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

GEMS SCIENCE TEAM MEETING
OCTOBER 11 2016

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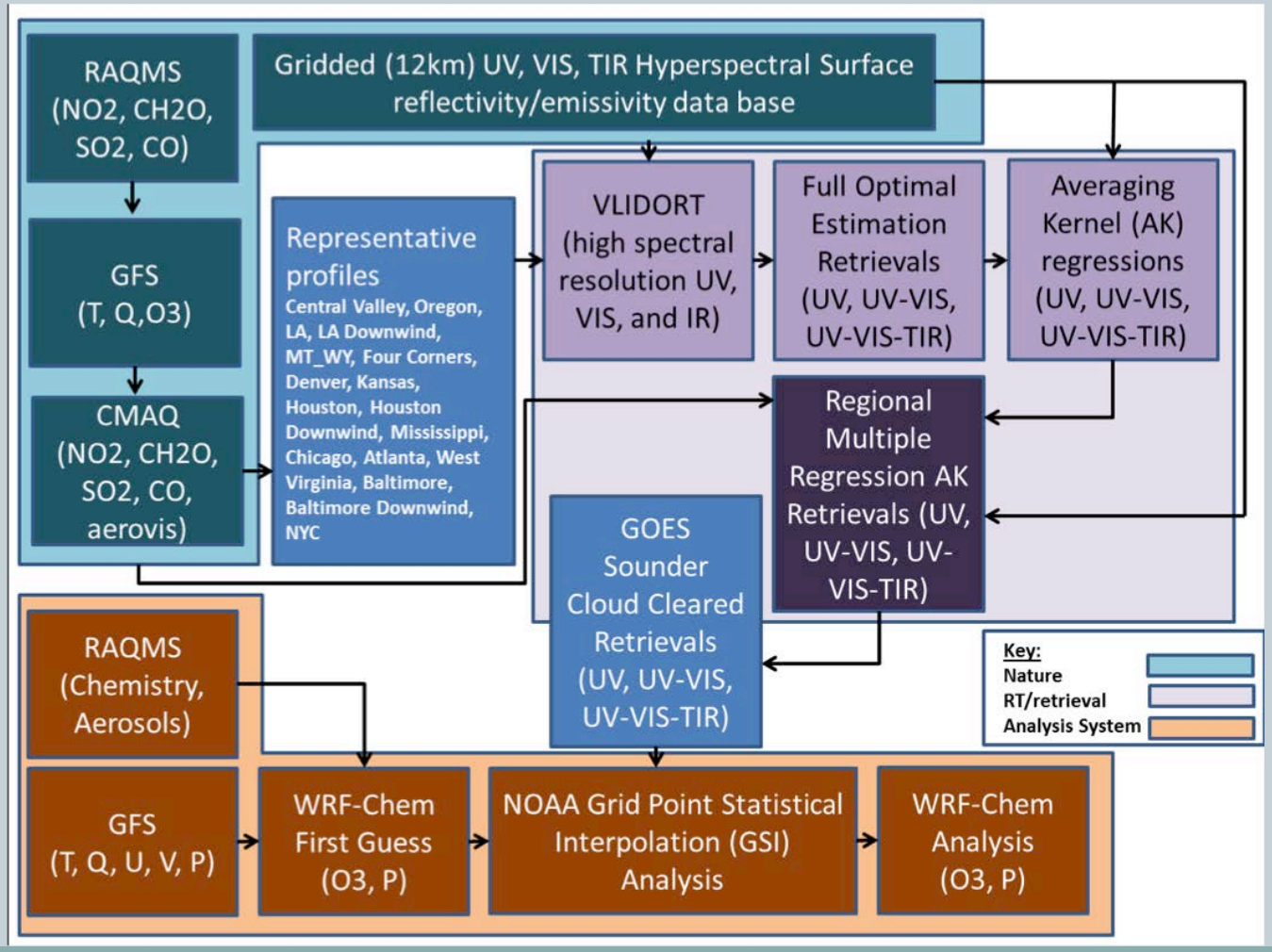
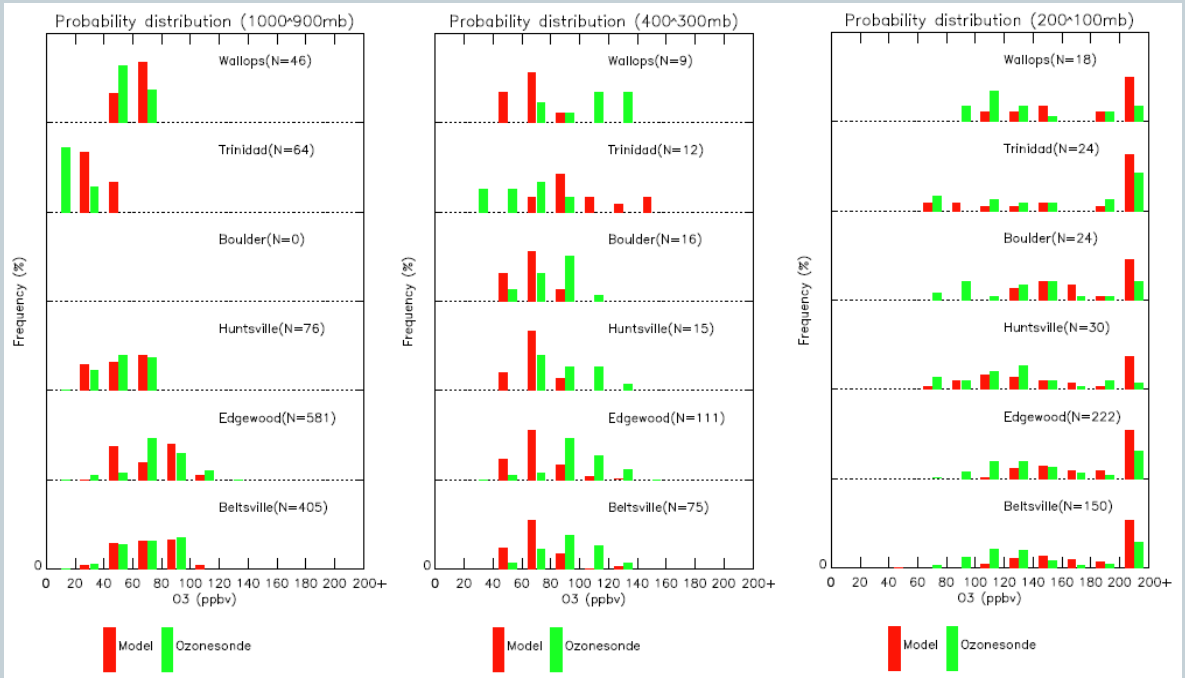
Goals

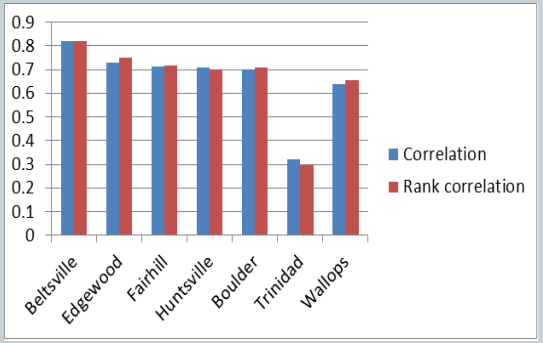
- Utilize independent modeling systems for generation of Nature atmosphere and conducting assimilation impact experiments
- Account for realistic atmospheric variability, which requires evaluation of the nature runs with respect to observations
- Include realistic variability in the synthetic radiances, 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

OSSE Flow Chart

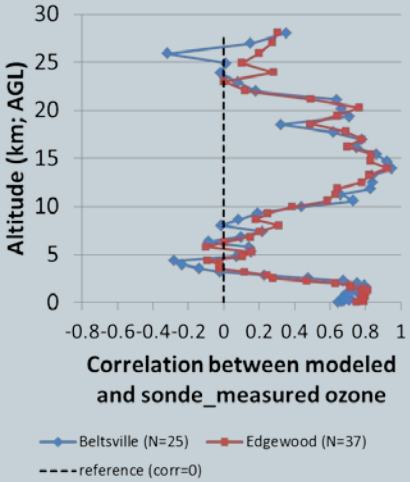


Quantifying Accuracy and Representativeness of Regional Nature Run





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

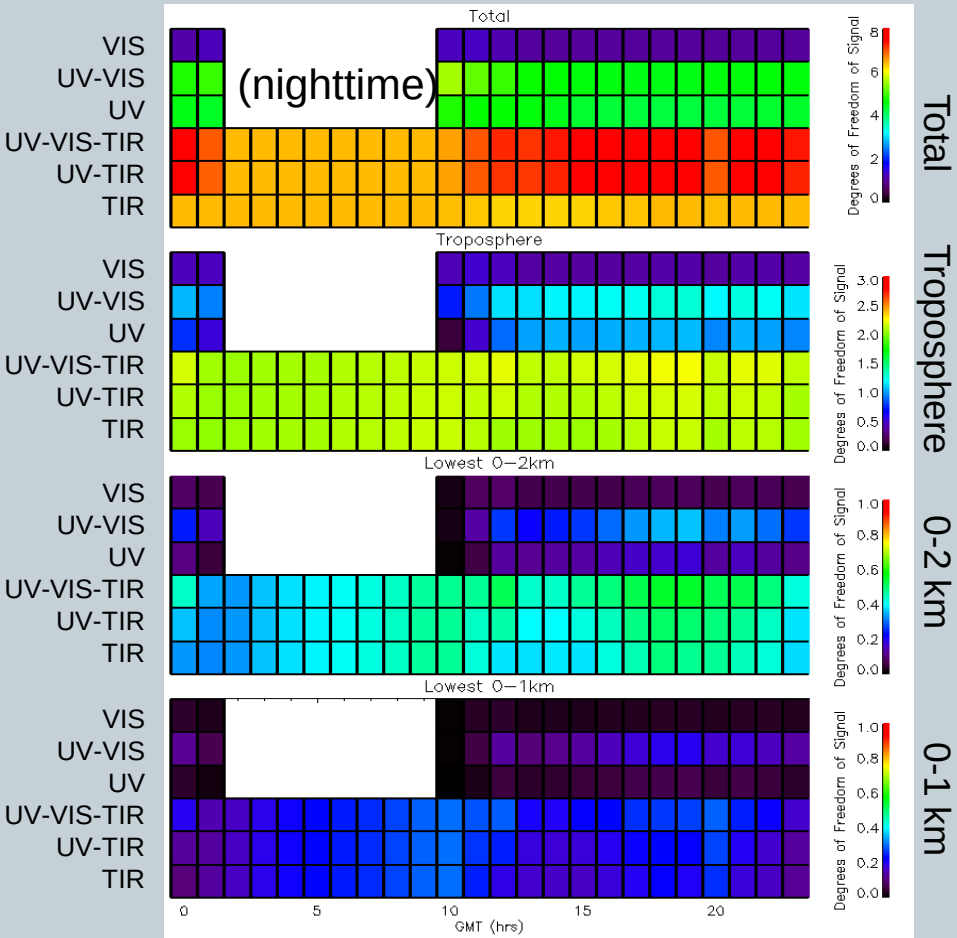


Correlation between model and ozonesondes at Beltsville and Edgewood

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

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)

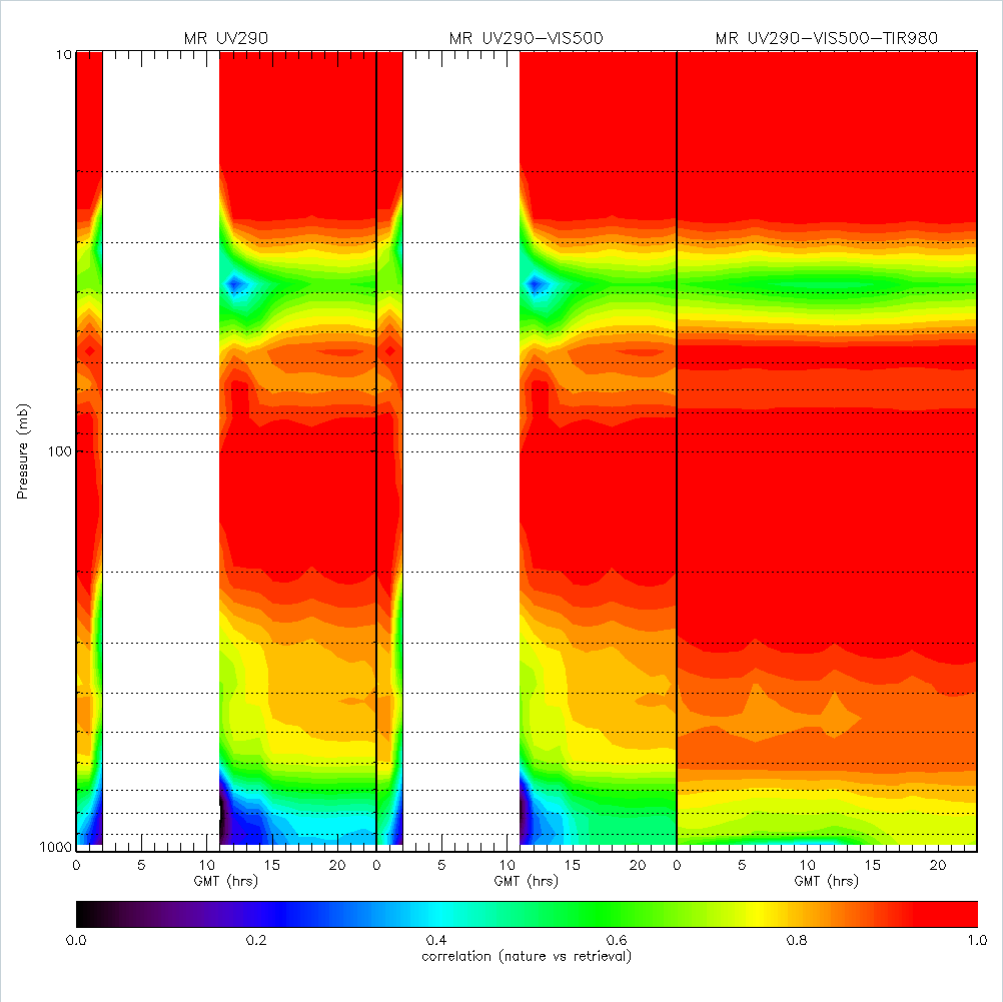
Note UV/VIS has the same spectral range and noise as TEMPO.

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



Data Assimilation

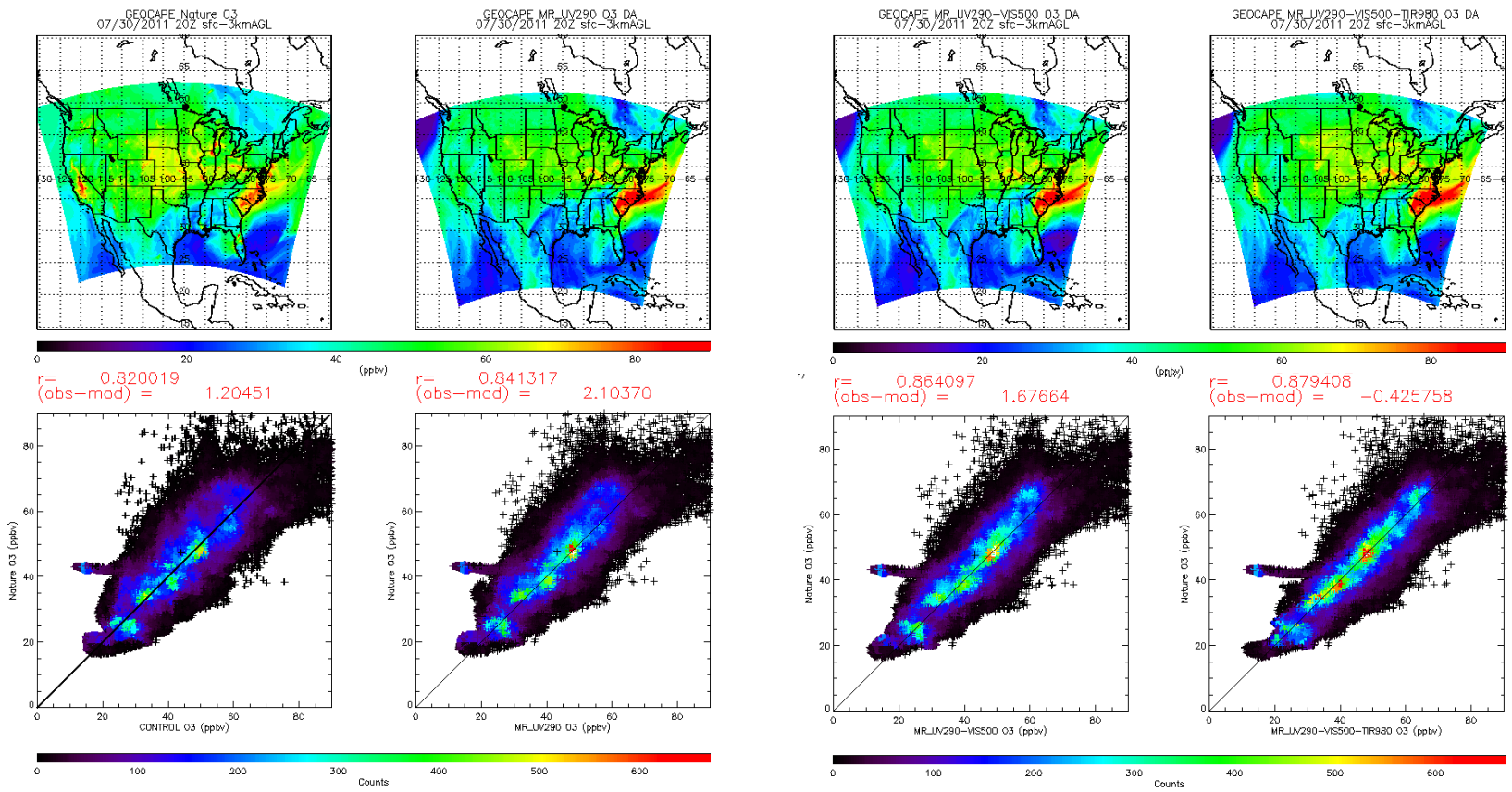
GEO-CAPE WRF-CHEM/GSI (3D-VAR) Regional/Urban O3 OSSE Study – July 2011

- Control
- Synthetic OMI (using retrieval efficiency factors and apriori)
- Multiple Regression GEOCAPE UV-VIS-TIR synthetic retrievals
- Multiple Regression GEOCAPE UV-VIS synthetic retrievals
- Multiple Regression GEOCAPE UV synthetic retrievals

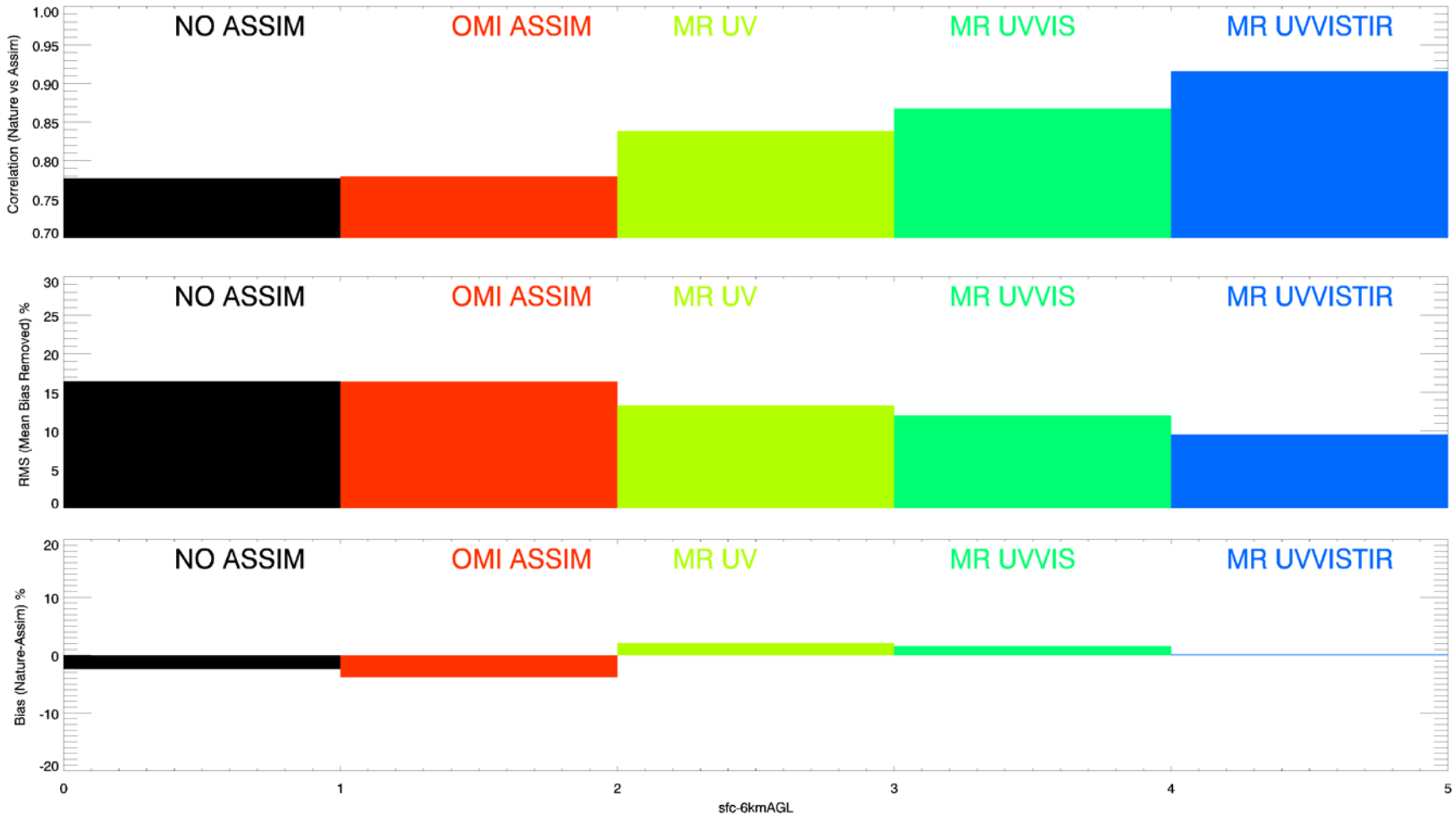
- All GEOCAPE experiments include:
  - 1 hour cycling
  - Inflation of background error covariances near surface
  - Application of tangent linear observation operator (AK) in GSI inner loop

- Results compared to nature run integrated over atmospheric layers

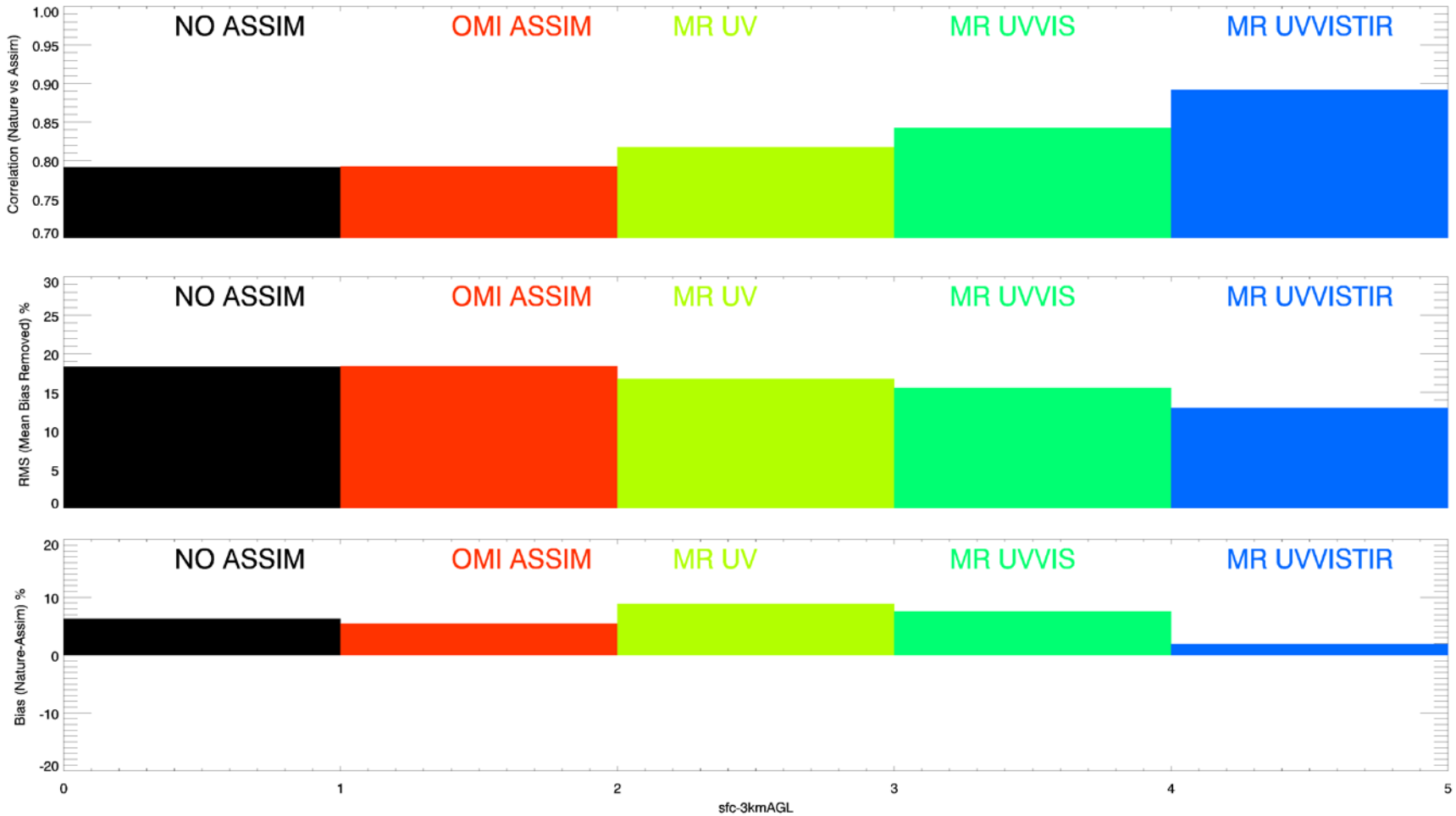
Impact of Assimilation: Layer Averages



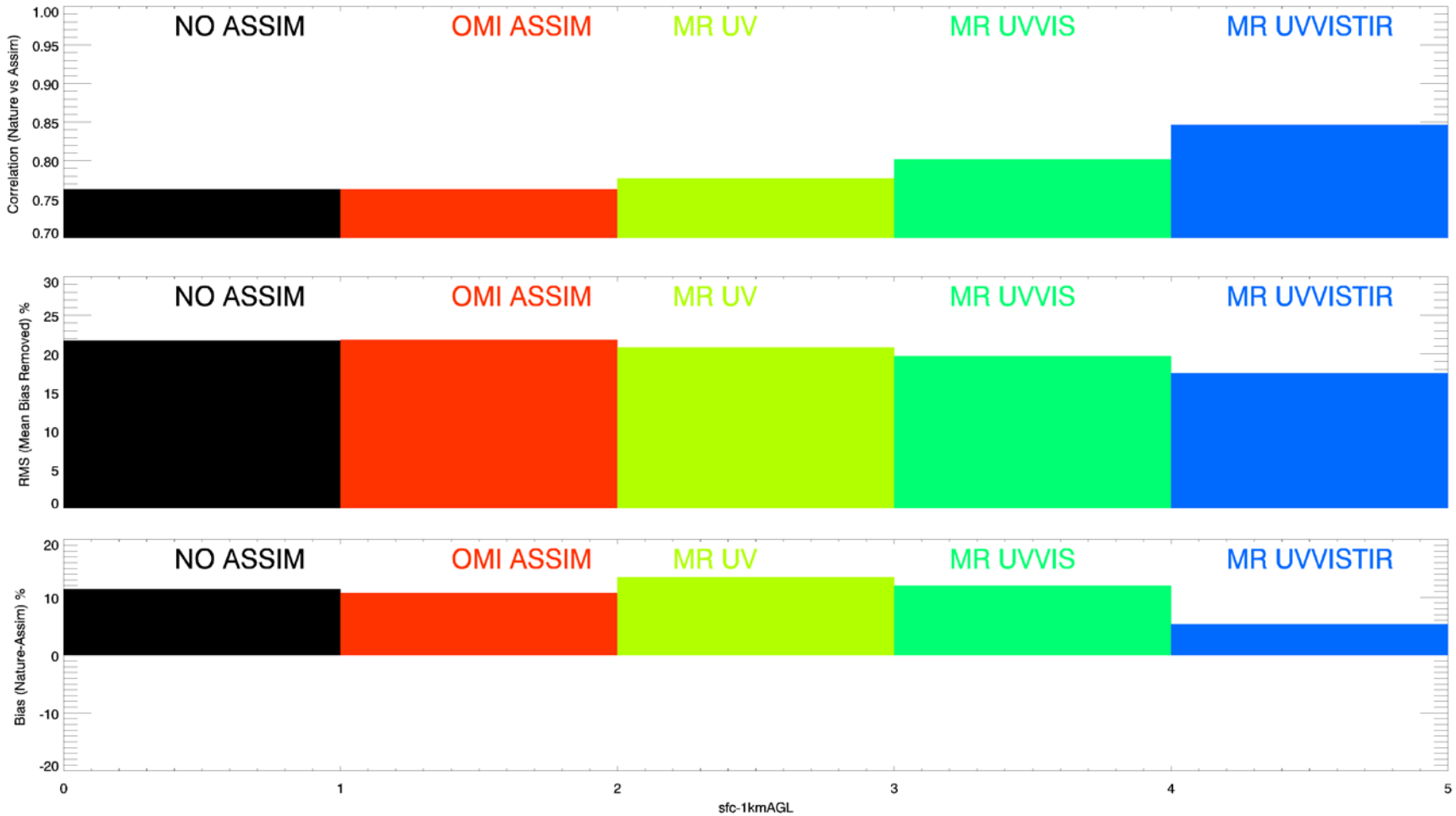
Impact of Assimilation: sfc-6km Results



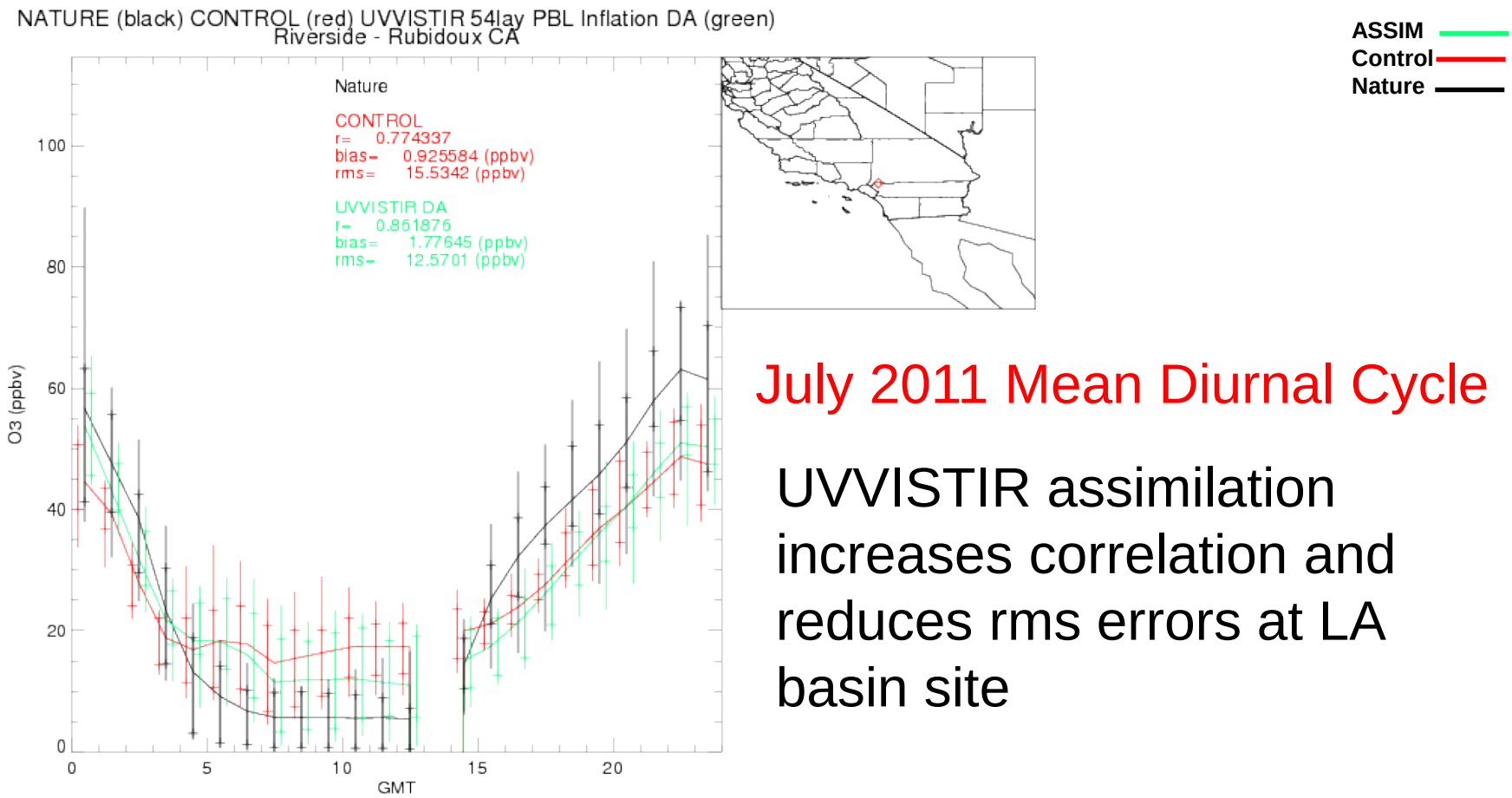
Impact of Assimilation: sfc-3km Results



Impact of Assimilation: sfc-1km Results



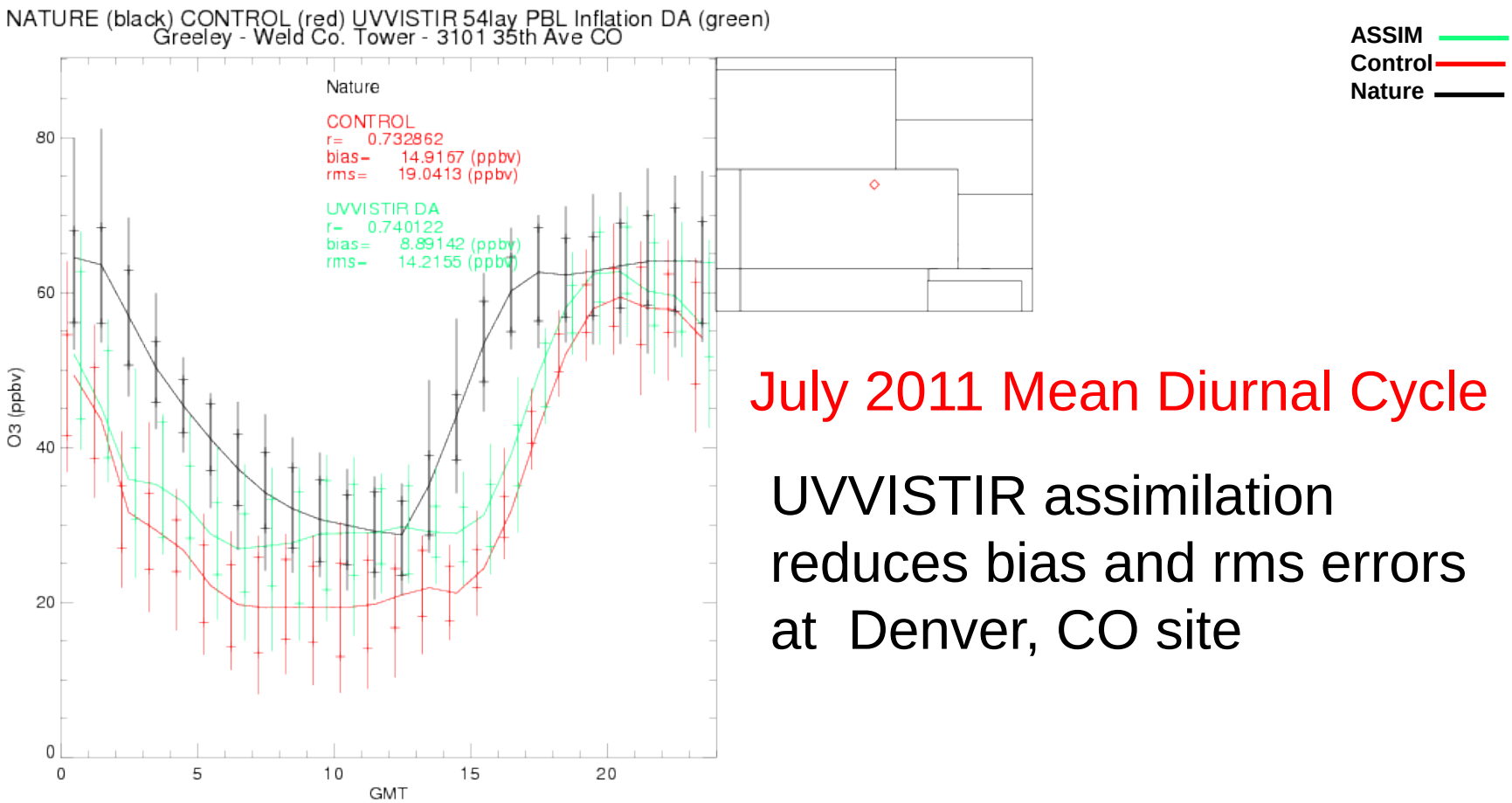
Impact of Assimilation: Selected Sites



July 2011 Mean Diurnal Cycle

UVVISTIR assimilation increases correlation and reduces rms errors at LA basin site

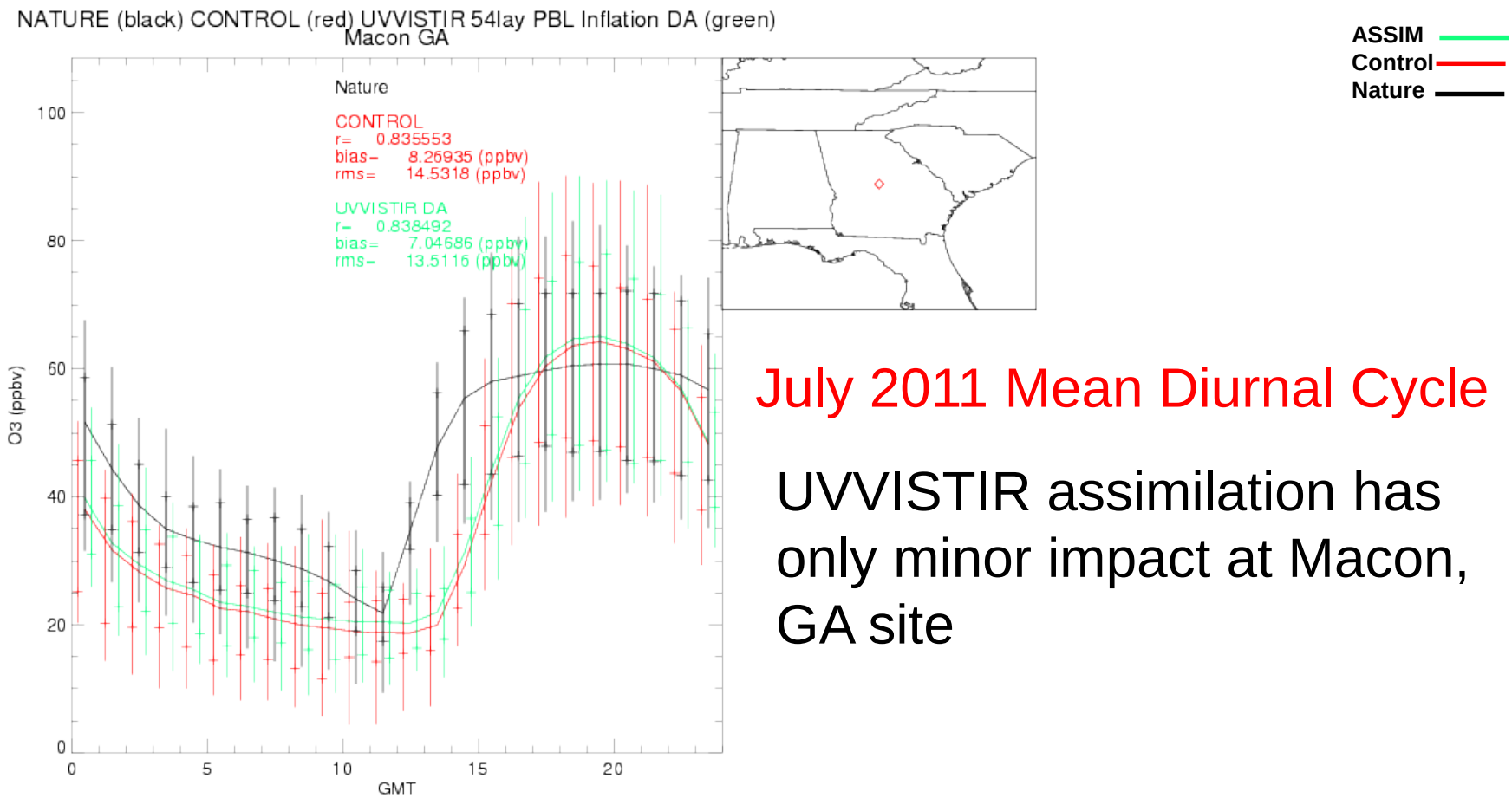
Impact of Assimilation: Selected Sites



July 2011 Mean Diurnal Cycle

UVVISTIR assimilation reduces bias and rms errors at Denver, CO site

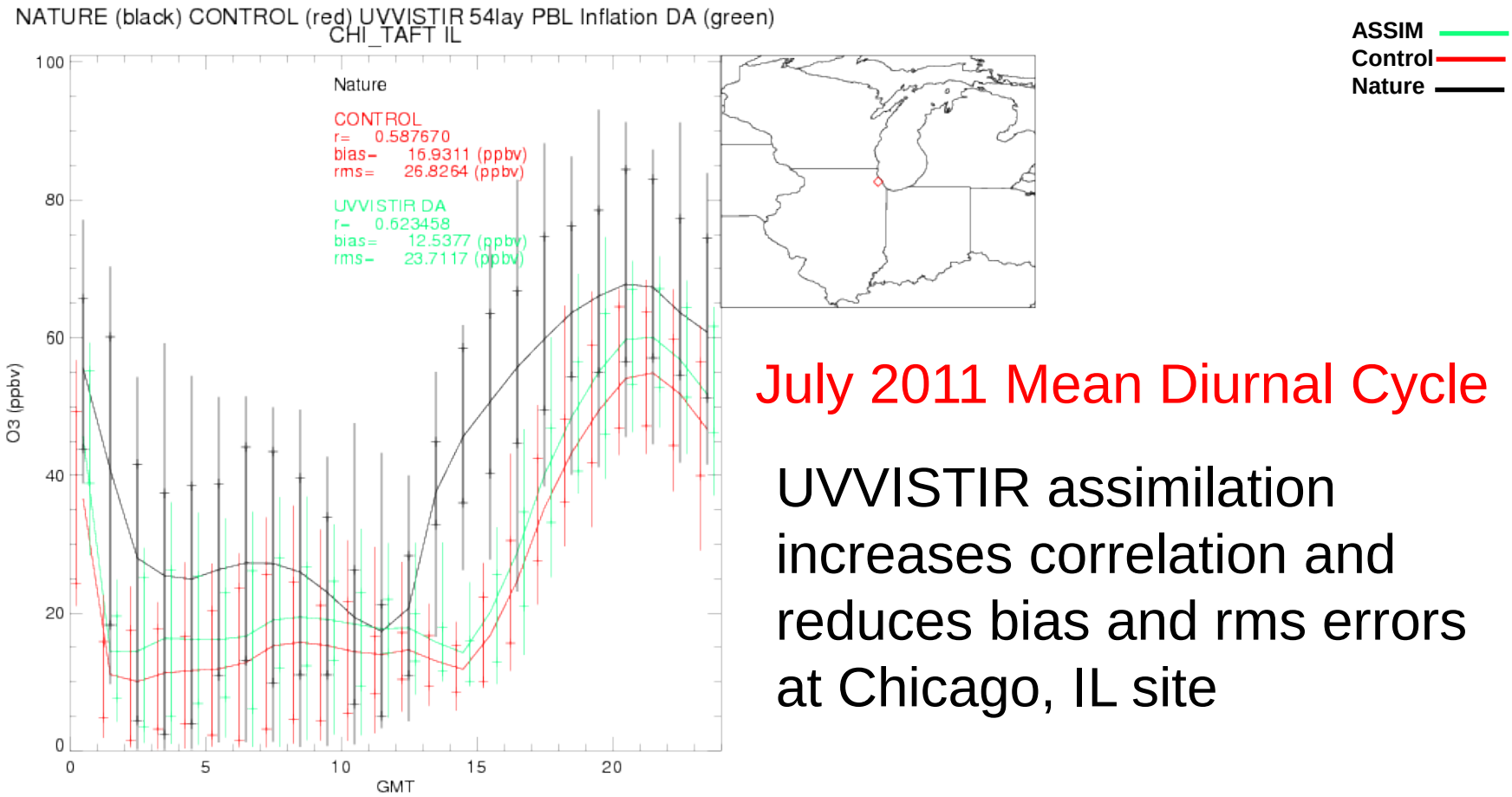
Impact of Assimilation: Selected Sites



July 2011 Mean Diurnal Cycle

UVVISTIR assimilation has only minor impact at Macon, GA site

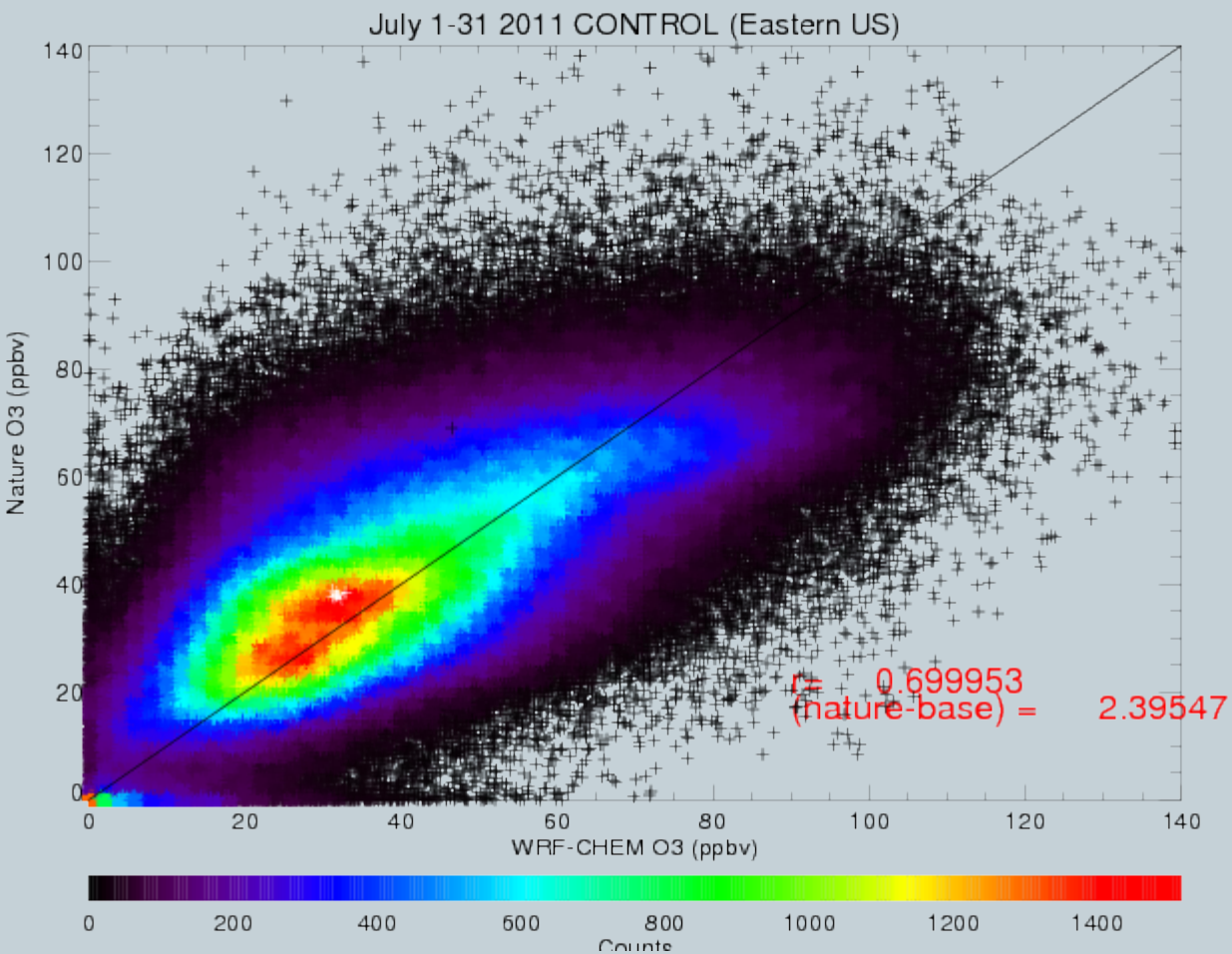
Impact of Assimilation: Selected Sites



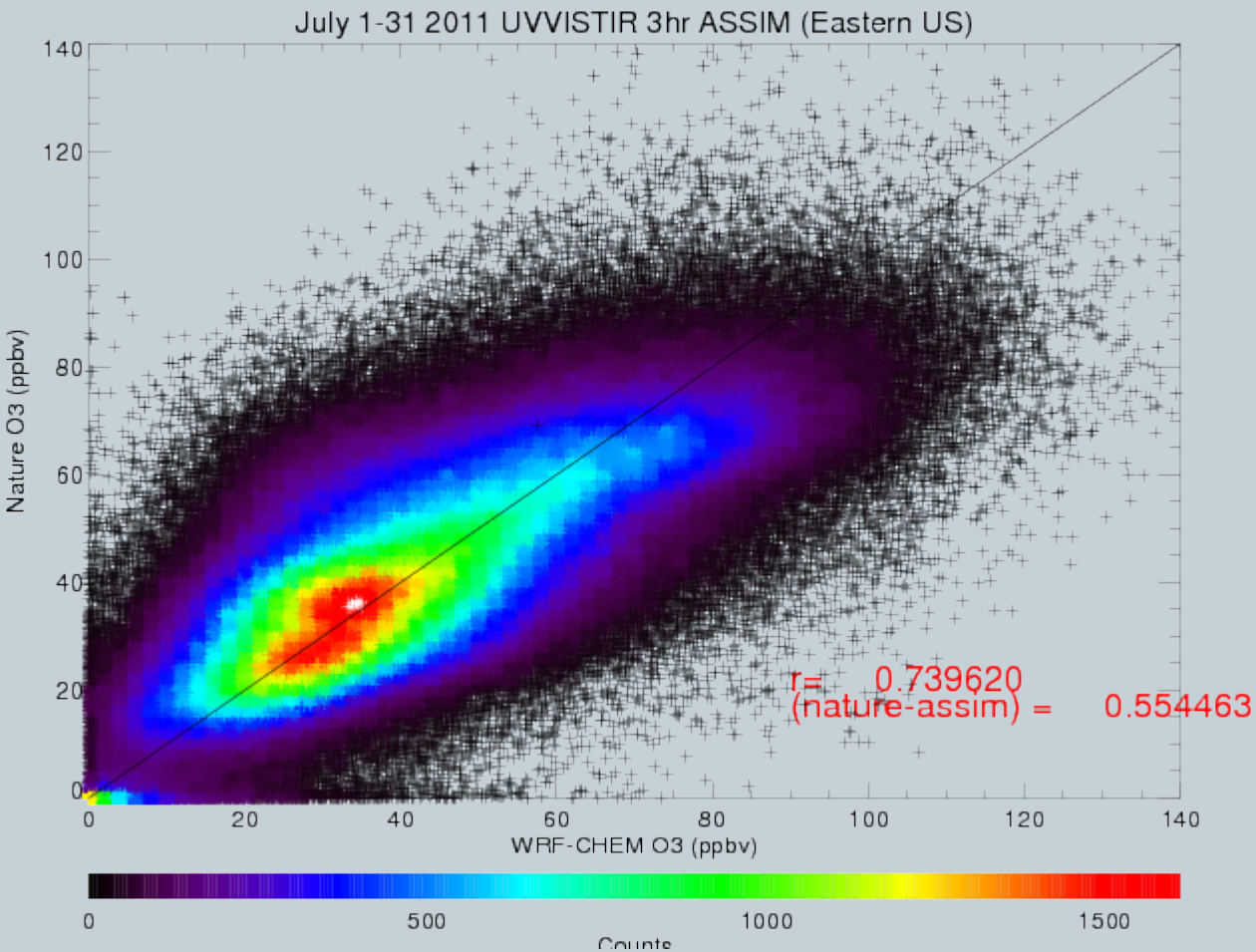
July 2011 Mean Diurnal Cycle

UVVISTIR assimilation increases correlation and reduces bias and rms errors at Chicago, IL site

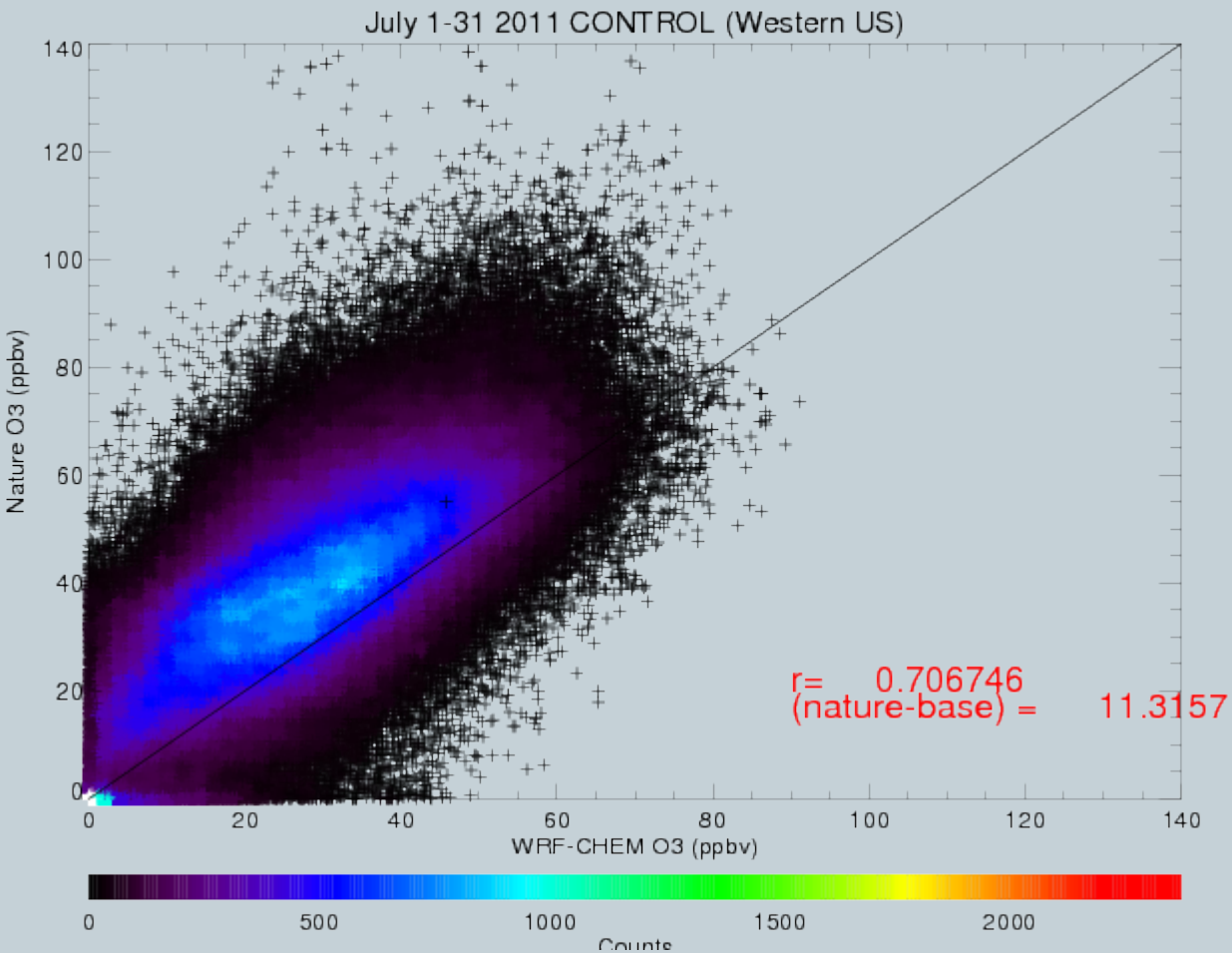
Impact of UVVISTIR Assimilation: All Eastern Sites



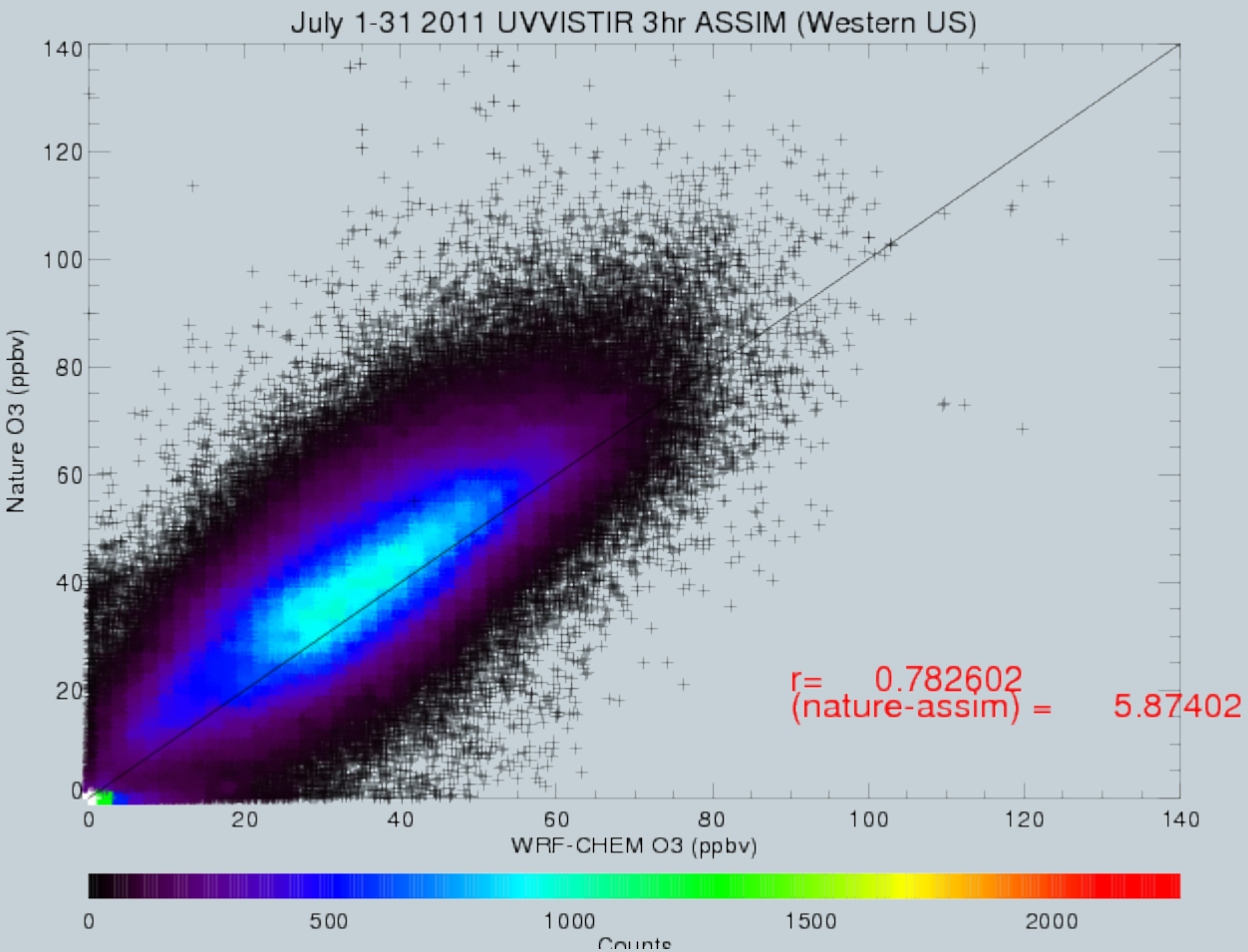
Impact of UVVISTIR Assimilation: All Eastern Sites



Impact of UVVISTIR Assimilation: All Western Sites



Impact of UVVISTIR Assimilation: All Western Sites



NO_2 OSSE Developments I

- 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)

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

NO_2 OSSE Developments III

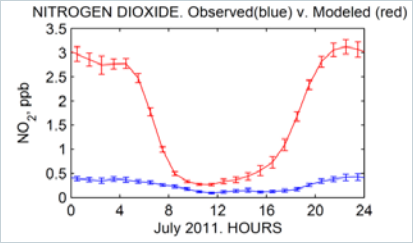
- Optimization to get 10x speedup
  - Optimized optical property initialization (mainly, aerosol phase function moments)
  - Removed redundant copying of data between variables
  - Separated operations that are the same for each profile (e.g. reading in of large aerosol optical property tables) from those that are different between profiles so that former needs to be done only once

NO_2 OSSE Developments IV

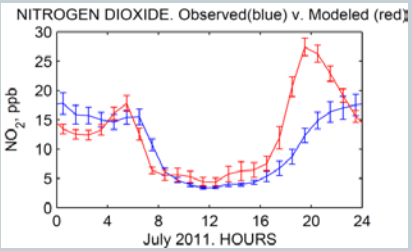
- Optimization to get 10x speedup
  - Implemented MPI interface to use multiple processors
  - Computed solar geometry early and only performed further calculations for daytime scenarios
  - Only took points without clouds that also had a surface albedo
  - Balanced the number of points on each processor to optimize processor utilization
  - Added option of only outputting data to netcdf file for clear and daytime scenarios

Quantifying Accuracy and Representativeness of Regional Nature Run

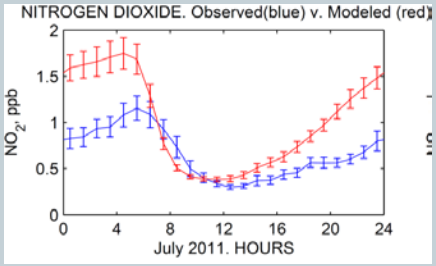
PINNACLE, NY. Park Forest



BIRMINGHAM, AL. Urban

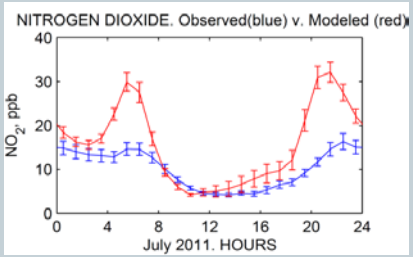


CENTERVILLE, AL. Rural

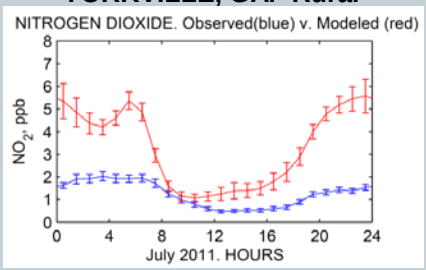


Observed & Modeled (Nature run) diurnal cycle of NO_2

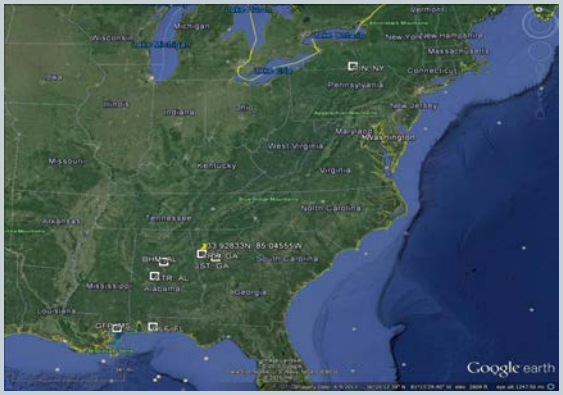
ATLANTA, GA. Urban



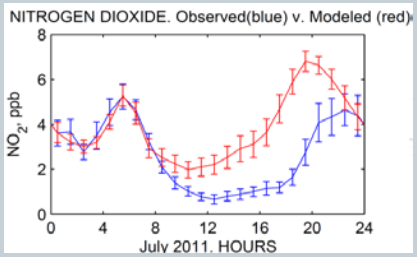
YORKVILLE, GA. Rural



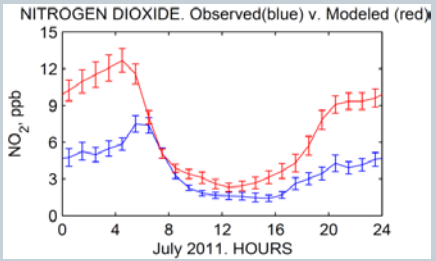
STATIONS MAP



PENSACOLA (OLF), FL. Urban



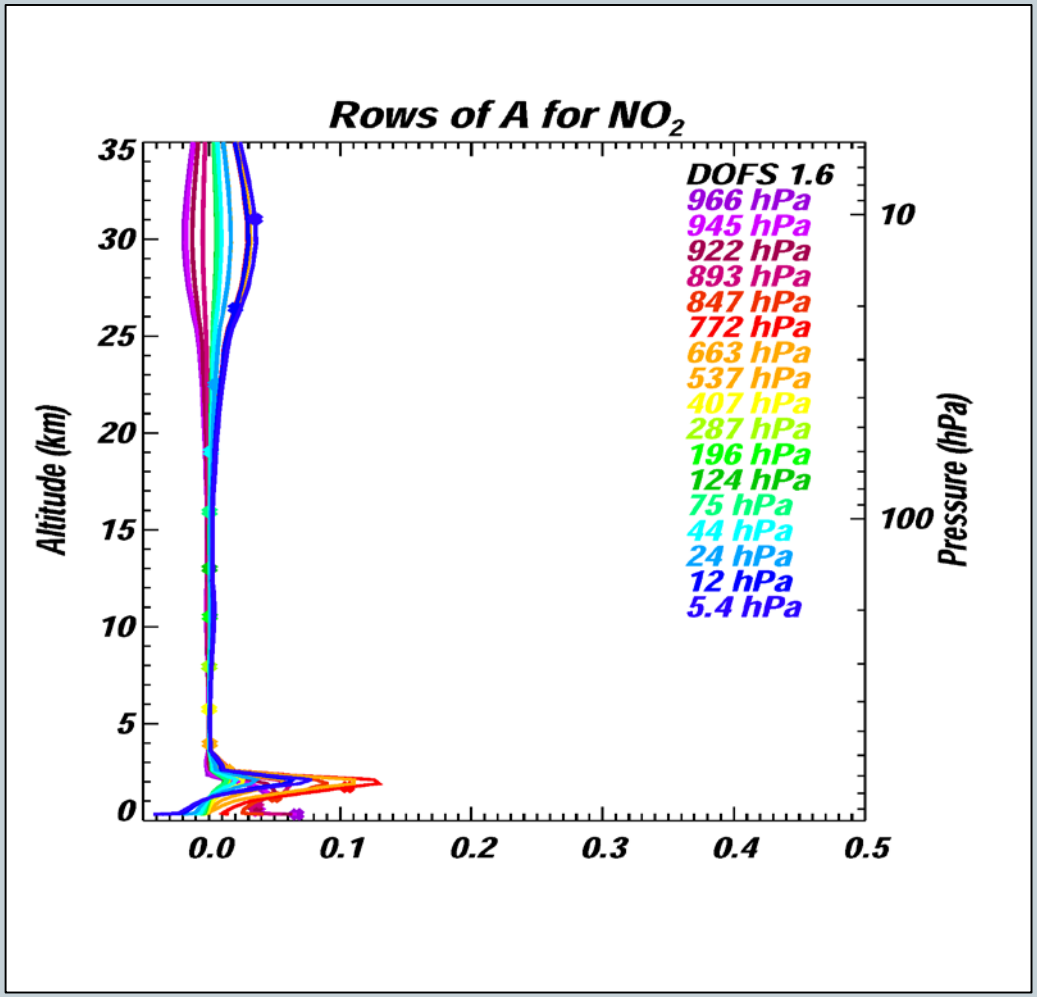
GULFPORT, MS. Urban



- **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



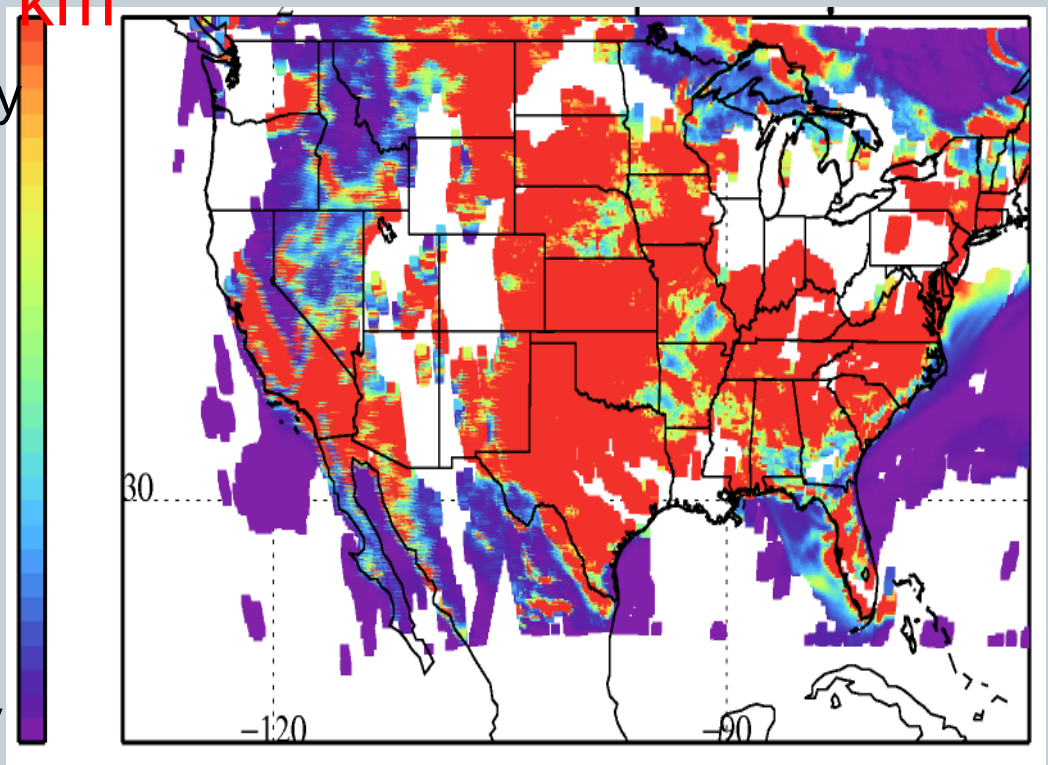
- Preliminary retrievals with TEMPO instrument characteristics meets GEOCAPE requirements for column precision
- We retrieve a profile and collapse into a column
- NO_2 has sensitivity in the lower troposphere and stratosphere
- There is limited profile information for NO_2

Real-time OSSE Estimates of Sensitivity

NO_2 sensitivity, surface to 2 km

Higher sensitivity

Lower sensitivity



July 18, 2011 2 pm local time

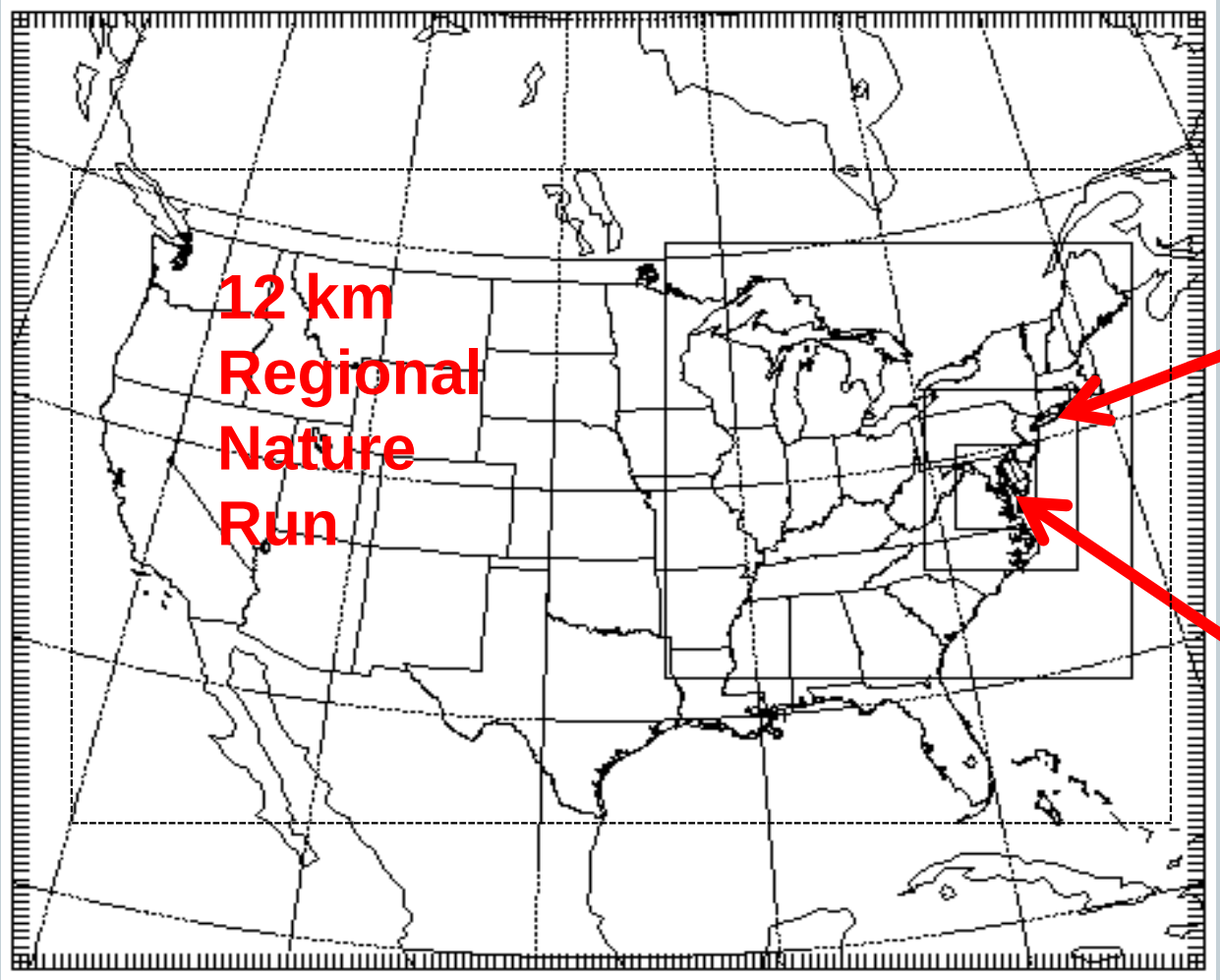
- Calculates Jacobians including aerosols and viewing geometry using fast RT system
- Better estimates what a satellite will actually see, which varies by location, time, and composition. Empty areas have thick cloud cover
- OSSEs will ingest results for better estimates of satellite performance

Conclusions

- O_3 Regional OSSE experiment underway
- Initial results promising
- Full UV-VIS-TIR retrievals showing positive impact on surface O_3
- Regional OSSE system showing realistic complexity
- NO_2 retrievals underway. Next step is to look at the distribution of aerosol and albedo true states to assess the cause of the variations in sensitivity.

Backup Slides

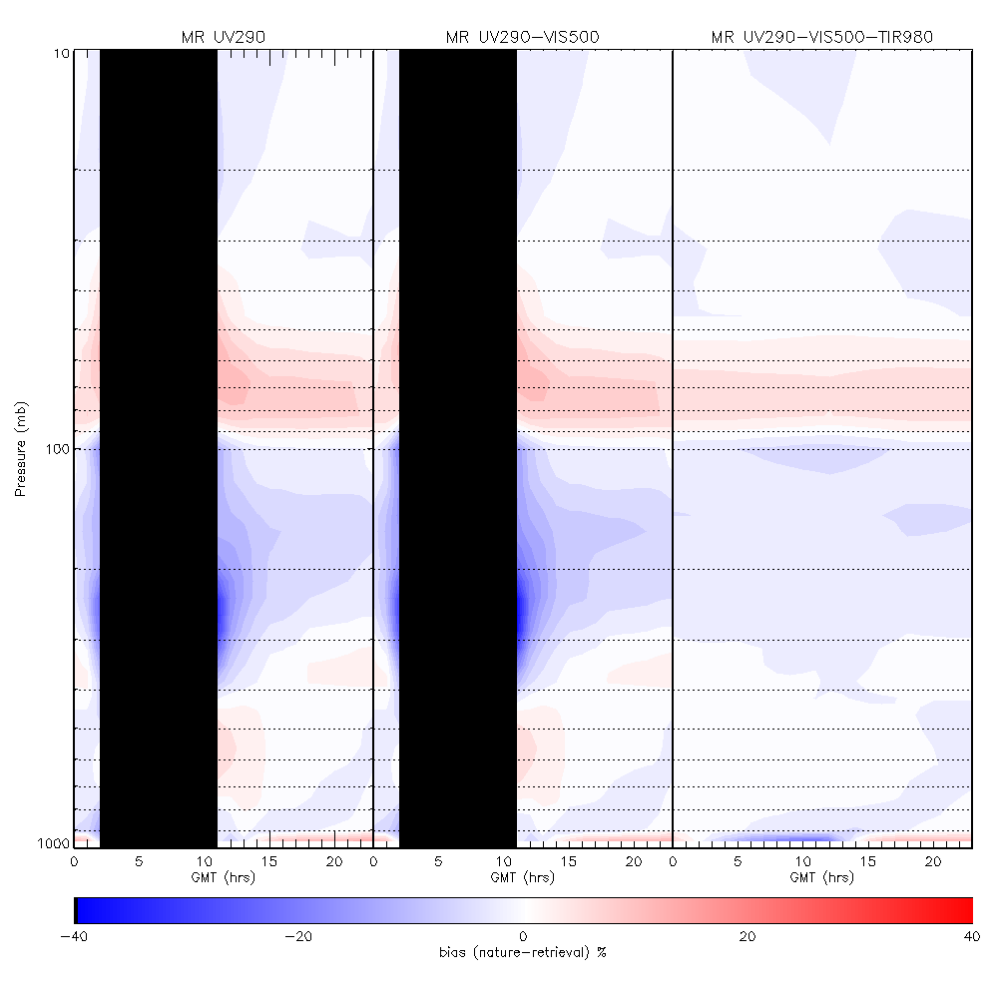
Nature Run



Courtesy: K. Pickering/C. Loughner

Retrieval Biases

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

Diurnally resolved biases between the Regional Nature Run and GEOCAPE O_3 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 O_3)