Ozone and NO_2 OSSEs on a Regional/Urban Scale for GEO-CAPE

AGU FALL MEETING
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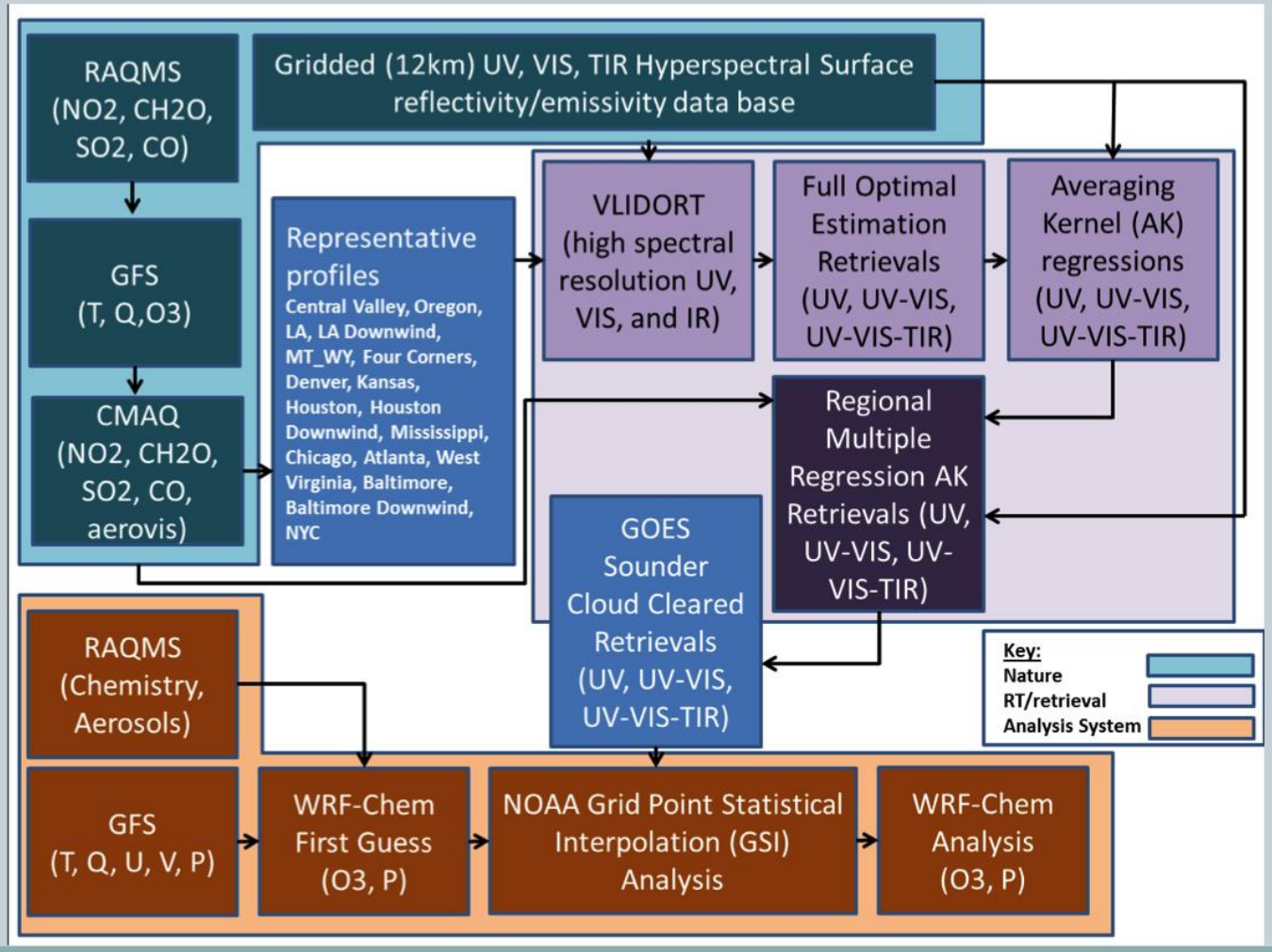
OSSE Flow Chart



Goals

- Utilize independent modeling systems for generation of Nature atmosphere and conducting assimilation impact experiments
- Account for realistic atmospheric variability, which requires evaluation of the nature runs with respect to observations
- Include realistic variability in the synthetic radiances, which requires using realistic albedos and emissivities
- Include realistic sensitivities, which requires generation of averaging kernels (AK) for each retrieval for use in assimilation studies

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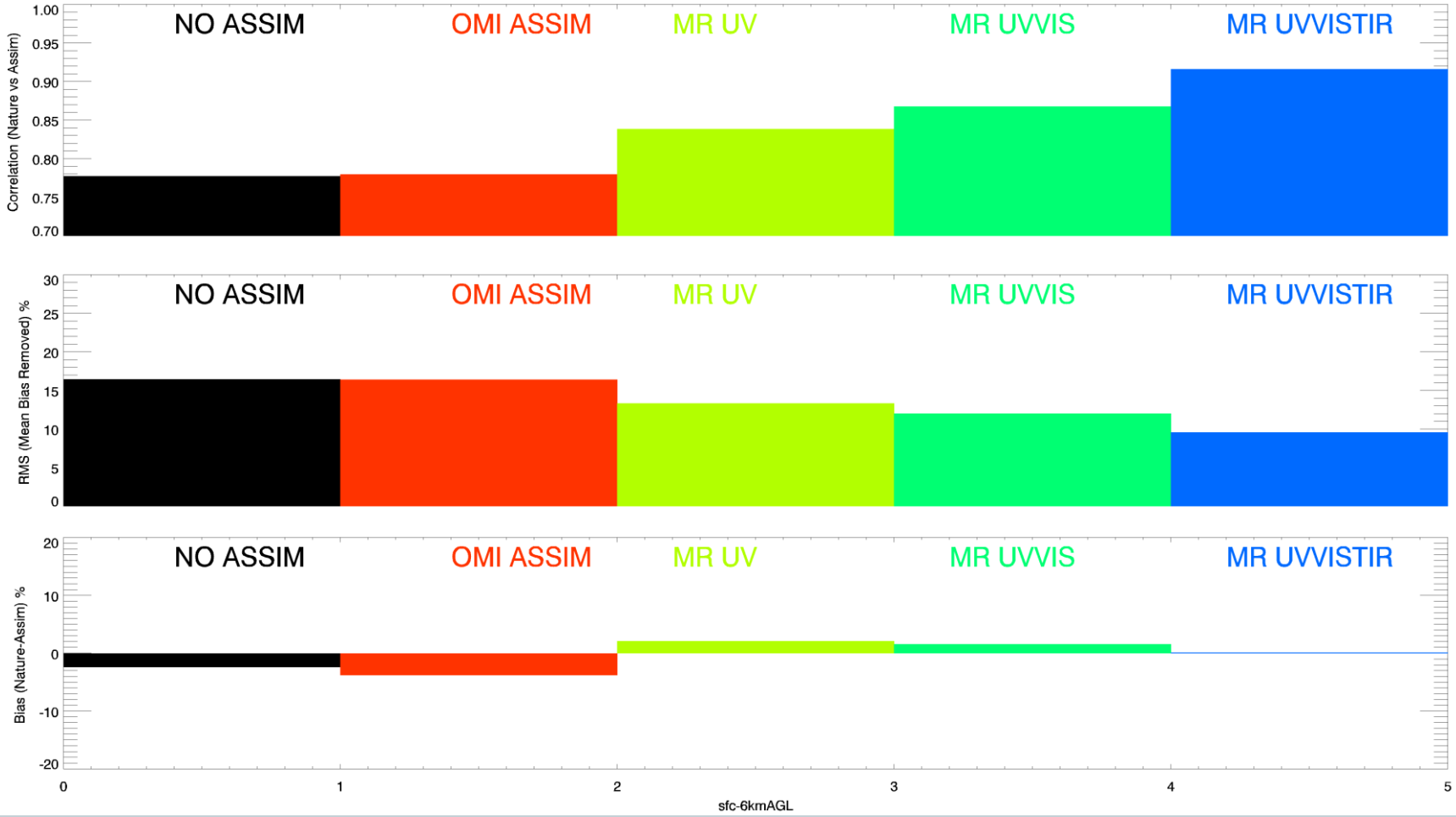
- Include realistic sensitivities, which requires generation of averaging kernels (AK) for each retrieval for use in assimilation studies

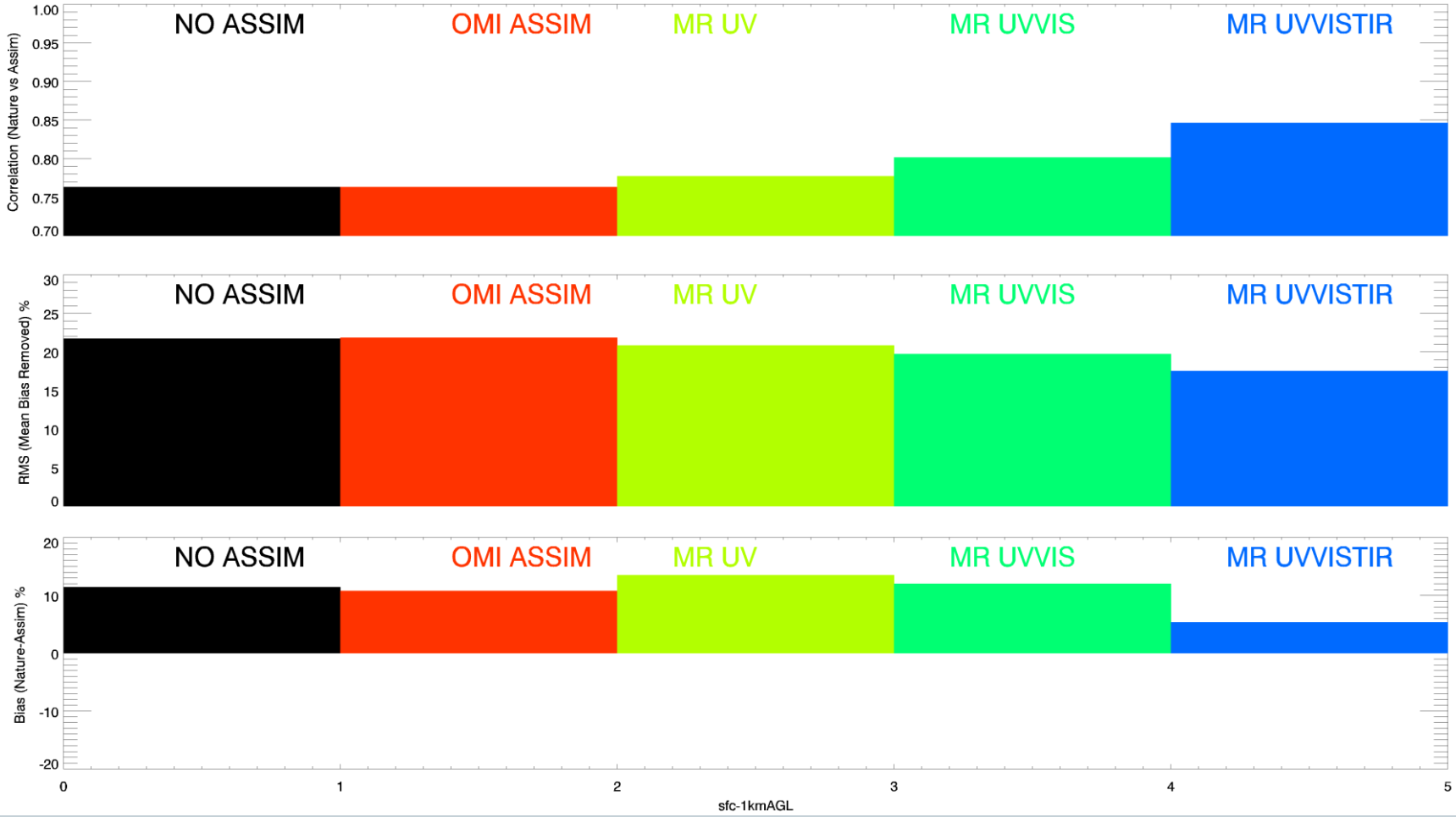
Forward Modeling for O_3

- Use a set of representative profiles from 17 sites (hourly, every 3rd day of July 2011)
- Perform full radiative transfer (using LIDORT)/Optimal Estimation
- Develop multiple regression estimate of the averaging kernels
- Use AK regressions for the full Nature atmosphere (CONUS, hourly, every day of July 2011) to generate the regional multiple regression AK retrievals

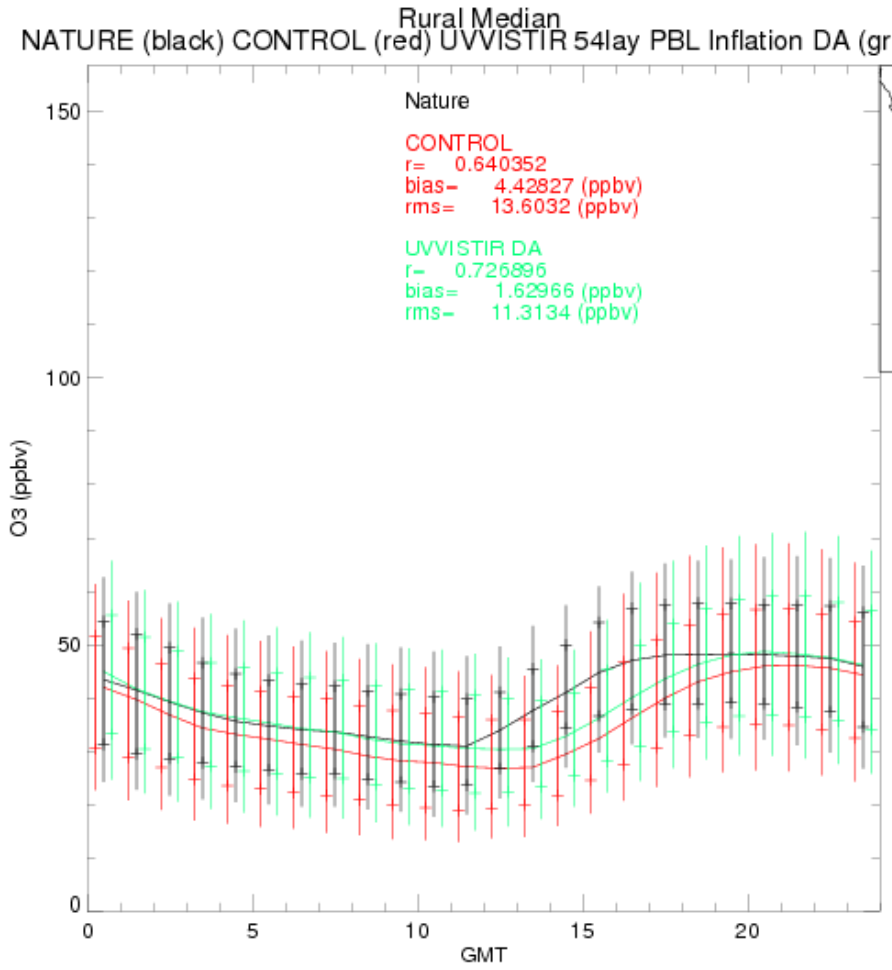
Impact of Ozone Assimilation: sfc-6km Results



Impact of Ozone Assimilation: sfc-1km Results



Impact of UVVISTIR Assimilation: Rural Sites

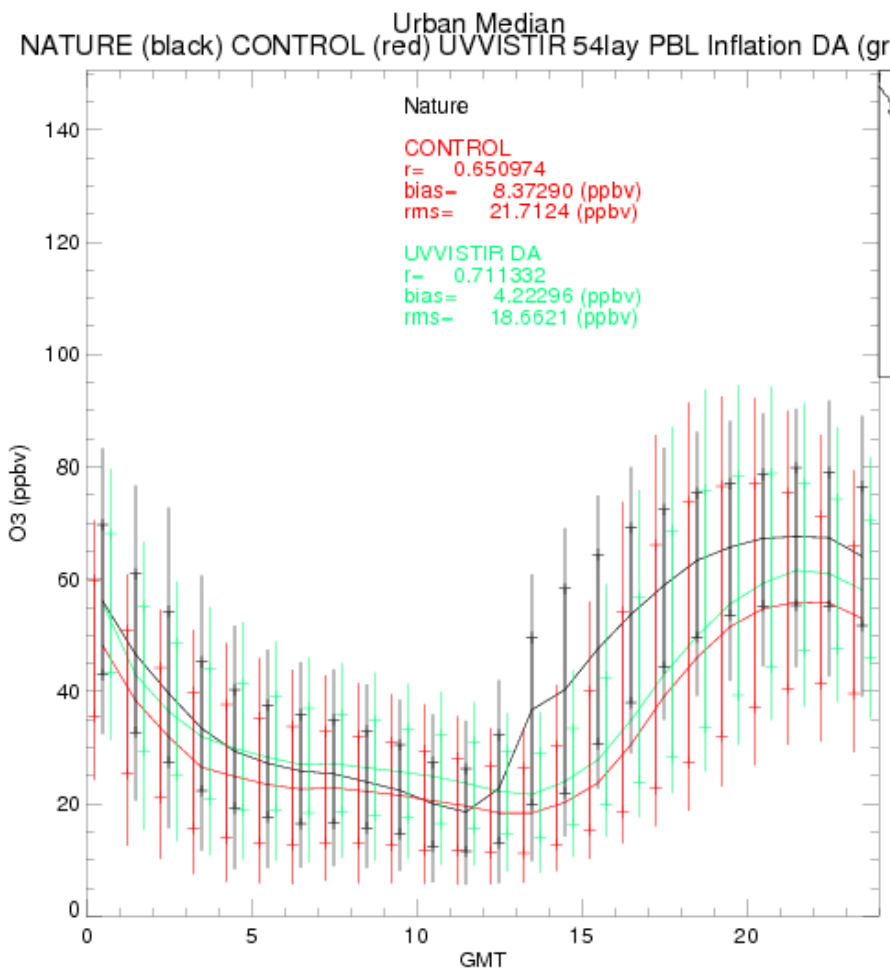


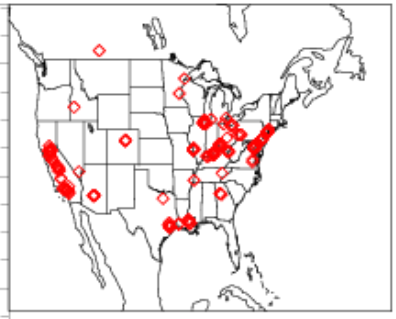
ASSIM
Control
Nature

July 2011 Mean Diurnal Cycle

UVVISTIR assimilation increases correlation by 13%, reduces bias by 63%, and reduces rms error by 17% at Rural sites

Impact of UVVISTIR Assimilation: Urban Sites





ASSIM
Control
Nature

July 2011 Mean Diurnal Cycle

UVVISTIR assimilation increases correlation by 9%, reduces bias by 50%, and reduces rms error by 14% at Urban sites

Forward Modeling for NO_2 I

- O_3 simulations required 8 hrs per day (~15 hrs daylight) per station using 44 CPUs
- NO_2 has significantly larger spatial variability
- AK regression unlikely to produce good results
- Need to investigate fast forward modeling approaches

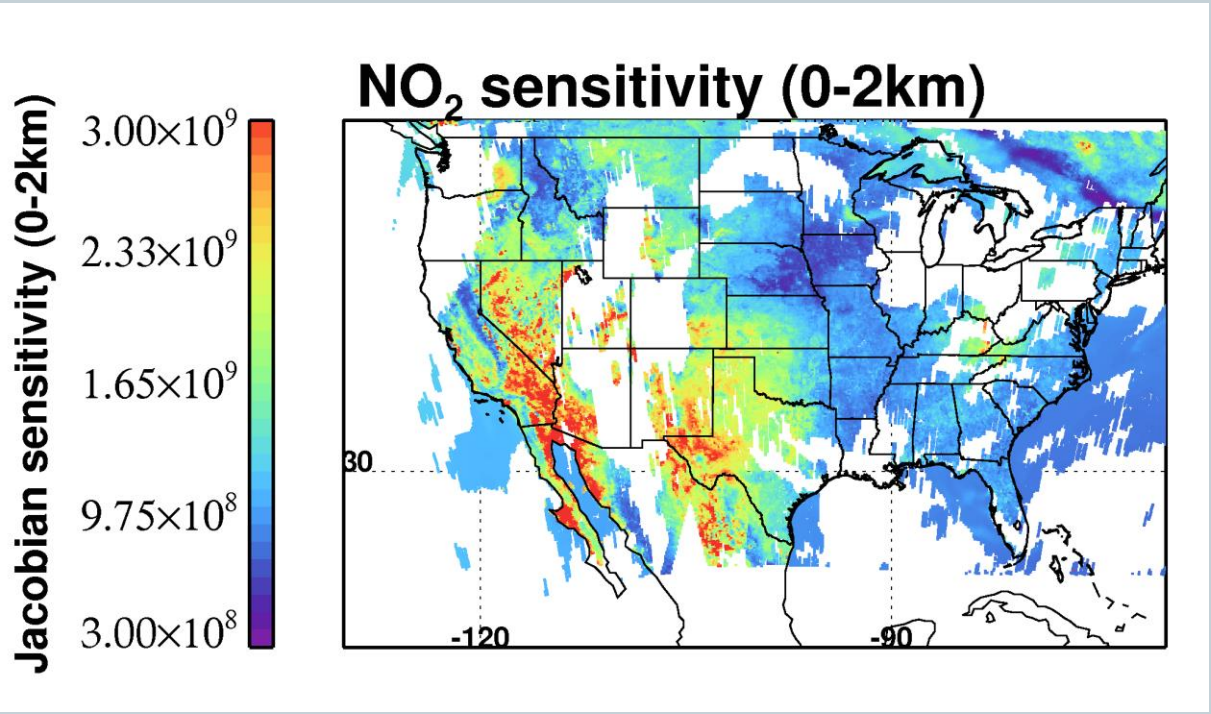
Forward Modeling for NO_2 II

- Spectral region: 400–490 nm (TEMPO spectral range)
- Forward modeling approaches
  - LIDORT
  - Exact single scattering + two-stream multiple scattering (2S-ESS)
  - 2S-ESS + cross sections convolved to TEMPO spectral resolution (2S-ESS convolved)

2S-ESS Model

- Exact computation of the single scattering using all moments of the phase function
- Two-stream approximation for multiple scattering
- Accurate single scatter calculation captures forward peak of aerosol phase function
- Two-stream model completely analytic except for BVP (which is also optimized)
- Technique used, e.g., for water vapor retrievals over LA basin from CLARS measurements

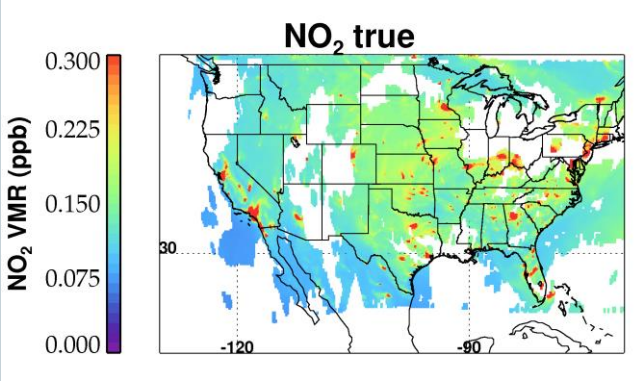
Real-time OSSE Estimates of Sensitivity

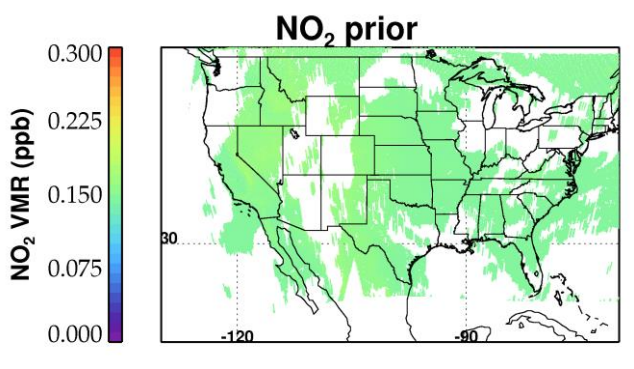


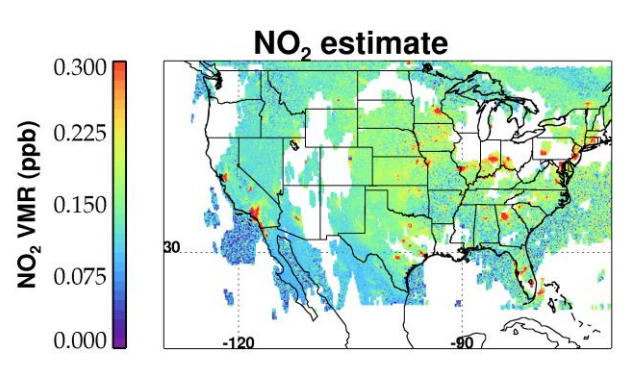
July 18, 2011 2 pm local time

- Calculates Jacobians including aerosols and viewing geometry using fast RT system
- Better estimates what a satellite will actually see, which varies by location, time, and composition. Empty areas have thick cloud cover
- OSSEs will ingest results for better estimates of satellite performance

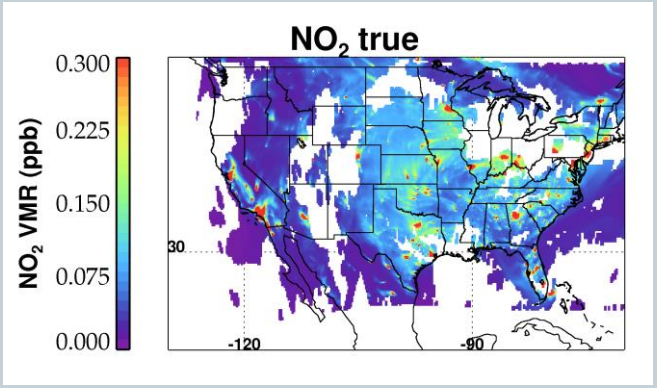
Total Column Retrievals

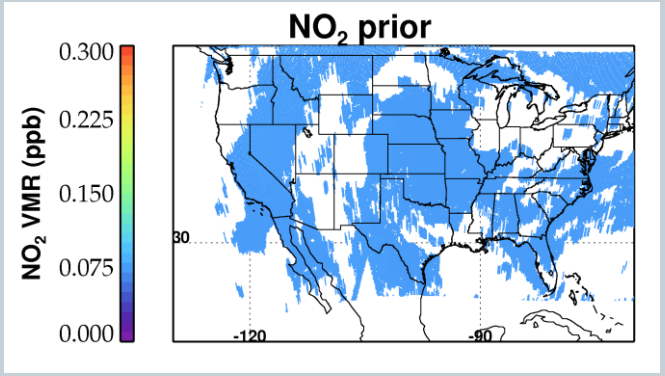


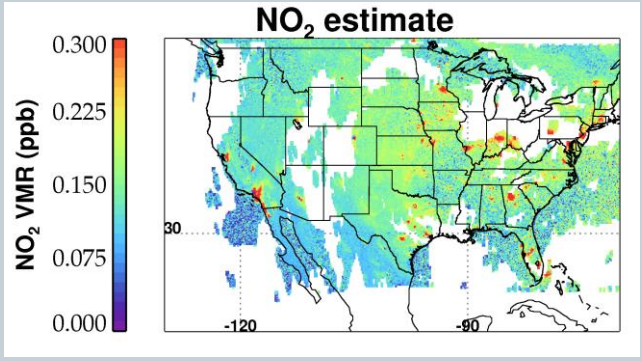




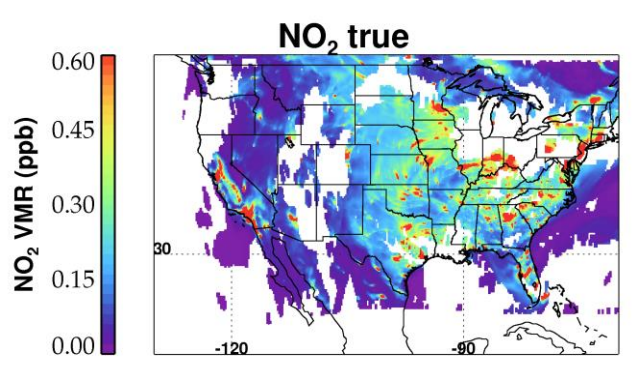
Tropospheric Column Retrievals

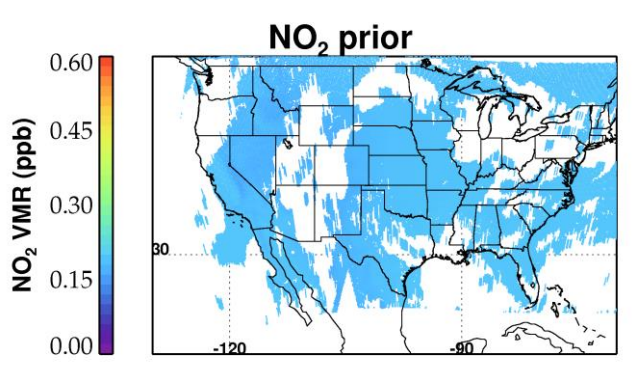


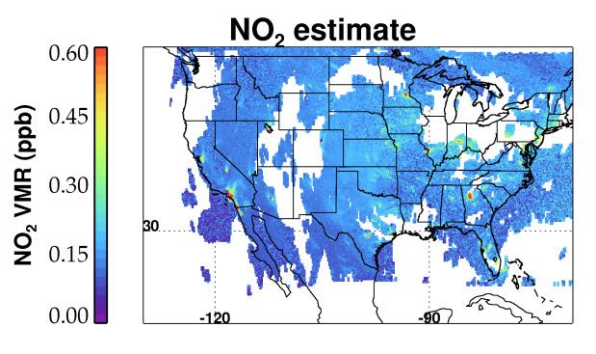




Lowermost Troposphere (0-2 km) Retrievals





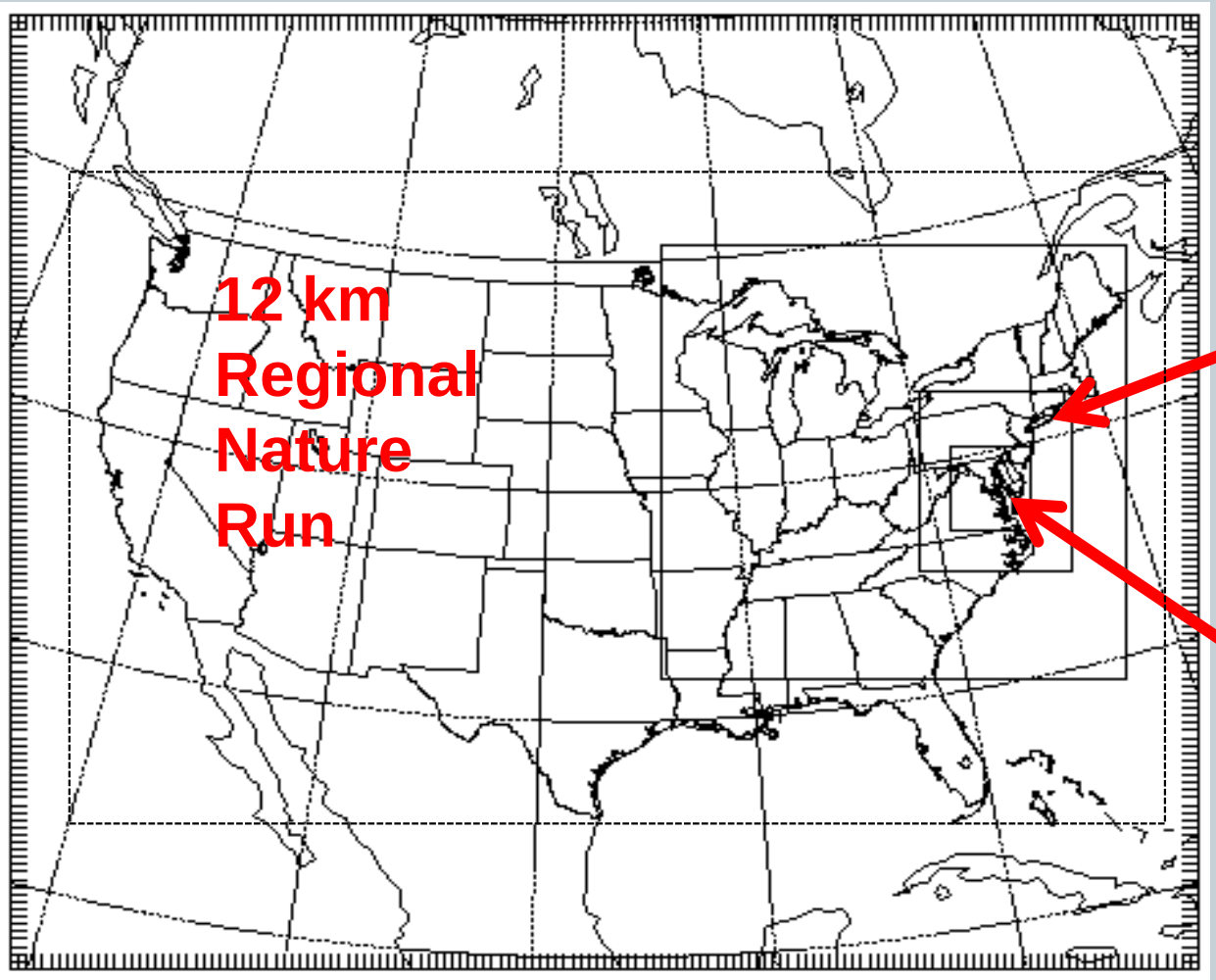


Conclusions

- Full UV-VIS-TIR retrievals showing positive impact on surface O_3
- Regional OSSE system showing realistic complexity
- NO_2 retrievals underway
- We find real satellite data sensitivity varies substantially, e.g. by aerosol optical depth, cloud cover, albedo, and viewing geometry
- Using a fast RT, we now estimate complete sensitivity (using scene dependent AKs) during OSSE simulations

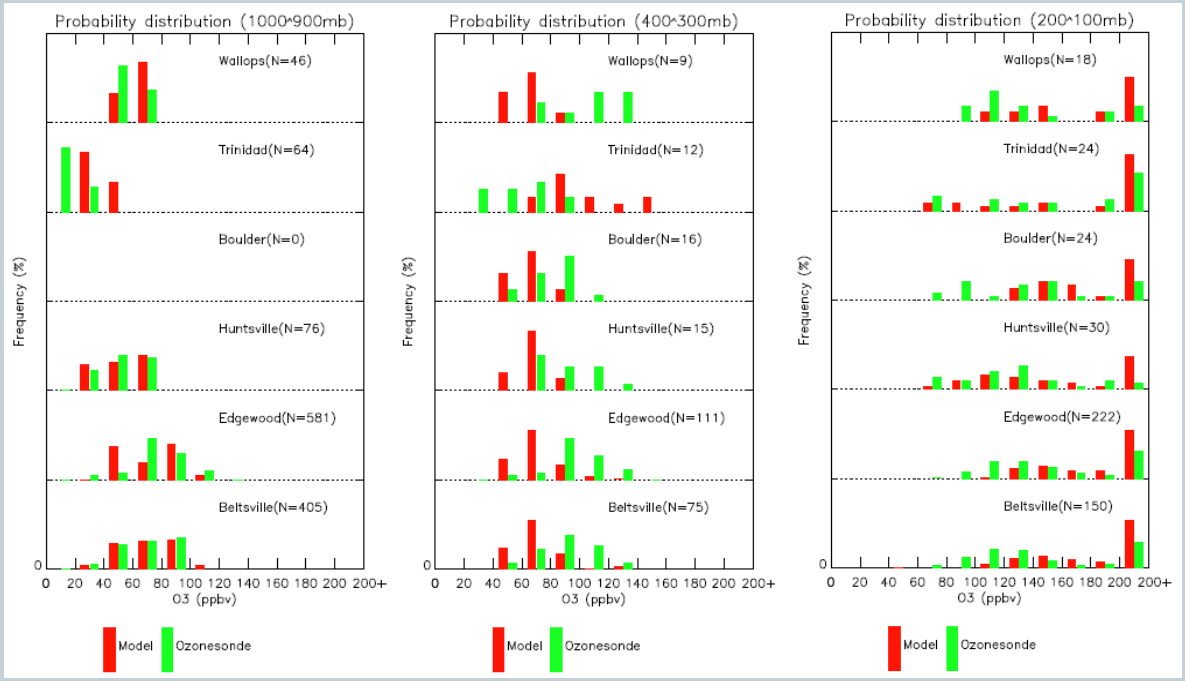
Backup Slides

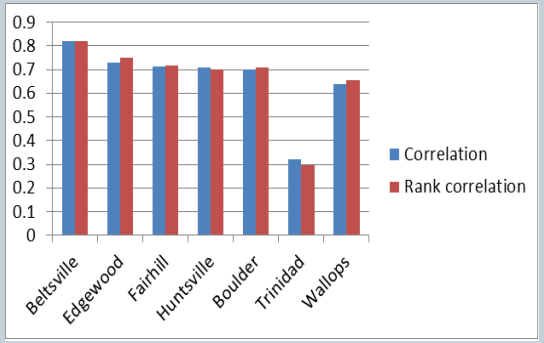
Nature Run



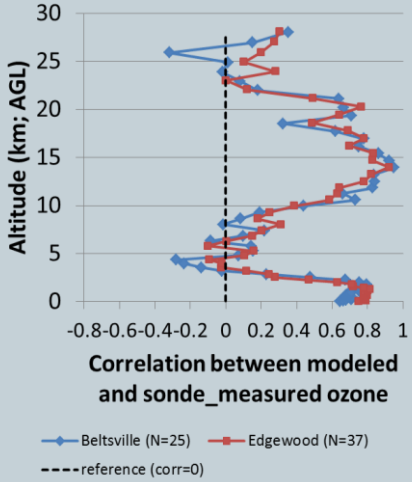
Courtesy: K. Pickering/C. Loughner

Quantifying Accuracy and Representativeness of Regional Nature Run





Correlation between model and EPA-monitored surface ozone (July 2011)



Correlation between model and ozonesondes at Beltsville and Edgewood

July 2011 Regional Nature run captures the variability of upper troposphere/lower stratosphere (200-100 mb) and boundary layer (1000-900 mb) ozone well but underestimates free tropospheric (400-300 mb) variance

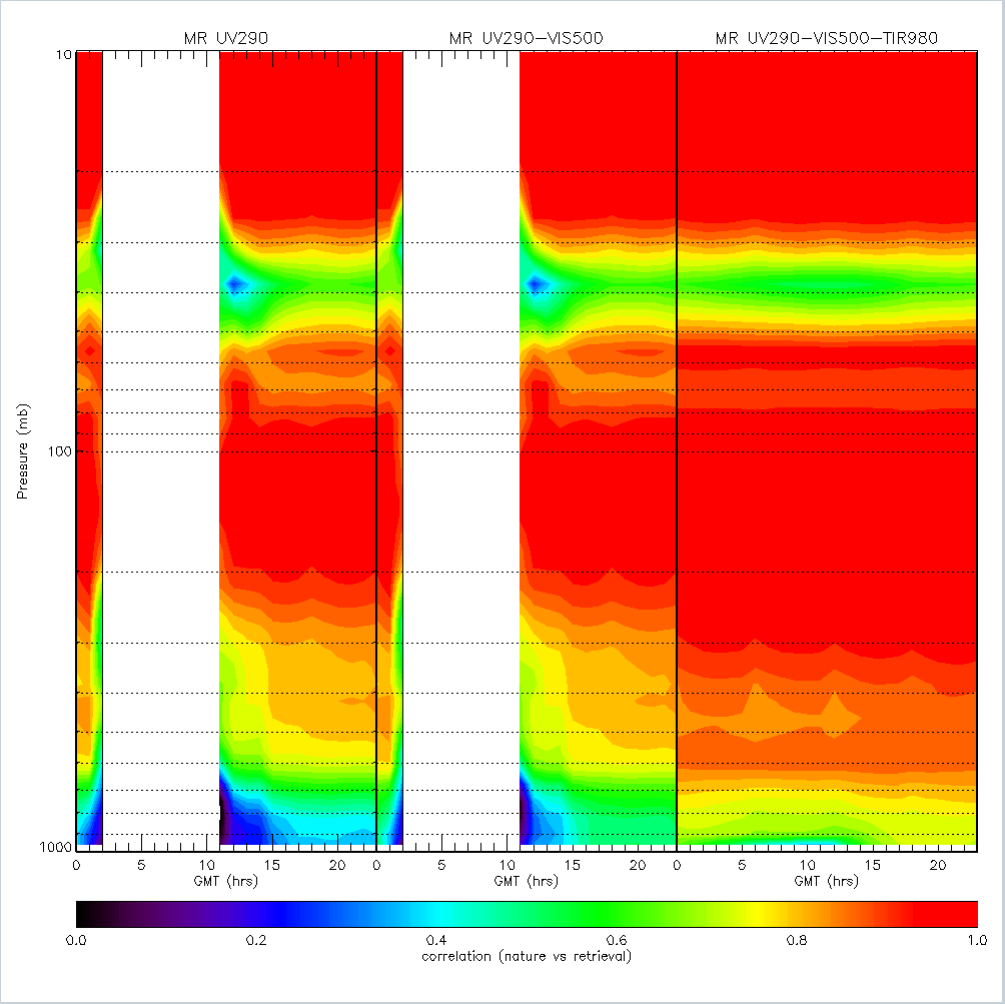
Courtesy: M. Newchurch/L. Wang

Nature/Retrieval Correlations

Regional Multiple Regression AK Retrievals (UV, UV-VIS, UV-VIS-TIR)

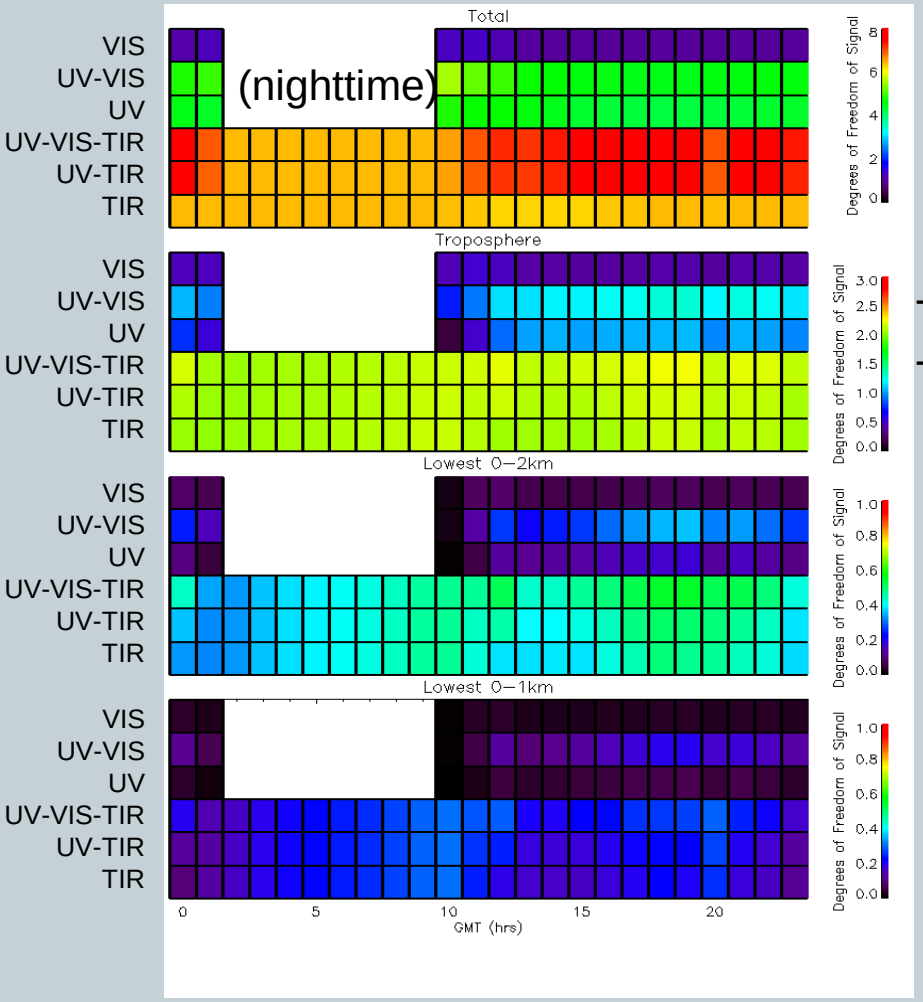
Diurnally resolved correlations between the Regional Nature Run and GEOCAPE O_3 retrievals for July 2011 show:

- UV-VIS-TIR shows the highest correlations in the mid and lower troposphere
- UV-VIS shows improvement over the UV only retrievals below 800mb



More details in H. Worden's poster

Multispectral O_3 Retrievals

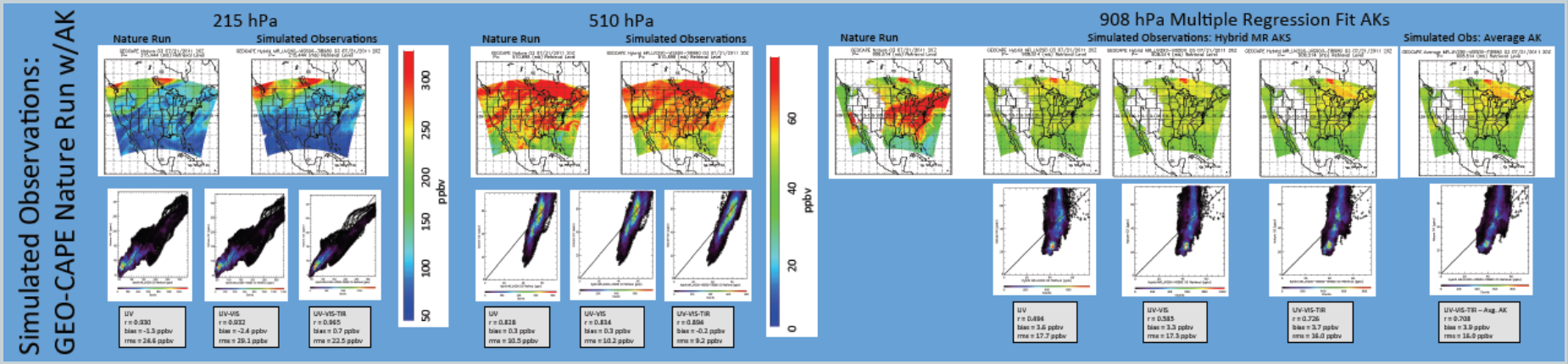


Full Optimal Estimation Retrievals (UV, UV-VIS, UV-VIS-TIR)

Diurnally resolved Degrees of Freedom for Signal (DOFS) for different pressure ranges and spectral combinations for all GEOCAPE Regional OSSE sites (no VIS, UV, or UV/VIS retrievals between 02-09Z)

Note UV/VIS has the same spectral range and noise as TEMPO.

AK Prediction



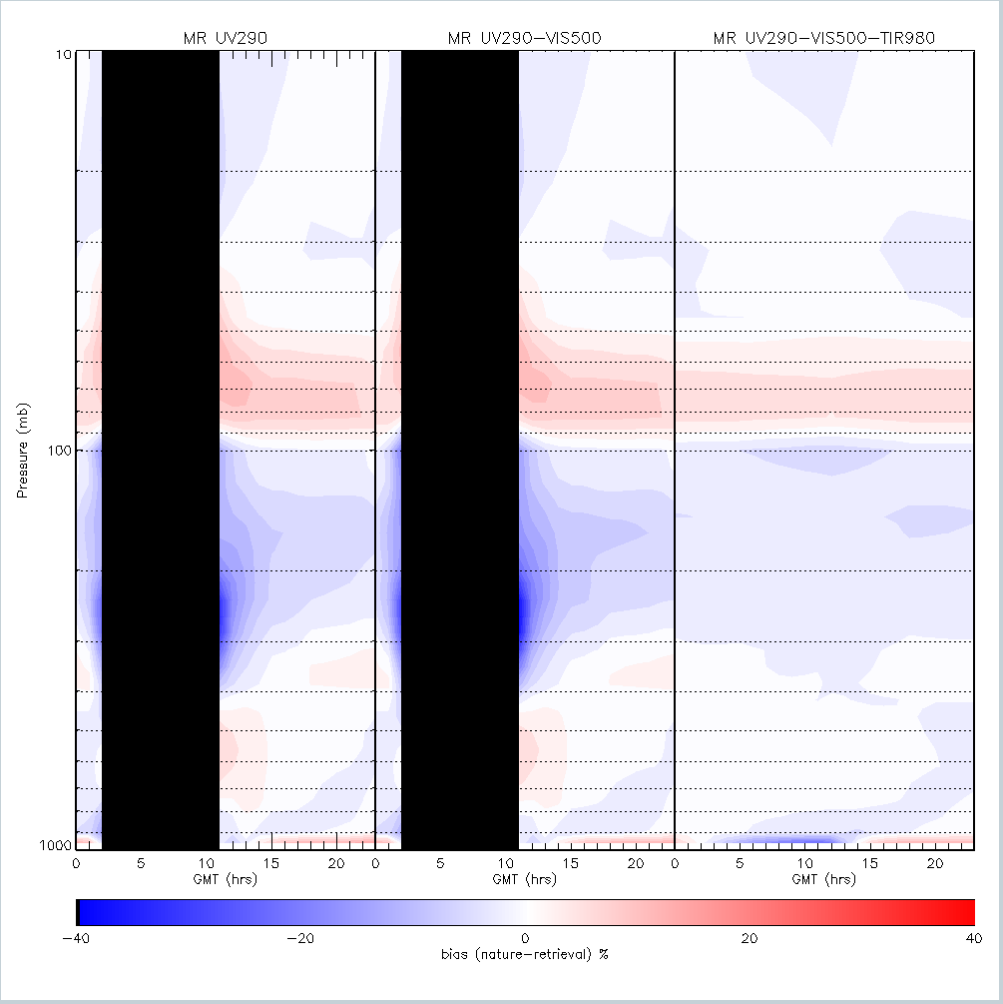
- Multiple regression works best for surface – 681 hPa
- Combinations of fit AK in lower troposphere and average AK above allow simulated observations for different wavelength combinations
- UV-VIS-TIR provides highest correlation between simulated observations and nature run

Retrieval Biases

Regional Multiple Regression AK Retrievals (UV, UV-VIS, UV-VIS-TIR)

Diurnally resolved biases between the Regional Nature Run and GEOCAPE O3 retrievals for July 2011 show generally low biases (<20%) except:

- between 200-300mb at sunrise and sunset (UV and UV-VIS only)
- at the surface (underestimate daytime and overestimate nighttime O3



Data Assimilation I

WRF-Chem Analysis (O_3, P)

- Initial RAQMS/WRF-CHEM/GSI GEOCAPE UV-VIS-TIR retrieval assimilation experiments have been conducted for early July, 2011
  - Currently assuming 30% observational errors and only assimilating retrievals below 100mb due to large initial adjustments in the lower stratosphere
  - Statistical analysis show positive impacts on surface ozone sampled at US EPA AIRNow sites

Data Assimilation II

WRF-Chem Analysis (O_3, P)

- Future plans
  - Improve observation error estimate using error estimates from Full Optimal Estimation retrieval for select stations
  - Assess impact of restricting assimilation of retrievals to below local tropopause to mitigate impact of poor vertical resolution in WRF-Chem in the lower stratosphere
  - Conduct regional UV and UV-VIS O_3 assimilation studies

Accomplishments for Ozone OSSE

- 12 km and 1 km Nature simulations were evaluated with respect to observations during the 2011 NASA DISCOVER-AQ campaign.

- Diurnally resolved high spectral resolution UV/VIS/TIR forward modeling at 14 representative sites using ozone, NO_2, HCHO, SO_2, aerosol, water vapor, and temperature profiles from the Regional Nature run has been completed.

- TIR, UV, VIS, UV/TIR, UV/VIS, and UV/VIS/TIR ozone retrievals have been generated and evaluated with respect to the Nature run profiles.

Accomplishments for Ozone OSSE

- Averaging Kernel (AK) regression based on instrument and observing parameters has been developed using retrievals from 14 representative sites.

- Data assimilation shows positive impacts on surface ozone sampled at US EPA AIRNow sites.

Backup Slides

NO_2 OSSE Developments II

- Computational time (one scenario):
  - LIDORT: 219 minutes
  - 2S-ESS: 295 seconds
  - 2S-ESS convolved: 78.5 seconds
- Computational time (one day, full domain):
  - LIDORT: > 8 years!
  - 2S-ESS: ~ 70 days
  - 2S-ESS convolved: 18 days
- With a 10x speed-up, we can perform calculations for one month for the entire domain in ~ two months

How do we get 10x speed-up?

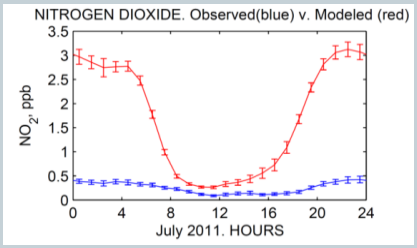
- Optimize optical property initialization (mainly, aerosol phase function moments)
- Perform interpolation of aerosol phase function instead of moments
- Perform profile-independent operations (e.g. reading in of large aerosol optical property tables) only once
- Remove redundant copying of data between variables

How do we get 10x speed-up?

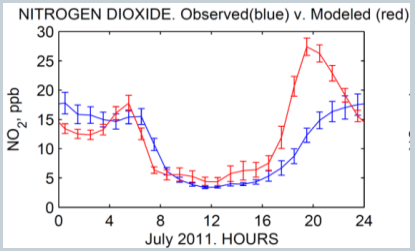
- Implement MPI interface to use multiple processors
- Compute solar geometry early and only perform further calculations for daytime scenarios
- Only consider cloud-free scenarios
- Balance the number of points on each processor to optimize processor utilization
- Only output data to netcdf file for clear and daytime scenarios

Quantifying Accuracy and Representativeness of Regional Nature Run

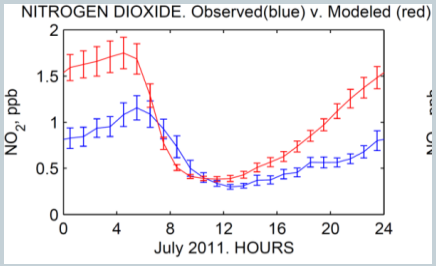
PINNACLE, NY. Park Forest



BIRMINGHAM, AL. Urban

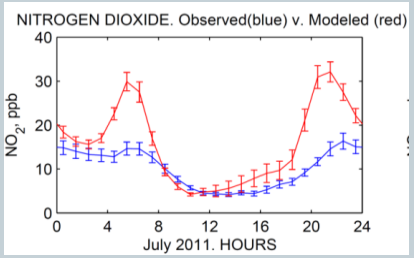


CENTERVILLE, AL. Rural

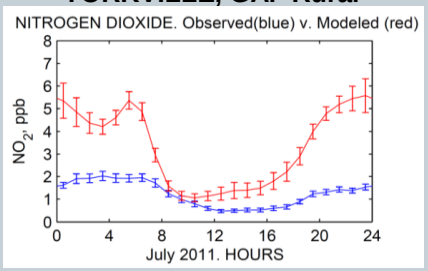


Observed & Modeled (Nature run) diurnal cycle of NO_2

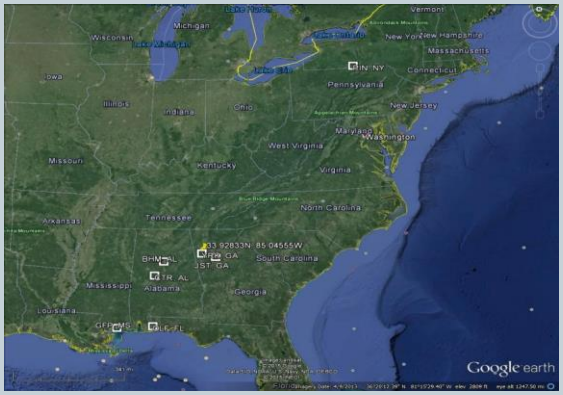
ATLANTA, GA. Urban



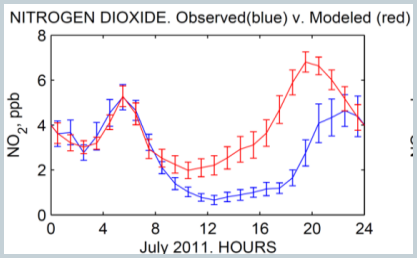
YORKVILLE, GA. Rural



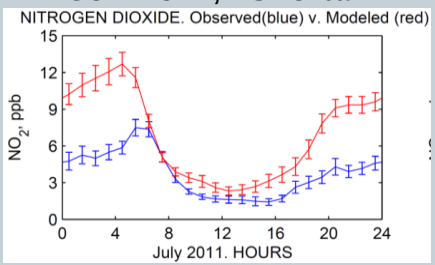
STATIONS MAP



PENSACOLA (OLF), FL. Urban



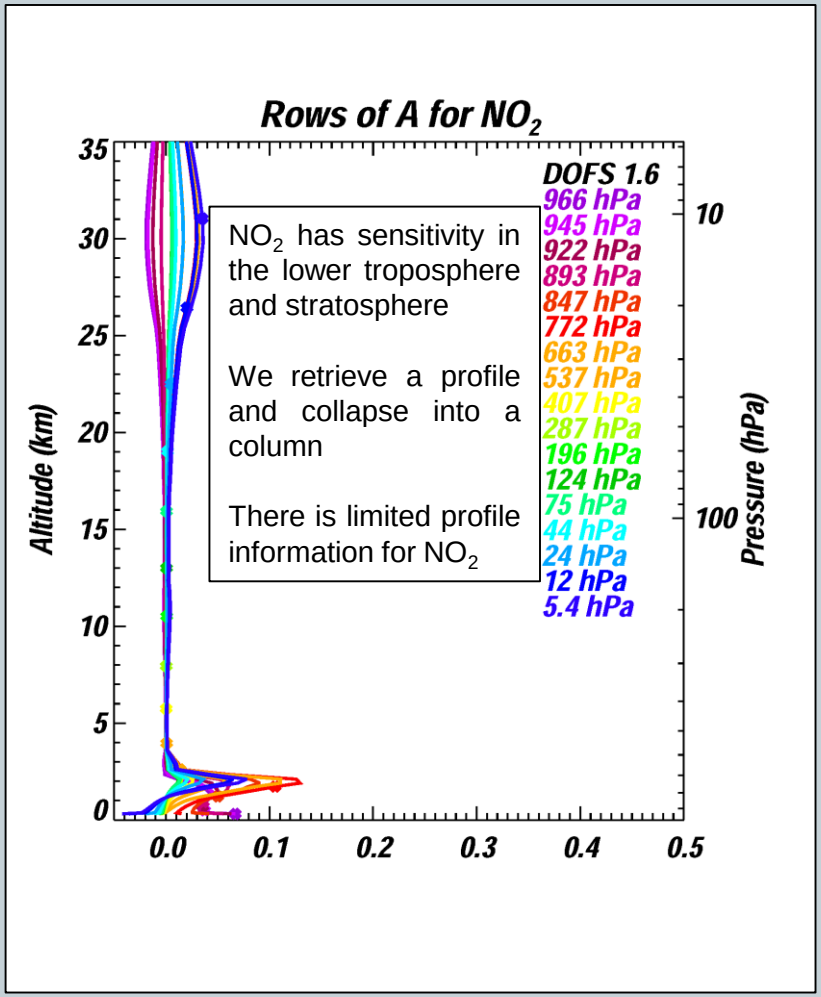
GULFPORT, MS. Urban

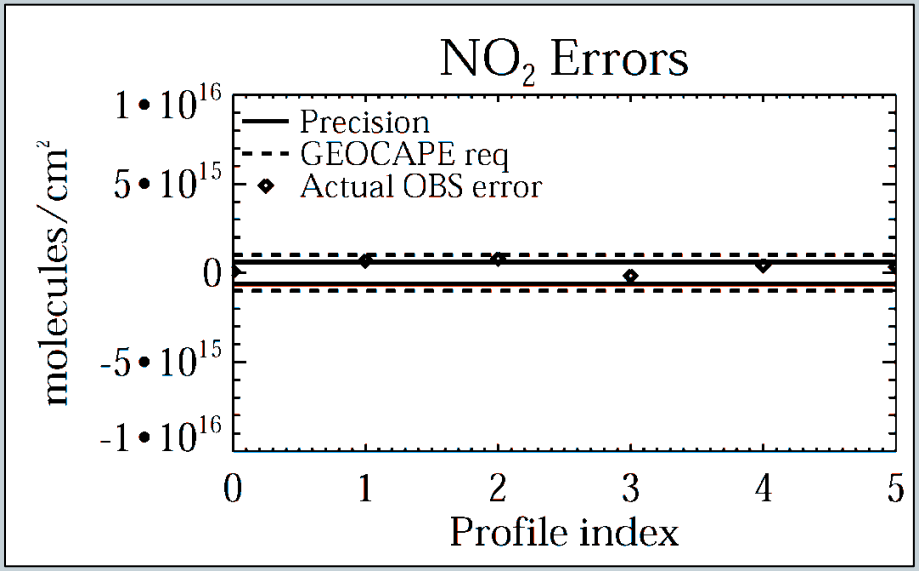


- **The model systematically overestimates NO_2 concentrations but correctly reproduces shape of diurnal cycle and differences of NO_2 concentrations between rural and urban locations.**
- **Modeled and observed daily variability in diurnal cycle of NO_2 concentrations are quite consistent.**

Courtesy: K. Vinnikov/R. Dickerson/N. Krotkov

NO_2 Retrievals: First Results





- Preliminary retrievals with TEMPO instrument characteristics meets GEOCAPE requirements for column precision (OBServation error includes precision and error from aerosols, albedo)
- Work underway on increasing computational efficiency to meet processing demands for full domain