A Simulation System for Panchromatic Retrievals of Trace Gases: Results for ozone and others

Presented by Annmarie Eldering

Jet Propulsion Laboratory
California Institute of Technology

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Contributors: Kevin Bowman, Meemong Lee, Zheng Qu, Mathew Yeates, John Worden, Ming Luo, Susan Kulawik

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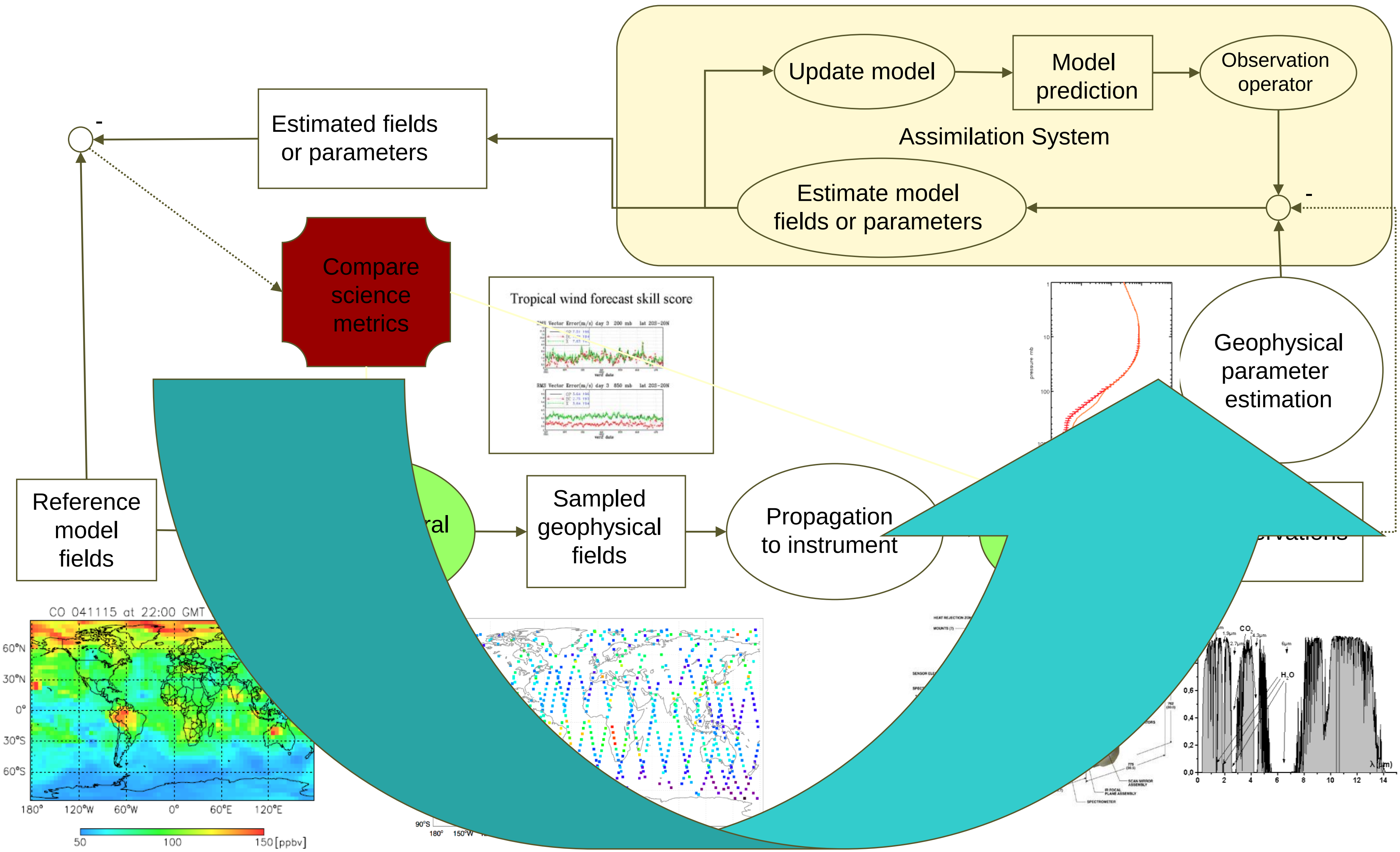
Outline:

- Motivation: Measuring tropospheric pollution and air quality from space for GEO-CAPE

2.1 Measure O3, CO, and PM to track pollution transport.	1. Tropospheric vertical spatial resolution	2 pieces of information in the vertical for O3 with sensitivity to the boundary layer	Separate the lower most troposphere from the free troposphere.
	Ozone : hourly for SZA<70	2.4×10^{16} cm^{-2} typical. 6×10^{15} cm^{-2} precision	Deleted HCHO, and CHOCHO for tracking pollution transport.

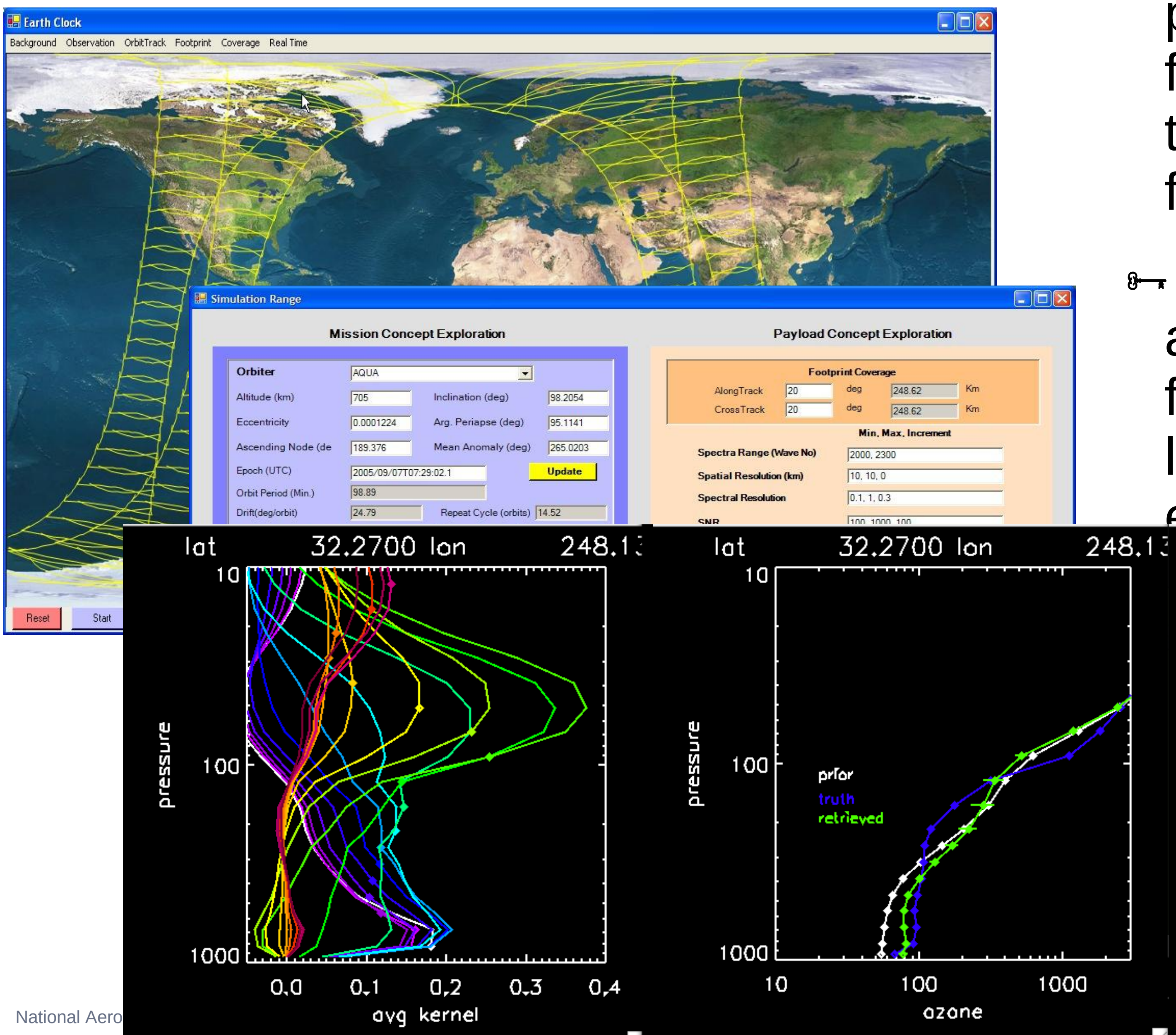
- Approach: Evaluation of possible approaches for ozone – focused on 825 hPa
- Conclusion
  - There are instrument designs that can measure boundary layer ozone
  - Use of uv/vis and high spectral resolution IR wavelengths together are needed to have low bias and low rms at 825 hPa
  - Assimilation of panchromatic ozone improves surface ozone and free troposphere estimates
  - In next steps, can look at freq of sampling and impact of LEO measurements

Exploiting OSSEs in the Mission Design Process



Sampling the field + retrievals

Orbiter-2D



- Can select orbit parameters and footprints, profiles then selected from field.
- Generate radiance, apply instrument function, and use linearized optimal estimation to generate simulated retrievals and error characterization (as well as averaging kernels).

Our experiments

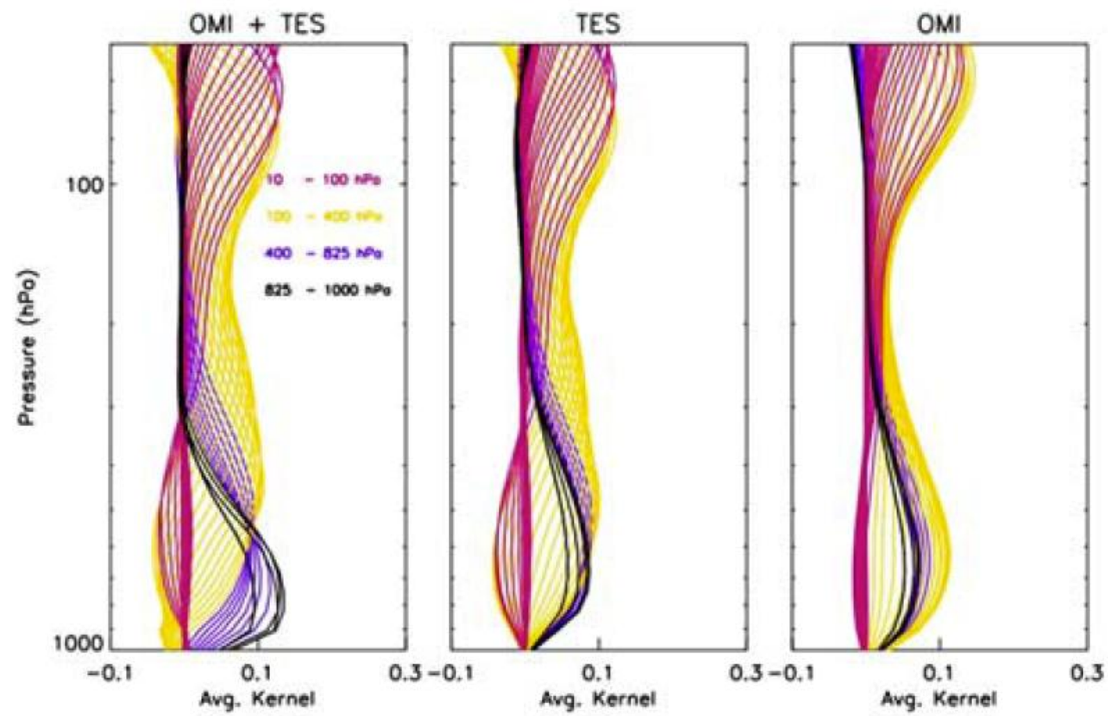
- This talk is focused on characterizing the retrieval sensitivity to instrument parameters and bands (primarily ozone, a little on other gases)
- Kevin will talk about assimilation/adjoint and implications for mission design in more detail

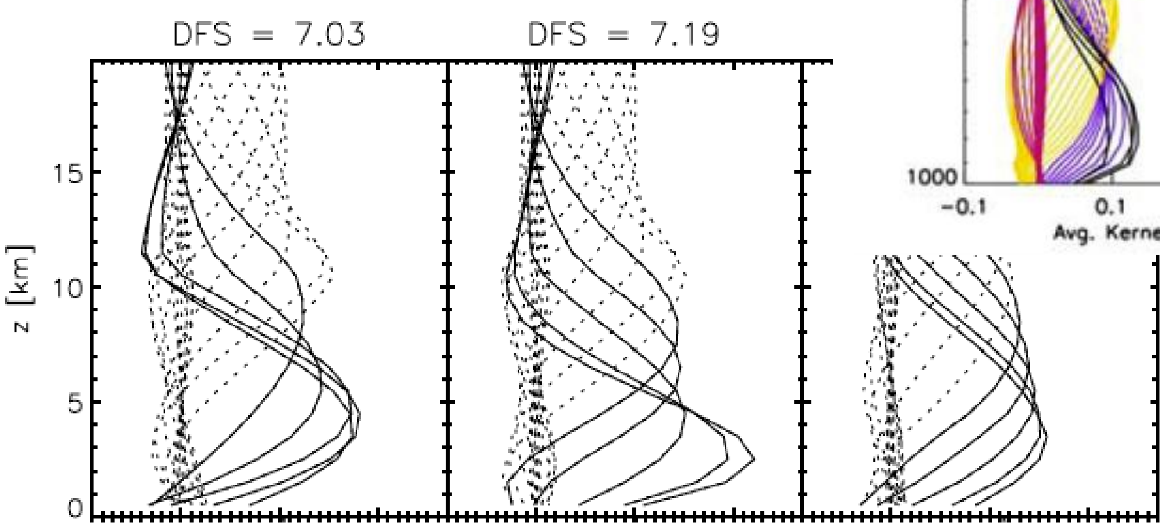
- How we compare instrument & mission ideas:
  - Averaging kernels - are they sensitive in the region of interest?
  - Bias statistics - does the bias meet the requirements?
  - Maps of characteristics - will the spatial characteristics meet science goals?
  - Assimilate into model - assess ability to capture features of interest

Suggestions in the literature

- Simulations based on existing instrument configurations (TES+OMI) show that combination of UV/vis and IR should have better sensitivity to the boundary layer.

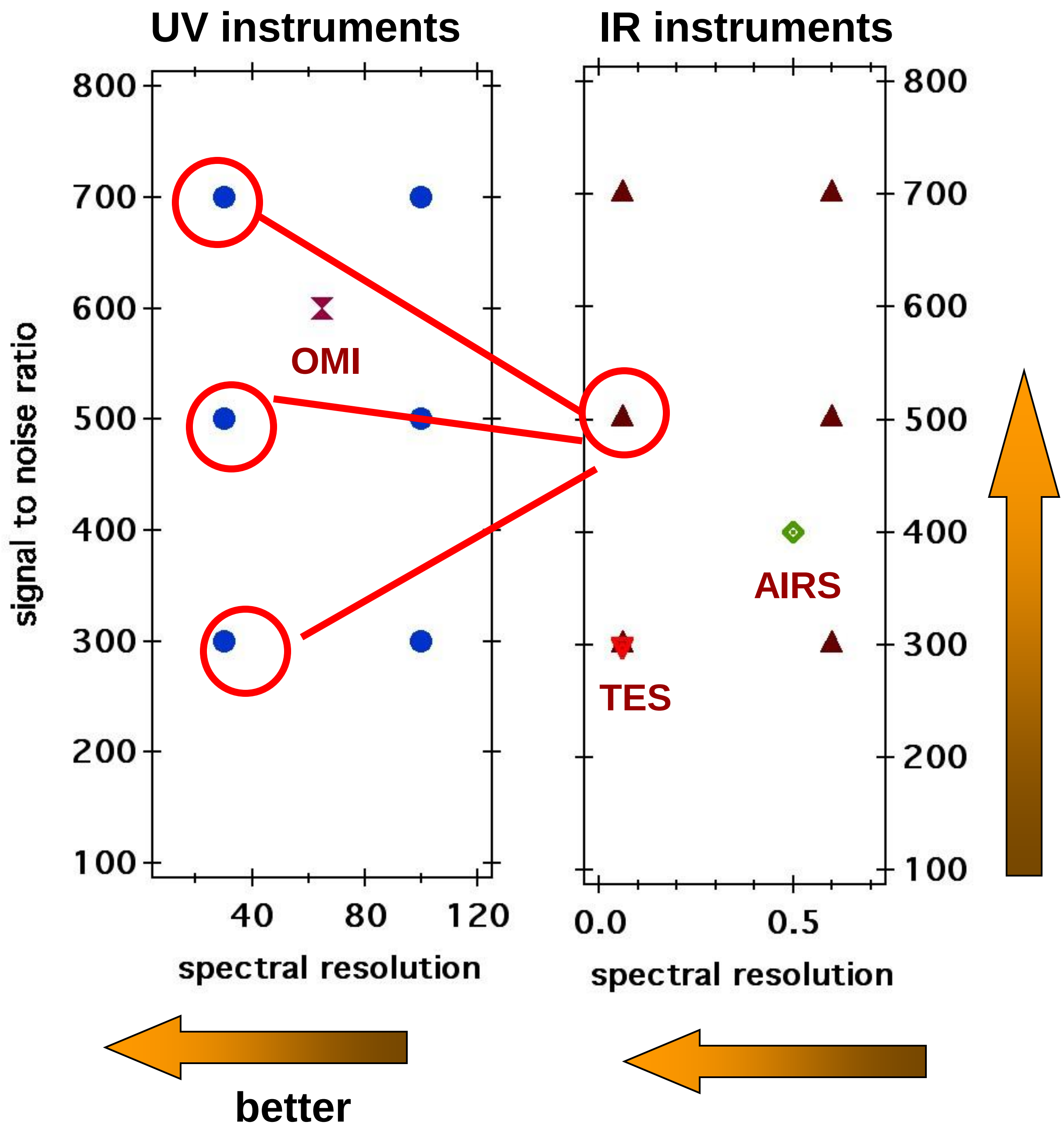
  - We have extended this to test in wide range of atmospheric conditions, range of mission designs, and in end-use science applications



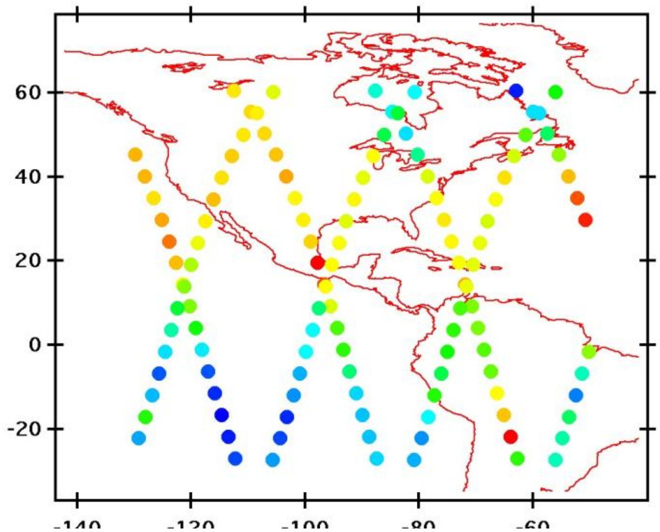


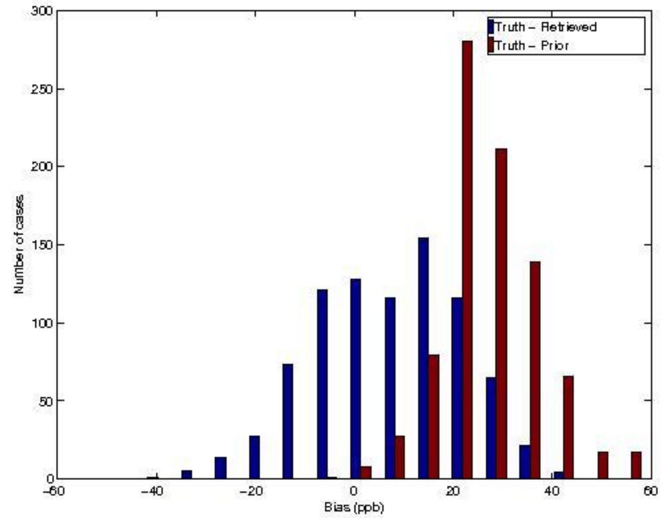
Instrument designs evaluated

- Using instrument designs in the realm of EOS capabilities.
- Looking at wide range of combinations
- IR: 970-1080 cm^{-1}
- UV/vis: 312-344 nm



Simulated retrievals used to derive metrics

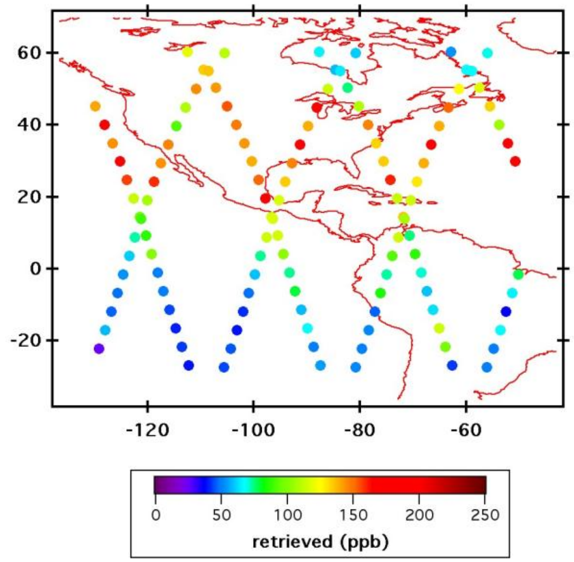


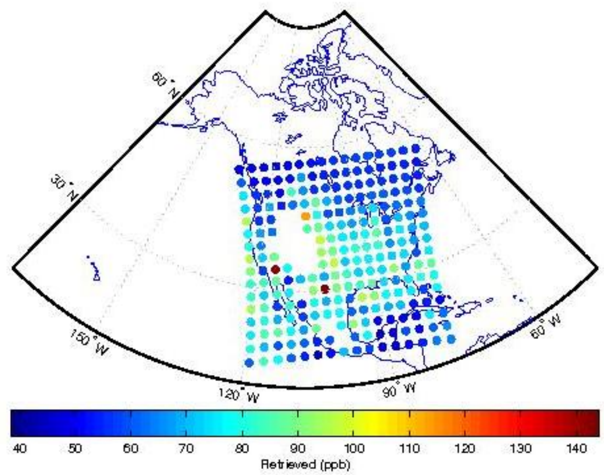


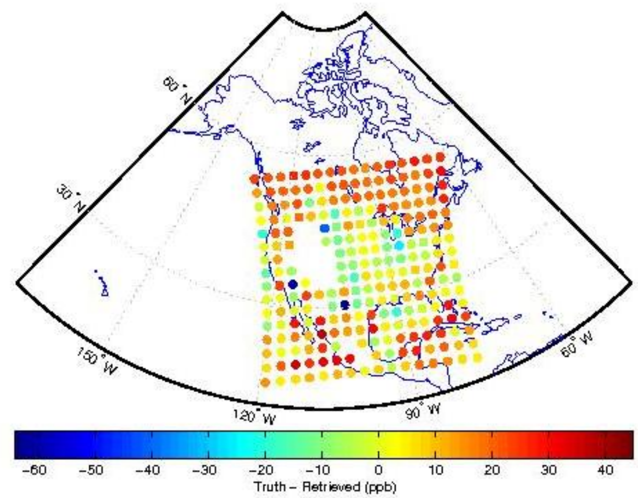
Pdf of truth – retrieved

-Used to derive bias (mean value of pdf)

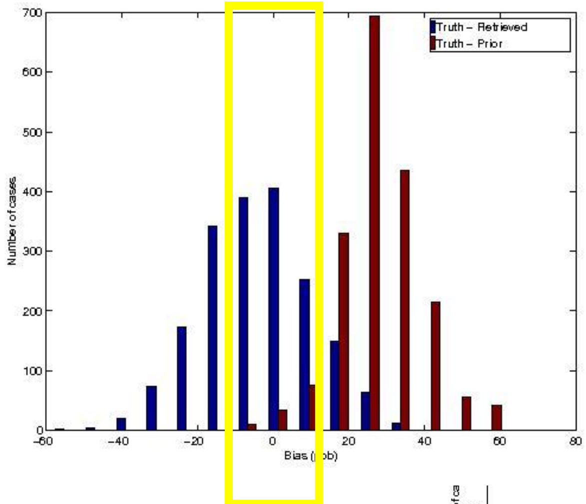
- And rms (rms of distribution)





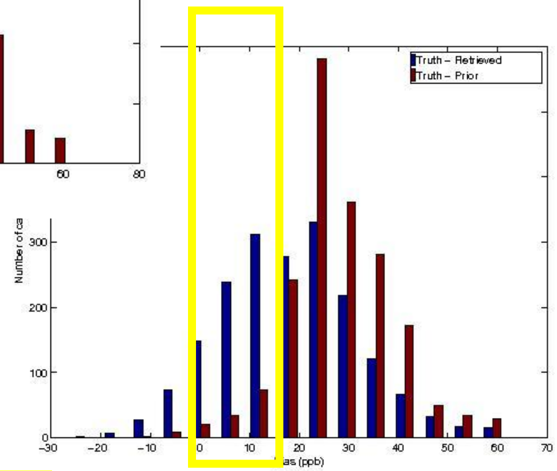


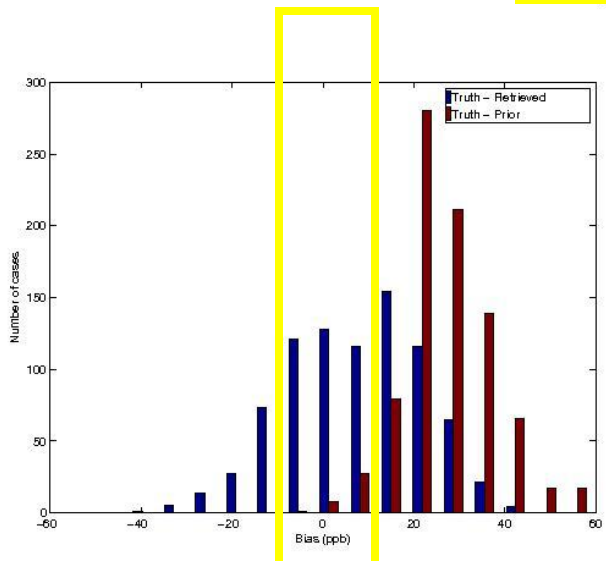
Can we design an instrument to measure O3 to 5ppb at 825 hPa??



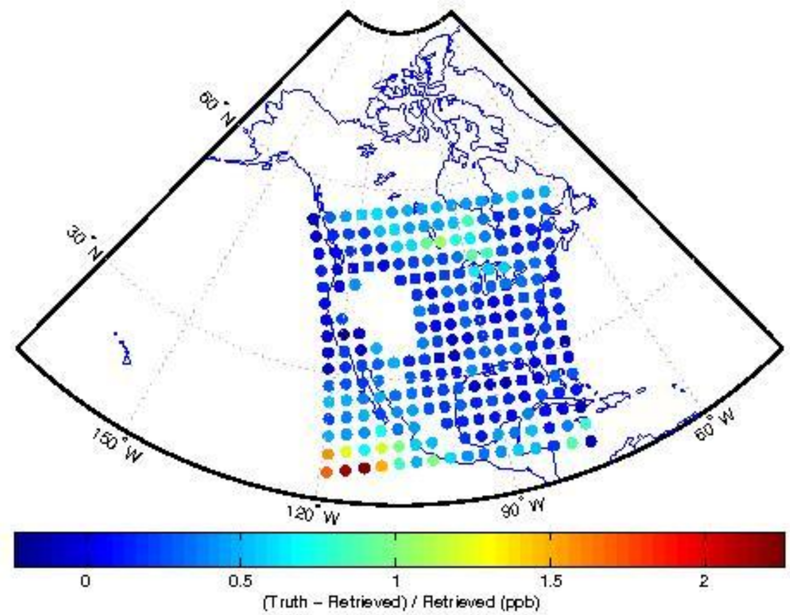
IR only – 0.06 cm^{-1} resolution

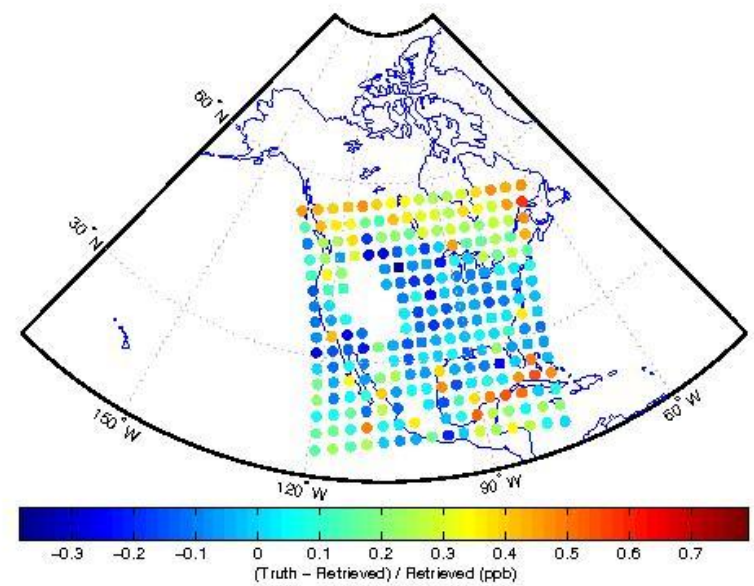
IR only – 0.6 cm^{-1} resolution



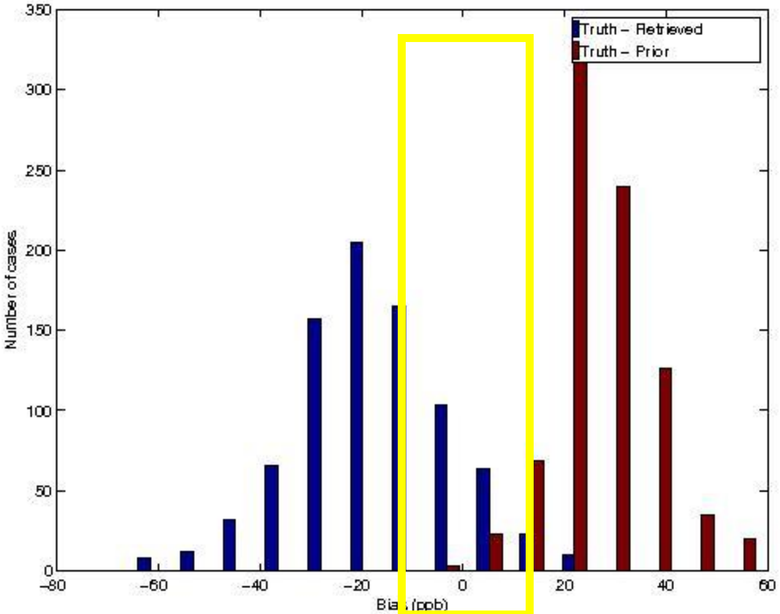


UV only – 30 cm^{-1} spacing

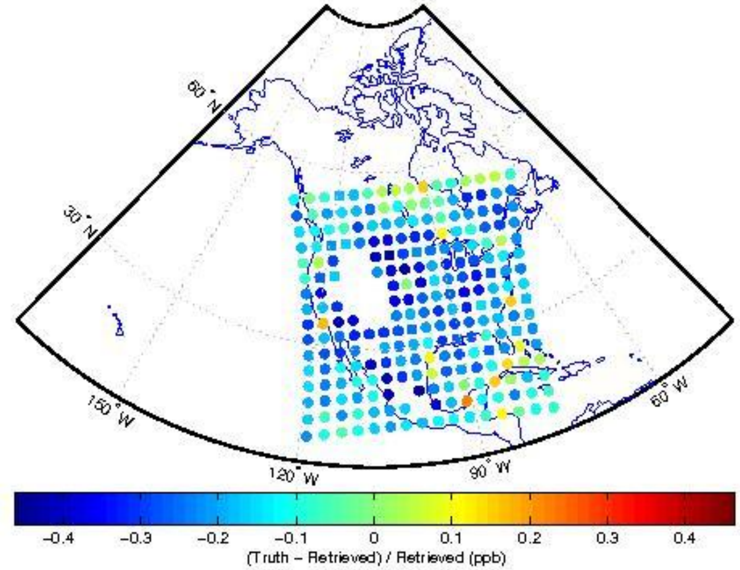


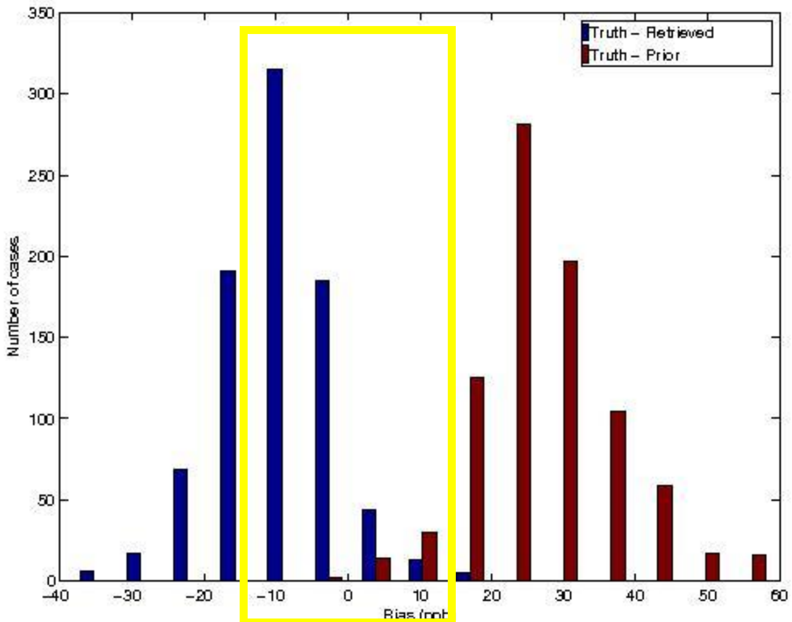


Combinations

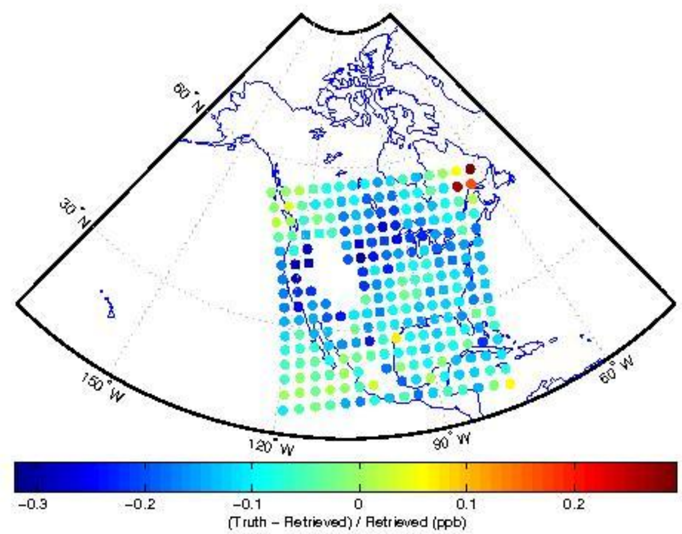


Combo – IR at 0.6 cm^{-1}, UV at 30





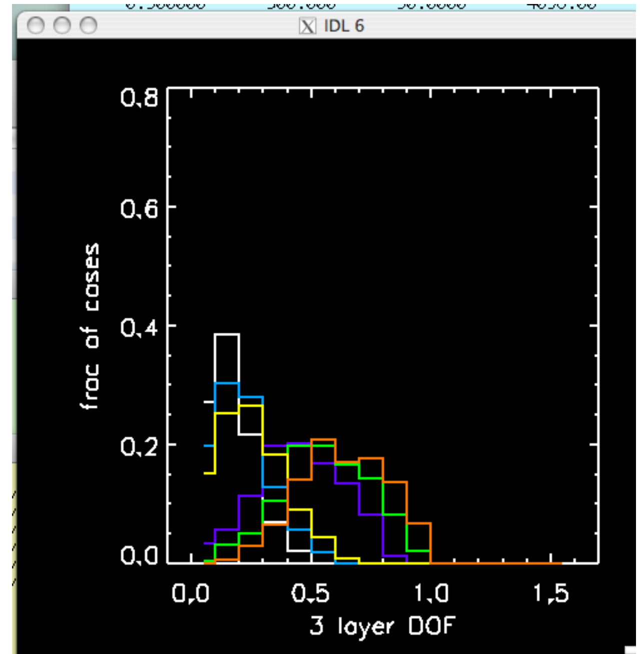
Combo – IR at 0.06, UV at 30 cm^{-1}

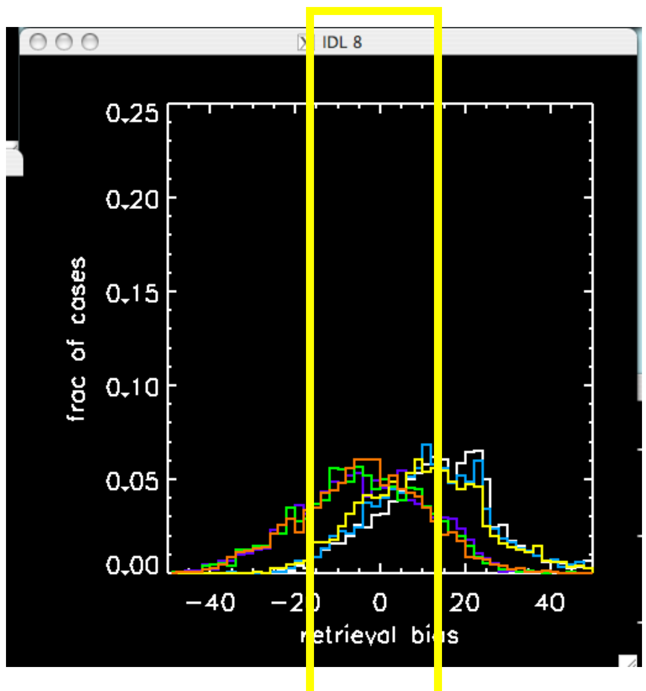


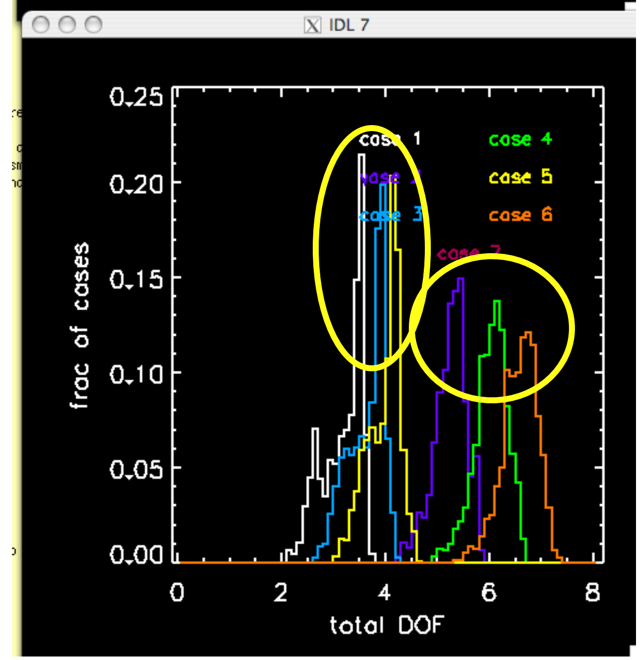
Sensitivity to noise characteristics: IR cases

✓In total degrees of freedom, the three cases with resolution 0.6 cm-1 group together, and the cases with resolution 0.06 cm-1 group together.
✓The spread across the groups is from the noise characteristics changing from SNR of 300 to 500 and 700.

✓Similar ordering is seen in the Degrees of Freedom for the lowest 3 layers of the atmosphere

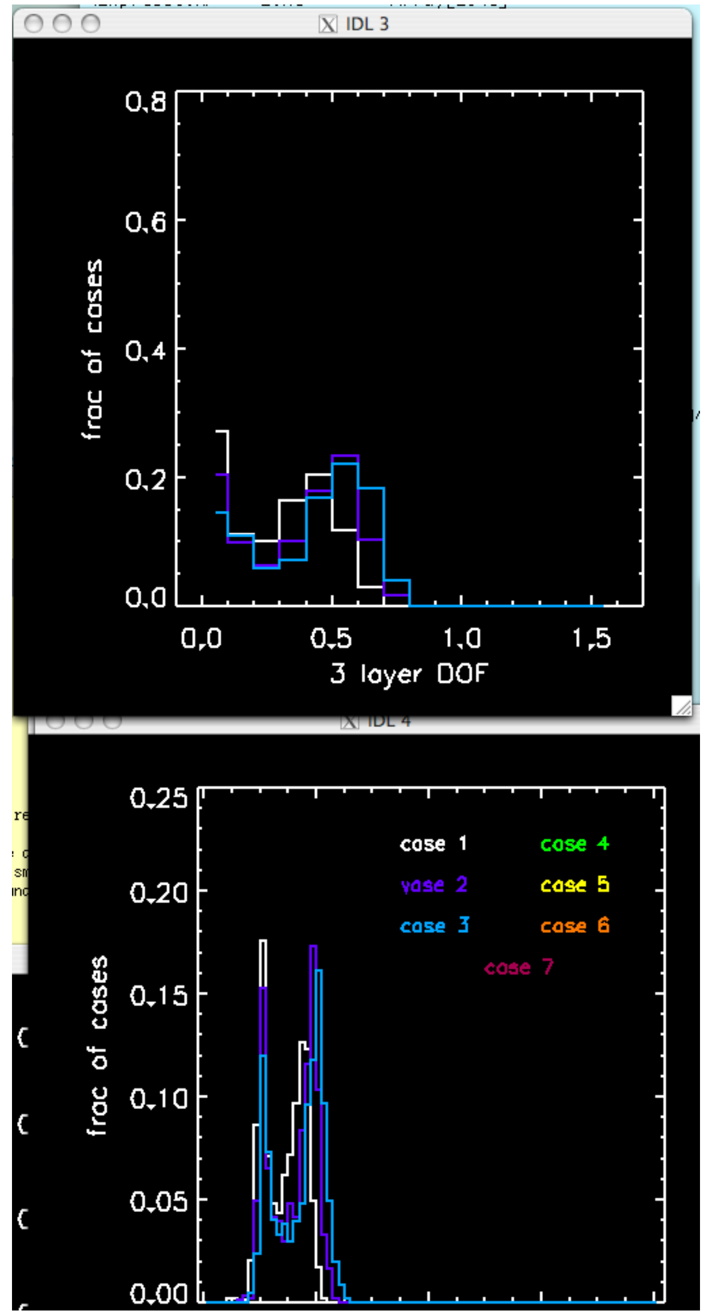






Sensitivity to noise characteristics: UV cases

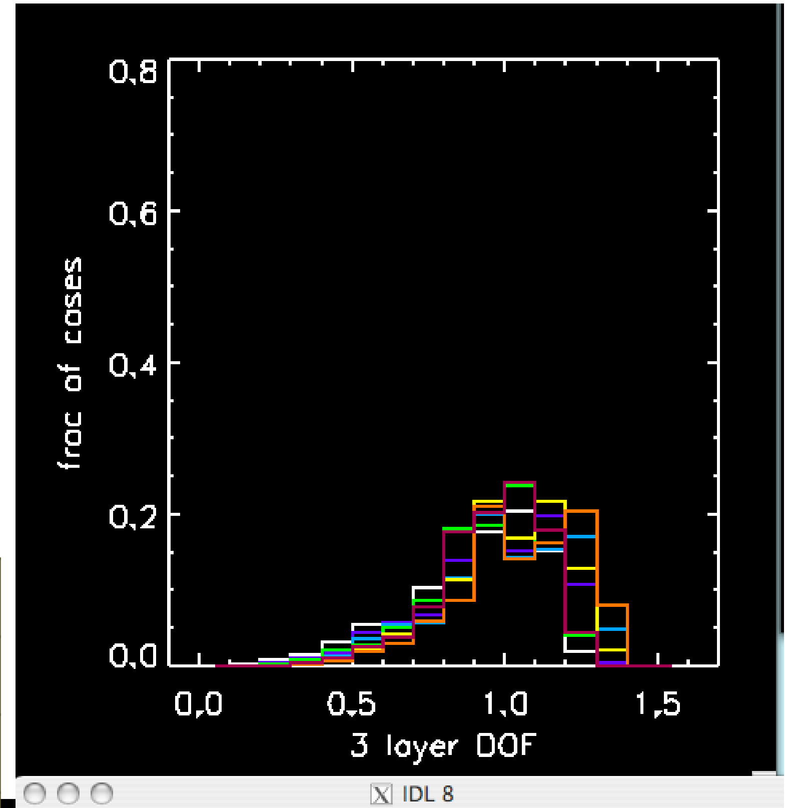
- Similar analysis – 3 UV cases with different noise characteristics
- Noise is less of a driver here

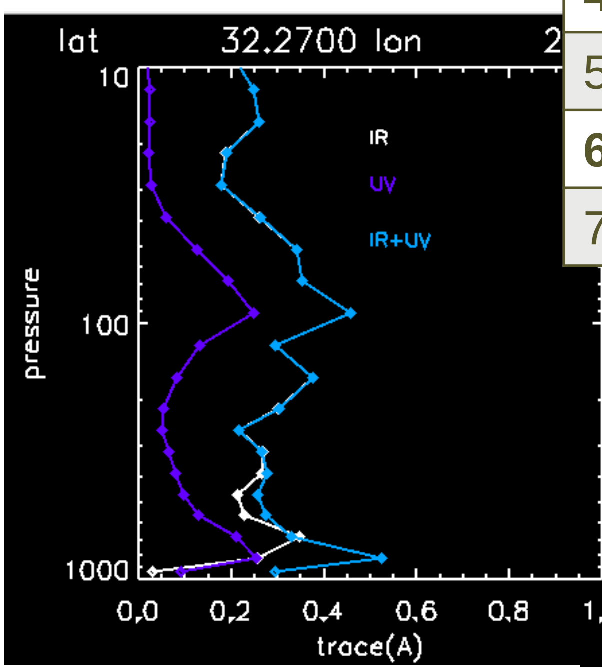


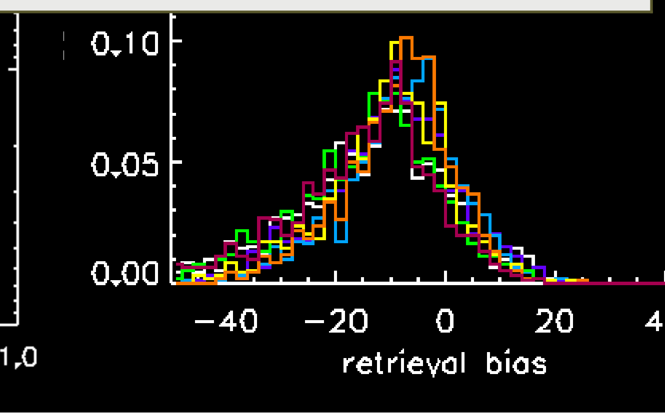
Now combining UV and IR

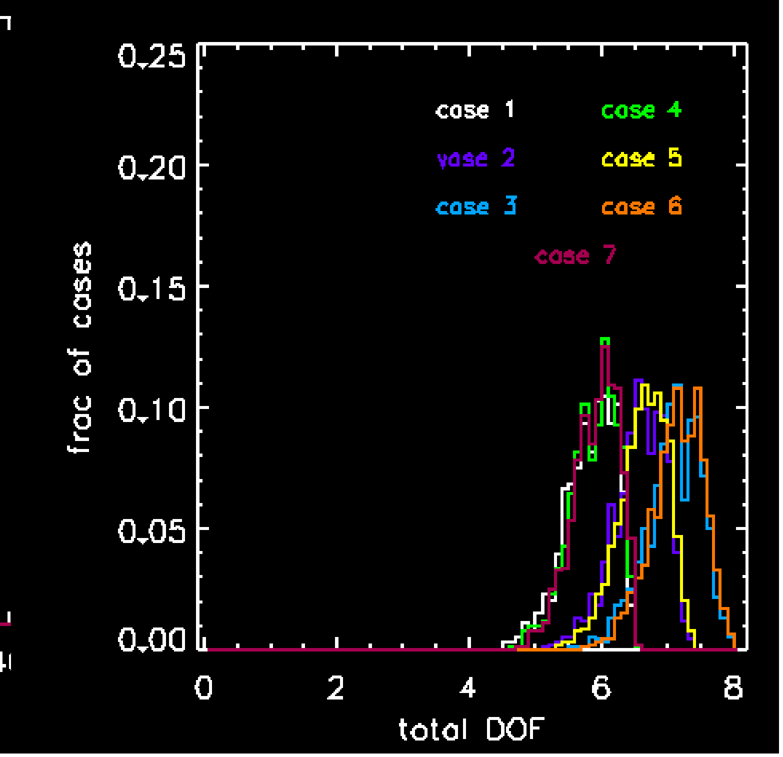
- Only include the high resolution IR cases here
- Grouping in total DOF driven by the infrared SNR
- Combination of wavelengths show needed sensitivity in boundary layer.

Case	UV SNR	IR SNR
1	300	300
2	300	500
3	**300**	**700**
4	500	300
5	500	500
6	**500**	**700**
7	700	300

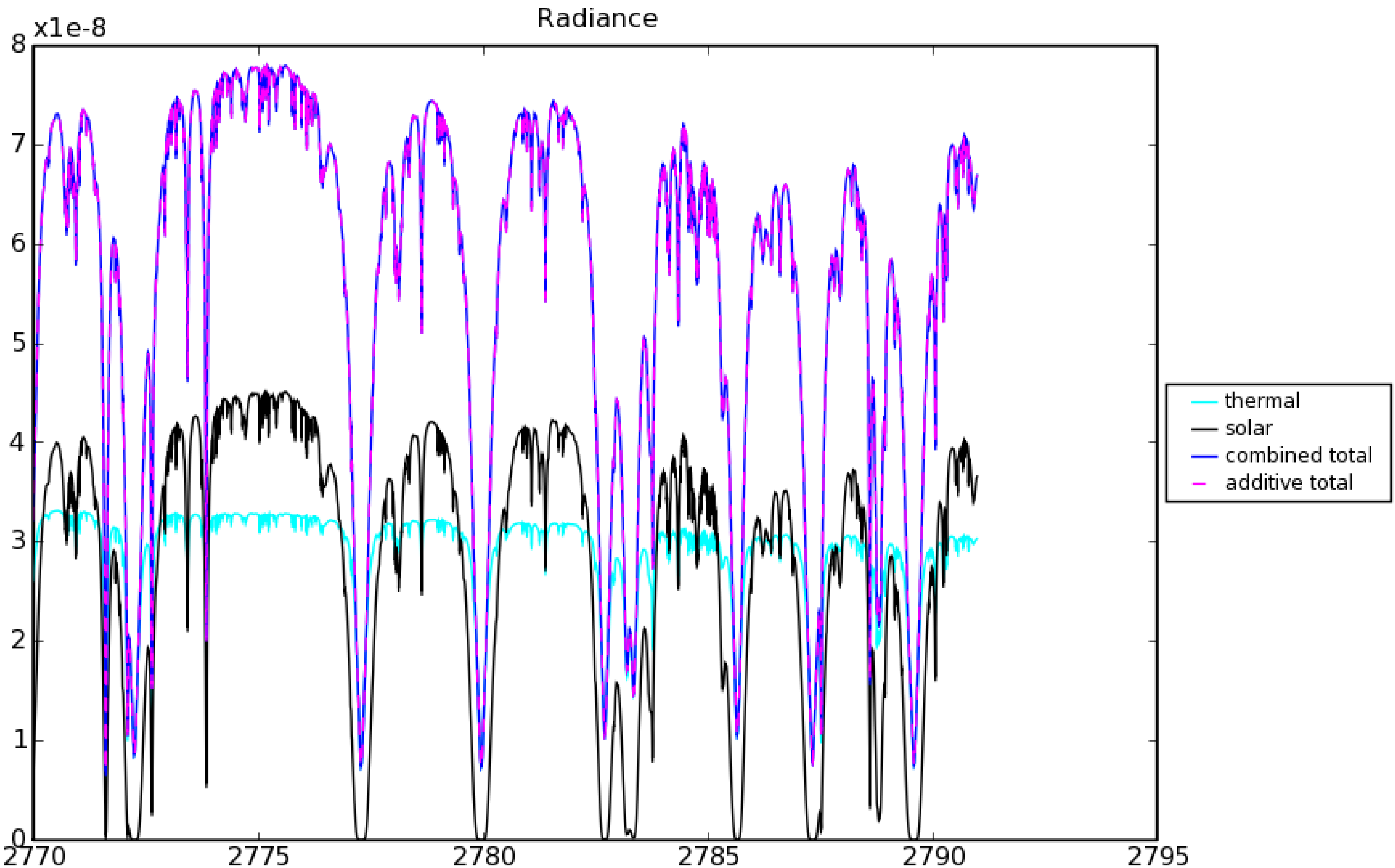






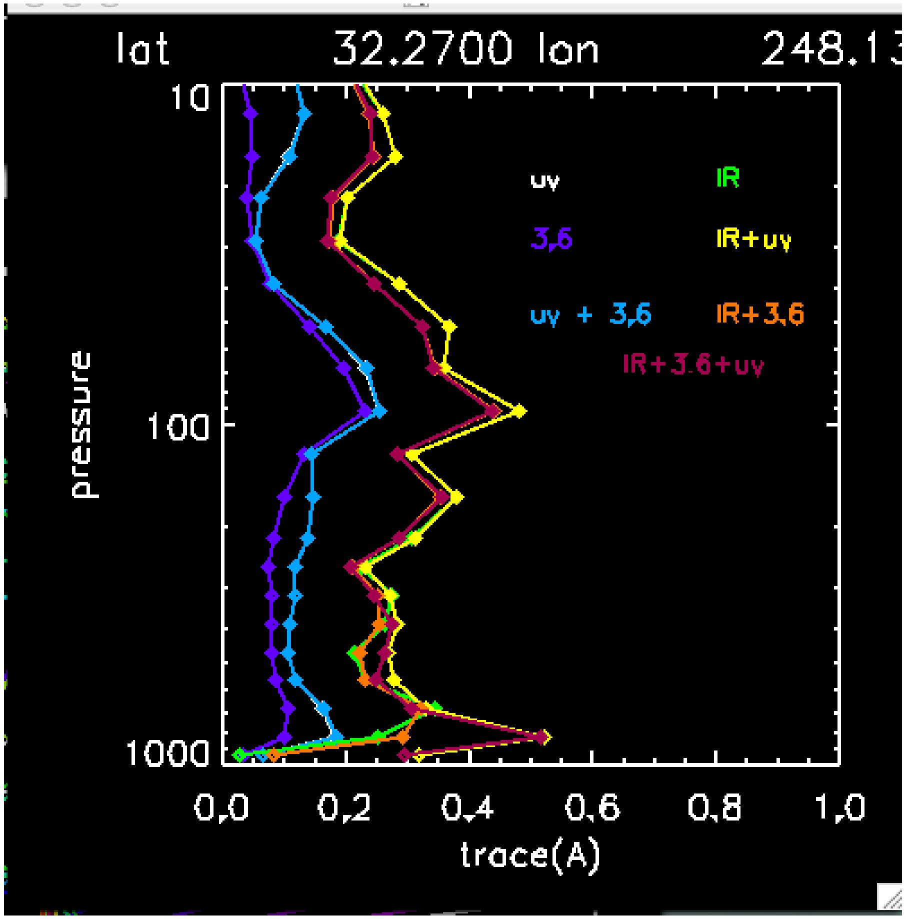


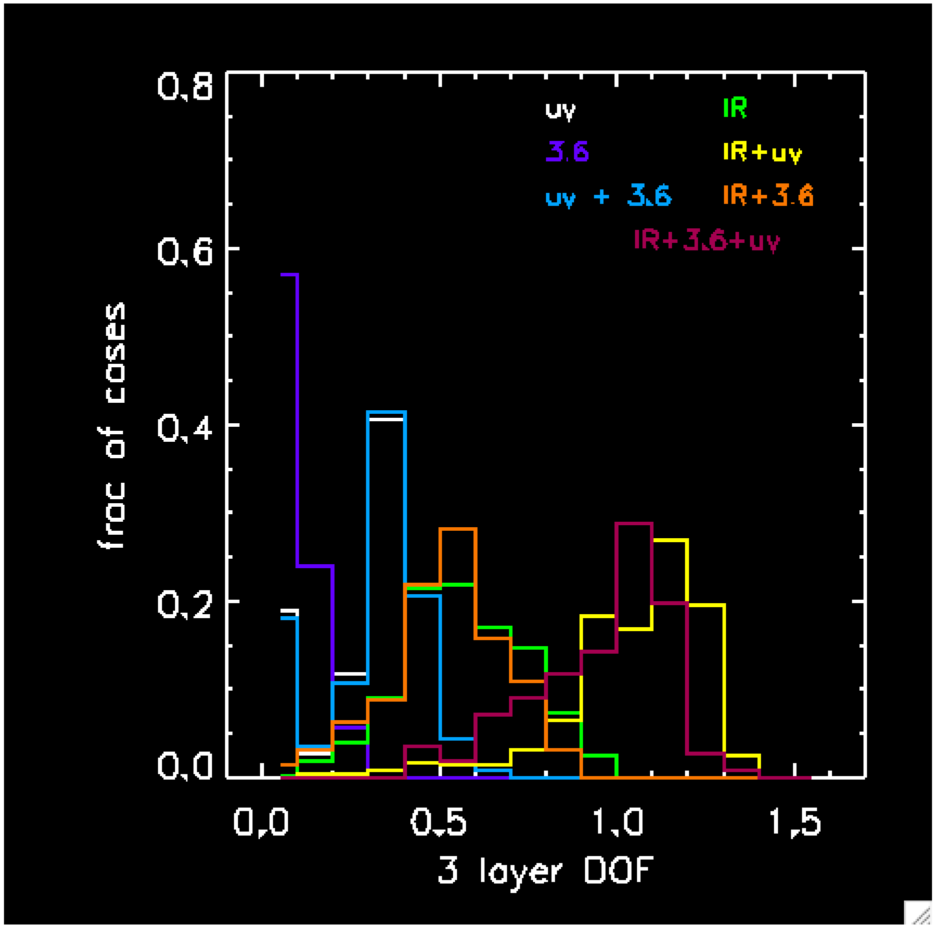
Verifying RT calculations in LIDORT for cross over region



Wavenumber (2778 cm^{-1} = 3.6 microns)

Adding 3.6 does not provide a boost

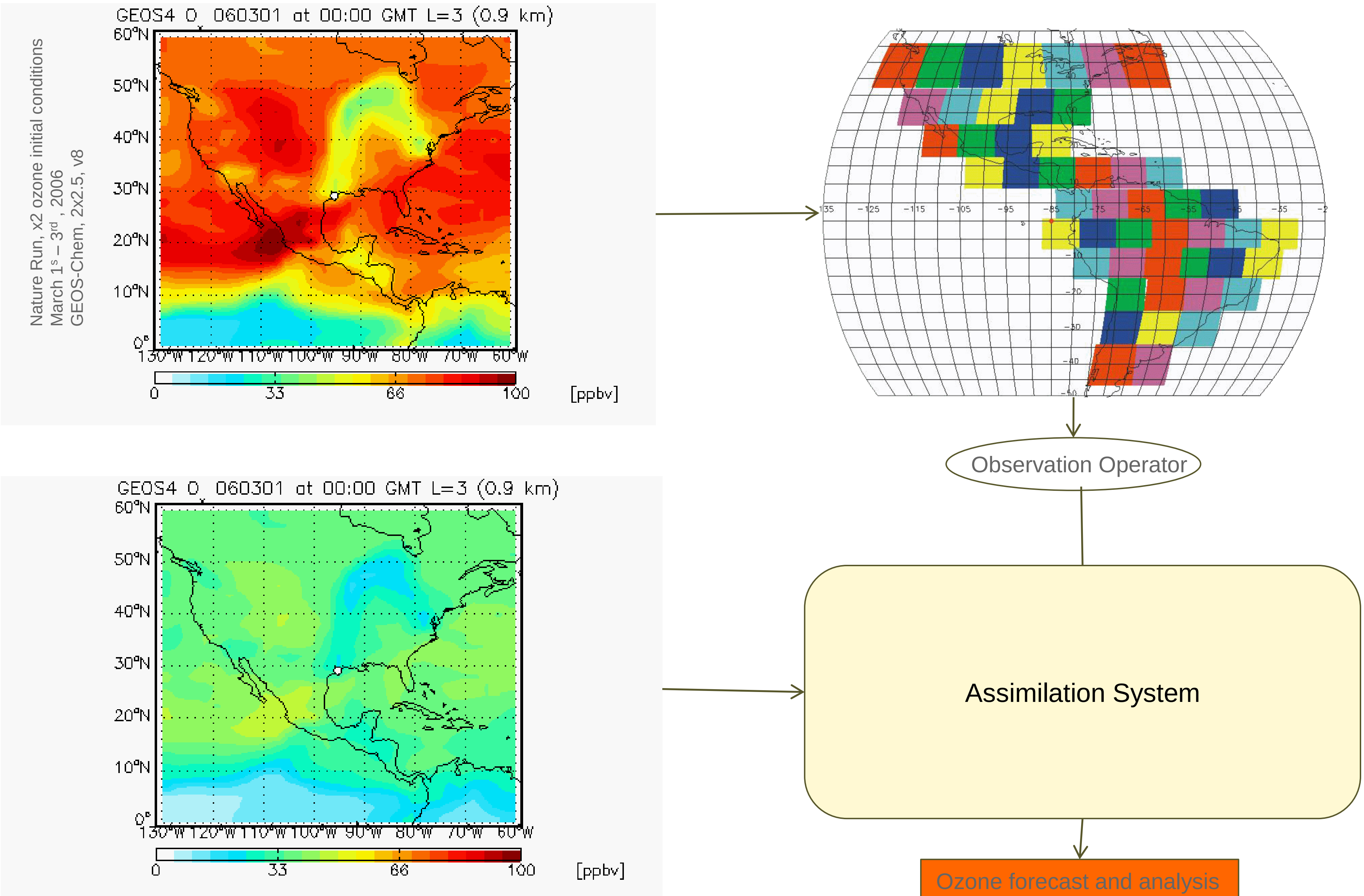




Assimilation and adjoint

- The retrieval statistics give us one measure of how sensitivity to ozone at 825 mb changes as a function of spectral resolution, noise characteristics, and the bands used.
- Now we show how assimilating that simulated data back into the model lets us test how well important features are captured with the simulated measurements

GEO-CAPE OSSE



Assimilation approach and instrument configuration

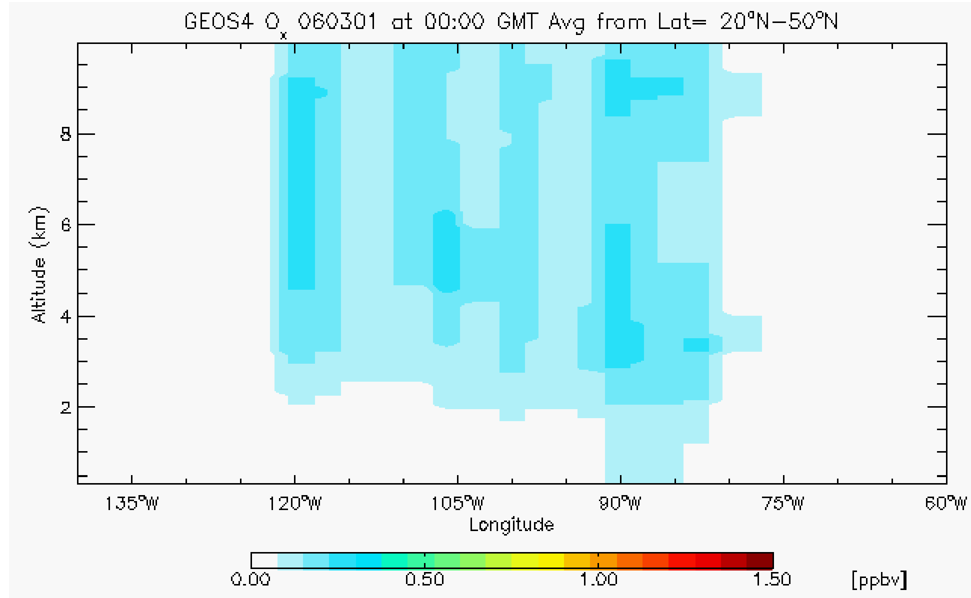
Sequential sub-optimal Kalman filter

$$\hat{\mathbf{x}}_k^a = \mathbf{x}_k^f + \mathbf{K}_k[\mathbf{y}^{\text{obs}} - \mathbf{H}_k\mathbf{x}_k^f]$$

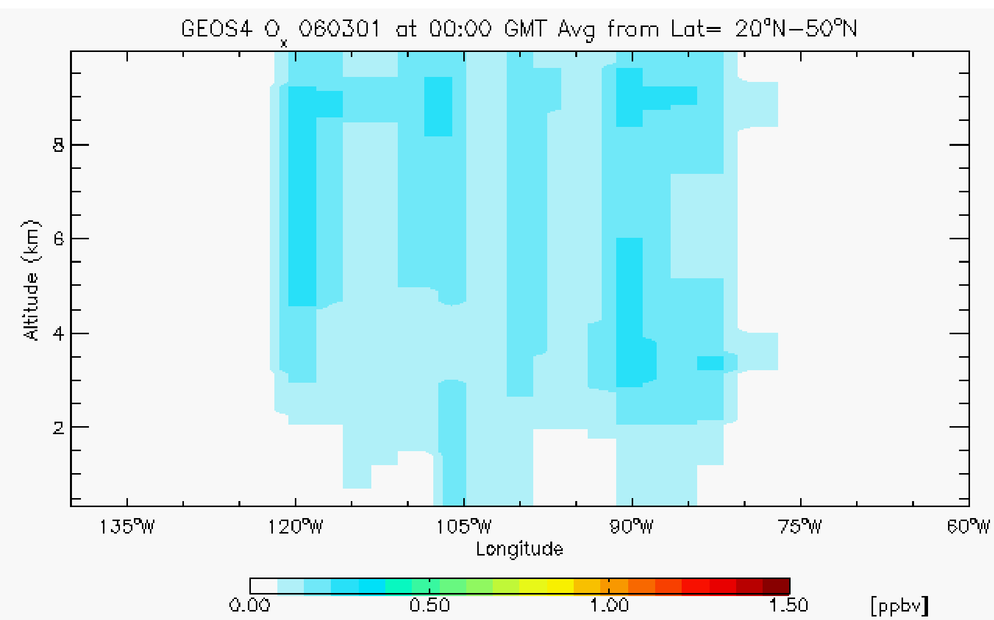
Assimilation metric: $$\frac{|\text{Assim-Model}|}{|\text{Nature-Model}|}$$

Instrument configuration:

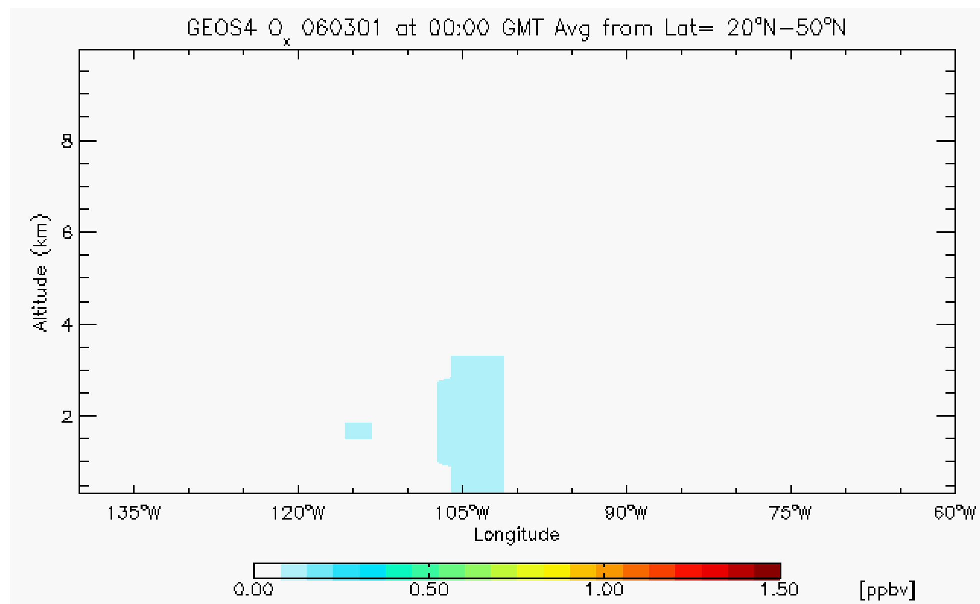
- IR 10 micron band, spec res. .09 cm^{-1}, SNR=700
- UV-Vis, 29000-32000 cm^{-1} , spec. res. 45 cm^{-1}, SNR=700
- UV-Vis+IR, same as above



IR



UV-Vis+IR

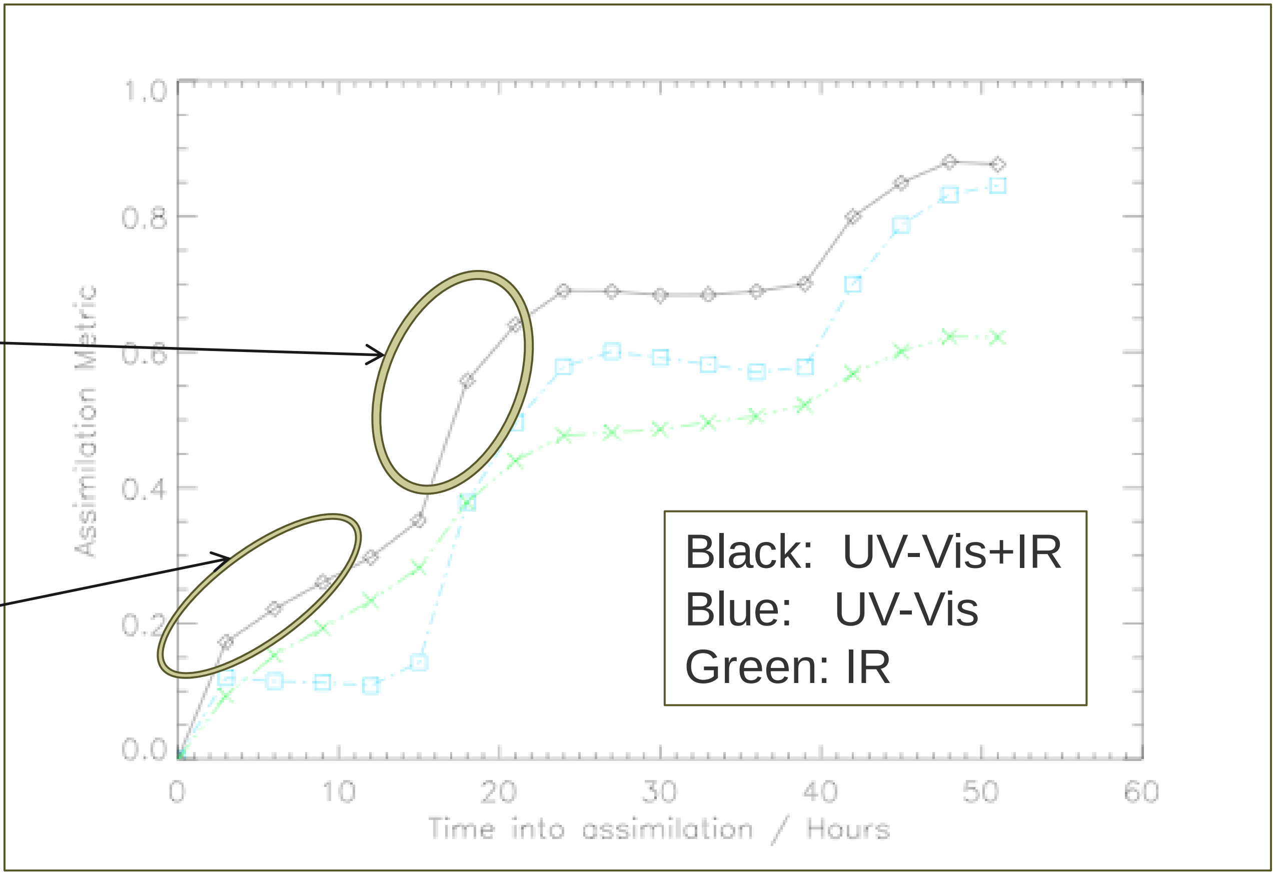


UV

Impact of spectral bands on surface ozone

Pan-spectral measurements provide surface ozone sensitivity during daylight hours resulting in steep improvement in assimilation

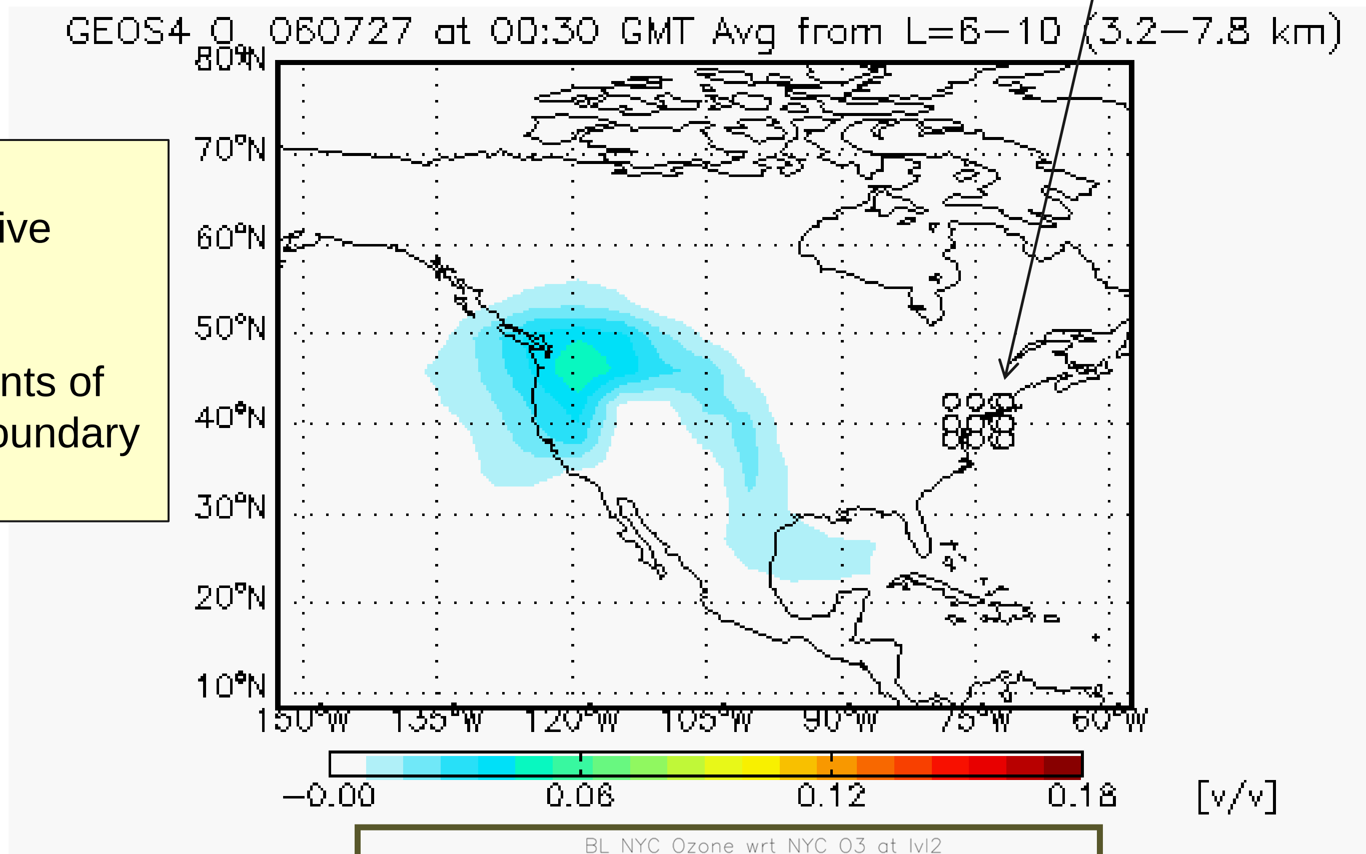
Pan-spectral measurements provide nocturnal and free tropospheric sensitivity



•UV-Vis+IR provides the best prediction of surface ozone over 48 hours
•IR bands significantly improves prediction through noctural and free tropospheric ozone assimilation
•UV bands provide highest gradient of assimilation performance

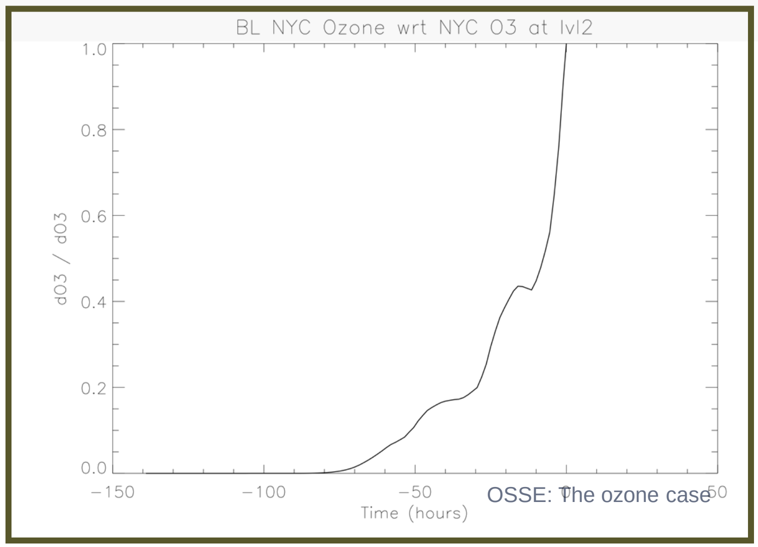
Diagnosing the contributions to surface ozone

target region



Adjoint sensitivity analysis suggests that NY boundary layer ozone is sensitive to free tropospheric ozone 2 days prior

Continuous, day and night measurements of free tropospheric ozone will improve boundary layer ozone prediction.

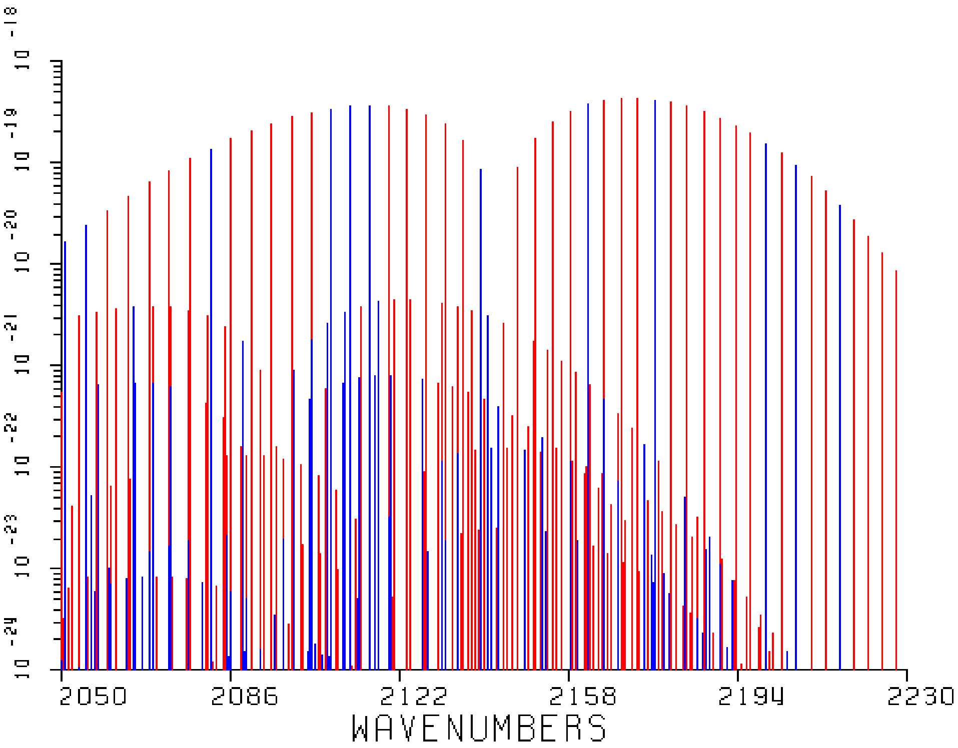


The sensitivity of ozone on 08/01/08 to boundary ozone on 07/31/08 is about a half

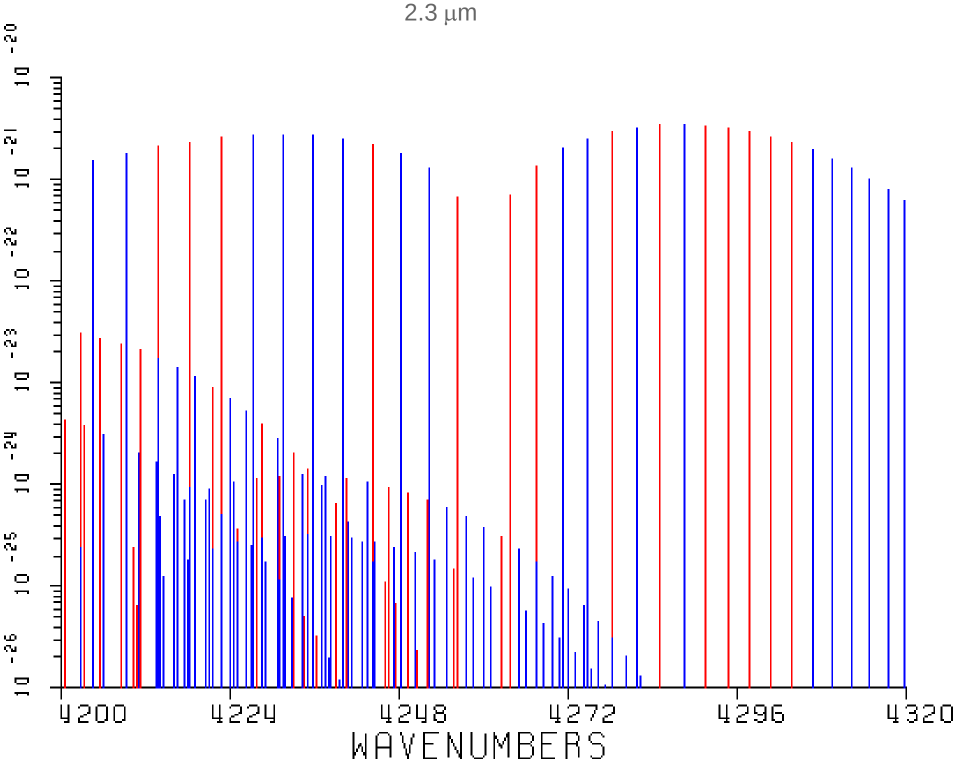
Daily, dirunal measurements of boundary ozone will signficiantly improve ozone forecasting

Extending analysis to other molecules

4.7µm



2.3 µm



Spectral window selections (limited by available filters etc):

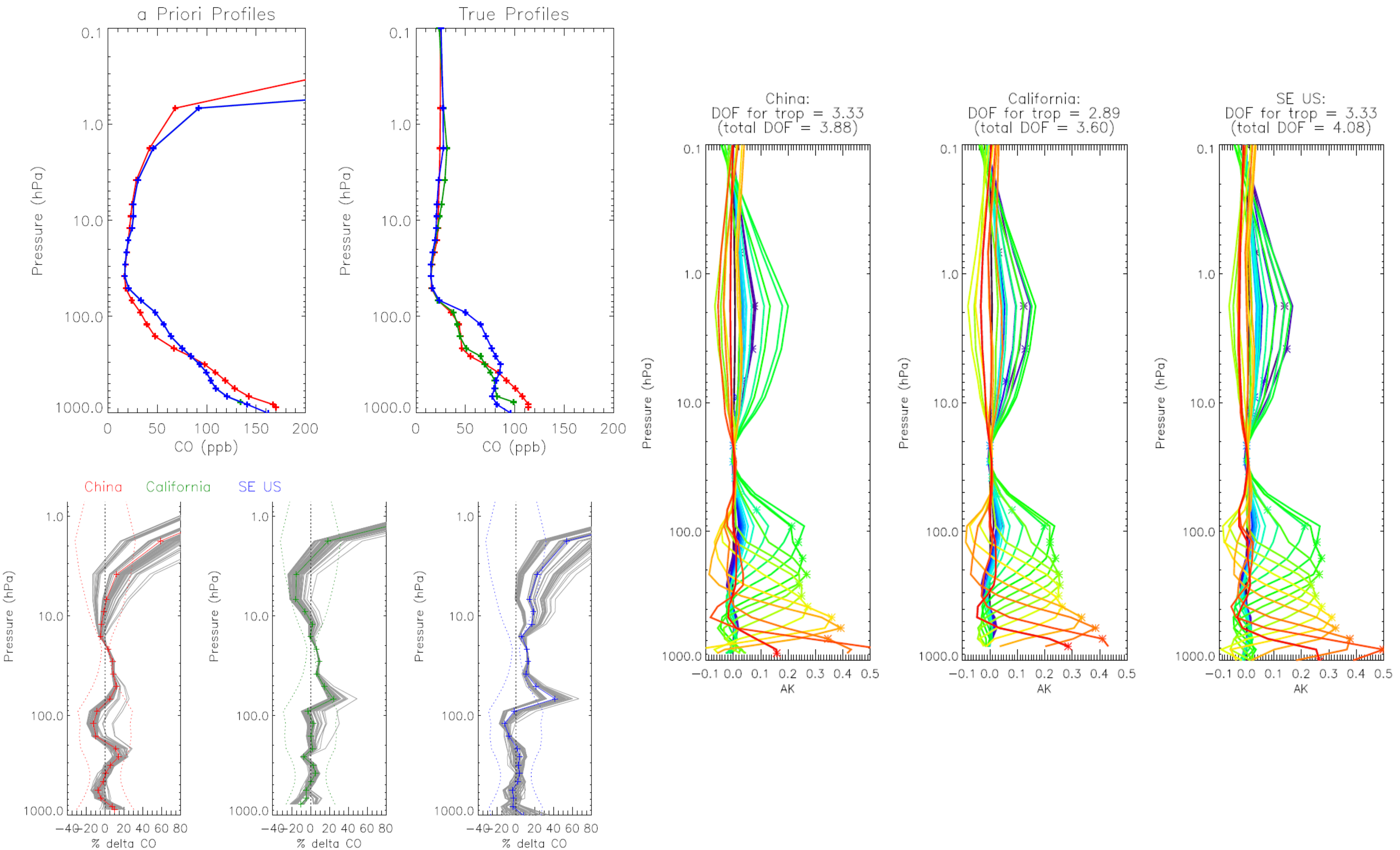
(red are those used for this study)

HITRAN CO line intensity plots

- TES: 11 micro-windows covering 2086.06 – 2176.66 cm-1, delta = 0.1cm-1.
- MOPITT: 2140-2192 cm-1 and 4265-4305 cm-1, eff delta = 0.04 cm-1.
- AIRS: ~2180-2220 cm-1 (has 2170-2674 available), delta = 1.8 cm-1.
- IASI: 2120-2200 cm-1, delta = 0.5 cm-1.

Start to investigate CO retrievals in spectral ranges of TIR and NIR

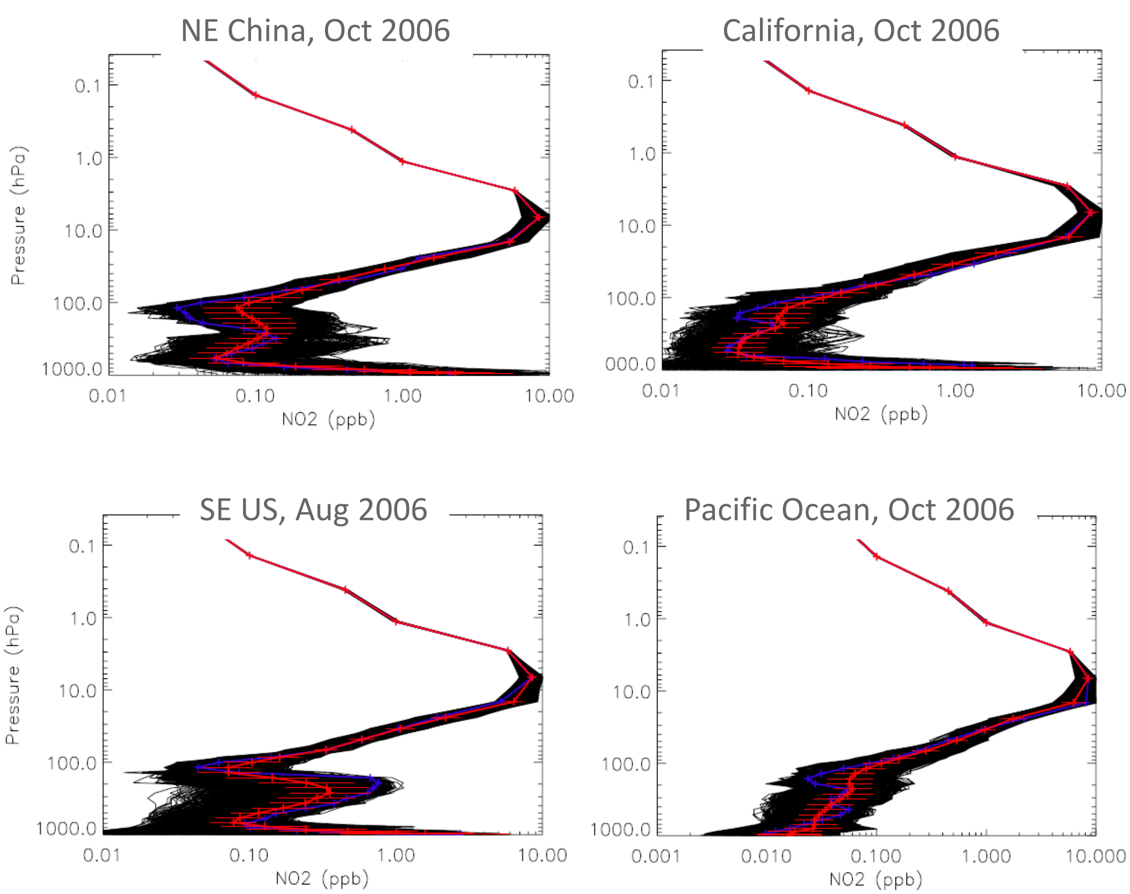
- Spectral range: 2086-2192 cm-1 (4.7 μm band) and 4265-4305 cm-1 (2.3 μm band)
- Typical atmospheres: China, California, SE US
- Varying instrument definitions: SNR & spectral resolutions.

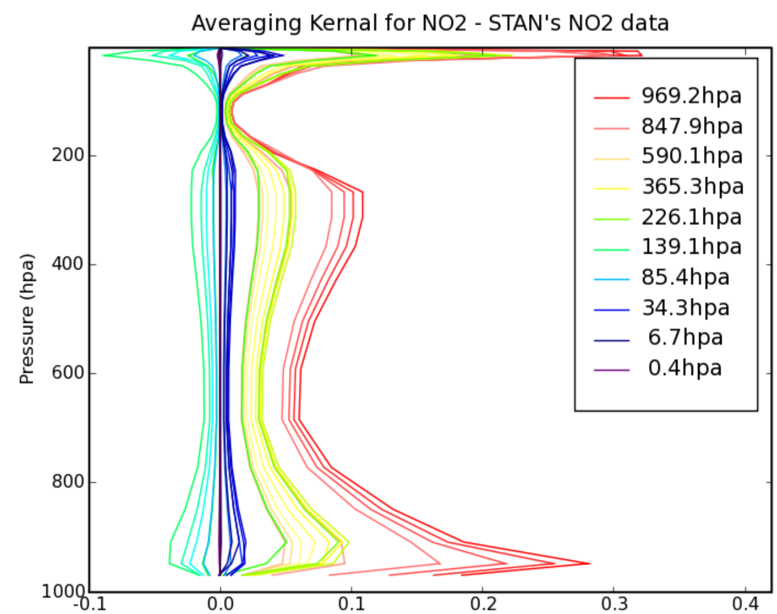


NO2 Retrieval Simulations

•Spectral windows to avoid solar lines: 20174-20474cm-1 (~ 493 nm) and 21926-21993cm-1 (~ 455 nm).

•Typical atmospheres: China, California, SE US (polluted), Pacific (unpolluted).
•Optimal retrievals of level NO2 in the troposphere.
•Examining the effect of spectral resolutions: high spectral resolution measurement doesn't provide an advantage in gaining vertical resolution in retrieved profile (boundary layer NO2, absorption lines overlap, scattering in the lower troposphere …).





SE US case:

DOF_trop = 1.06; DOF_total = 1.16

Conclusions

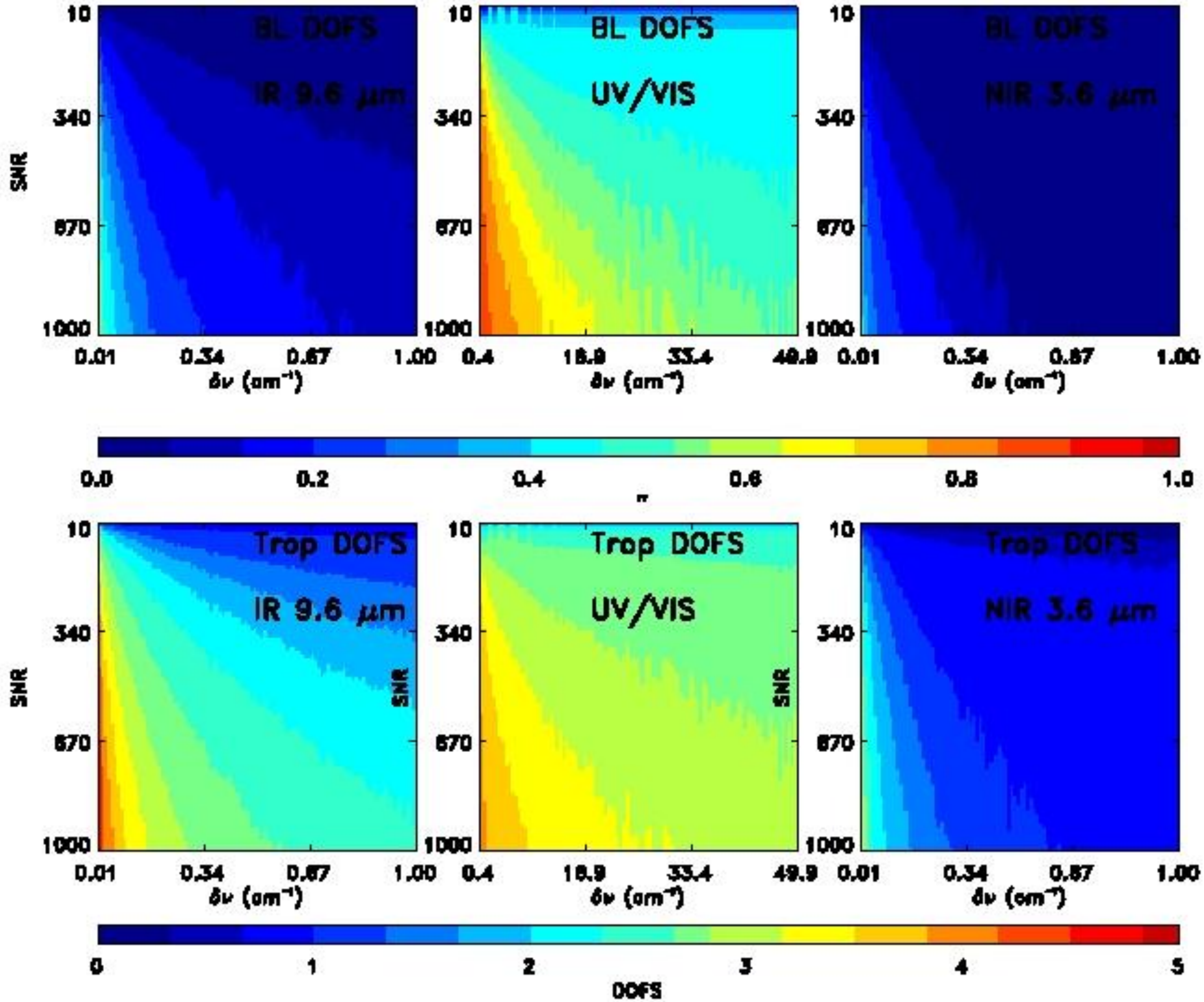
- OSSE tool provides powerful tool for generating simulated datasets, comparing retrieval statistics, and linking to model assimilation
- Has been used to characterize ozone retrievals for a geostationary view, ready to look at frequency of sampling and coverage tradeoffs
- Next steps include CO, SO2, CH4 and integration of regional modeling dataset
- Assimilation of IR ozone significantly improves free tropospheric ozone
  - Implications for continental transport, outflow, and radiative forcing
  - nocturnal ozone assimilation matters to surface ozone prediction
- Assimilation of the UV-Vis improves surface ozone prediction
- Assimilation of UV-Vis+IR combines the advantages of both and provides the best overall prediction
- Adjoint sensitivity analysis shows
  - diurnal measurements of free tropospheric ozone will improve surface ozone prediction
  - daily local measurements of ozone will improve ozone forecasting.

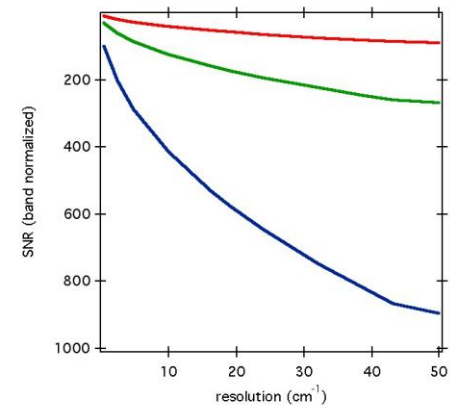
Future directions

- Analysis of frequency of sampling and application to additional species
- Perhaps integration of the RT tool that subgroup is using
- Incorporation of 4D-variational adjoint assimilation into OSSE framework
  - Investigation of multi-constituent assimilation on surface ozone estimation
  - How important are diurnal measurements of NOx to ozone relative to LEO, e.g., GOME-2?
- Development of nature run for summer 2006
- Investigate implications of GEO-CAPE measurements for instantaneous ozone radiative forcing
- Incorporation of information theoretic techniques to assess instrument impact.

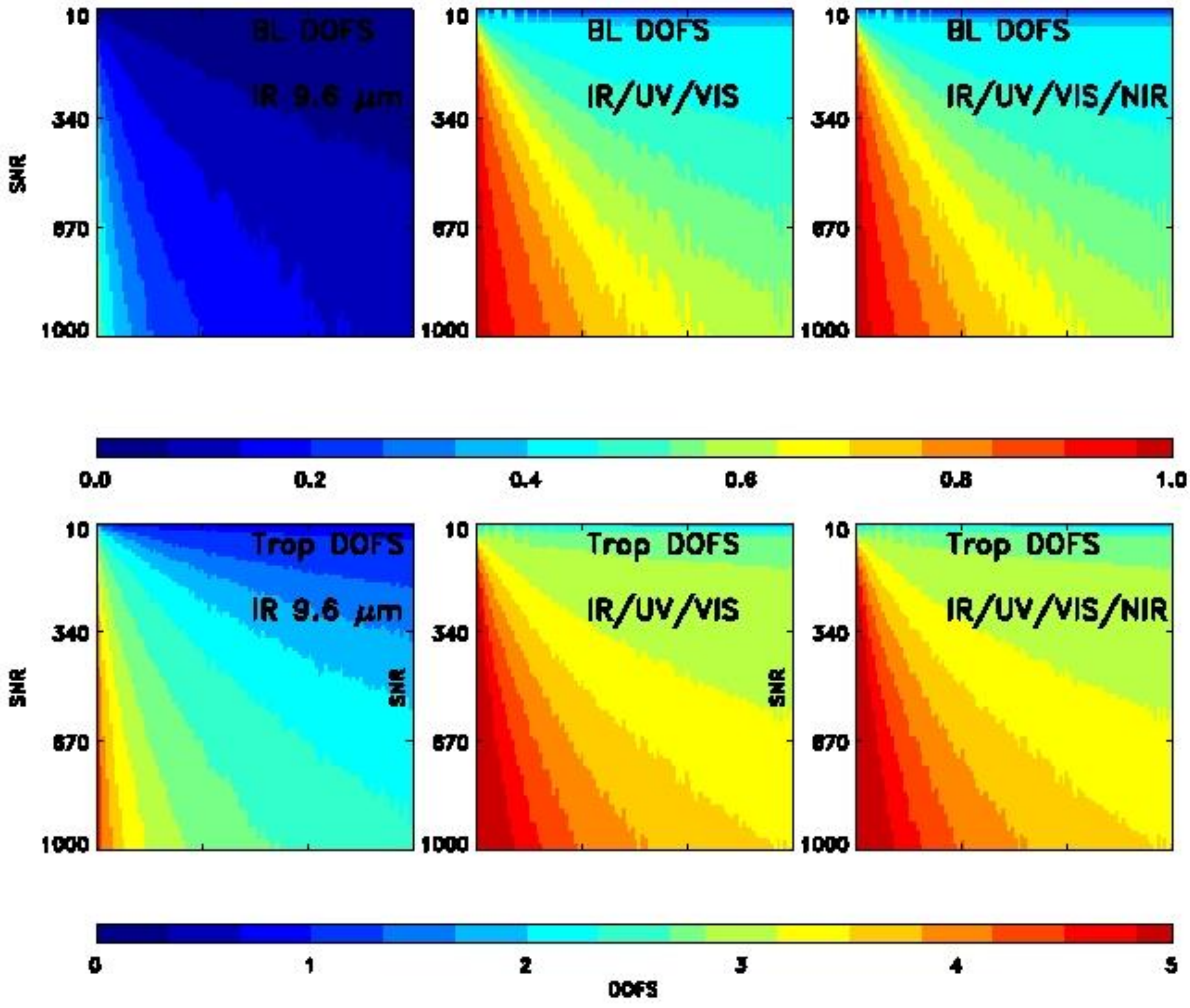
THANK YOU!

Building on the single case analysis

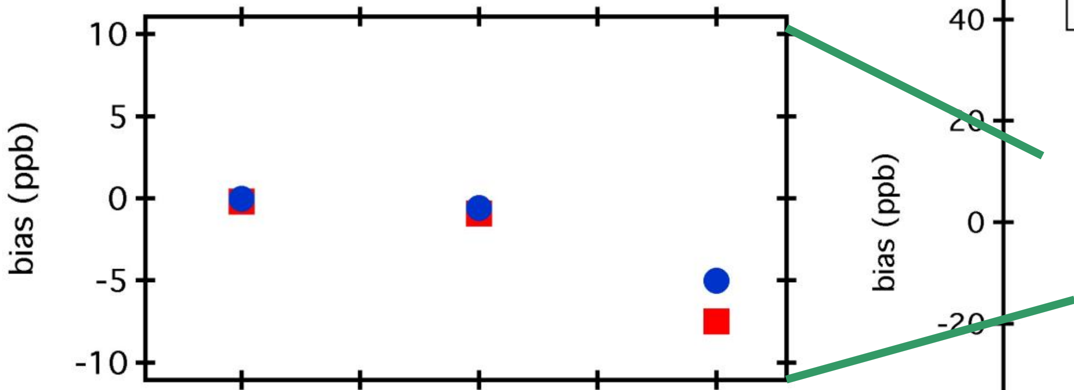


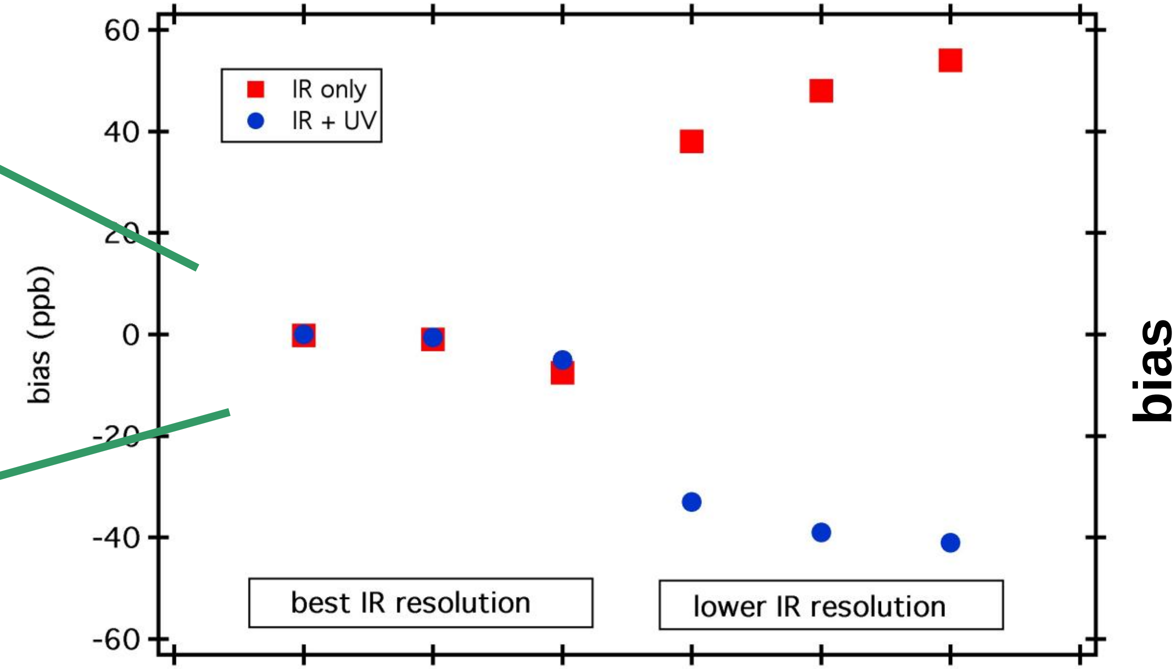


Starting to look at joint retrievals

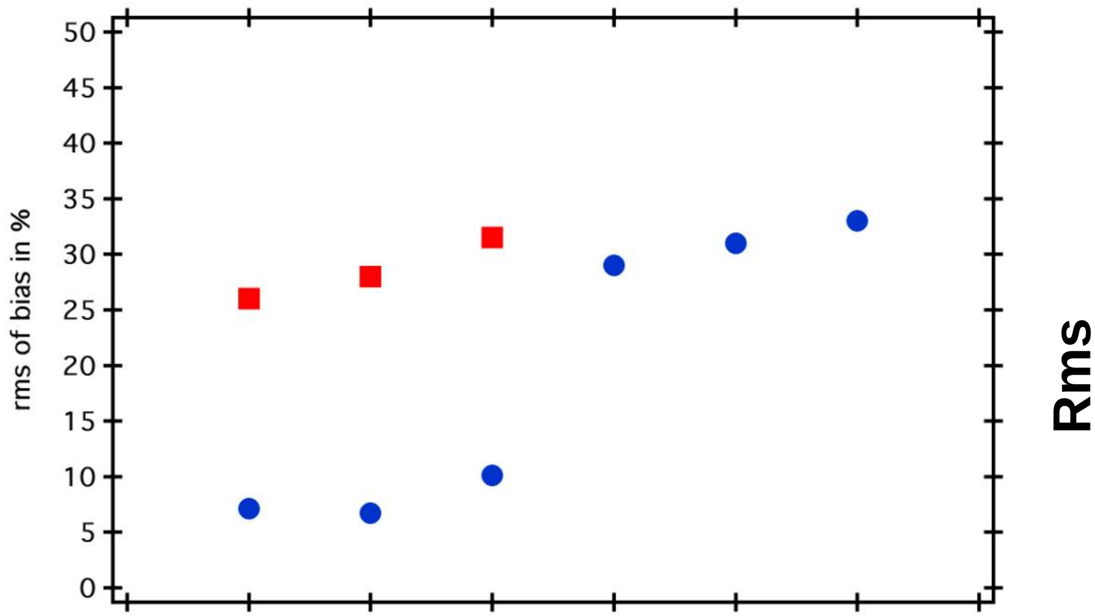


Looking over the range of cases





- Lower spectral resolution IR instrument (used alone or in combination with UV/vis) have large bias and rms
- Combined high-spectral resolution IR and uv/vis have low bias and rms

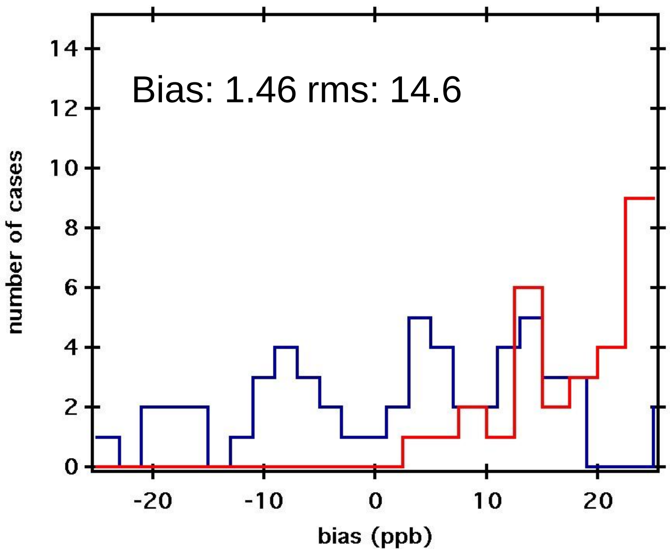


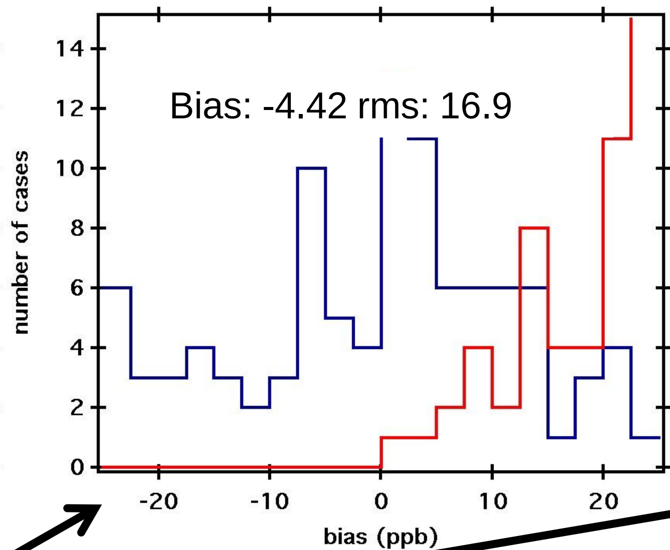
Comparing statistics: varying width of IR window

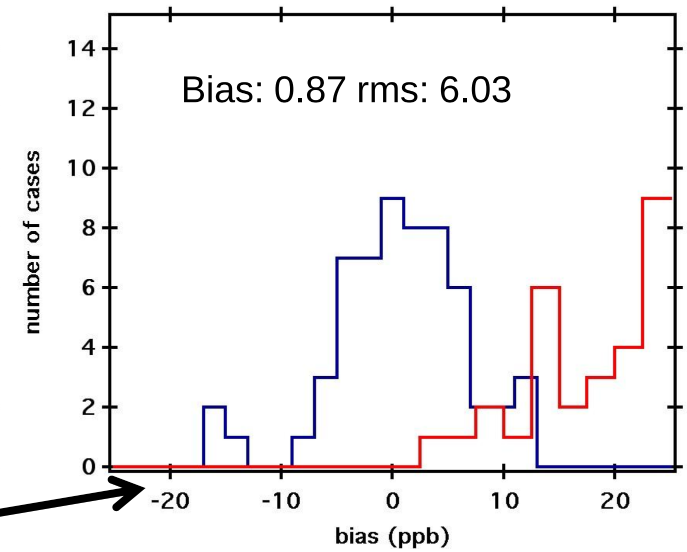
UV only

IR only

UV + IR





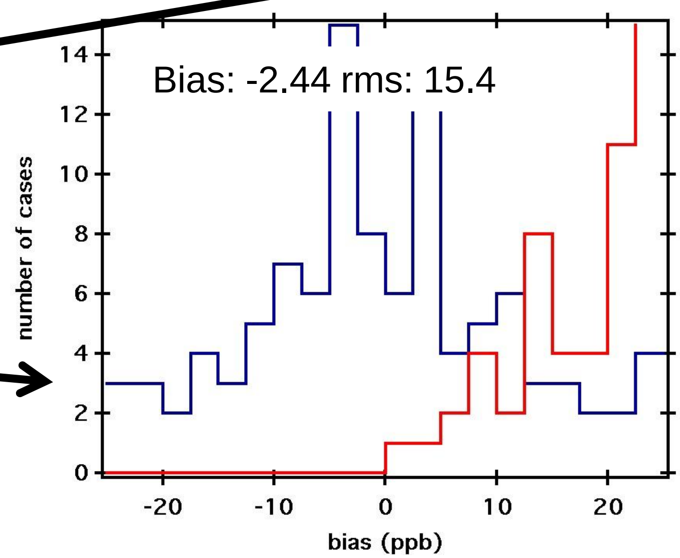


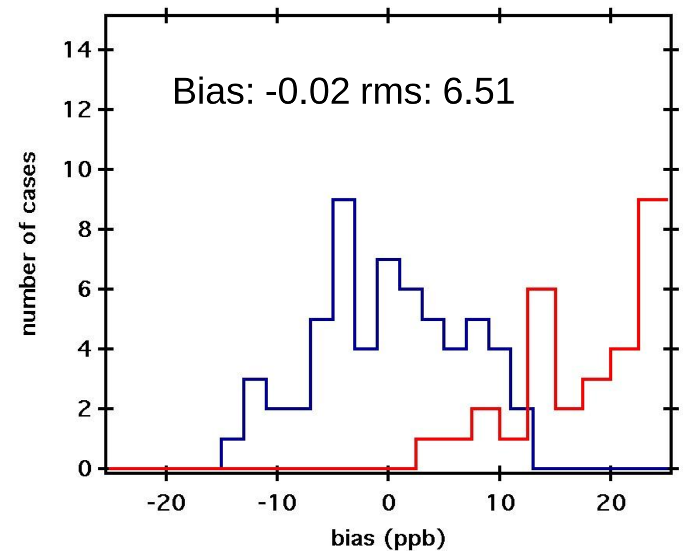
Narrow window

1043-1075

wider window

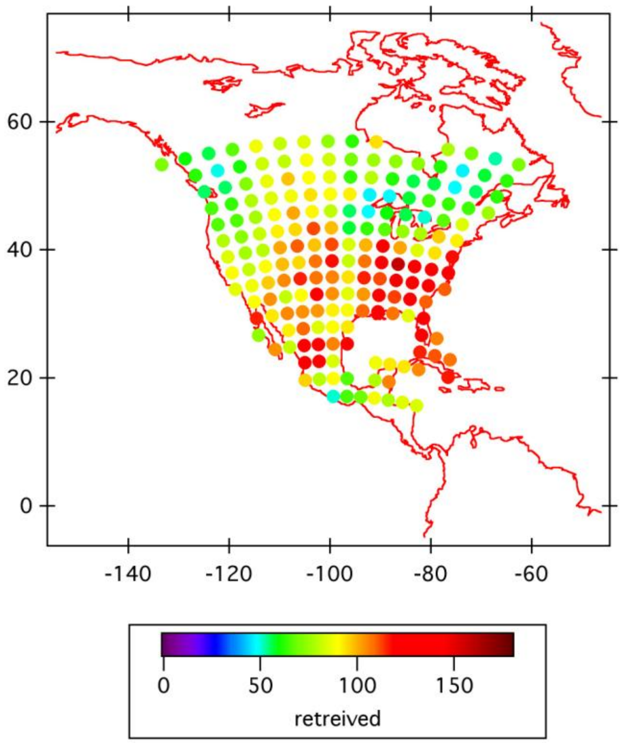
970-1080

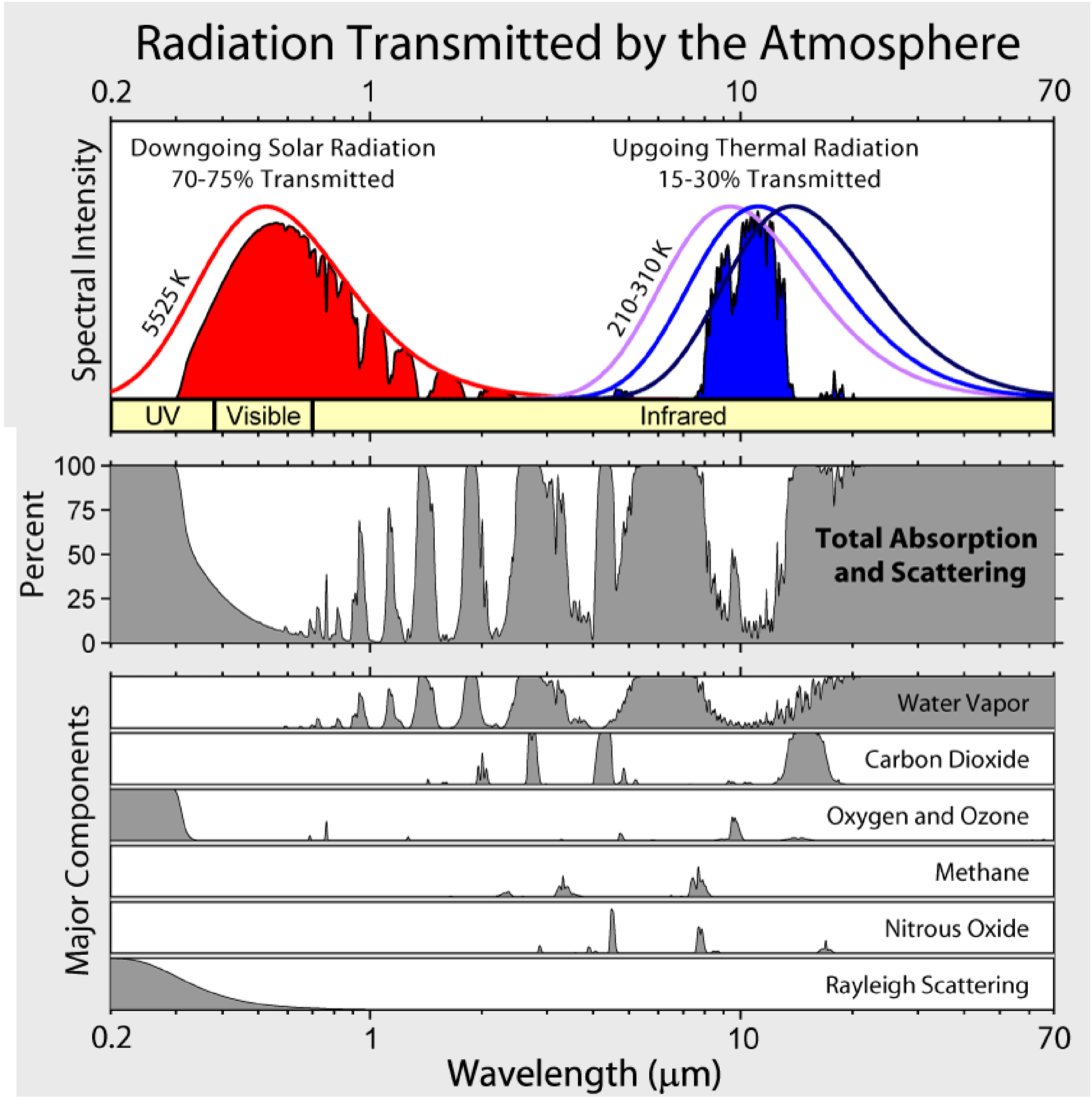




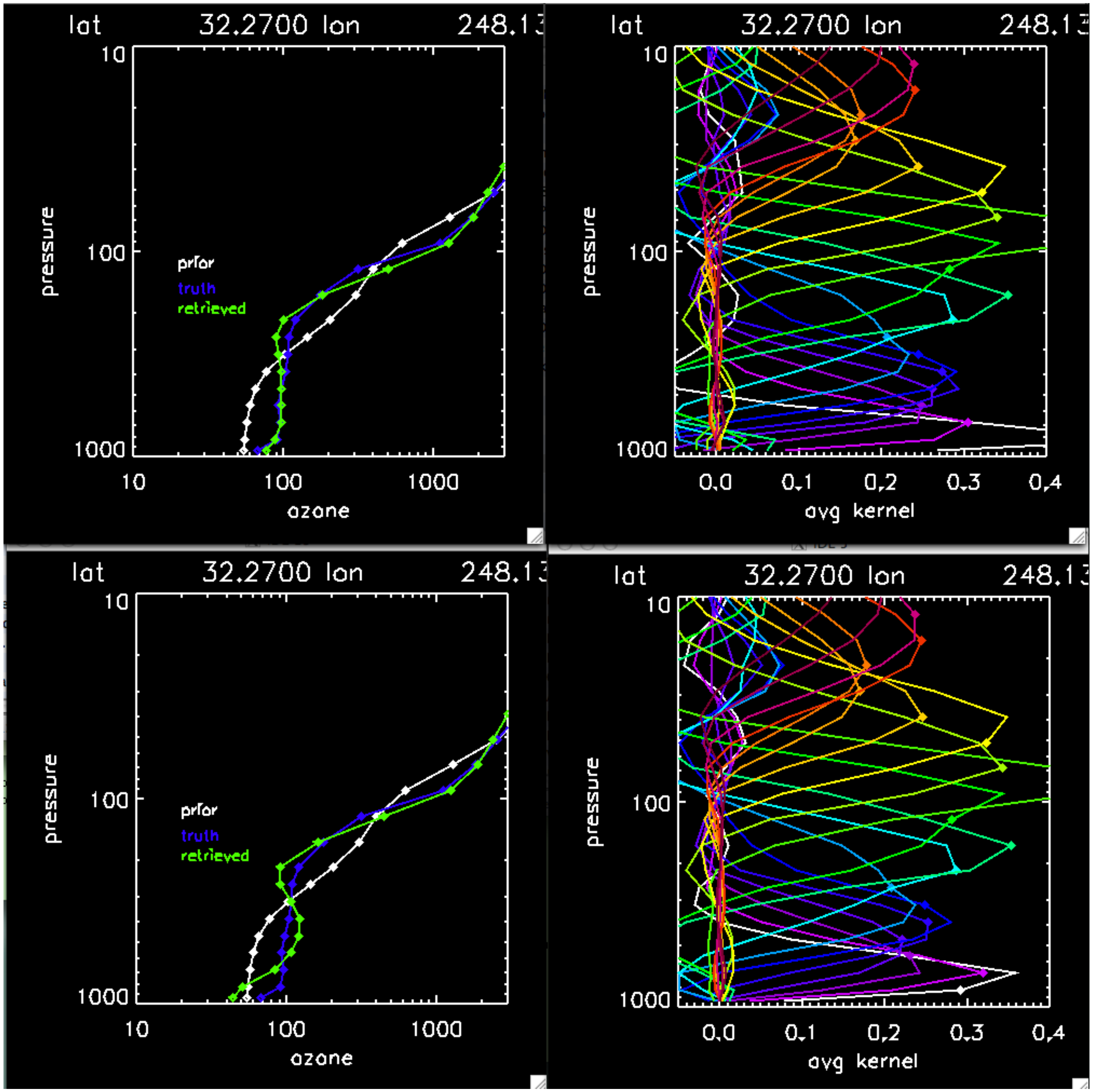
Upgrades include 3.6 microns

- Need to perform radiative transfer calculations with both solar terms and thermal emission



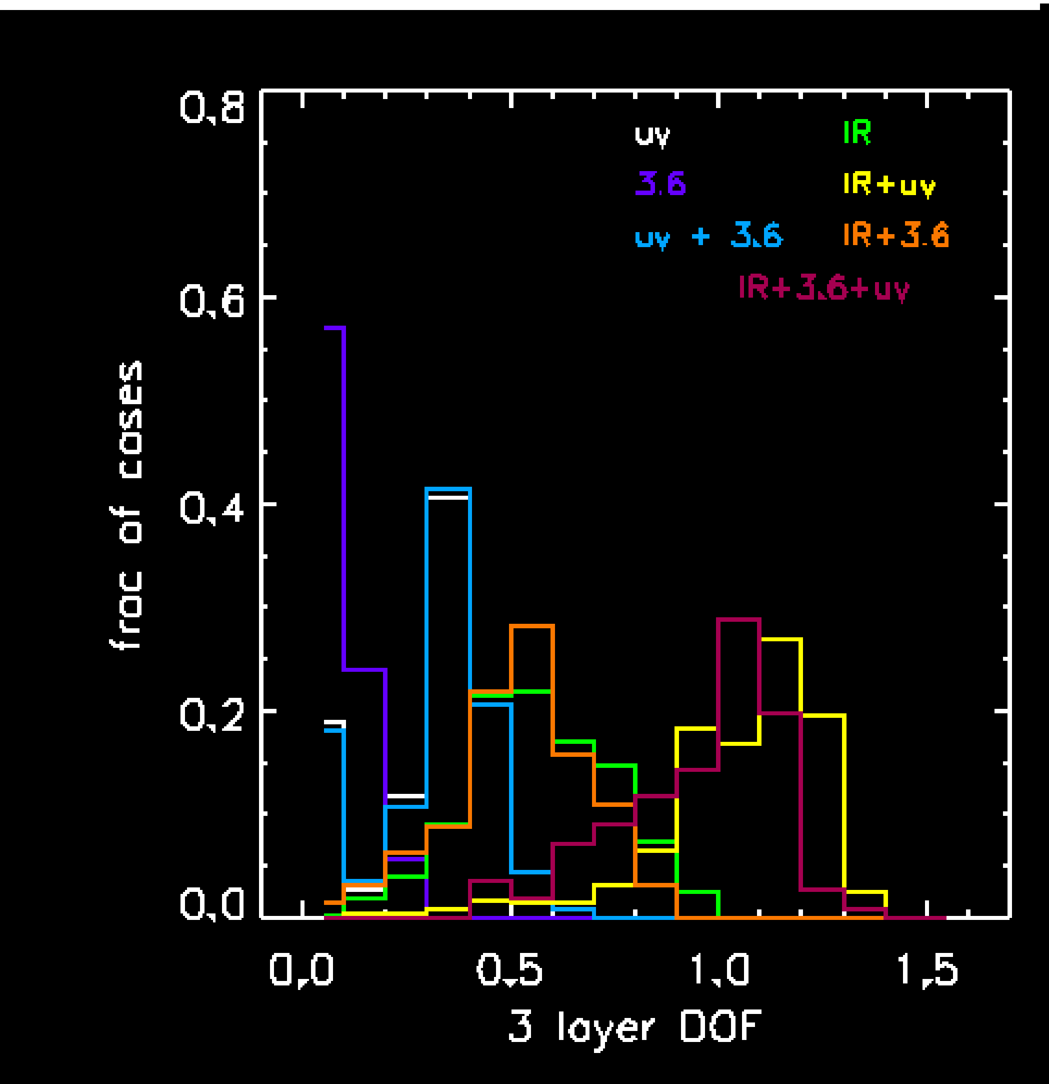


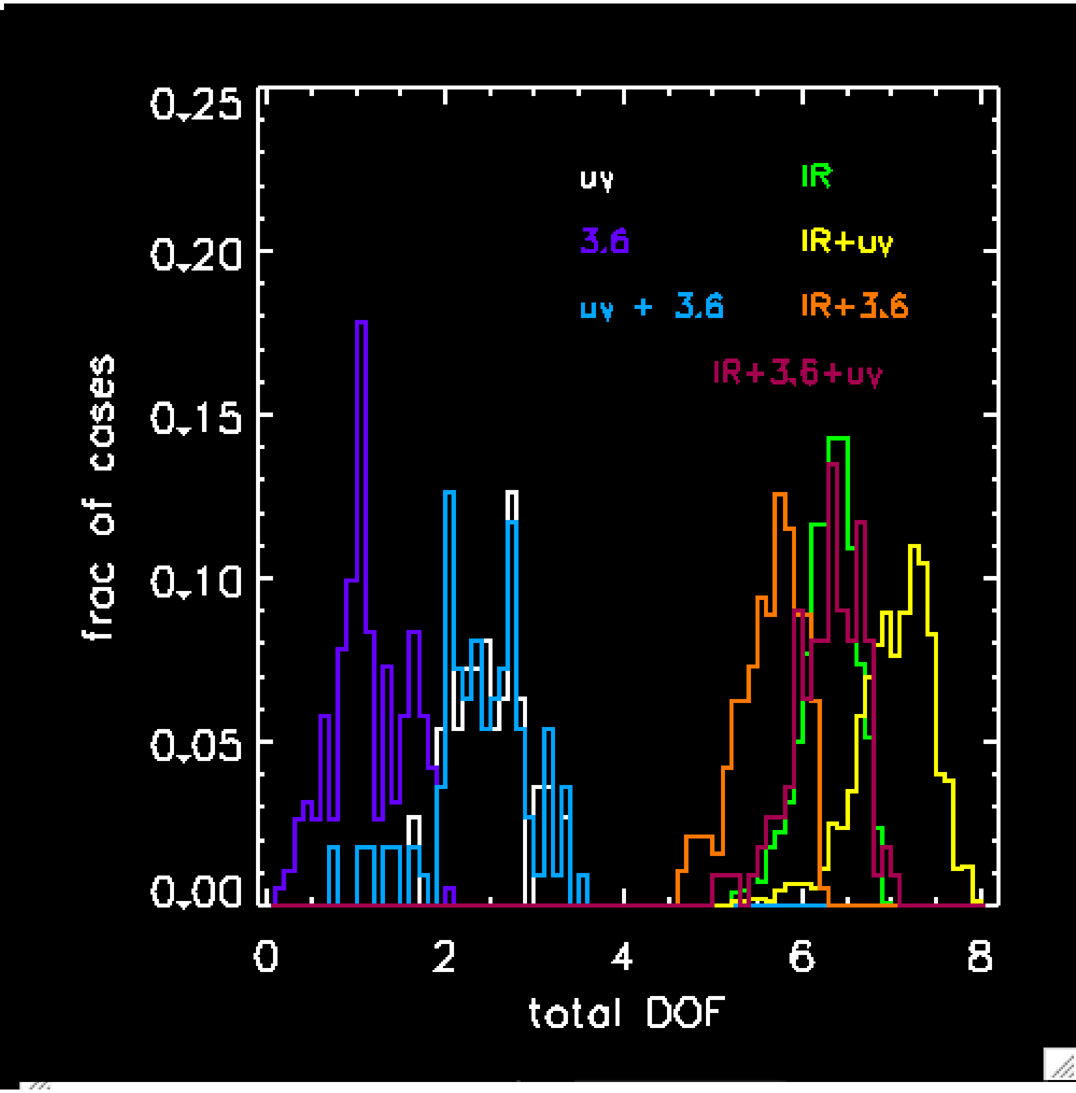
Results



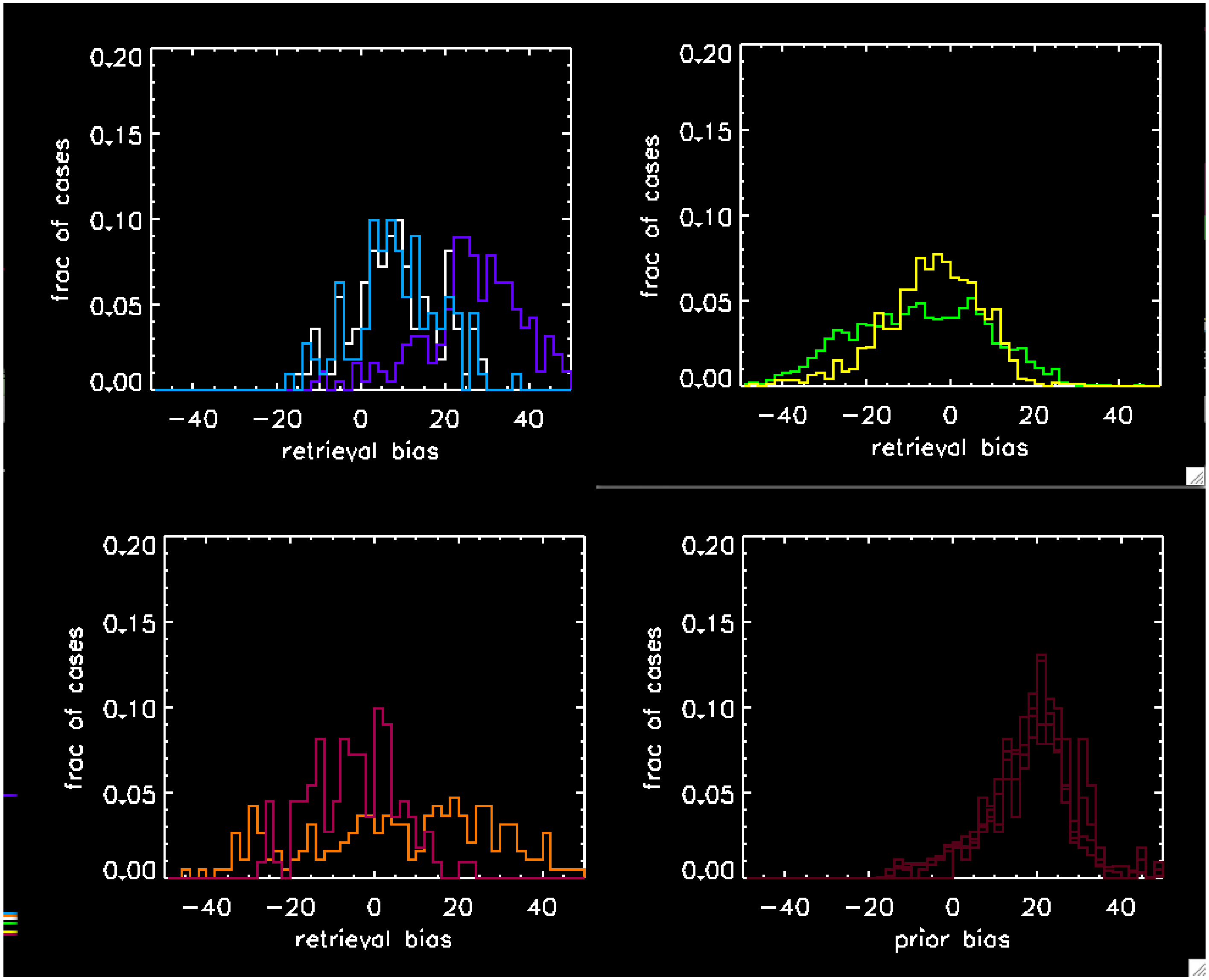
lat 32.2700 lon 248.13
pressure
azone
prior
truth
retrieved
avg kernel

More Results - DOF





More Results – bias statistics



Comparing requirements to simulated performance

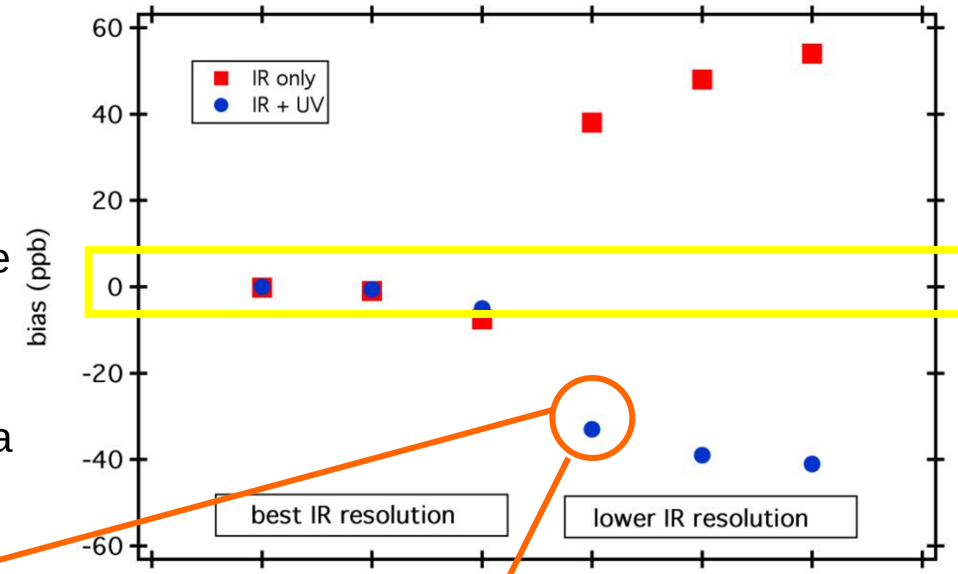
Table 1 Mission sensitivity analysis. Measurement needs for science translate into required column density measurement capability.

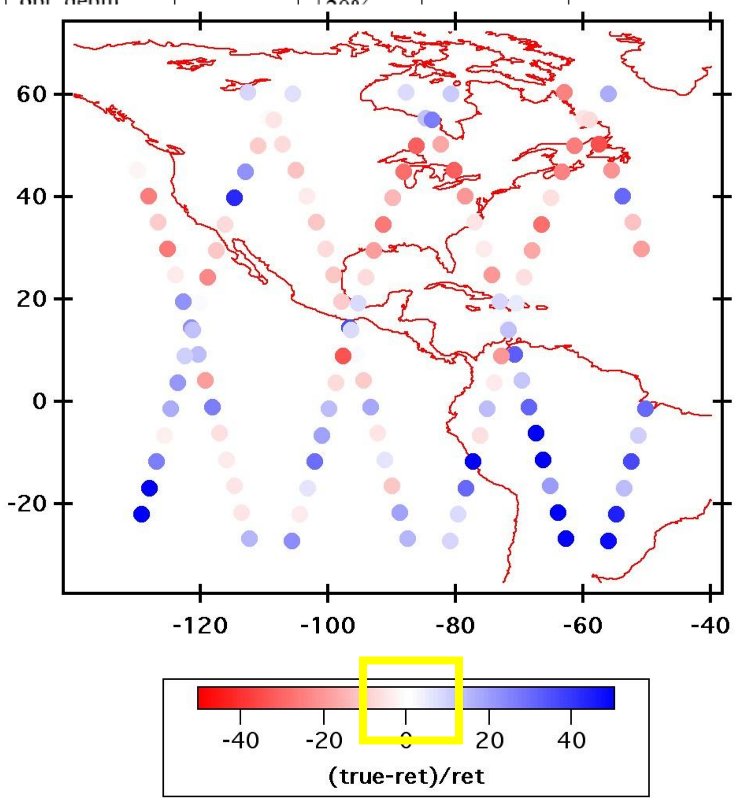
Level 3 data Products	Needed mixing ratio precision (Δ)	Needed Accuracy	Column density capability* mol.cm^{-2}
NO_2	0.2 ppbv	±20%	5.0×10^{14}
CH_2O	1.0 ppbv	±20%	2.5×10^{15}
O_3	5 ppbv	±10%	1.3×10^{16}
CO	10 ppbv	±20%	1.0×10^{17}
aerosol opt. depth	0.02	±0.05 or ±20%	N.A.

Focus on the ozone requirements from the NRC white paper - JANZ

All figures for 825 hPa

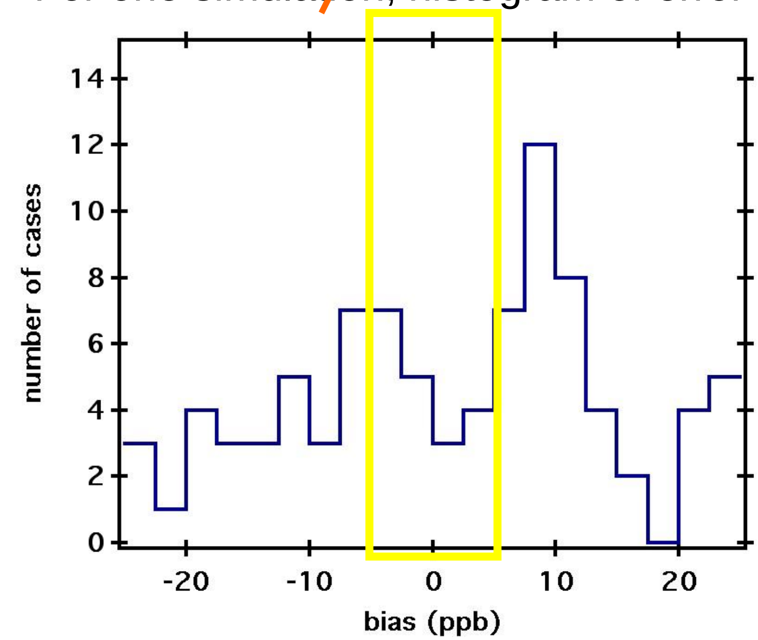
Mean bias @ 825hPa for all simulated instruments





For one simulation, distribution of error

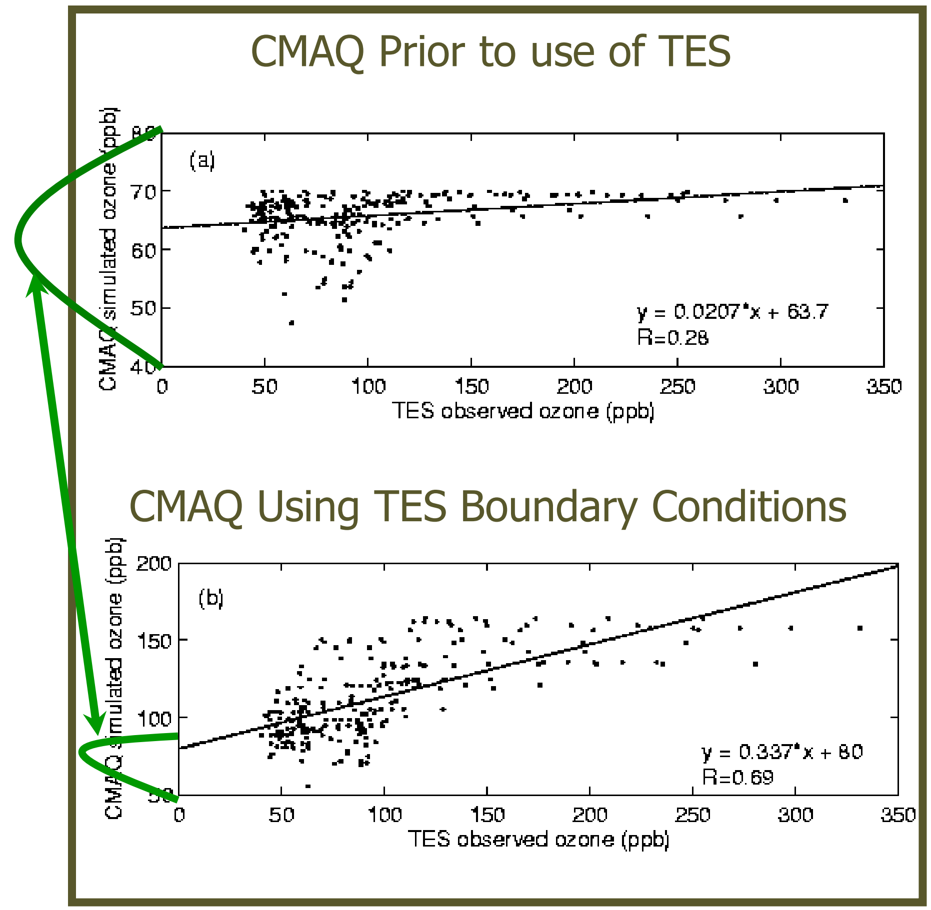
For one simulation, histogram of error

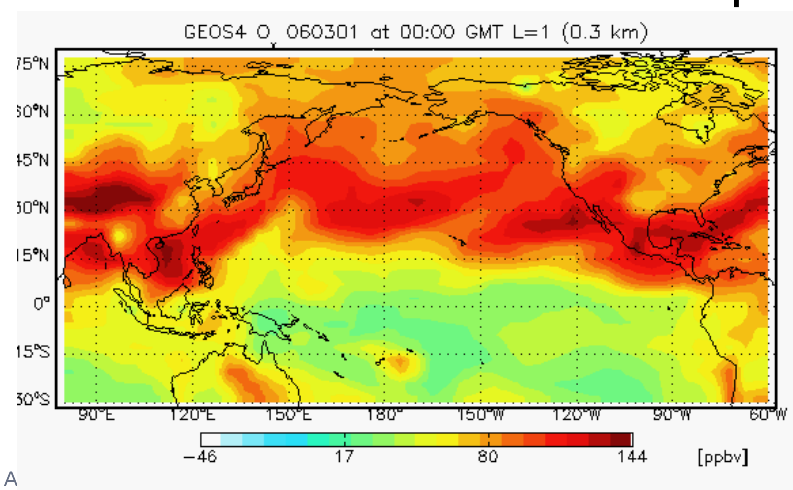


Yellow box marks requirement

Where do we go from here?

- Important science questions with societal impacts push us towards a new way of measuring ozone (GEO-CAPE)
  - Improve air quality forecast skill
  - Quantify impacts of pollution transport on regional to continental scales
  - Monitor pollution emissions
- Current measurements fall short for these science goals
  - Limited sensitivity to the lower layers of the atmosphere
  - Observations at best twice per day





Using OSSEs to more fully evaluate possible approaches (getting to the right design for the INSTRUMENT and the MISSION):

Science question used to define measurement requirements

↓

Instrument designed to meet measurement requirements (sensitivity)

↓

Mission designed to meet measurement requirements (frequency of samples)

↓

Thoroughly test in simulated science analysis

Measuring ozone from Space

- We have a long history of space based measurements
- Many nadir viewing approaches, key for tropospheric measurements
  - Total column ozone from SBUV, TOMS, and OMI based on uv/vis
  - GOME, SCIAMACHY, GOME-2
  - Infrared sounder measurements
    - » AIRS total column
    - » TES - profiles with ability to differentiate the upper and lower troposphere
    - » IASI - total columns and some thick layer vertical information