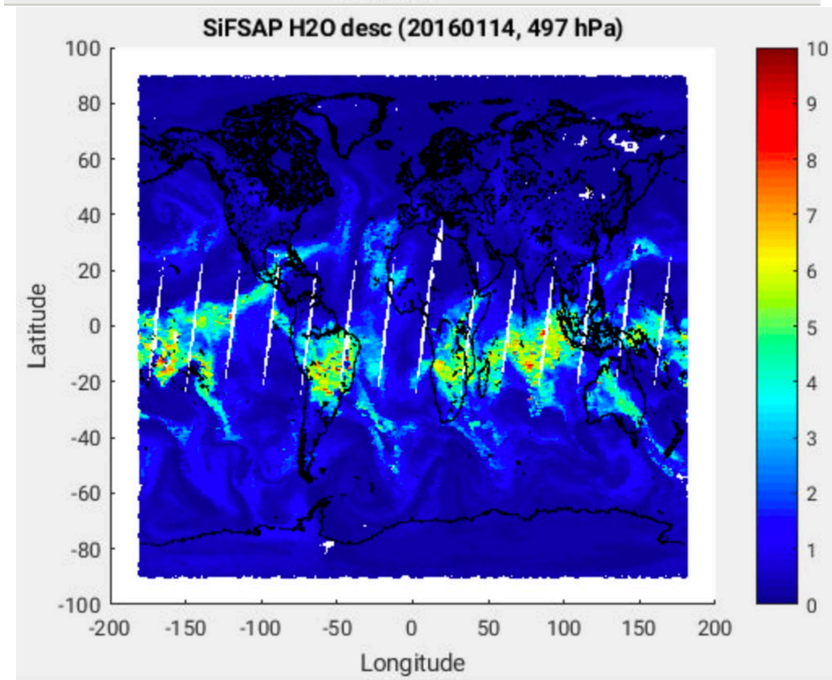


Consistent Daily Products from both SiFSAP and ClimFiSP



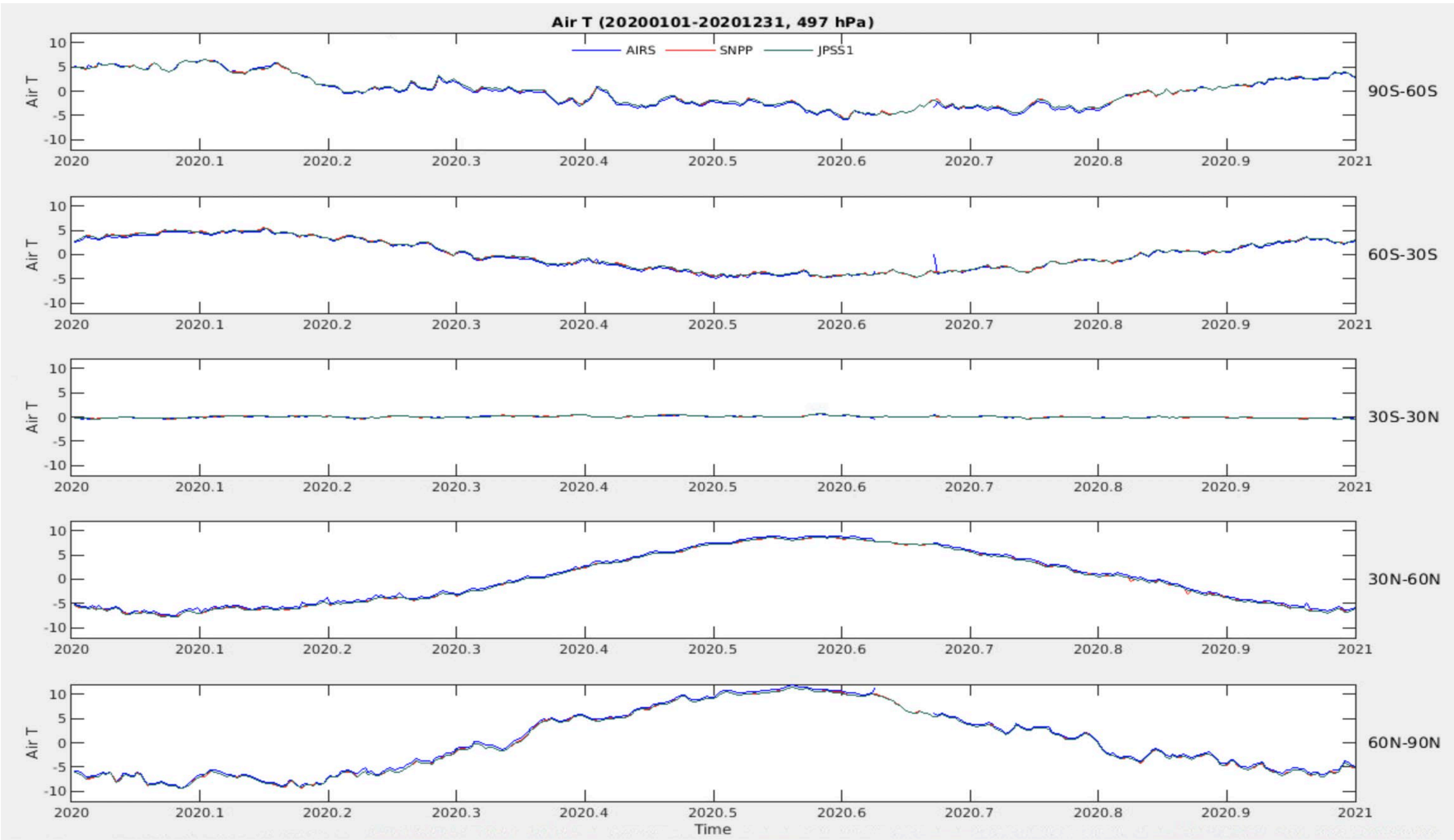






Consistent ClimFiSP Products from Aqua/AIRS, SNPP/CrIS, and NOAA20 CrIS (2020)

500 hPa Temperature from Aqua/AIRS (Blue) SNPP/CrIS (Red), and NOAA20/CrIS (Green)

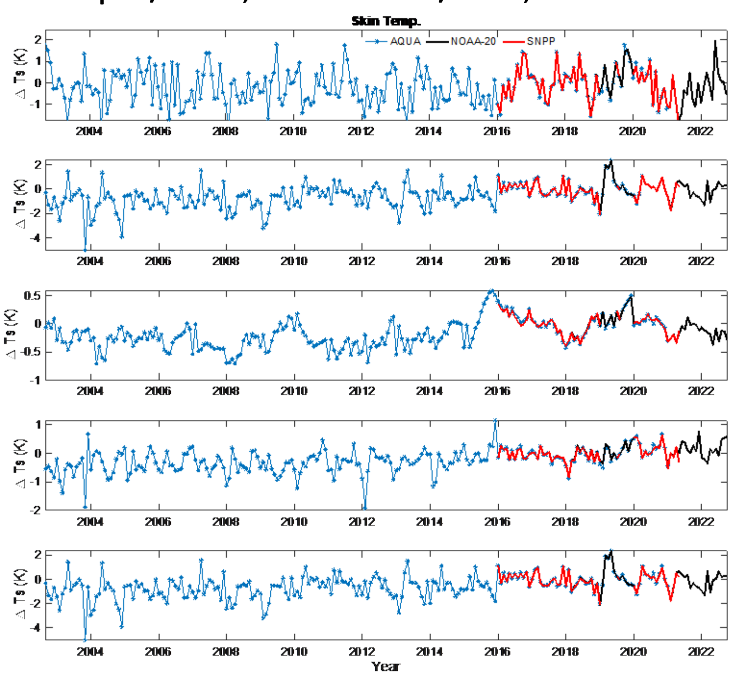


Applying the ClimFiSP Algorithm to CHIRP

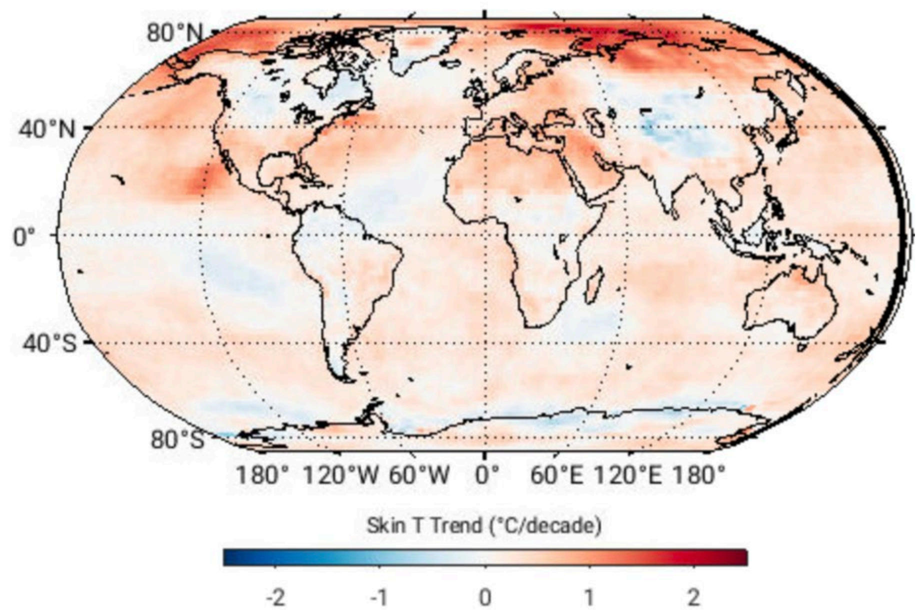
- CHIRP - Climate Hyperspectral Infrared Radiance Product
  - ➢ Bias-corrected radiance (L1) time series for Aqua/AIRS, SNPP/CrIS, and NOAA20/CrIS
  - ➢ Generated by Larrabee Strow et al (2021)
  - ➢ Available at NASA Sounder SIPS and DACC

- We have applied the ClimFiSP algorithm to CHIRP data from 2003-2022
  - ➢ Obtained climate time series for:
    - o atmospheric temperature, water vapor, O3, and other trace gas vertical profiles
    - o cloud optical depth, cloud height, and cloud particle size
    - o surface skin temperature, and surface emissivity

Example of ClimFiSP derived global surface temperature time series for different latitude bins
Blue:Aqua/AIRS, Red: SNPP/CrIS, Black: NOAA20/CrIS

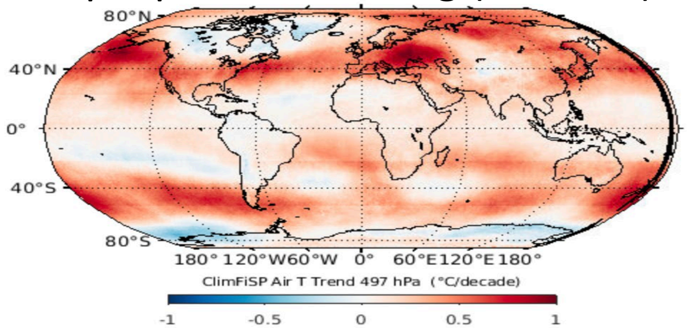


Example of ClimFiSP derived global surface temperature trend from 20 years of sounder data

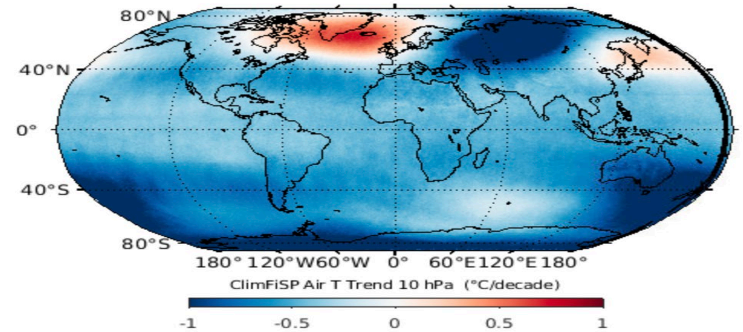


20-year Climate Trends from ClimFiSP

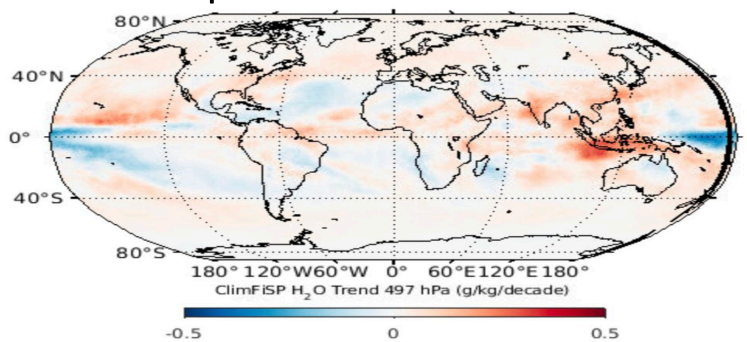
Tropospheric warming (500 hPa)



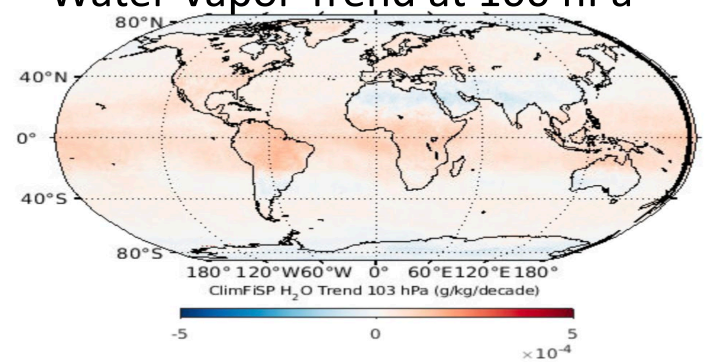
Stratospheric cooling (10 hPa)



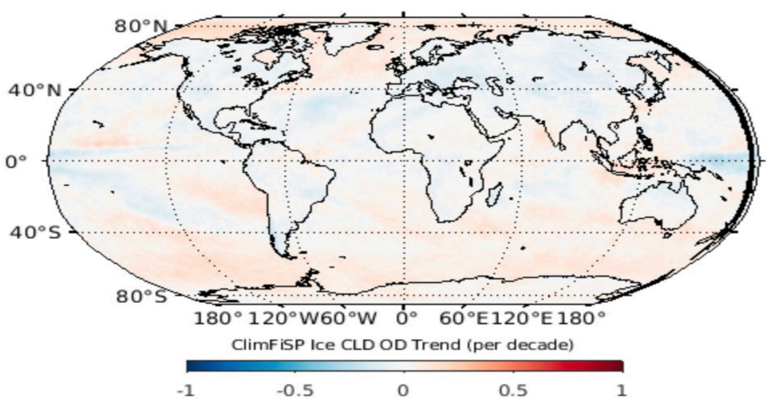
Water Vapor Trend at 500 hPa



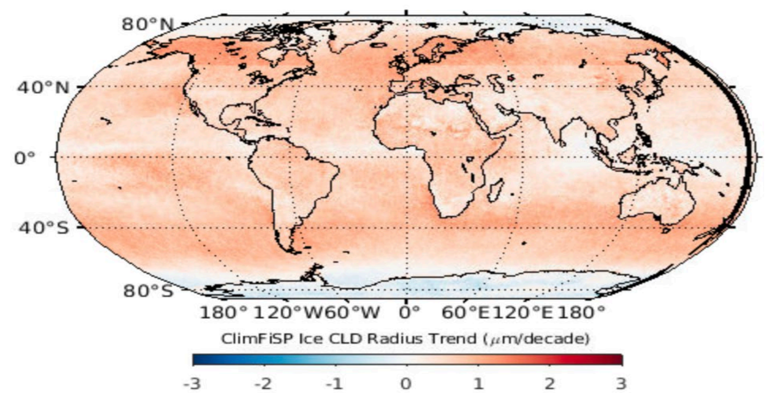
Water Vapor Trend at 100 hPa

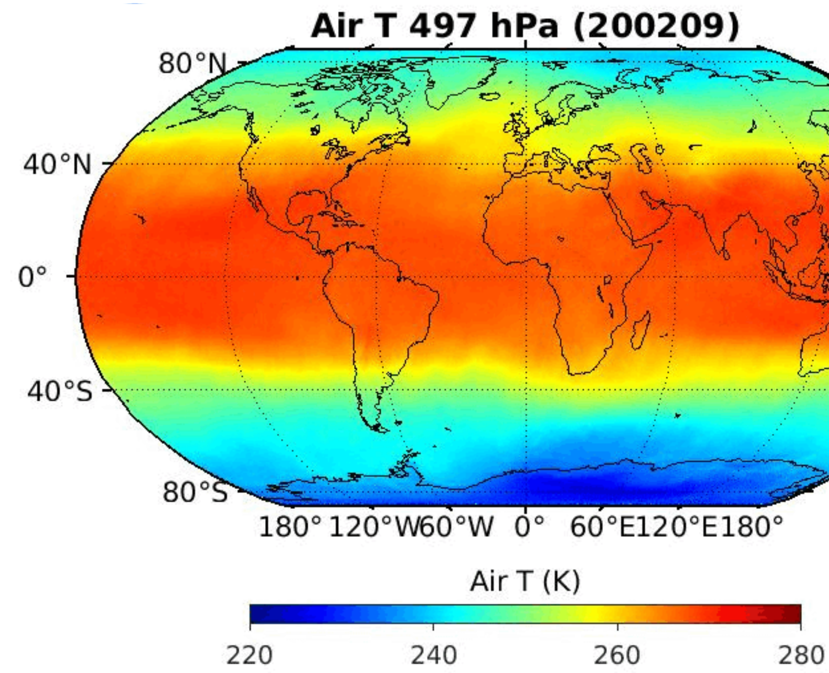


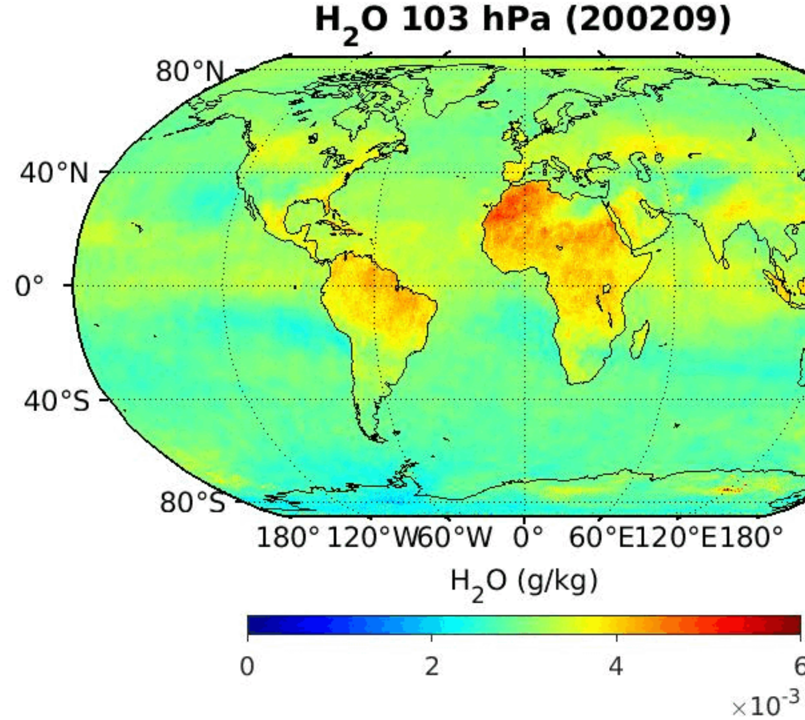
ClimFiSP Ice Cloud Optical Depth Trend

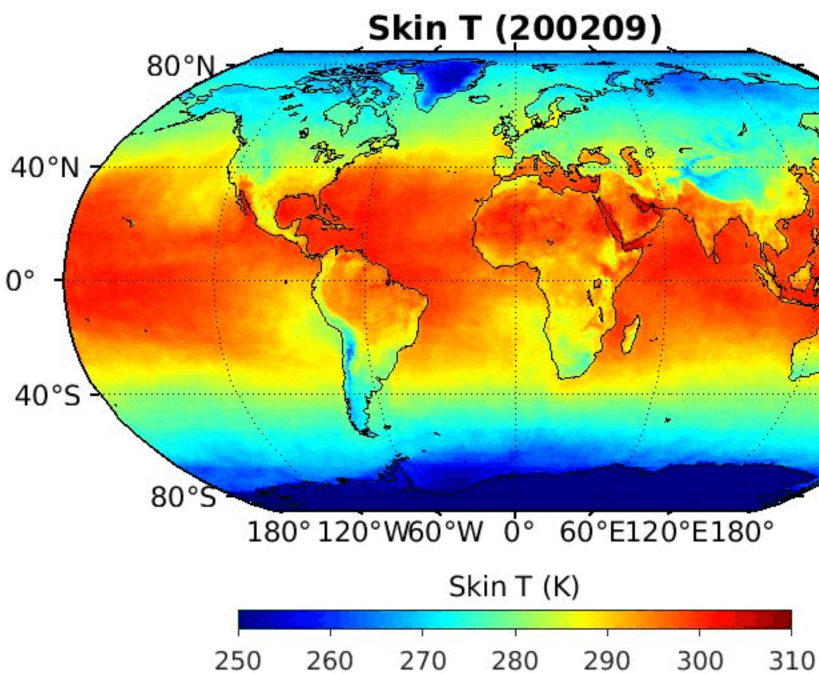


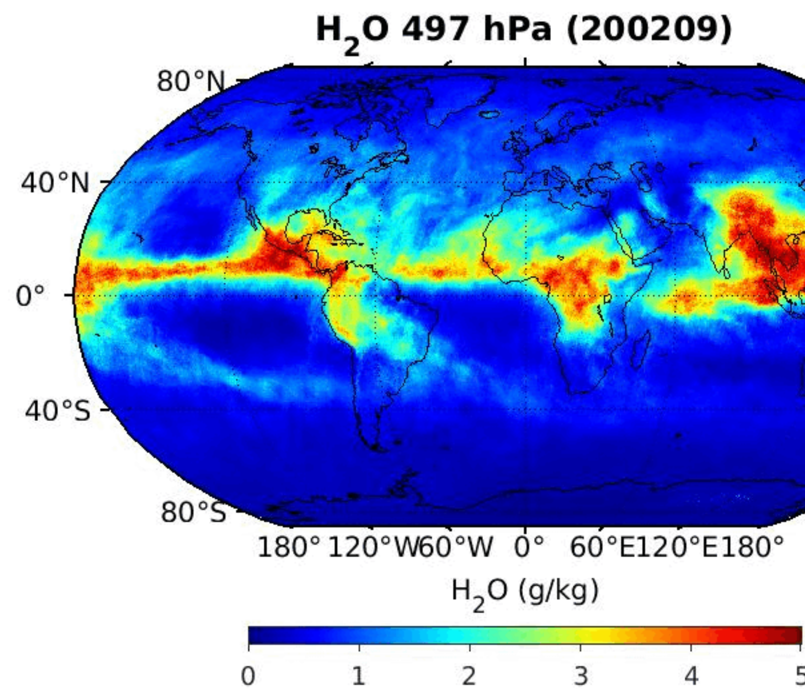
ClimFiSP Ice Cloud Effective Radius



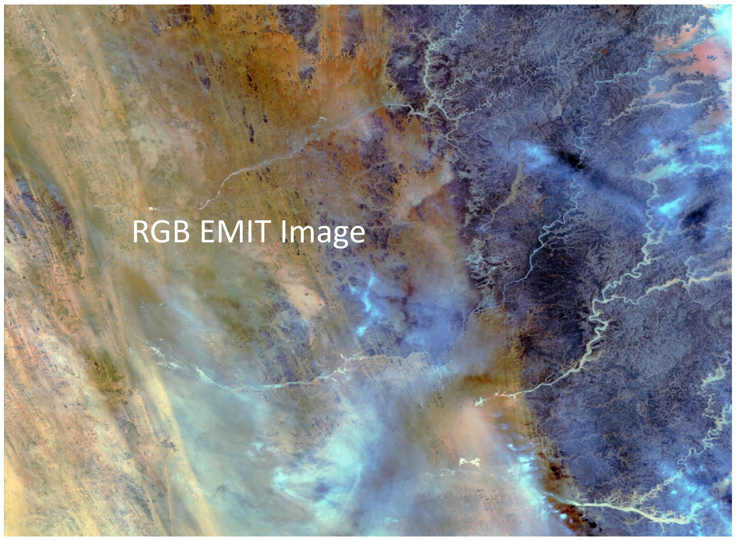

Air T 497 hPa (200209)
80°N
40°N
0°
40°S
80°S
180° 120°W60°W 0° 60°E120°E180°
Air T (K)
220
240
260
280

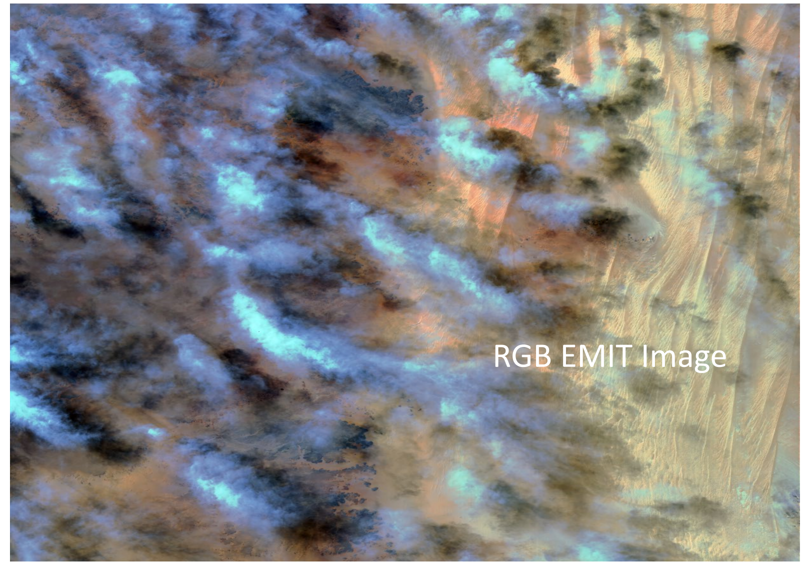

H_2O 103 hPa (200209)
80°N
40°N
0°
40°S
80°S
180° 120°W60°W 0° 60°E120°E180°
H_2O (g/kg)
0
2
4
6
$\times 10^{-3}$

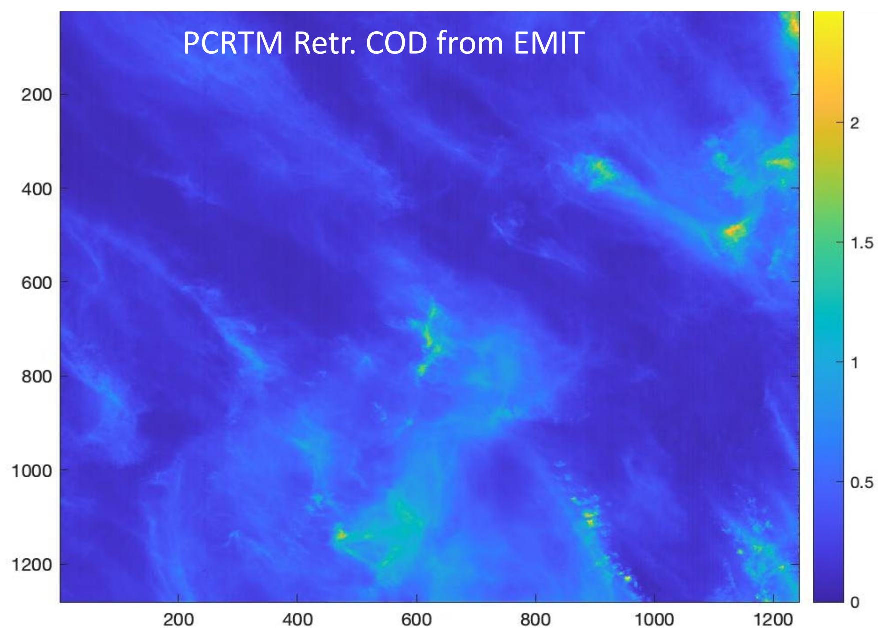

Skin T (200209)
80°N
40°N
0°
40°S
80°S
180° 120°W60°W 0° 60°E120°E180°
Skin T (K)
250
260
270
280
290
300
310

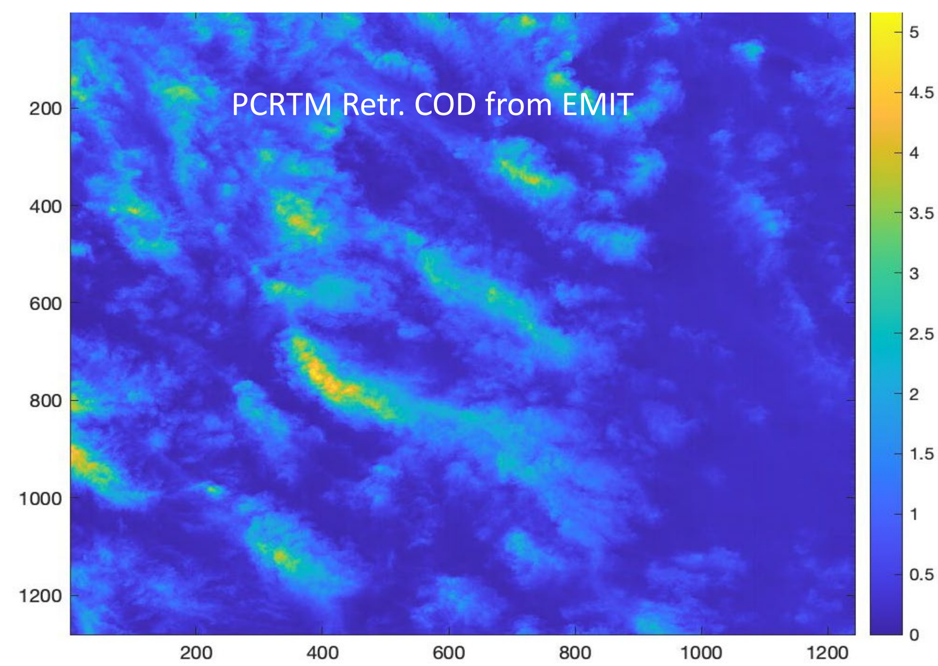

H_2O 497 hPa (200209)
80°N
40°N
0°
40°S
80°S
180° 120°W60°W 0° 60°E120°E180°
H_2O (g/kg)
0
1
2
3
4
5

PCRTM generated data are used to train an AI Cloud Retrieval algorithm for EMIT and applied successfully using EMIT data









Summary and Conclusions

- PCRTM is ideal for dealing with hyperspectral satellite remote sensors
- Both SiFSAP and ClimFiSP produce daily products from hyperspectral IR remote sensors
  - Temperature, water vapor, O_3, CO, CH_4, N_2O, CO_2 atmospheric profiles
  - Cloud temperature, pressure, optical depth, phase, and effective size
  - Surface skin temperature and surface emissivity spectra
- SiFSAP (L2) is available at NASA GES DISC
  - 9-times area spatial resolution relative to current cloud-clearing products
  - Radiometric closure condition met
- ClimFiSP (L3) is in the process of being transitioned to NASA GES DICS
  - 20 years of Climate Data Records from Aqua/AIRS, SNPP/CrIS, and NOAA20/CrIS
- PCRTM has a wide range of applications such as high fidelity satellite sensor simulator, forward model for atmospheric correction, AI-based algorithm etc.