

# Progress on Tiger Team Project: Air Quality Reanalysis

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**School of Civil & Environmental Engineering,  
Georgia Institute of Technology**

**With thanks to project leaders Greg Carmichael and Pius Lee and other members**

**GT-Emory ACAST Meeting, August 28<sup>th</sup>, 2015**

*Georgia Institute of Technology*

# Part 1: Project Team and Major Goals

# Air Quality Reanalysis (Configuration for 2010 HTAP production)

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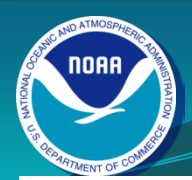
<sup>8</sup> Corporation for Atmospheric Research, Boulder, CO

<sup>9</sup> Atmospheric Chemistry and Dynamics Lab., NASA, Greenbelt MD



## Concept of Reanalysis

A 'reanalysis' is a climate or weather model simulation of the past that includes data assimilation of historical observations. The observations can be very comprehensive (satellite, in situ, multiple variables) or relatively sparse (say, sea level pressure only), and the models themselves are quite varied. Generally these models are drawn from the weather forecasting community (at least for the atmospheric components) which explains the odd terminology. An 'analysis' from a weather forecasting model is the 6 hour (say) forecast from the time of observations. Weather forecasting groups realized a decade or so ago that the time series of their weather forecasts (the analyses) could not be used to track long term changes because their models had been updated many times over the decades. Thus the idea arose to 're-analyze' the historical observations with a single consistent model. These sets of 6 hour forecasts using the data available at each point are then more consistent in time (and presumably more accurate) than the original analyses were. - See more at: <http://www.realclimate.org/index.php/archives/2011/07/reanalyses-r-us/#sthash.WKOIKeHl.dpuf>



# Applications of Reanalysis

## Environments



- Climate Change
- Outdoor Air **NEW**
- Water
- More

## Health Effects



- Asthma
- Cancer
- Childhood Lead Poisoning
- More Health Conditions

## Population Health



- Population Characteristics
- Health Impact Assessments **NEW**
- Children's Environmental Health
- More

## Info by Location



Select State:

Select ▼

GO

Reanalysis would be able to provide PM2.5 speciation data with national coverage at county level

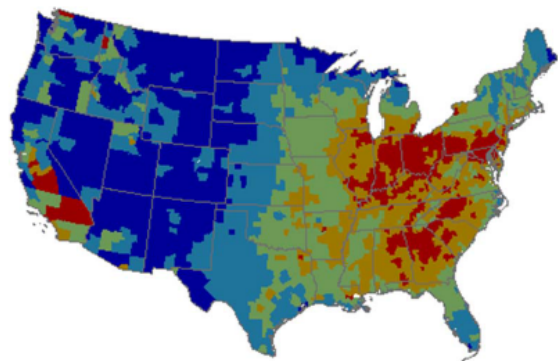
Courtesy: Dan Costa

“New Directions in Air Quality Research at the US EPA”

# Public Health Burden of PM<sub>2.5</sub>

(Fann et al., 2011)

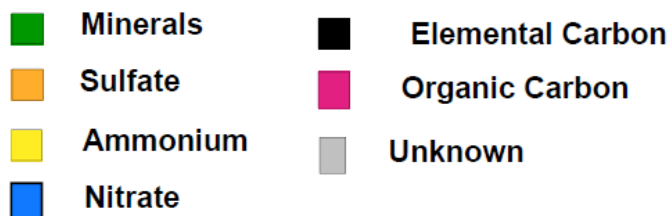
Percentage of PM<sub>2.5</sub> related deaths due to 2005 air quality levels by county



Los Angeles



Eastern US



Summary of National PM <sub>2.5</sub> impacts due to 2005 air quality	
Excess mortalities (adults) <sup>A</sup>	130 to 320,000
Percentage of all deaths due to PM <sub>2.5</sub> <sup>B</sup>	5.4%
<b>Impacts among Children</b>	
ER visits for asthma (<18 yr)	110,000
Acute bronchitis (age 8-12)	200,000
Exacerbation of asthma (age 6-18)	2,500,000

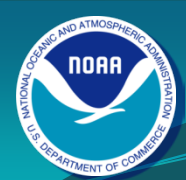
<sup>A</sup> Range reflects use of alternate PM mortality estimates

<sup>B</sup> Population-weighted value using Krewski et al. (2009) PM mortality estimates

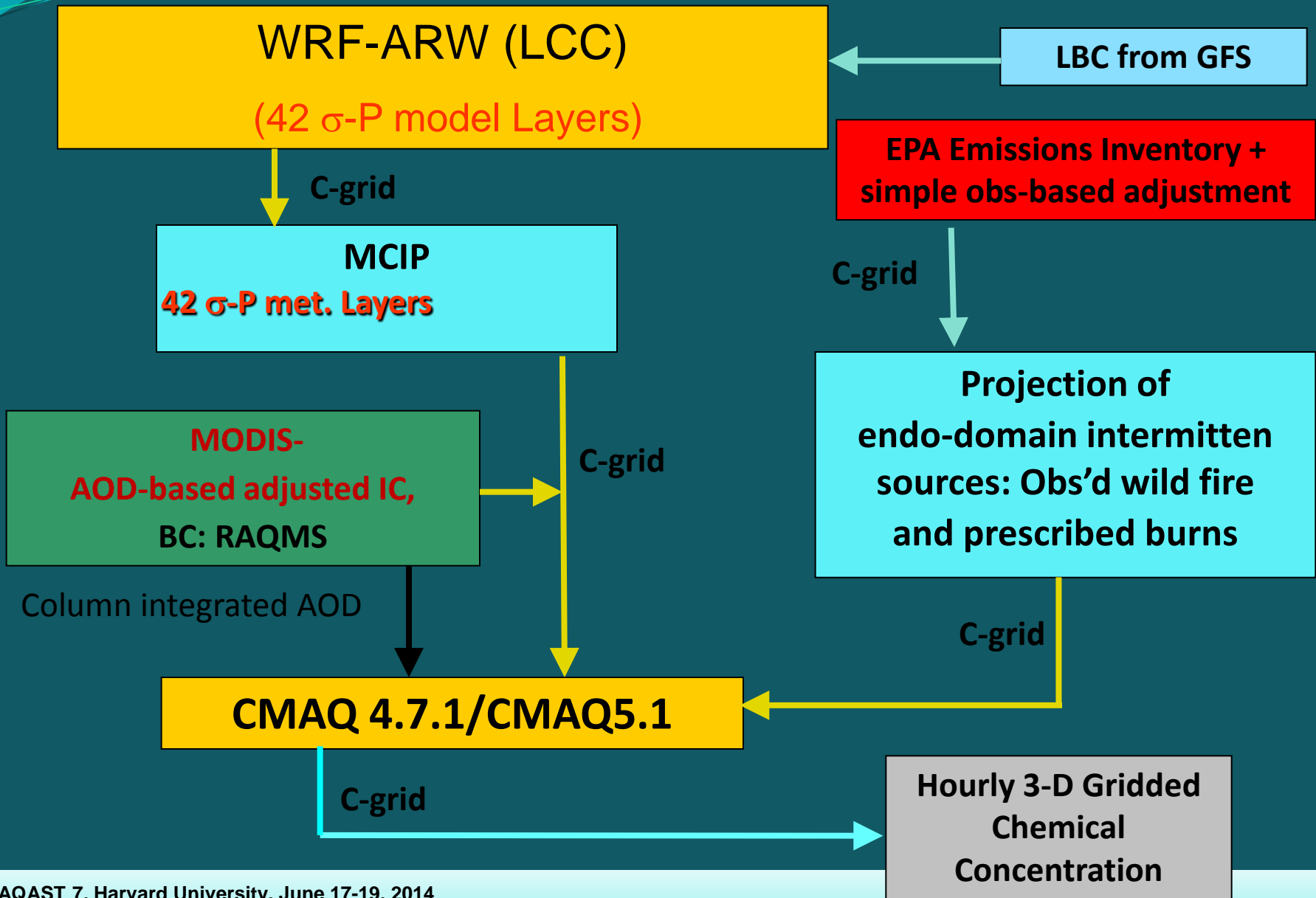


# Part 2: Tasks to make the model more robust

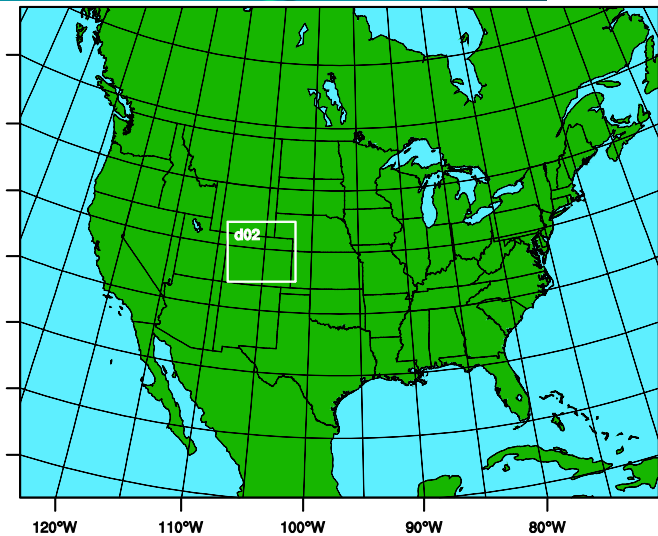




# WRF\_ARW-MCIP-CMAQ forward model

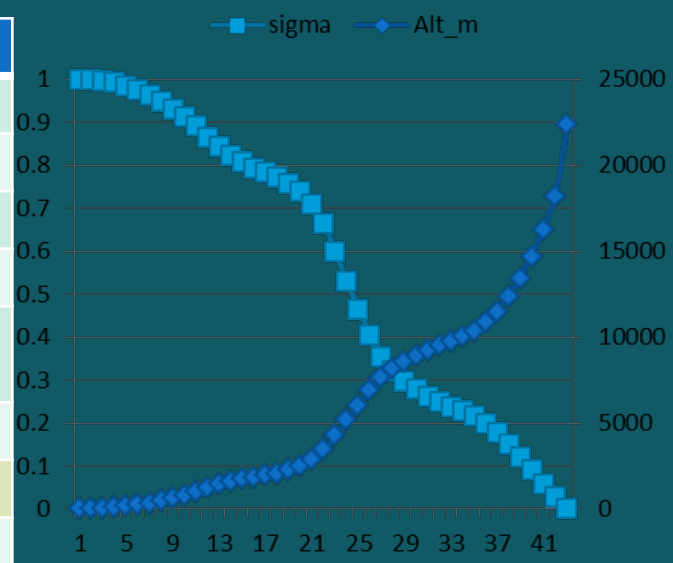


<b>WRF-ARW</b>	<b>Both North America (12 km) &amp; CONUS (4 km)</b>
<b>Map projection &amp; grid</b>	<b>Lambert Conformal &amp; Arakawa C staggering</b>
<b>Vert. co-ordinate</b>	<b>42 <math>\sigma</math>-p unevenly spaced levels</b>
<b>advection</b>	<b>RK3 (Skamarock and Weisman (2008))</b>
<b>SW &amp; LW radiation</b>	<b>RRTMG (Iacono et al. 2008))</b>
<b>PBL Physics</b>	<b>Mellor-Yamada-Janjic (MYJ) level 2.5 closure</b>
<b>Surface layer scheme</b>	<b>Monin-Obukhov Similarity with viscous sub-layer</b>
<b>Land Surface Model</b>	<b>NCEP Noah</b>
<b>Cloud Microphysics</b>	<b>Thompson et al. (2008)</b>
<b>Cloud convective mixing</b>	<b>Betts-Miller-Janjic Mass adjustment</b>



**AQ forecast: ^12 km nested to 4 km**

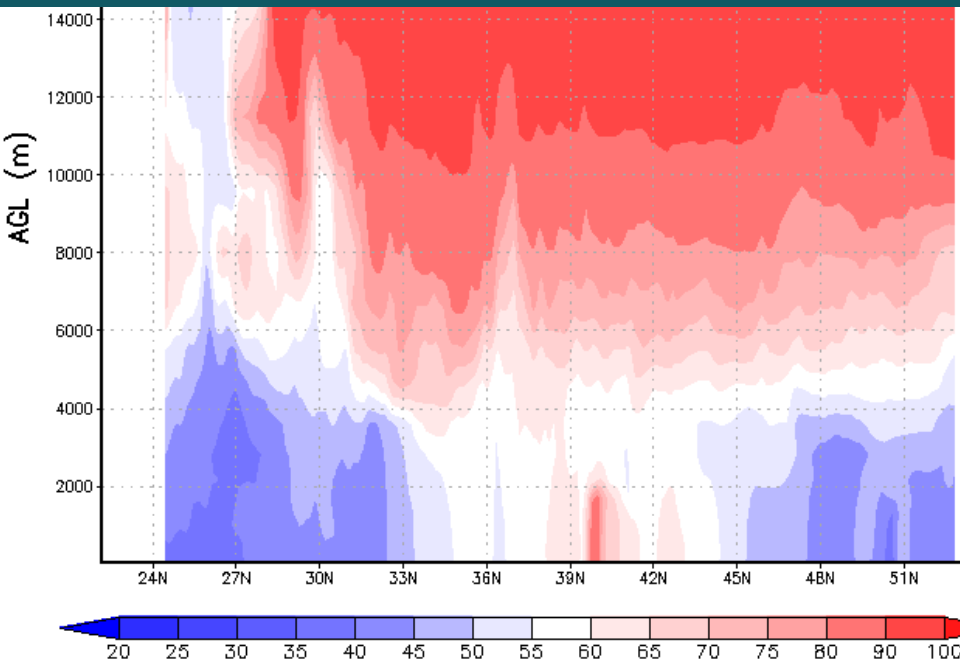
<b>CMAQ4.7.1</b>	<b>Both CONUS(12 km) &amp; SENEX (4 km)</b>
<b>Map projection &amp; grid</b>	<b>Lambert Conformal &amp; Arakawa C staggering</b>
<b>Vert. co-ordinate</b>	<b>42 <math>\sigma</math>-p unevenly spaced levels</b>
<b>Gas chemistry</b>	<b>Cb05 with 156 reactions</b>
<b>Aerosol chemistry</b>	<b>Aero5 with updated evaporation enthalpy</b>
<b>Anthropogenic emission</b>	<b>2005NEI as base year, mobile projected using AQS*, area and off-road used CSpr^, point source uses 2012 CEM data</b>
	<b>WRAP oil and gas emissions data</b>
<b>Biogenic emission</b>	<b>BEIS-3.14</b>
<b>Lateral BC</b>	<b>RAQM (B. Pierce)</b>



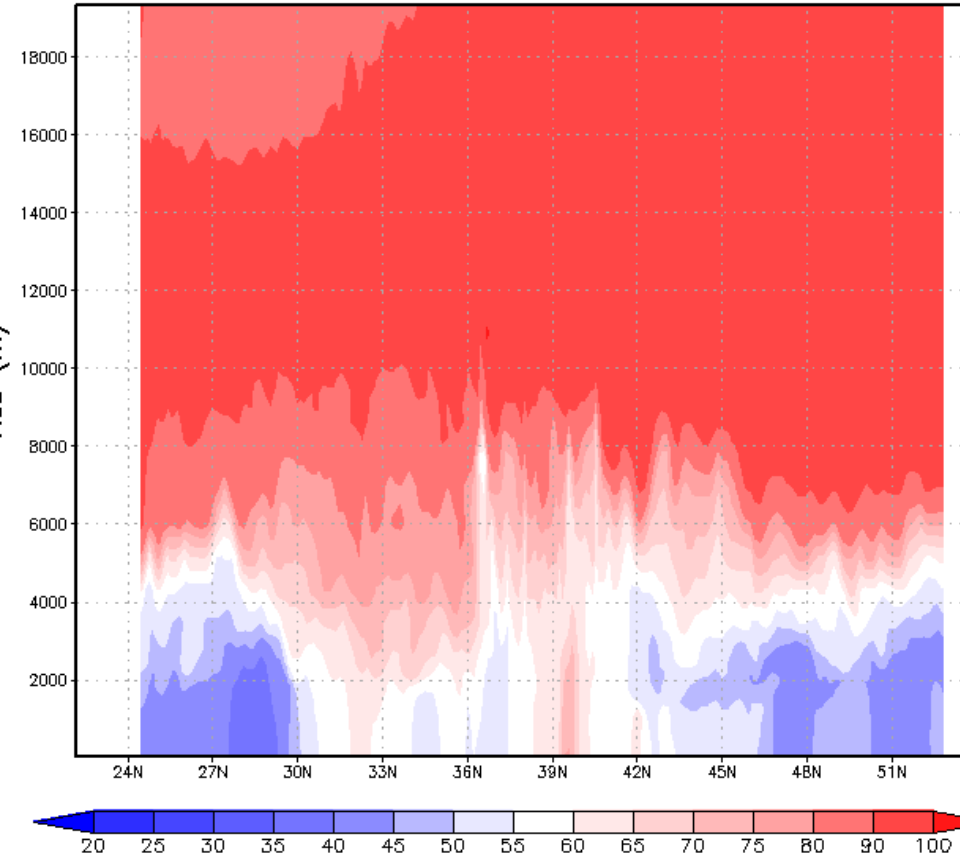
**42 vertical layers**



## NMMB-CMAQ4.7.1 (22L)



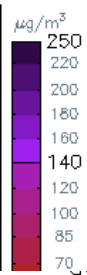
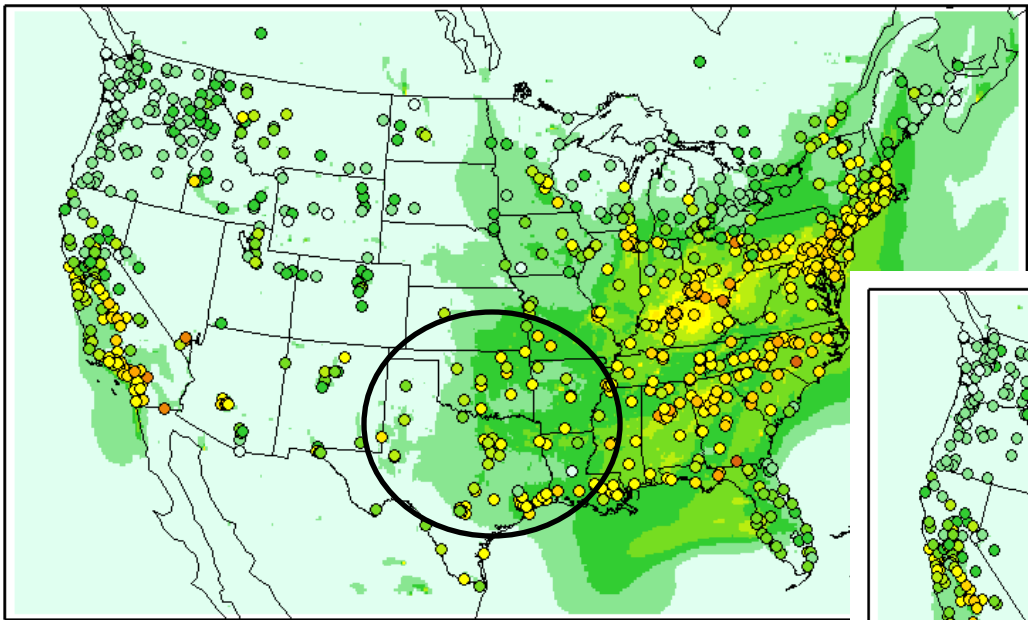
L42 O<sub>3</sub> (ppbv) over Lon=-105W at 20Z, 07/02/



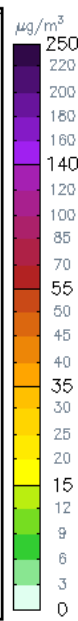
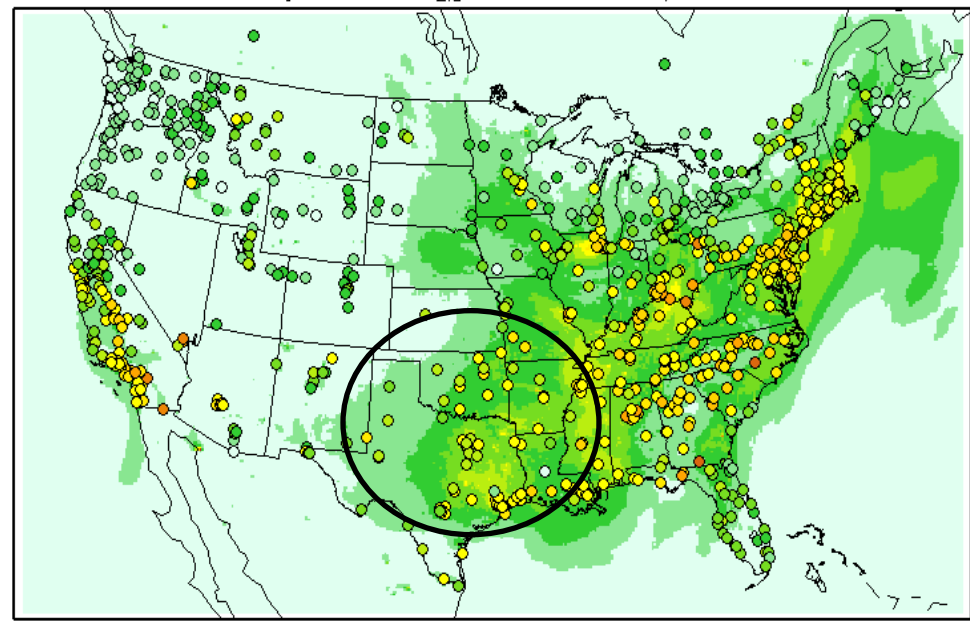
Longitudinal cross-section along Denver (105W) at 20 UTC July 2, 2011  
No spurious spikes of vertical gradients over complex terrain for O<sub>3</sub> concentration

# NMMB-CMAQ4.7.1 (22L)

daily mean PM<sub>2.5</sub> 20110703 LT / 22L



# WRF ARW-CMAQ4.7.1 (42L)



24 h averaged surface PM<sub>2.5</sub> on July 3 2011

A mixed result as a general lower predicted value by 42L exacerbated under-bias, but the higher predicted values by 42L in Lower Middle helped.

# Outline on progress

- *The Regional Chemical Analysis TT started in 2013:*
- *Deliverable in 2014: Analysis fields for July 2011 provided for GaTech and UMD for SIP modeling*
  - *Assimilated exo-domain wild fire, O<sub>3</sub> using RAQM*
  - *Upgrade emission based on NEI2011*
  - *Assimilated wild-fire using NESDIS obs, PM<sub>2.5</sub> constraints using MODIS AOD & AQS PM<sub>2.5</sub>*
  - *Assimilated cloud attenuated photolytic rate*
  - *Mimicked SIP reduced RMSE by 400% for PM<sub>2.5</sub>*
- *Deliverable in 2015: Analysis fields for 2010, support HTAP*
  - *Assimilate lightning NO<sub>x</sub>, PAR, DYNAMO Isoprene*
- *User friendly portal and archive for chemical analysis fields over Continental U.S.*



# Lightning Process currently used in CMAQ 5.0\*

NLDN (National Lightning Detection Network) data

Model's convective  
Precipitation rate

Map to CMAQ grid

Calculate Total monthly Lightning flash  
Count over each grid

Model's strike count  
(monthly total)

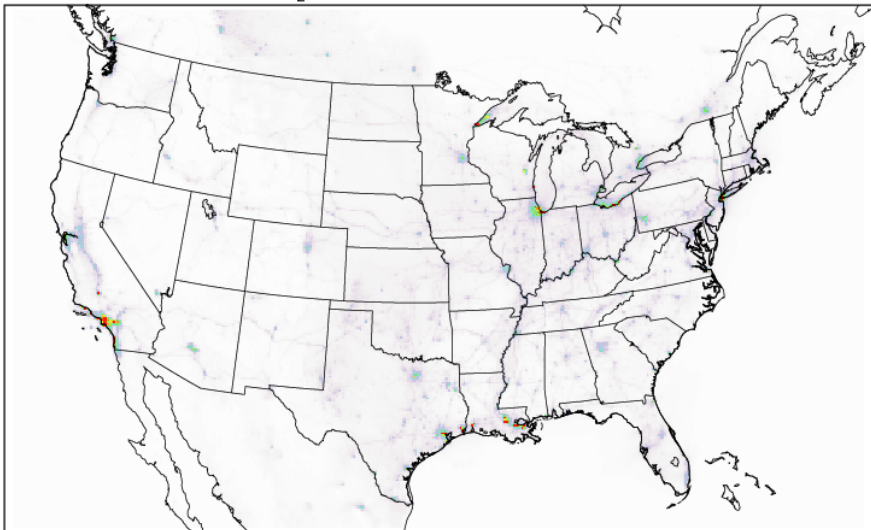
Mean LRatio used in  
CMAQ NLDN/Model

\*CMAQ Version 5.0 and higher contains a scheme based on Allen et al. (2012, ACP) that was funded under NASA Applied Sciences Air Quality Program project (Ken Pickering, PI):

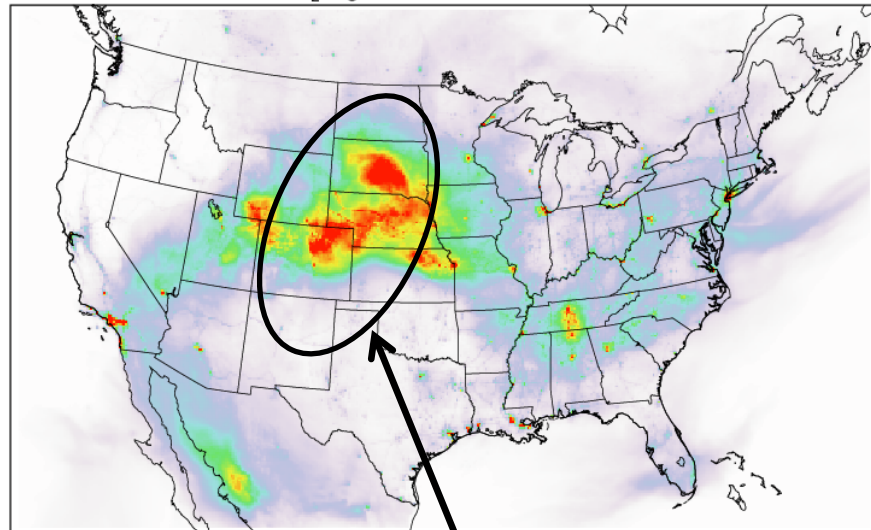
- Method for estimating lightning flash rates
- $LNO_x$  production per flash
- Method of allocating  $LNO_x$  production in the vertical

# July 1-10, 2011 NO<sub>2</sub> (Left) Base (Right) with LNOx, (Bottom) Difference

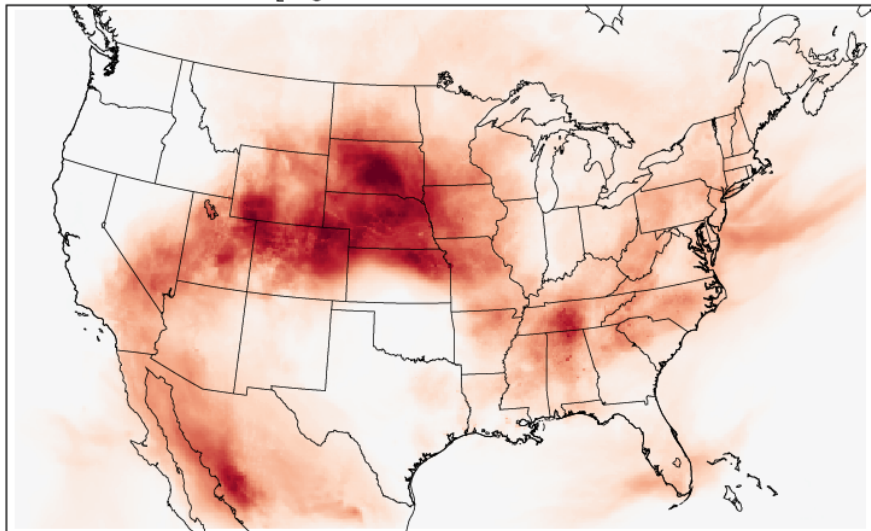
NO<sub>2</sub> BASE 20110701 - 20110710



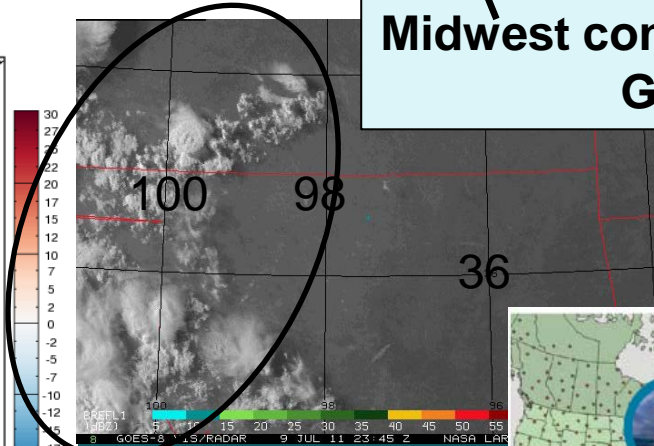
NO<sub>2</sub> Ltgn 20110701 - 20110710



NO<sub>2</sub> Ltgn-Base 20110701 - 20110710



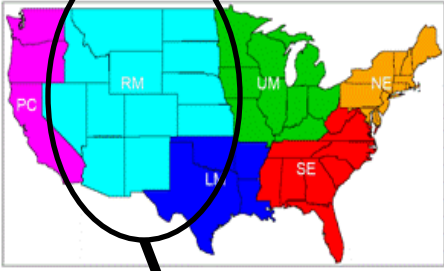
**Midwest convections.  
GOES13**



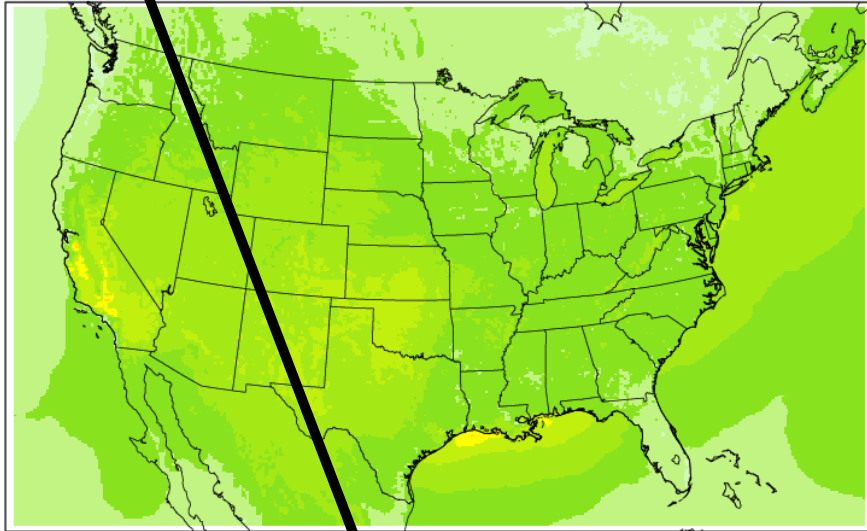
*U.S. NLDN consists of more than 114 remote, ground-based lightning sensors.*

*Sensors instantly detect the electromagnetic signals created when lightning strikes the earth's surface.*

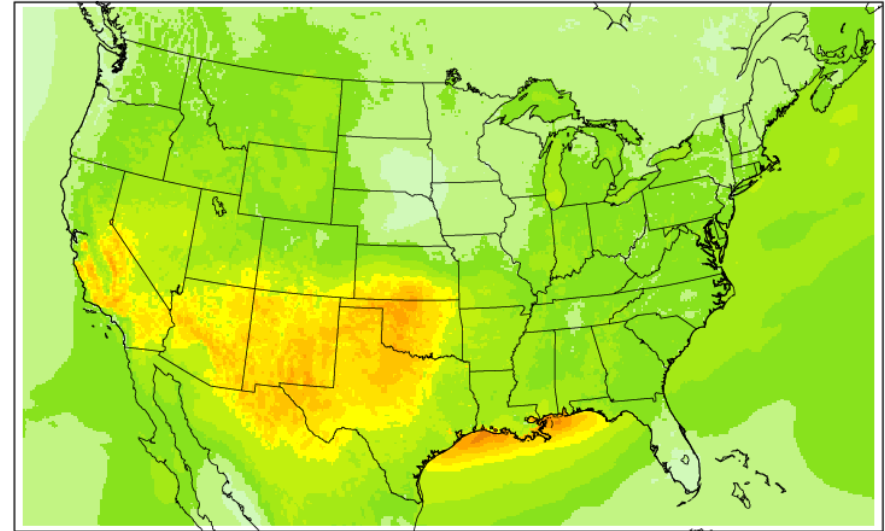
# July 1-10, 2011 O<sub>3</sub> (Left) Base (Right) with LNOx, (Bottom) Verification



O<sub>3</sub> BASE 20110701 - 20110710



O<sub>3</sub> Ltgn 20110701 - 20110710

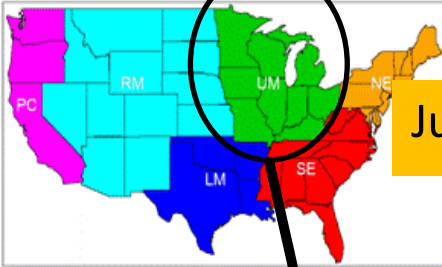


O <sub>3</sub> 10 days avg	Stations	Obs mean	Mean bias	RMSE	Corr. Coef.
Base	3222	36.45	-0.17	15.81	0.66
		36.45	2.90	24.54	0.53

O <sub>3</sub> 10 days avg (RM)	Stations	Obs mean	Mean bias	RMSE	Corr. Coef.
Base	483	42.36	1.32	13.32	0.61
Include LNOx		42.36	6.61	29.60	0.48

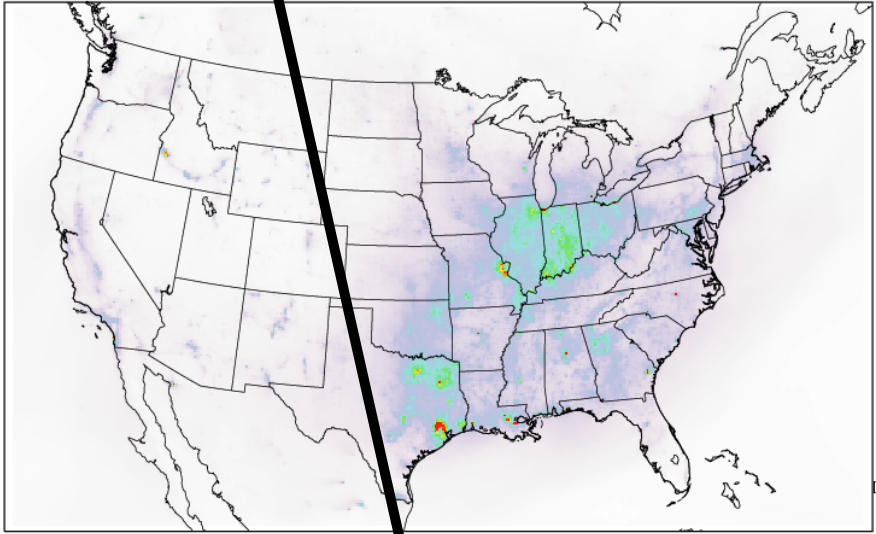




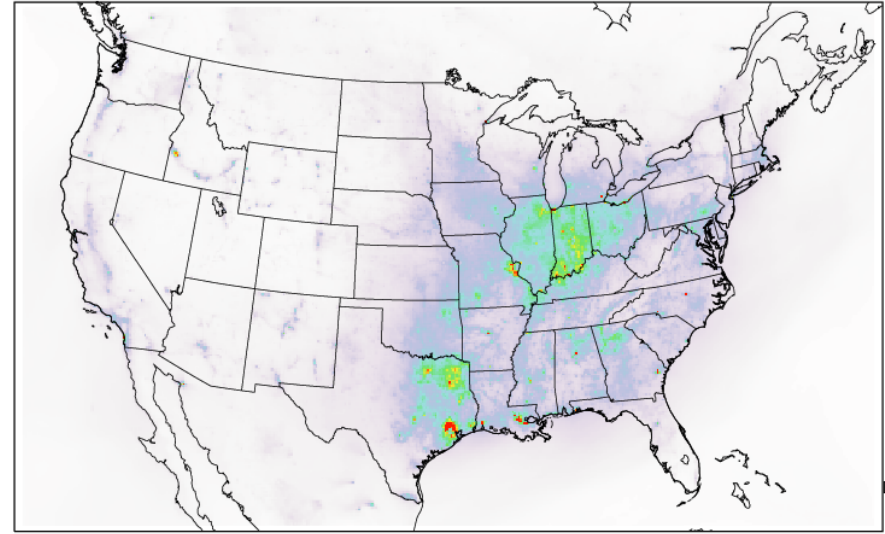


July 1-10, 2011 PM<sub>2.5</sub> (Left) Base (Right) with LNOx, (Bottom) Verification

PM<sub>2.5</sub> BASE 20110701 - 20110710



PM<sub>2.5</sub> Ltgn 20110701 - 20110710



PM <sub>2.5</sub> 10 days avg	Stations	Obs mean	Mean bias	RMSE	Corr. Coef.
Base	1801	12.67	-3.47	13.22	0.25
		12.67	-3.07	13.58	0.24
PM <sub>2.5</sub> 10 days avg (UM)	Stations	Obs mean	Mean bias	RMSE	Corr. Coef.
Base	276	17.71	-3.66	16.40	0.23
Include LNOx		17.71	-2.61	17.08	0.22

# Part 3: Data Assimilation Methodology



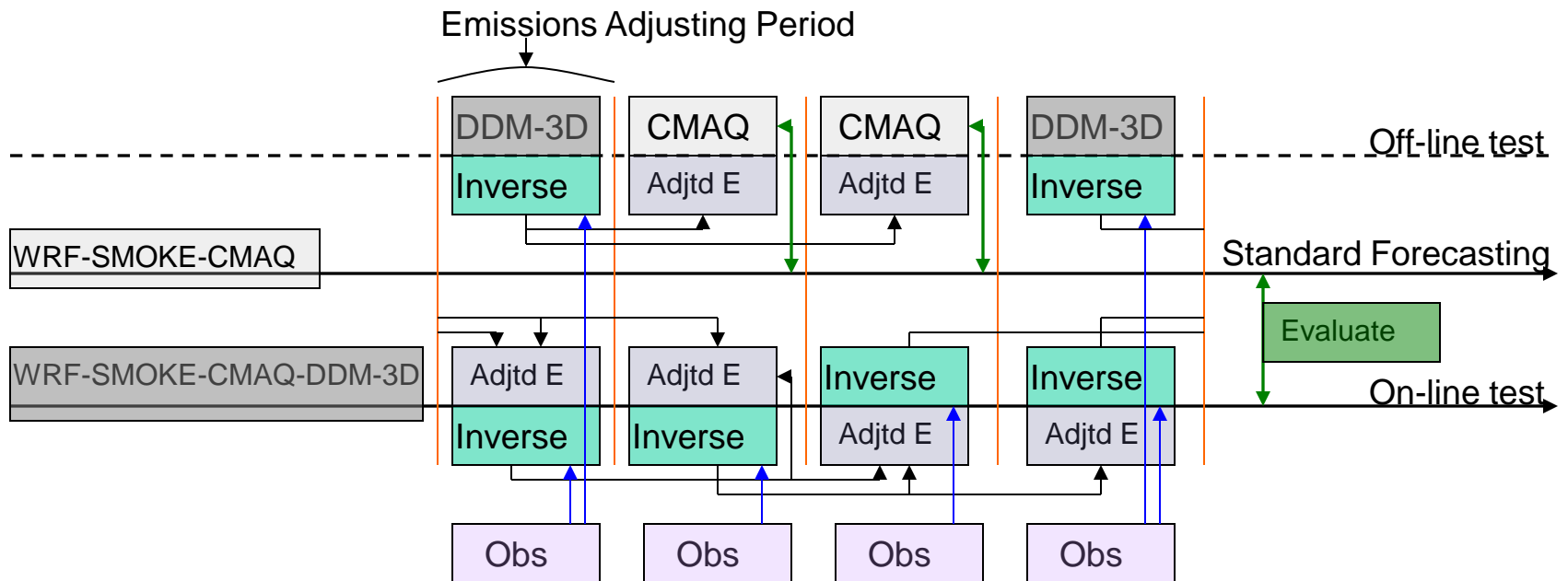
# Optimal Interpolation (OI)

- OI simplifies the extended Kalman filter formulation (Dee et al. *Q. J. R. Meteor. Soc.* 1998) by limiting the analysis problem to a subset of obs.

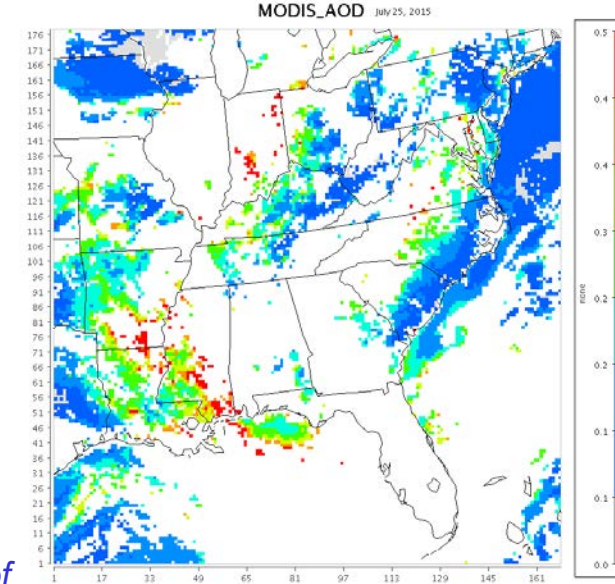
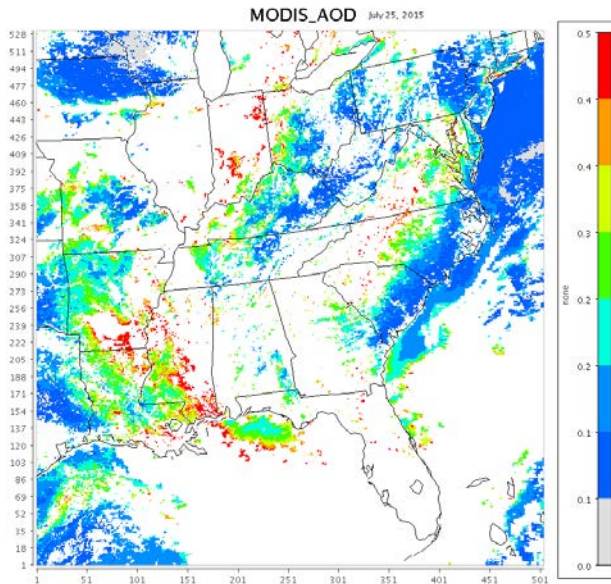
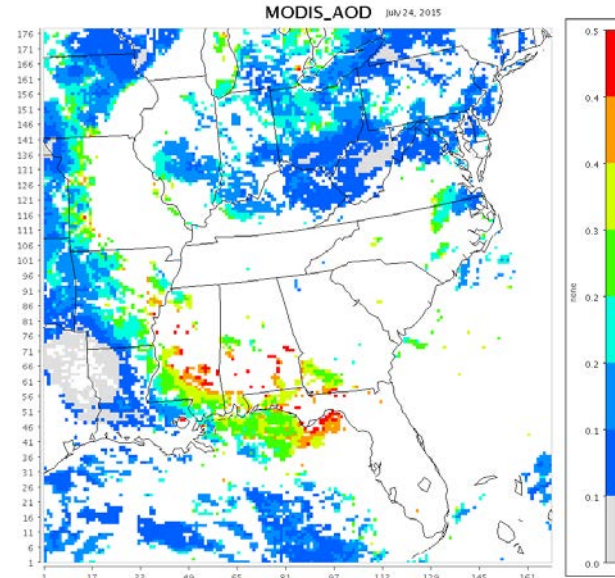
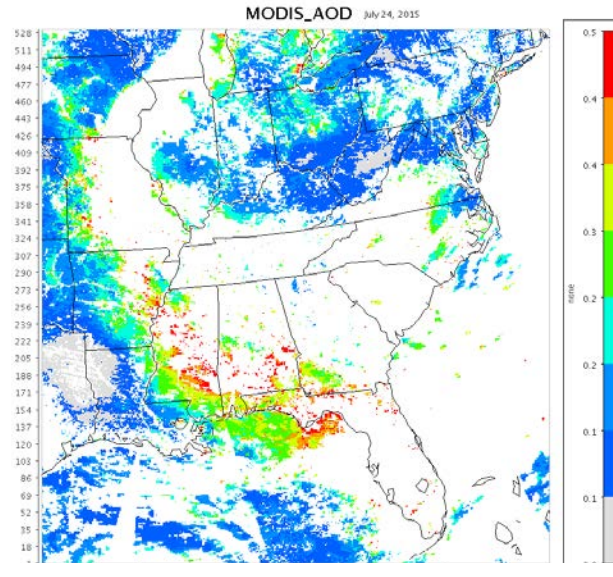
$$X^a = X^b + BH^T (HBH^T + O)^{-1} (Y - HX)$$

- Obs far away (beyond background error correlation length scale) have no effect in the analysis.
- Injection of Obs through OI takes place at 1800 UTC daily.

# Alternative methods: Emissions adjustments and model results based data fusion



# MODIS L2 C6 AOD Re-gridded Near Real-Time HiRes2 Products: 12-km versus 4-km



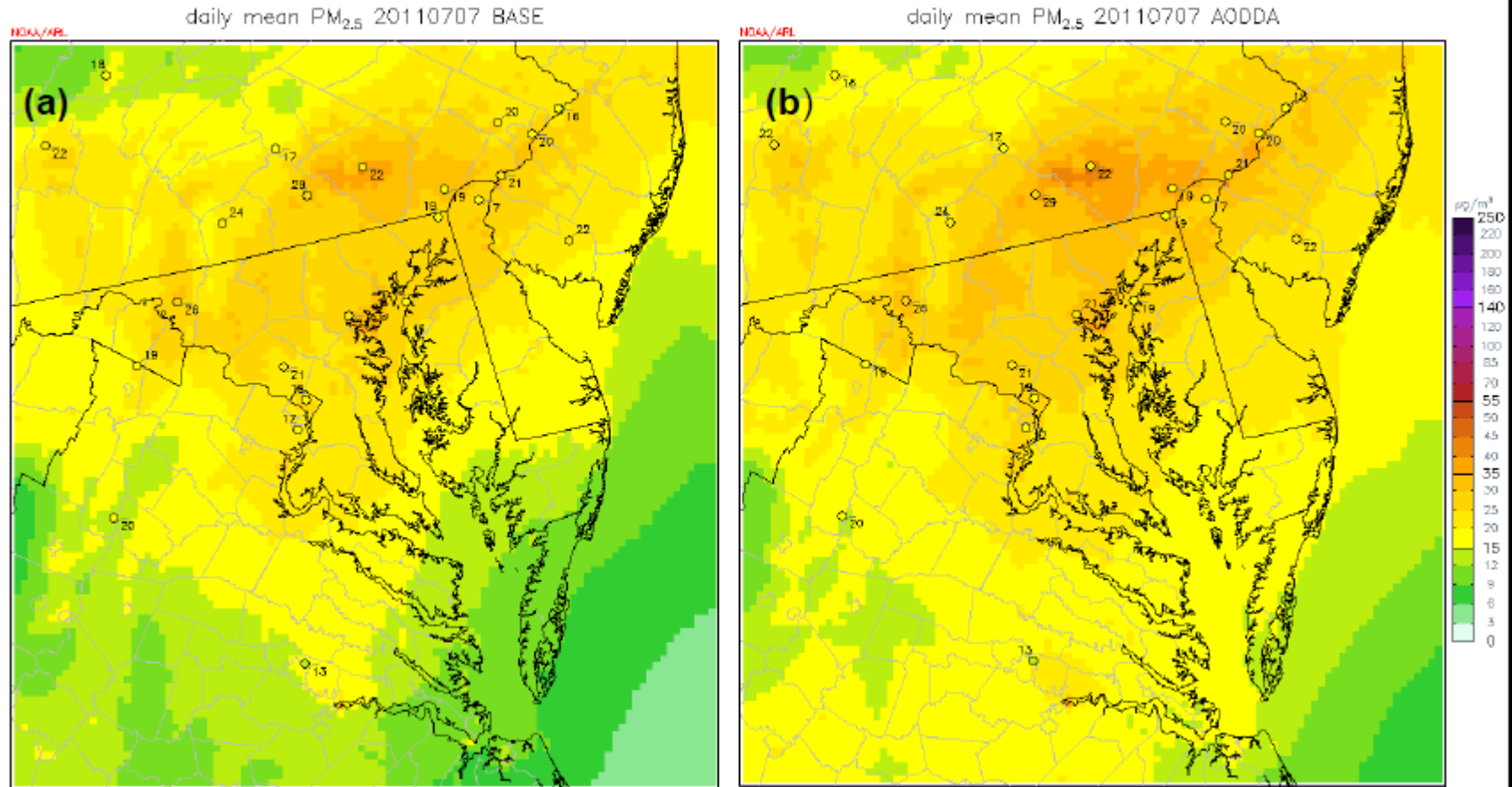
stitute of



# Part 4: Reanalysis fields for SIP modeling and health studies

# Use Reanalysis fields for SIP modeling's initial and boundary conditions

24 h PM<sub>2.5</sub> on 07/07/2013 (a) Base, (b) AOD\_DA for DISCOVER-AQ GA\_Tech 4 km



## DISCOVER-AQ

GA\_Tech  
4 km

PM2.5 24h avg	Obs mean	Mean bias	RMSE	Corr. Coef.
Base	17.36	-5.88	22.50	0.40
With re-analysis field to derive LBC	17.36	-3.48	22.19	0.42



# Summary

- Decision on matching the GFS vertical structure **42-L** was made for the chemical reanalysis forward model
  - The reanalysis forward model showed reasonable ozone cross-section in complex terrain
- The reanalysis forward model is **tested** and used to generate July 2011 reanalysis fields for MDE for SIP modeling
- **July 2011** analysis fields was used by Georgia Tech for a 14-day SIP simulation and showed significant improvement in RMSE
- **Data Set assimilated:** RAQMS (MLS, OMI O<sub>3</sub>, MODIS AOD); HMS Fire; GOES cloud fraction for photolytic rate correction; MODIS AOD; AQS O<sub>3</sub>, PM<sub>2.5</sub>
- **Assimilate lightning NOx:** Use NOAA hourly reporting of the National Lightning Detection Network to derive and distribute LNOx
- Preliminary surface NOx and O<sub>3</sub> verification showed over-estimation
- Further improvement of LNOx assimilation algorithm is being test
- Analysis configuration also includes **observation set on biogenic emission** from the DYNAMO team
- **Production FY2010** in conjunction with HTAP support
- Portal via RSIG is being tested

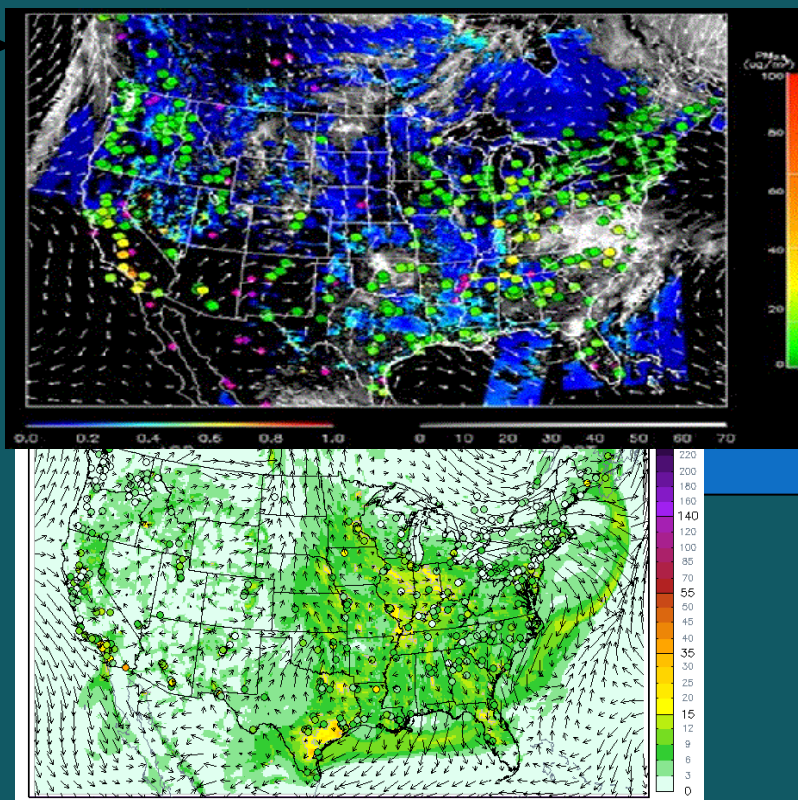
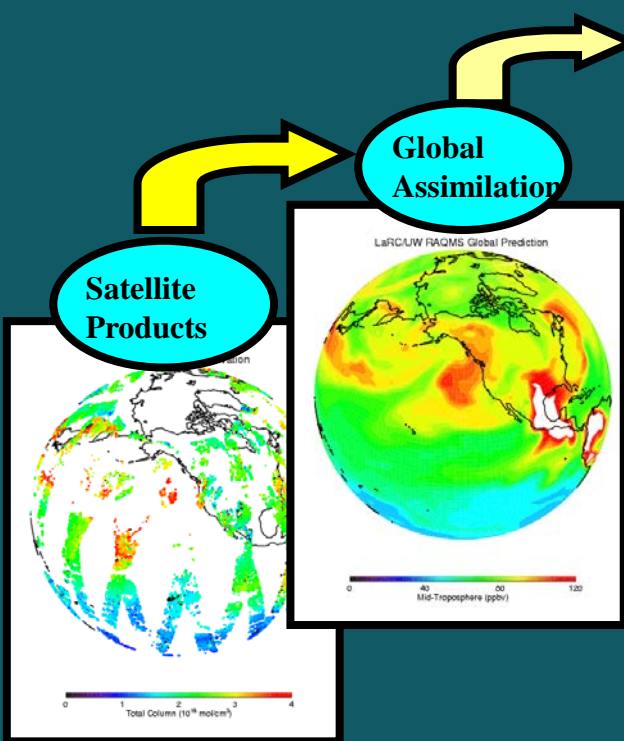


# Supplement



# AQAST Project: Air Quality Reanalysis

(*Translating Research to Services*)



- + AQ Assessments
- + State Implementation Plan Modeling
- + Rapid deployment of on-demand rapid-response forecasting; e.g., new fuel type, ..., etc.
- + Health Impacts assessments
- + Demonstration of the impact of observations on AQ distributions
- + Ingestion of new AQAST products into operations



3:30-5:00 Session

Yang Liu: MODIS C6

Alvarado & Hegarty:  $\text{NH}_3$

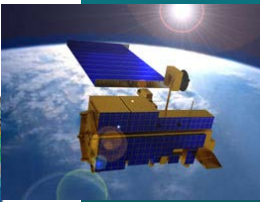
Huang, McNide, Lee :  $T_{\text{skin}}$

<http://acmg.seas.harvard.edu/aqast/projects.html>



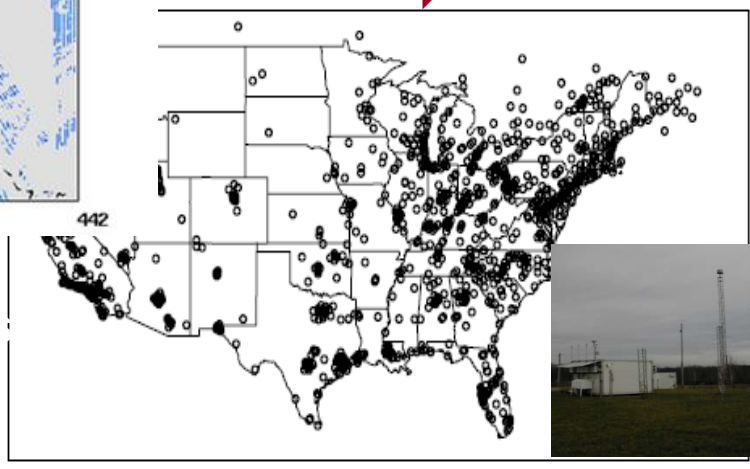
done →

# MODIS obs



done →

# AIRNow



done →

# Cloud-obs Photolysis rates

## GOES-MCIP INTERFACE

Cloud transmissivity (calculated from satellite retrieved cloud albedo), cloud top pressure, and cloud fraction are prepared for input to MCIP

## MODIFIED MCIP

GOES retrievals replaces MM5 cloud information being passed to CMAQ. Cloud fraction, transmissivity, cloud base and top heights are passed to CMAQ.

## PHOT in CMAQ

In subroutine PHOT, clear sky photolysis rates will be adjusted for cloud cover based on GOES cloud fraction and cloud transmissivity information.

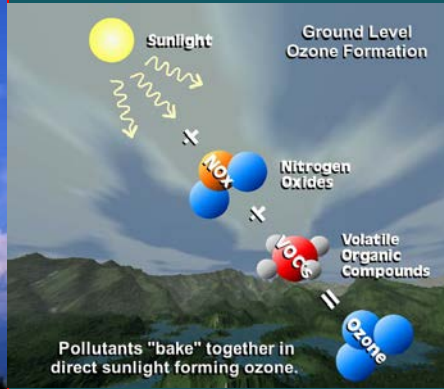
Interpolated in between.

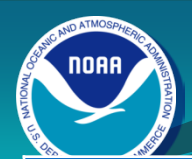
Cloud Base According to Lifting Condensation Level

$$T_c = B \ln \left[ \frac{A \varepsilon}{w p_s} \left( \frac{T_s}{T_c} \right)^{1.8} \right]$$



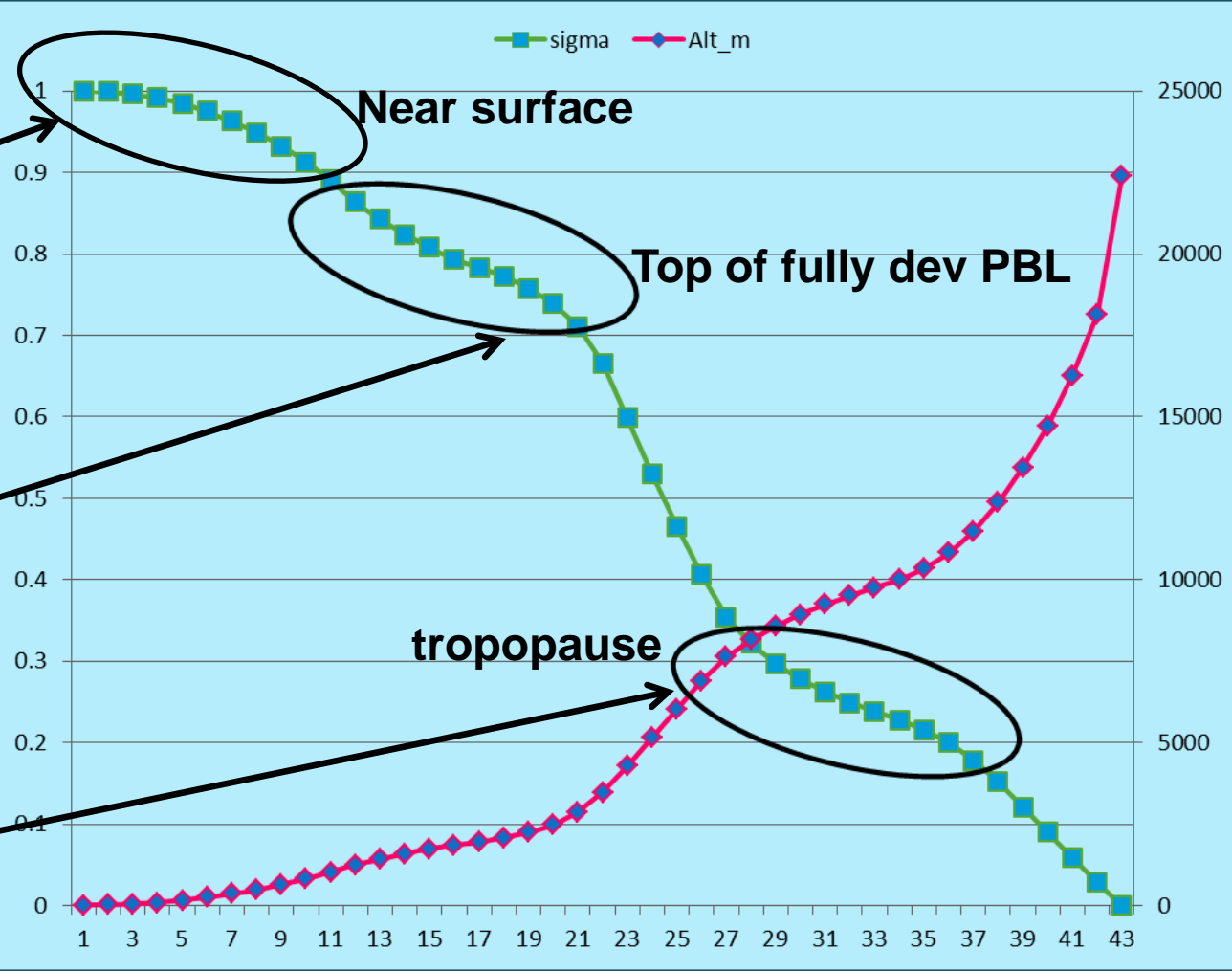
# Yet to do Isoprene & PAR



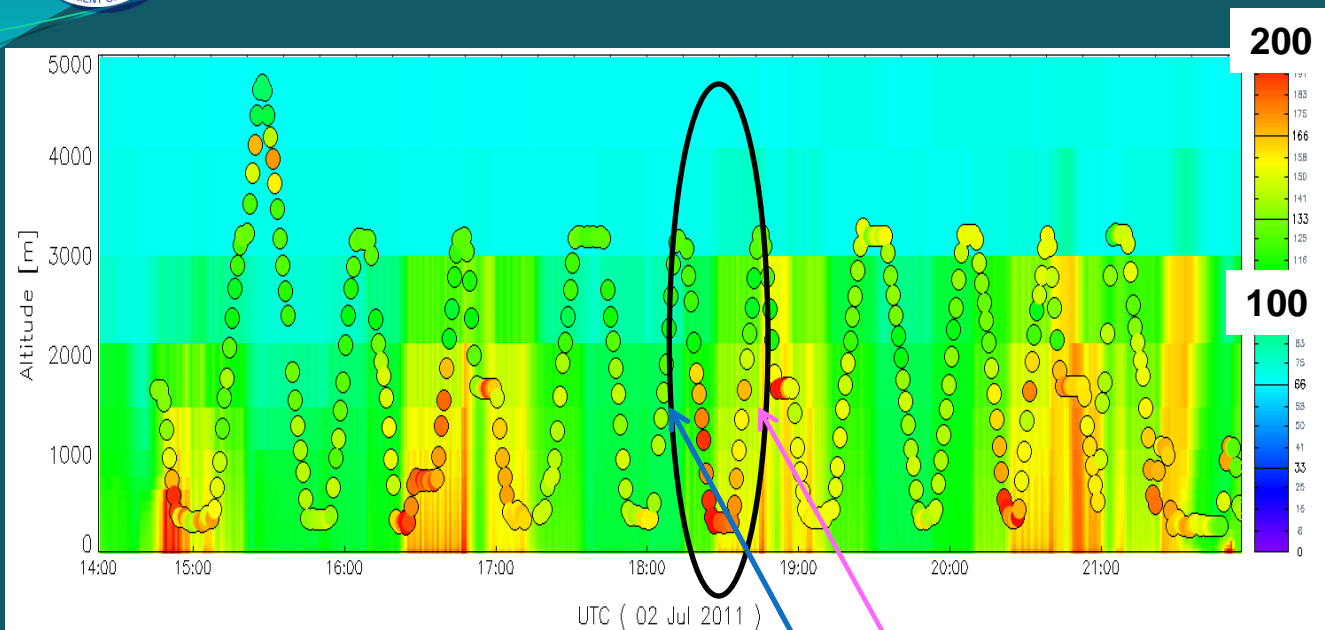


# Re-configuration of vertical structure: Decision to match GFS (NCEP)

sigma	Pres (hPa)	Z (m)
1	1013	0
0.999	1012	4
0.996	1010	20
0.992	1007	48
0.985	993	92
0.864	872	1245
0.843	852	1430
0.824	836	1590
0.808	821	1735
0.322	348	8150
0.297	326	8580
0.278	310	8940
0.262	296	8580



# CO (ppb) along the P3 Flight – July 2 2011: AOD\_DA case vs. Obs

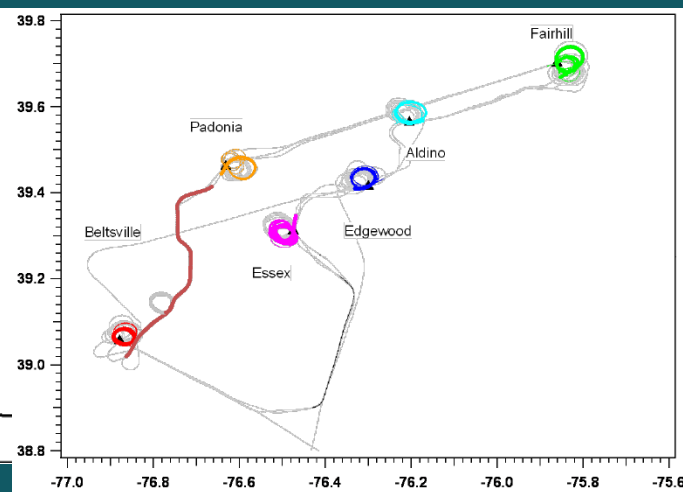
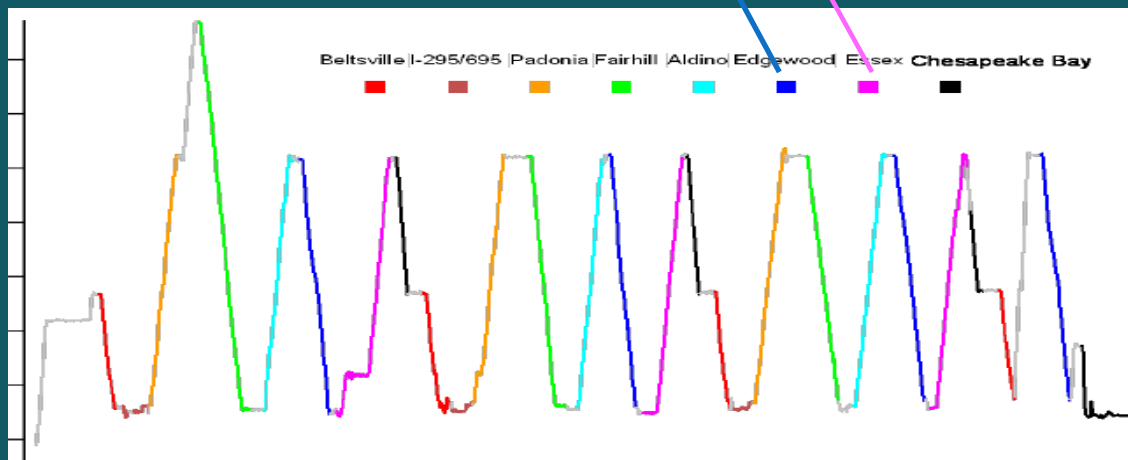


P3 Three and a half loops:

- Beltsville
- Padonia
- Fairhill
- Aldino
- Edgewood
- Essex
- Chesapeake Bay

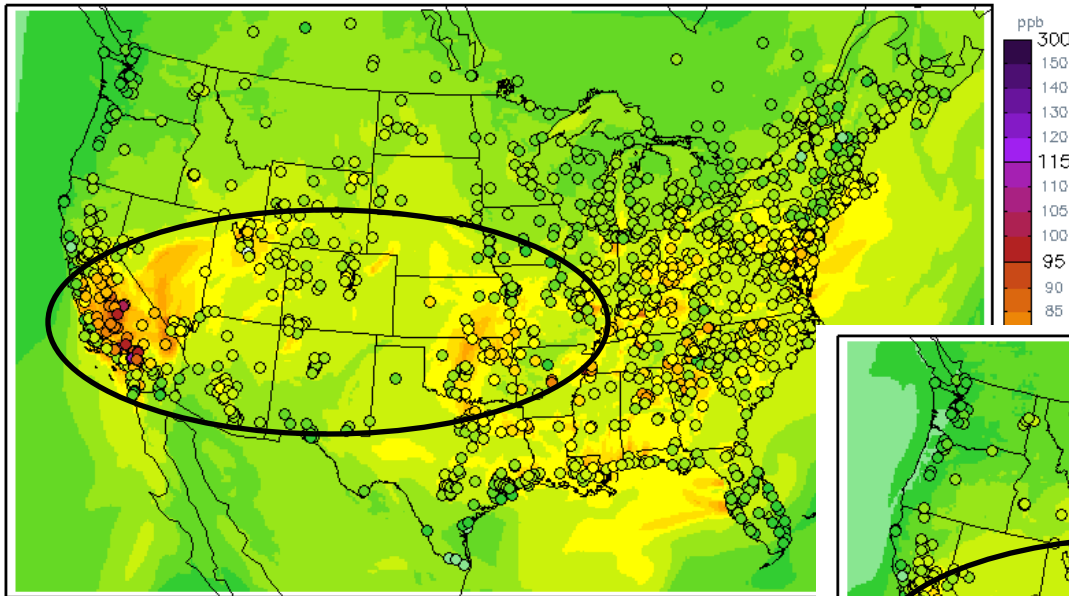


★ Pan & Lee et al.,  
AE 2014

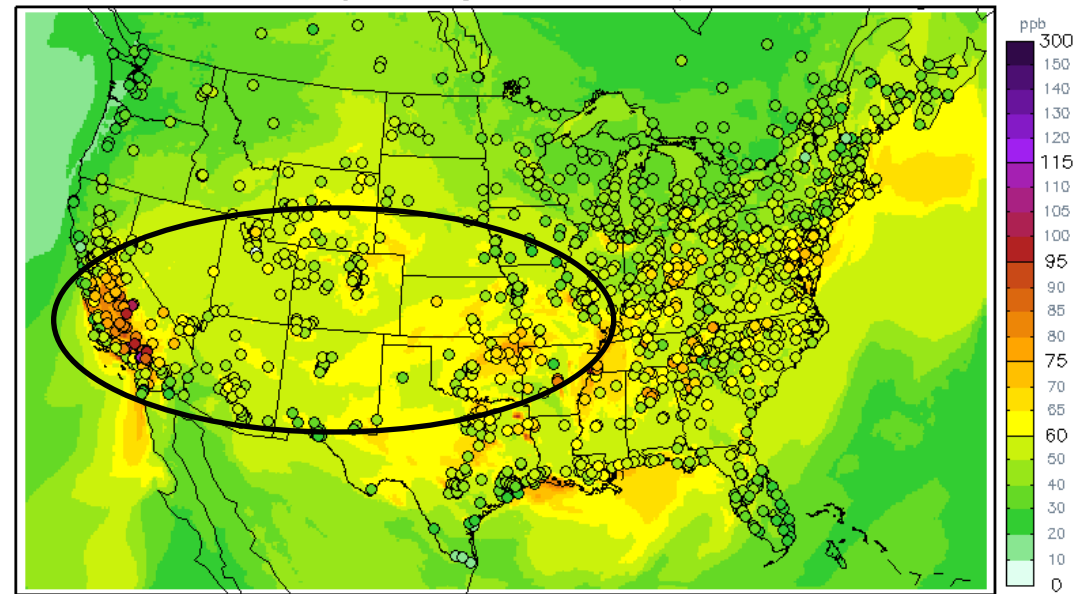


# NMMB-CMAQ4.7.1 (22L)

8h daily max O<sub>3</sub> 20110703 LT / 22L



# WRF\_ARW-CMAQ4.7.1 (42L)

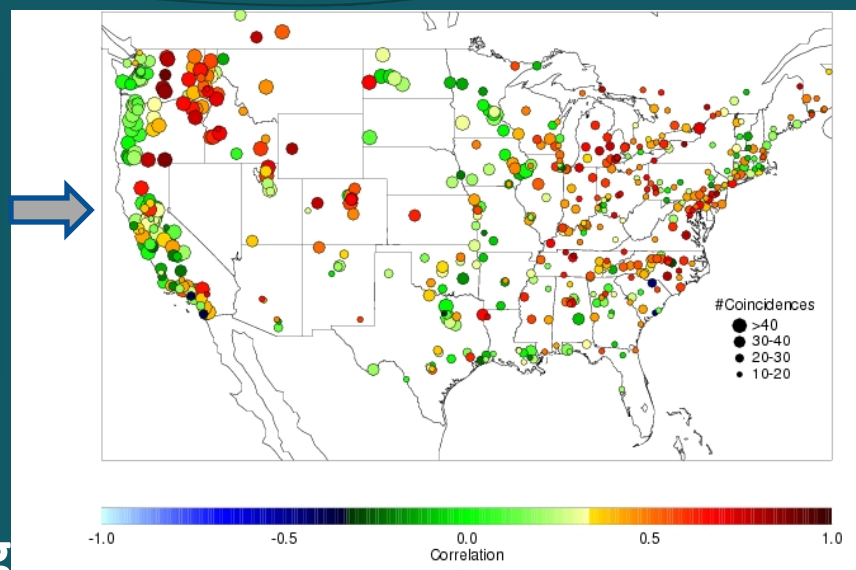


Daily maximum 8 h averaged surface O<sub>3</sub> on July 3 2011  
The over bias across a large swath in the Southern U.S. was reduced by 42L



# National correlation map between AIRNow measurement and MODIS AOD

Typically good correlation between surface PM<sub>2.5</sub> and AOD retrieved by MODIS



## MODIS (Moderate Resolution Imaging Spectroradiometer) AOD

Courtesy :NESDIS

- Orbit:** 705 km, 10:30 a.m. descending node (Terra) or 1:30 p.m. ascending node (Aqua)
- Swath Dimensions:** 2330 km (cross track) by 10 km (along track at nadir)
- Spatial Resolution:** 250 m (bands 1-2)  
500 m (bands 3-7)  
1000 m (bands 8-36)

<http://terra.nasa.gov/About/>

