Source-Specific Forecasting of Air Quality Impacts with Dynamic Emissions Updating

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Georgia Institute of Technology

AQAST
NASA AIR QUALITY APPLIED SCIENCES TEAM

Motivation and Objective

- Motivation
  - Air quality models providing backbone of regional and national air quality forecasting systems
    - Ozone forecasting with UAM began for Olympics
    - CMAQ then used for regional and national ozone forecasting
    - CMAQ now being used for PM2.5
  - Improved AQM forecasting performance desired
  - Source specific air quality impacts potentially usable for air quality management and improve forecasting performance.
    - Prediction with 3-D models relies on accuracy of emissions
      - Uncertain (particularly for smaller sources)
      - Change with time
- Objective
  - Provide information that can assist air quality management and exposure assessment
    - Source impact forecasting in addition to air quality forecasting
    - Improve air quality forecasting accuracy using near real time measurements through dynamic adjustment of emissions
      - Utilize measurements (gases, PM, AOD and PM composition)
    - Use source-specific impacts to improve air quality management
      - Recent PNAS paper showing use with electricity dispatch modeling

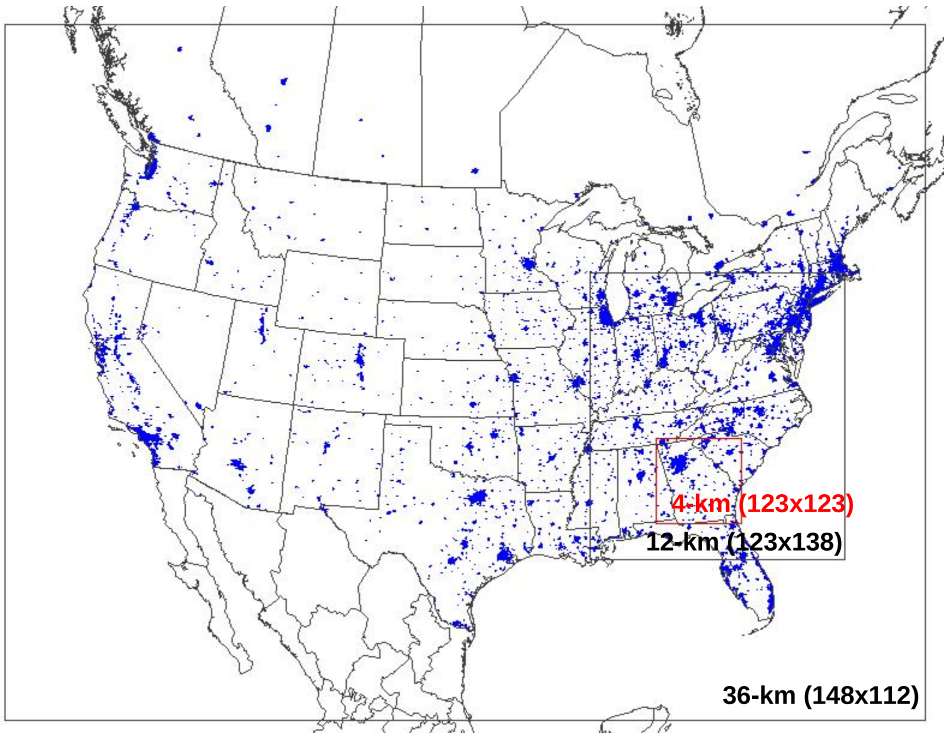
IMPROVED AIR QUALITY IMPACT FORECASTING

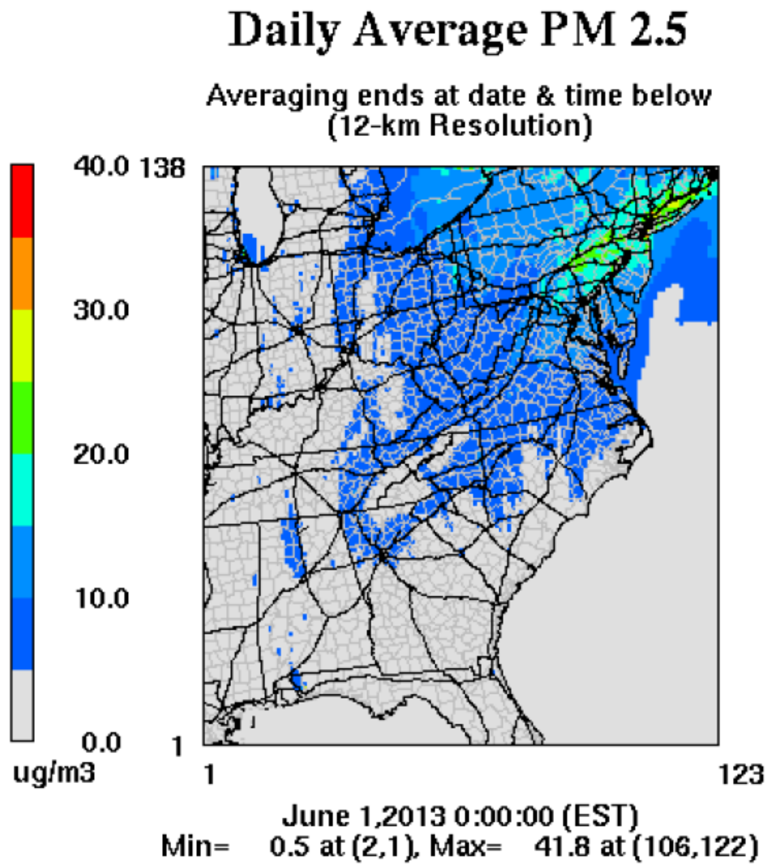
Air Quality Forecasting Enhancements

- Objective
  - Improve regional air quality forecasts
  - Provide more information on sources of air pollutants for potentially more effective air quality management
- Approach
  - Advance the Hi-Res forecasting system
    - Outgrowth of activities starting before 1996 Olympics
  - Improve air quality forecasting system (Hi-Res2) inputs
    - Use observations (ground & satellite) to adjust model inputs and parameters
      - Emissions updating
    - Use advanced model capabilities to provide link between simulated and observed concentrations
      - Advanced sensitivity analysis (DDM-3D)

Hi-Res: forecasting ozone and $PM_{2.5}$
48 hr forecast @ 4-km resolution for Georgia and @ 12-km for most states of eastern US

Hi-Res Modeling Domains



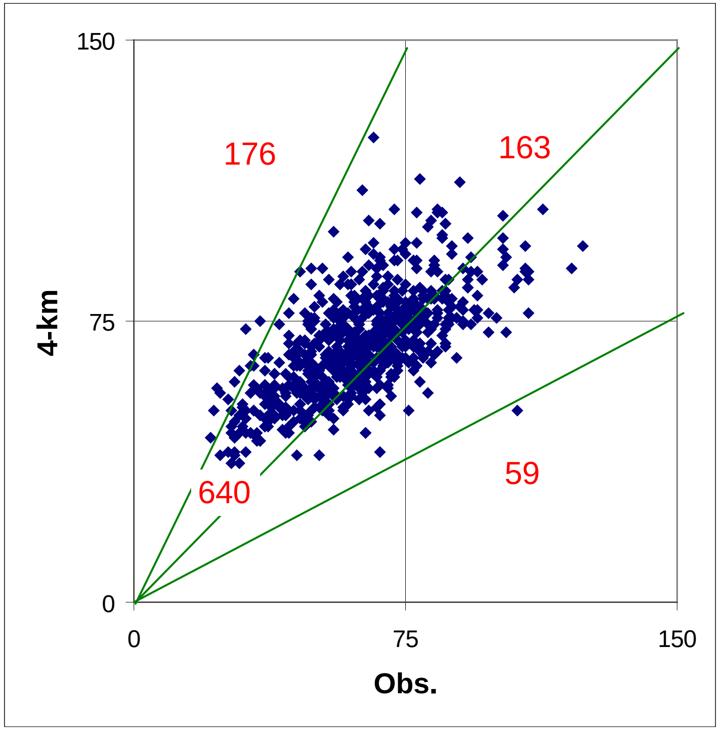


Hi-Res forecasting products are in use by Georgia EPD assisting their local AQI forecasts for multiple metro areas

Hi-Res forecasting products are potentially useful elsewhere

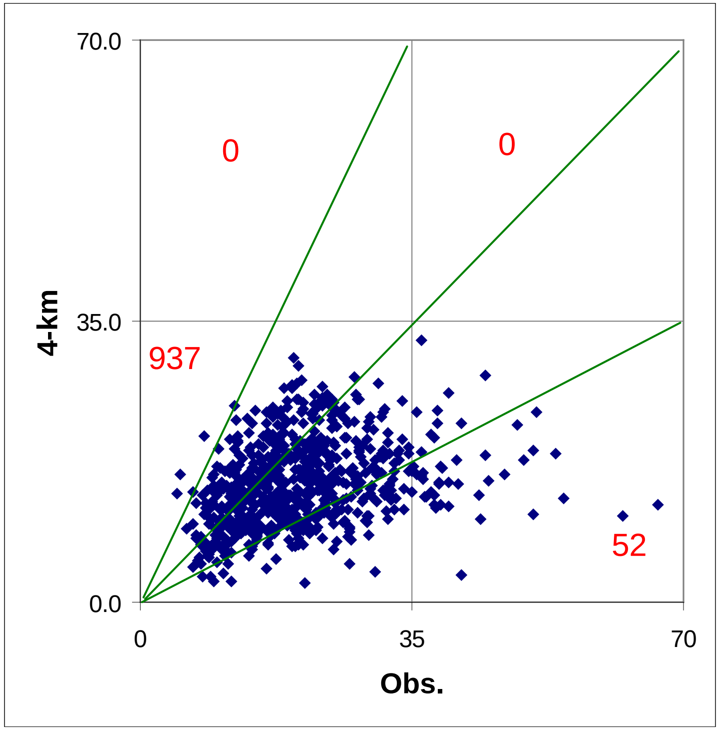
Overall 2006-2012 Performance (Ozone Season): Atlanta Metro

Ozone



MNB	19%
MNE	24%

$PM_{2.5}$



MNB	-13%
MNE	31%

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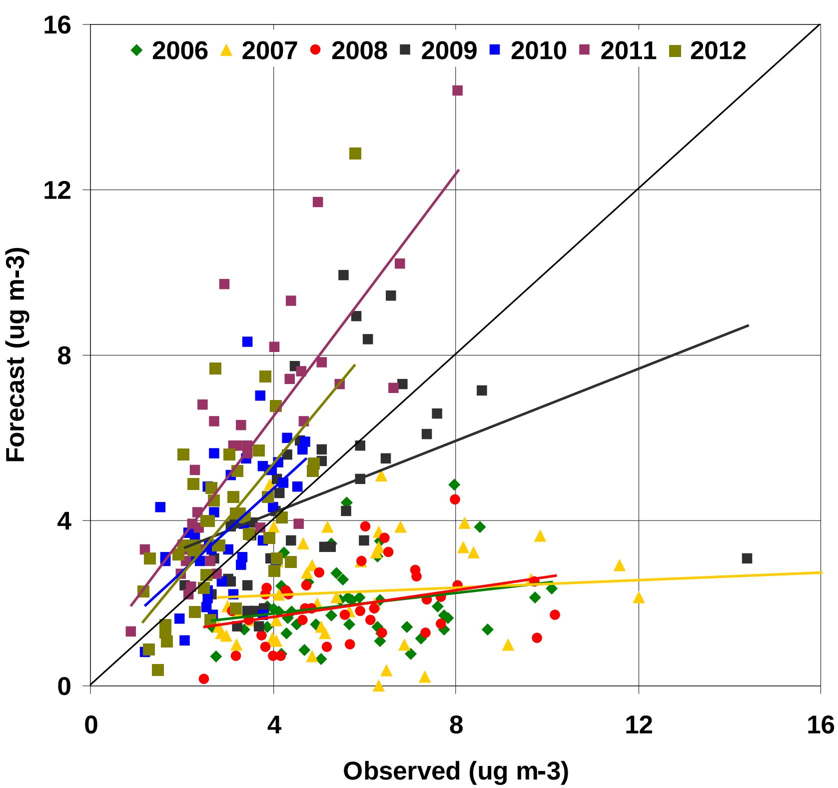
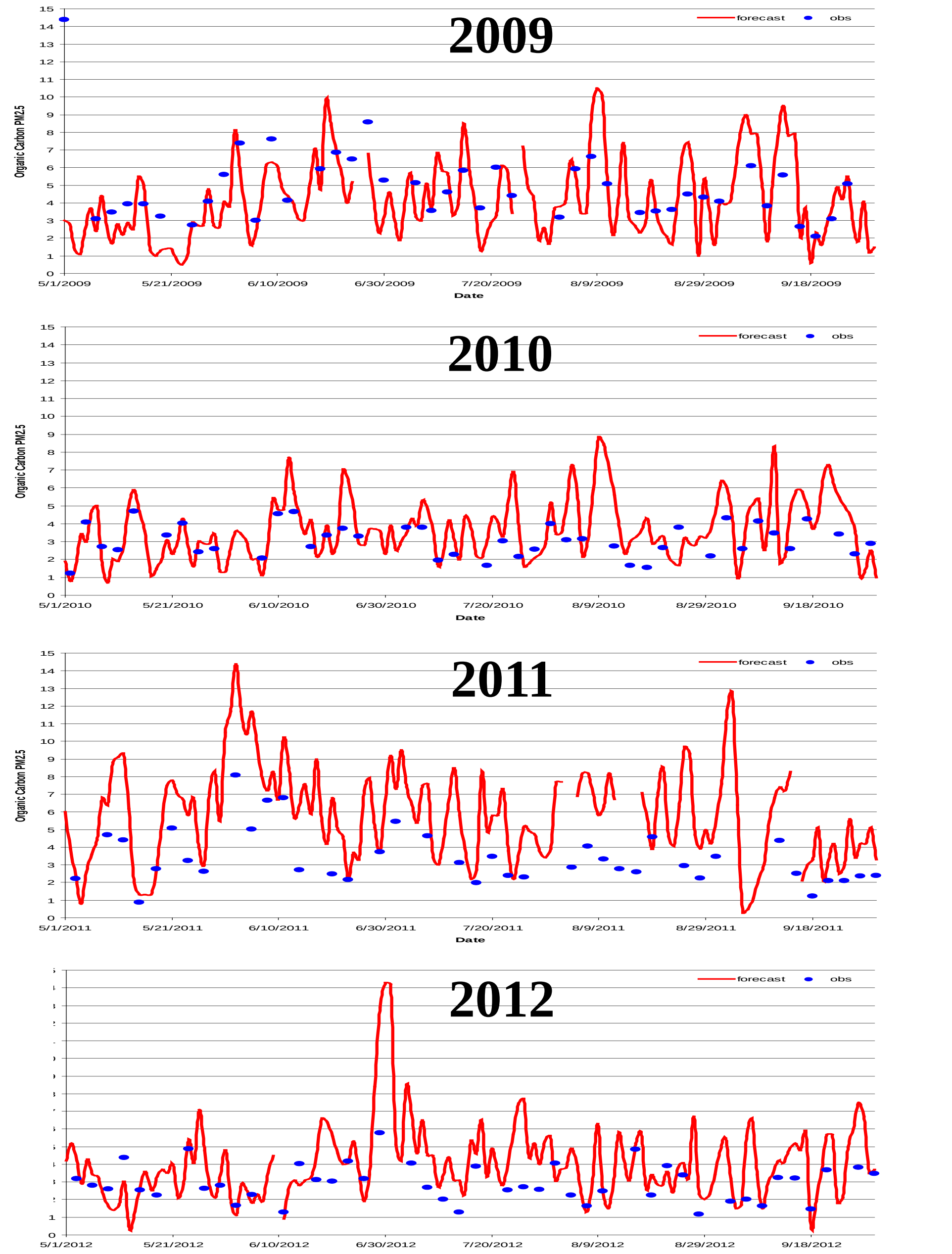
Forecast vs. Observed OC at South DeKalb

- Implemented multigenerational OC formation in 2009 (Baek et al. 2011)

Ozone Season May-September

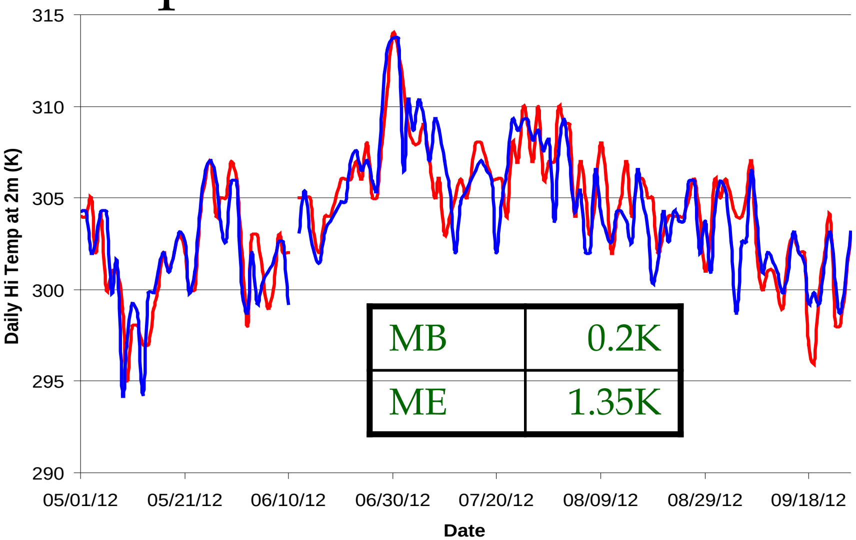




Forecast vs. Observed 2012 Ozone Season

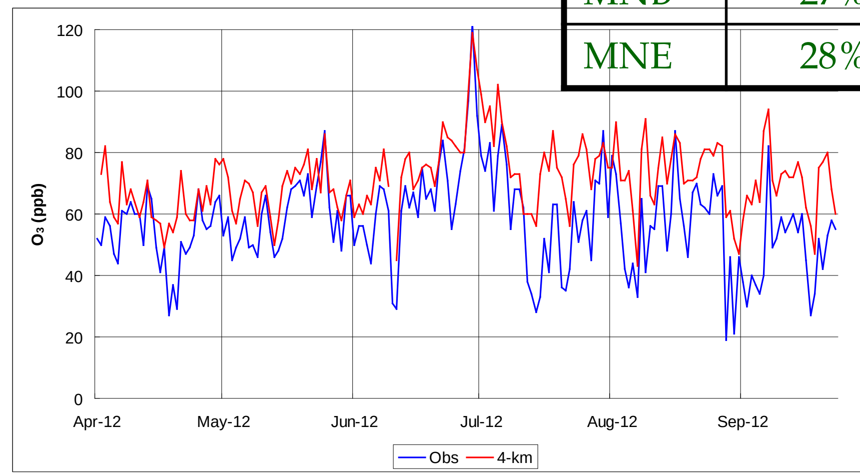
Metro Atlanta

Temperature 2012



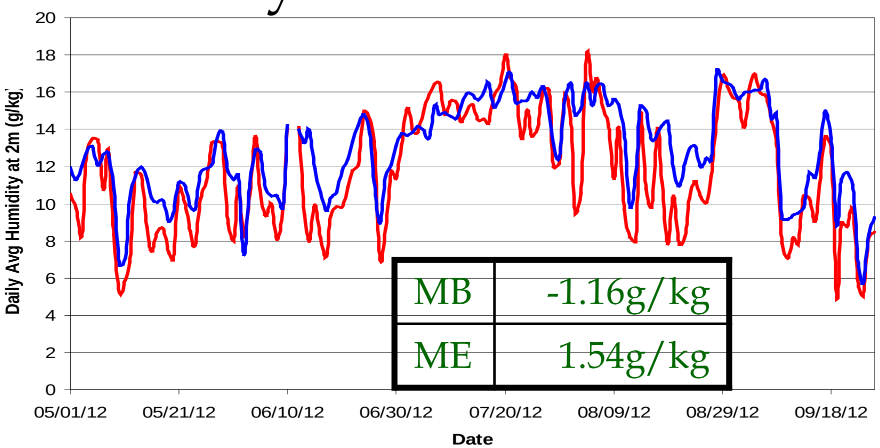
MB	0.2K
ME	1.35K

O3



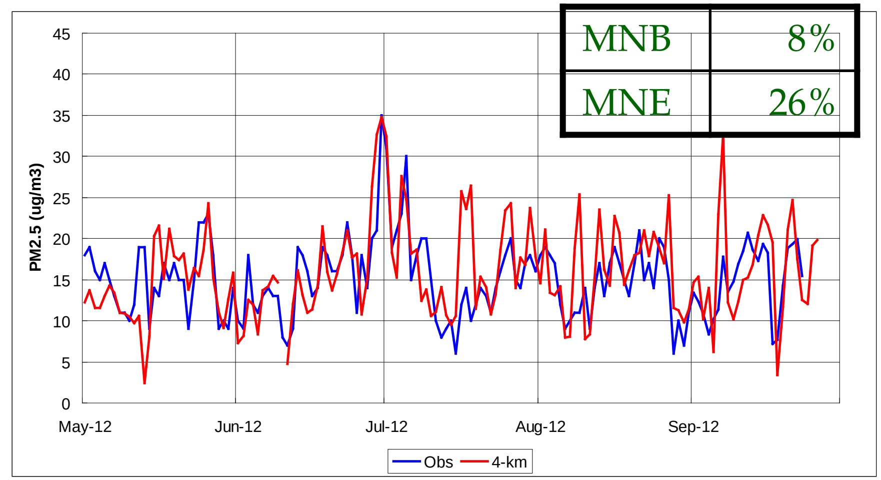
MNB	27%
MNE	28%

Humidity 2012



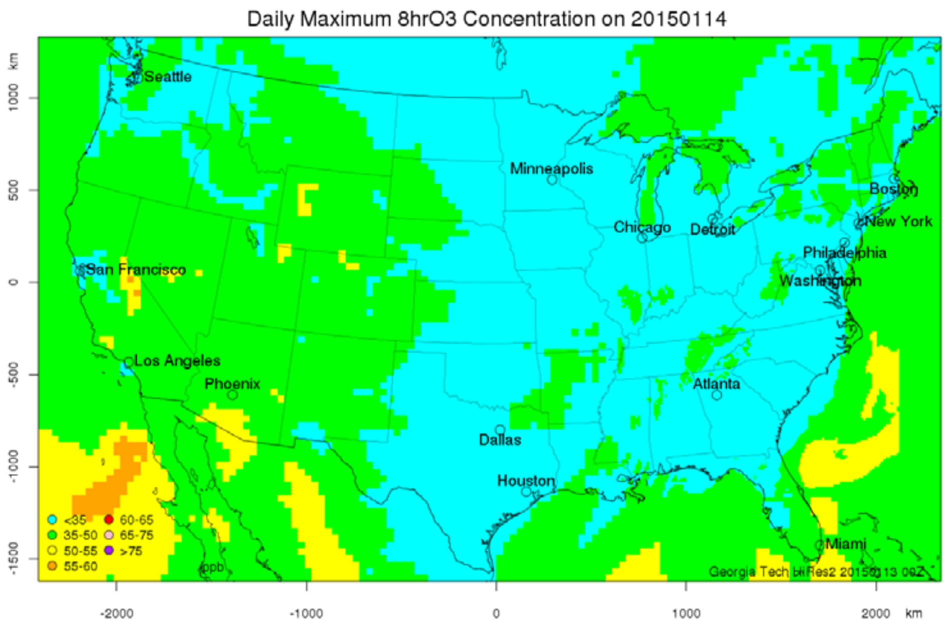
MB	-1.16g/kg
ME	1.54g/kg

PM2.5



MNB	8%
MNE	26%

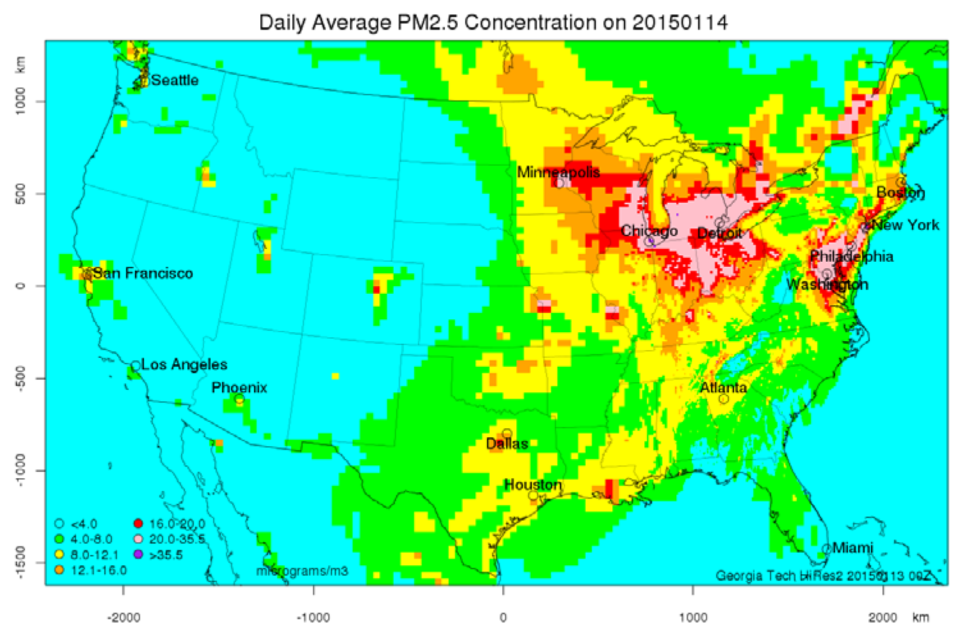
Hi-Res2 Forecasting System



Forecasting Air Quality for CONUS

(https://forecast.ce.gatech.edu open since November 28th,2014)

- Updated base emissions to 2011NEI
- WRF3.6.1 and CMAQv5.02 used
- 72-hour forecasts at 4-km resolution for Georgia and surrounding states, 12-km for most of Eastern states and 36-km for the rest of CONUS



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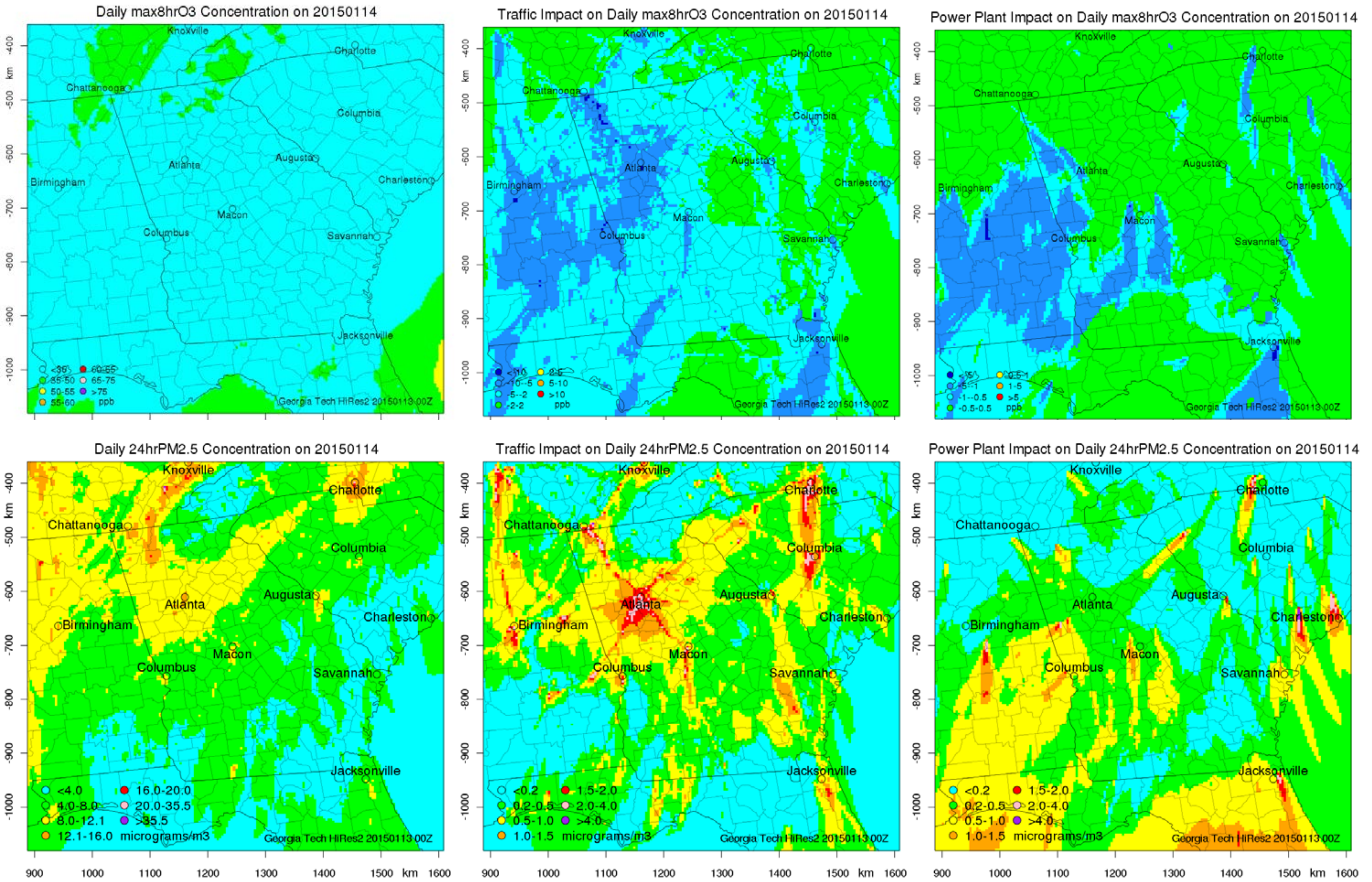
SOURCE-SPECIFIC AIR QUALITY IMPACT FORECASTING

Source Specific Air Quality Impact Forecasting

- Forecasting system calculates impacts of mobile sources and power plants impact air quality in region
  - CMAQ DDM-3D
- Adjust emissions, dynamically, to improve model performance
  - Calculate optimal emission strength to minimize model error
  - Use new emissions in forecasts

Forecasting Source Impacts at 4-km for Georgia

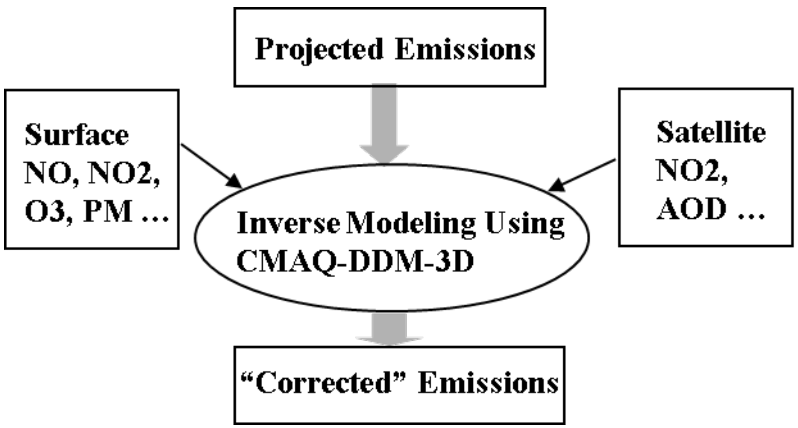
(https://forecast.ce.gatech.edu open since November 28th,2014)



Hi-Res2: Online Auto-Emissions-Adjustment

Inverse Modeling Approach for Adjusting Emissions

An emissions and air quality auto-correction system utilizing near real-time satellite and surface observations



Currently working with $PM_{2.5}$ measurements at ~20 sites in Georgia and Soon with MODIS C6 AOD

- Minimizes the differences between forecast and observed concentrations
- Minimal adjustment to source emissions
- Uses impacts of emission sources calculated by CMAQ-DDM-3D
  - Source impacts can be used for dynamic air quality management.(e.g., traffic and fires)

Inverse Model Formulation

- Solve for the Adjustment Factors, R_j, that minimize χ^2

DDM-3D calculated sensitivity of concentration *i* to source *j* emissions

emission adjustment ratio

$$\chi^2 = \underbrace{\sum_{i=1}^{N} \left[\frac{\left(c_i^{obs} - c_i^{sim} - \sum_{j=1}^{J} S_{i,j}(R_j - 1) \right)^2}{\sigma_{C_i^{obs}}^2} \right]}_{\chi_{Ci}^2} + \underbrace{\Gamma \sum_{j=1}^{J} \frac{(\ln R_j)^2}{\sigma_{\ln R_j}^2}}_{\chi_{Rj}^2}$$

weight

Remaining Error

Amount of Change in Source Strengths

L-BFGS algorithm is used for the optimization (R package nloptr)

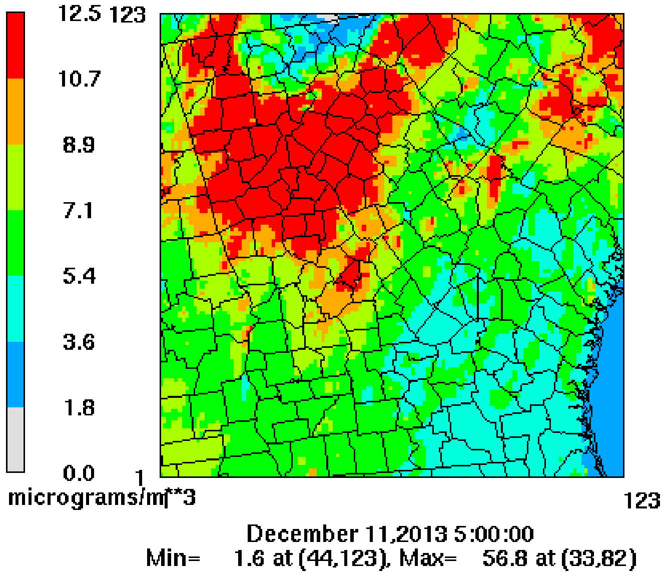
Offline Test: week1 Dec.1-7, 2013 & week2 Dec. 08-14, 2013

Dec. 1-7,2013	Area	On-road	Non-road	Point
Adjustment	0.17	0.83	0.85	0.97

In online system, traffic and power plant emission adjustments are forced within 30% and 10%, respectively

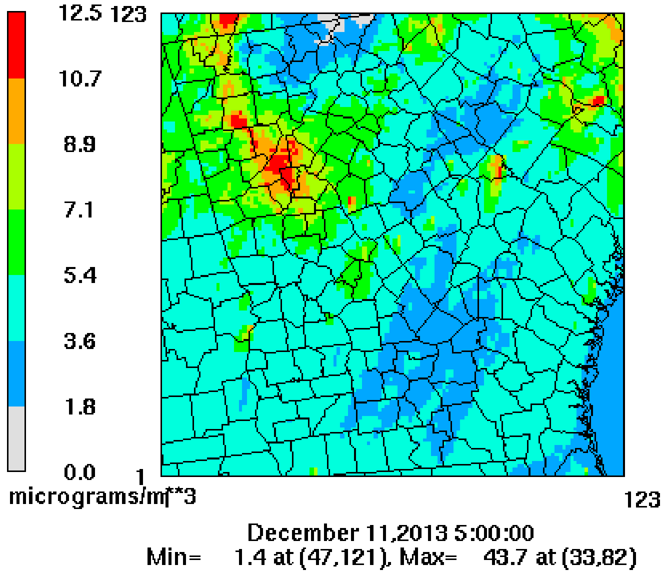
without emissions adjustments

Dec. 11, 2013 $PM_{2.5}$ Concentration



with emissions adjustments

Dec.11, 2013 $PM_{2.5}$ Concentration

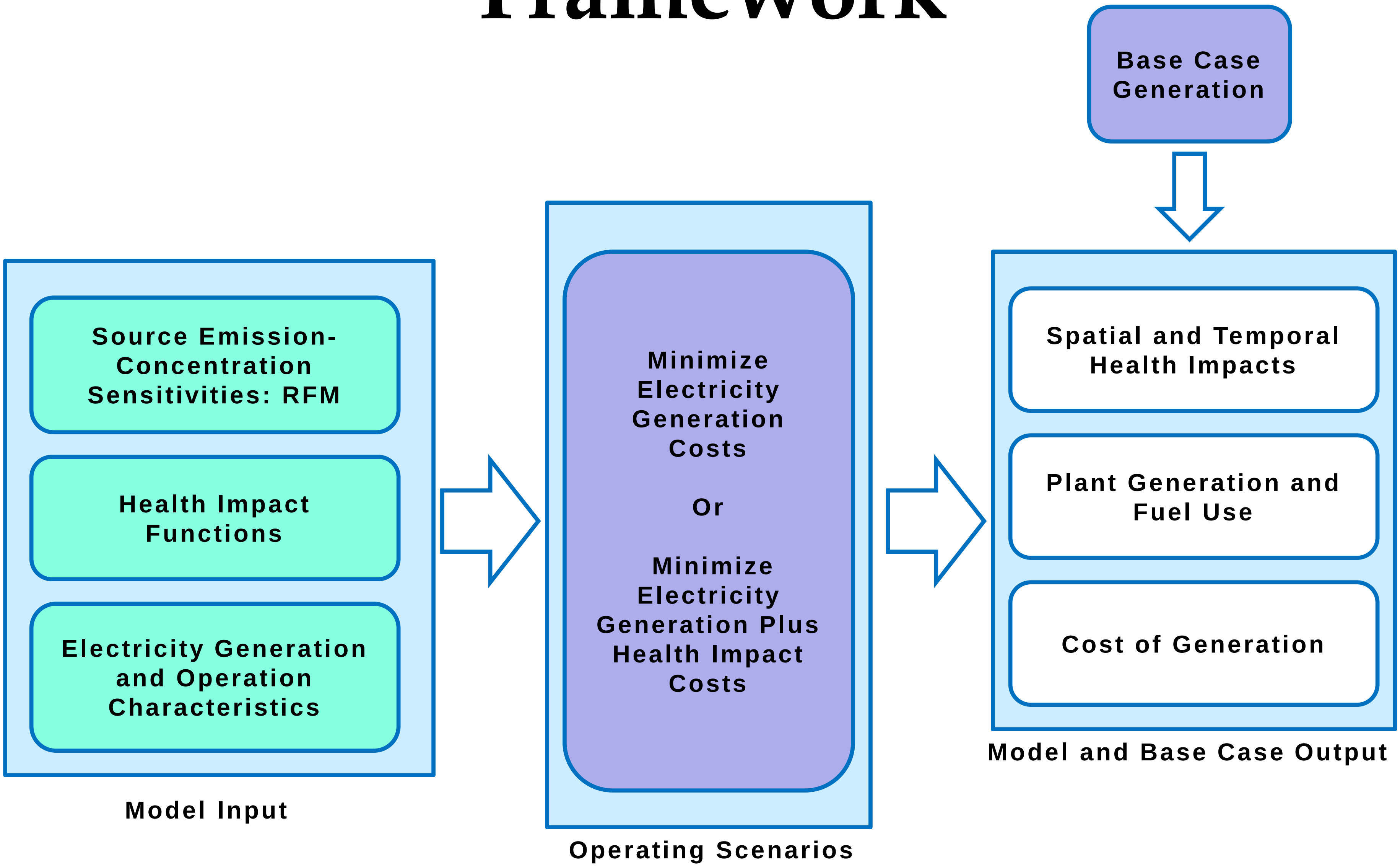


Dec. 8-14, 2013	Obs (ug/m3)	Sim (ug/m3)	NFE	NFB
Original	4.64	10.04	86%	85%
Emis adjusted		5.62	54%	39%

Use of Forecast Source Impacts in Air Quality Management

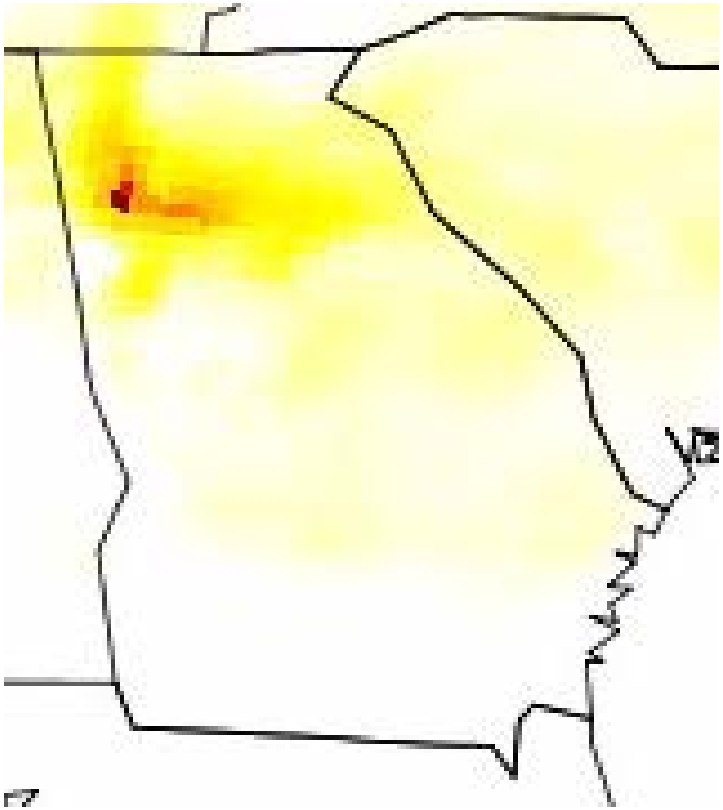
- Motivation
  - Electricity dispatch modeling conducted to optimize multiple objectives (e.g., cost minimization)
    - Typically does not include potential health impacts
      - Environmental justice
  - Source impacts on air quality & health highly variable
    - Fuel use, source location, time of day, …
- Goal
  - Link a reduced form air quality model (CMAQ-DDM/3D-RF) with a dispatch model to assess the potential of integrating forecast air quality impacts in decision making
    - Assess incorporating temporally finer scale relationships between emissions and air quality
    - Show how changes in unit emissions impact results

Framework

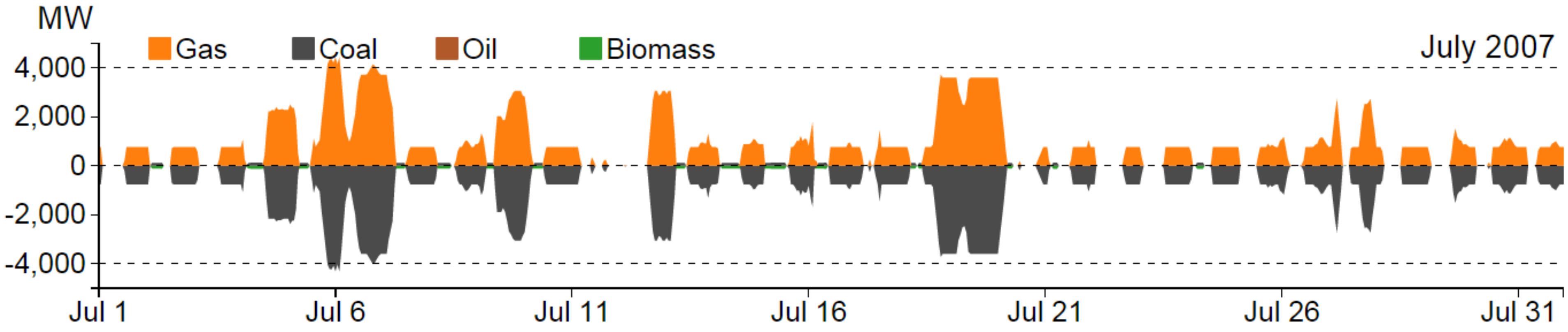

Base Case Generation
Source Emission-Concentration Sensitivities: RFM
Health Impact Functions
Electricity Generation and Operation Characteristics
Model Input
Minimize Electricity Generation Costs
Or
Minimize Electricity Generation Plus Health Impact Costs
Operating Scenarios
Spatial and Temporal Health Impacts
Plant Generation and Fuel Use
Cost of Generation
Model and Base Case Output

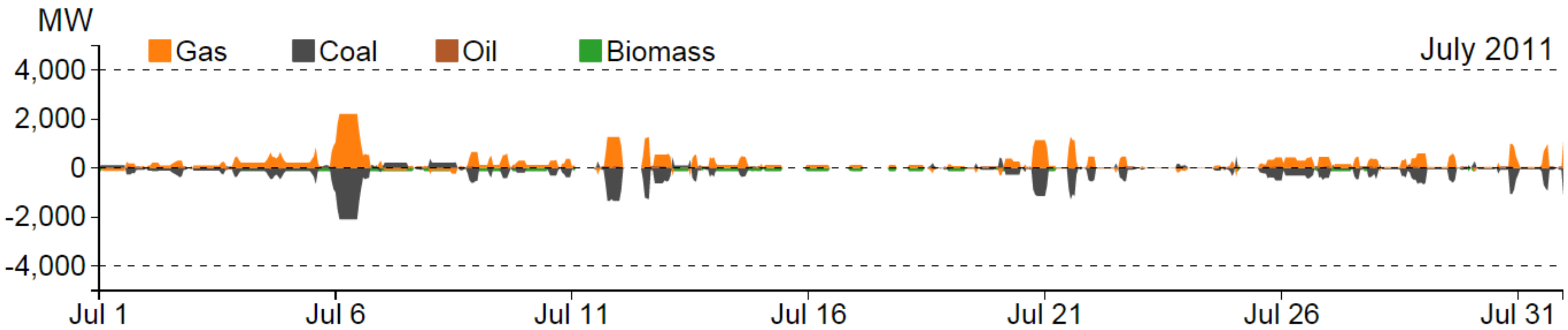
Power Plant Impact Simulation

- PM2.5 impact from Plant Bowen emissions



Shift in Fuel Use 2007 vs. 2011





Plant Bowen July 2007 $PM_{2.5}$ Optimization with/without Potential Exposure Changes

Demographic	$PM_{2.5}$ Scenario Without Health Impacts	$PM_{2.5}$ Scenario With Health Impacts	$PM_{2.5}$ Reduction	% Reduction
Total Population	0.201 μg/m^3	0.109 μg/m^3	0.092 μg/m^3	**45.9%**
Black	0.151 μg/m^3	0.082 μg/m^3	0.069 μg/m^3	**46.0%**
Hispanic / Latino	0.256 μg/m^3	0.129 μg/m^3	0.127 μg/m^3	**49.5%**
White	0.215 μg/m^3	0.119 μg/m^3	0.097 μg/m^3	**45.0%**

Summary

- PM and ozone forecasting system (Hi-Res2) operational with source impact forecasting and dynamic emission adjustments
  - Supports dynamic air quality management through providing source specific information
  - Currently for traffic, power plant and prescribed-burn (Talat's talk) emissions
  - Expansion to include other species measurements underway
  - Improved approach to assimilating AOD and PM measurements underway (Utilizing data-fused fields)
- Source-specific forecasting capability, combined with dispatch model, can provide additional pathways to reducing human exposure
  - Can be applied to other sources, other locations
- Source-specific impact analysis with data-driven adjustment also being used for advanced, hybrid source impact modeling
  - Hu et al., (2014), Ivey et al., (2015)
  - To be used in health studies

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- Georgia EPD
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- US Forest Service
  - **Scott Goodrick, Yongqiang Liu, Gary Achtemeier**
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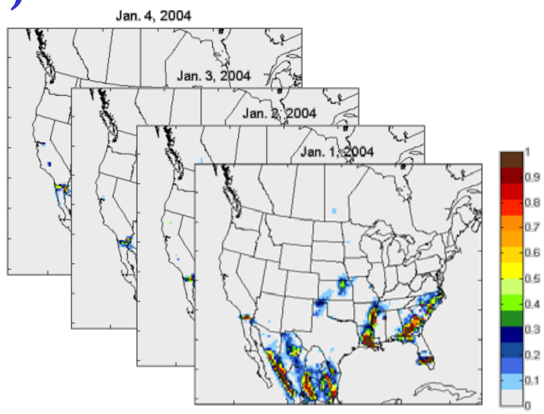
- Atlanta Regional Commission (ARC)
- GT Strategic Energy initiative

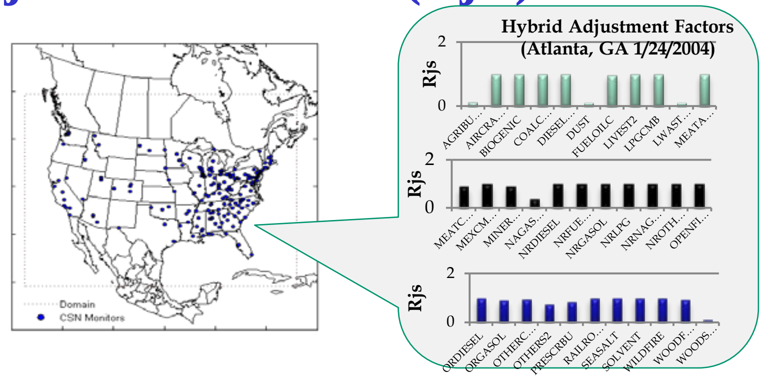
HYBRID SOURCE APPORTIONMENT

Spatial Hybrid Approach (Ivey et al, *GMDD,* 2015)

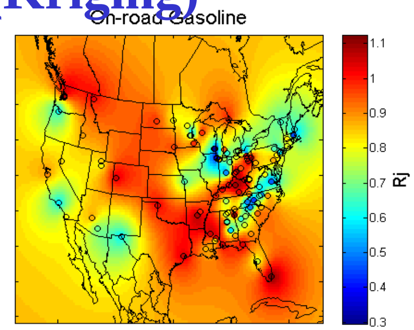
1. CMAQ-DDM Source Impacts (~30 sources, daily)



2. Hybrid Analysis at Monitors to find Adjustment Factors (Rj's)

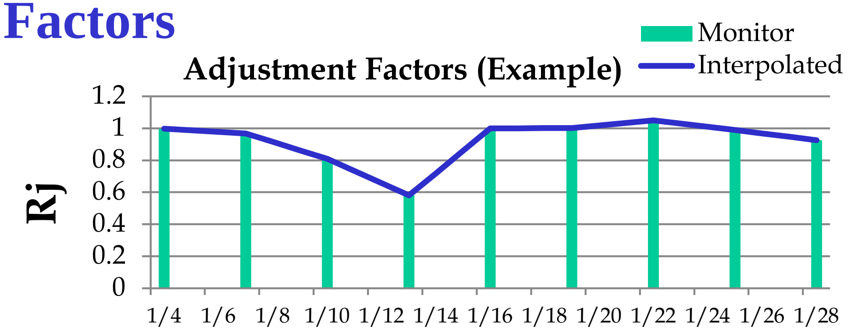


3. Spatial Interpolation of Adjustment Factors (Kriging)

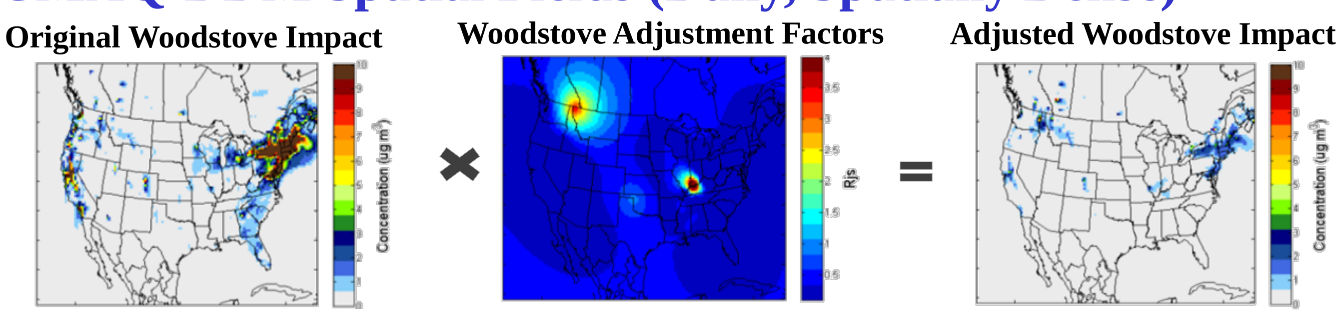


January 4, 2004

4. Temporal Interpolation of Adjustment Factors



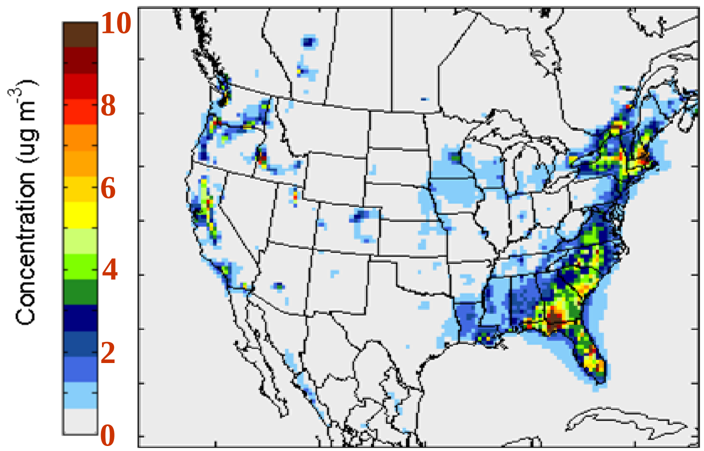
5. Adjust CMAQ-DDM Spatial Fields (Daily, Spatially Dense)



Biomass Impact: Before/After Assimilation of Observations

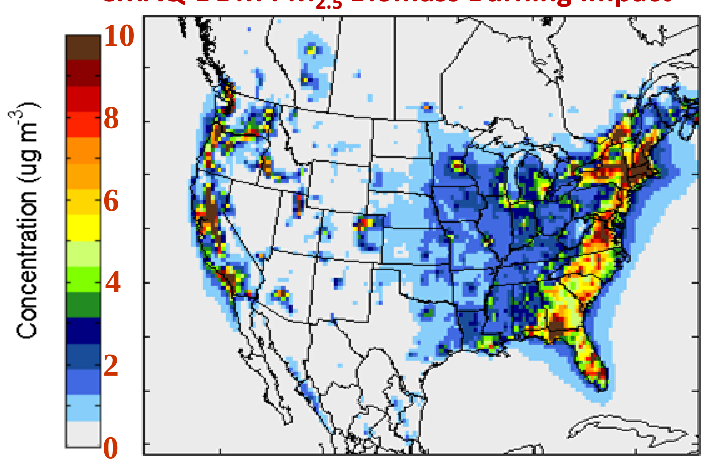
- Many sources are highly variable leading to significant differences between observations and simulations
  - Biomass
  - Dust
  - Agriculture
- Seasonal results in much better agreement

Adjusted $PM_{2.5}$ Biomass Burning Impact

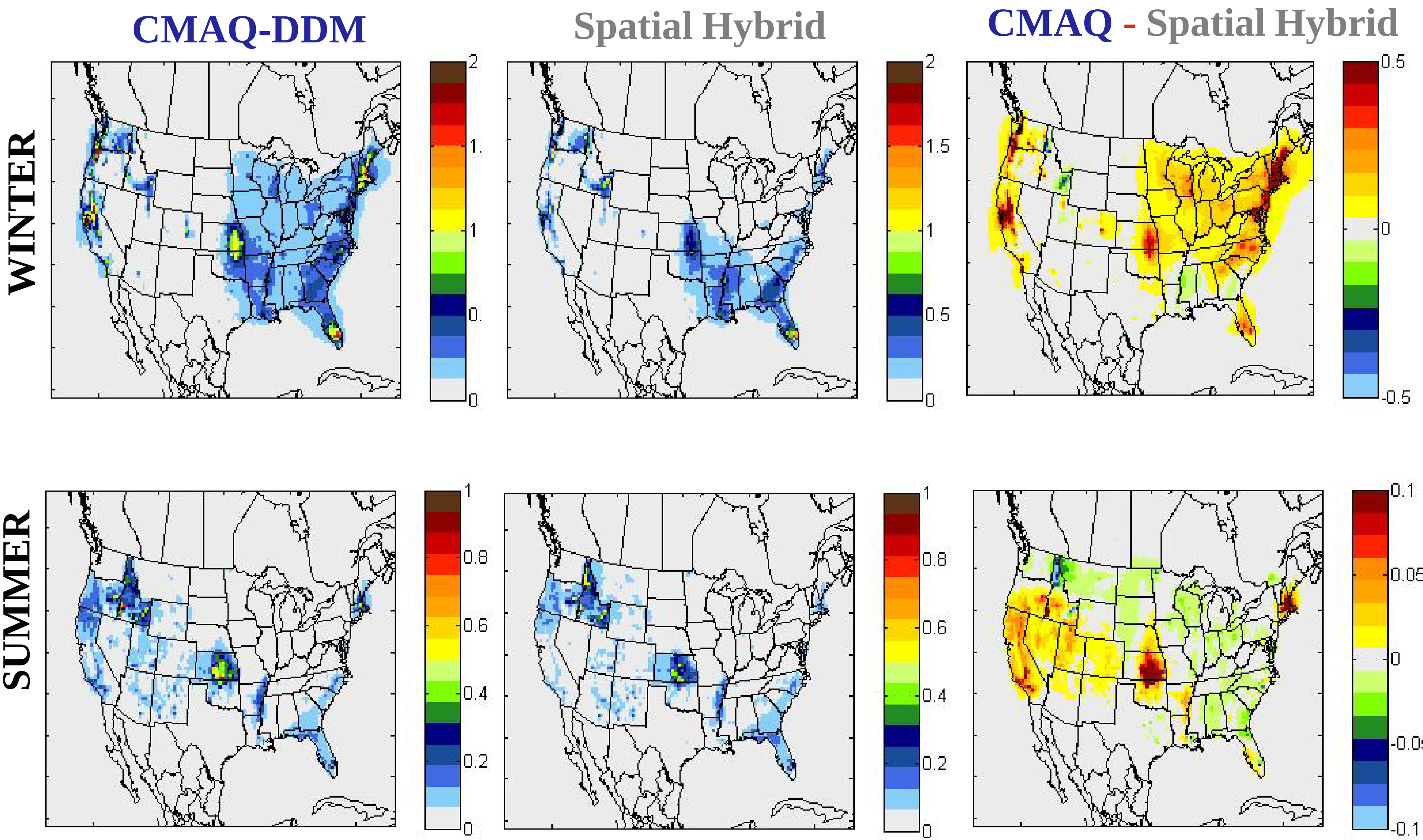


04/01/04

CMAQ-DDM $PM_{2.5}$ Biomass Burning Impact



2006 Seasonally-Averaged PM2.5 Impacts (ug/m3): Biomass Burning (2006)



IMPROVING ORGANIC AEROSOL SIMULATIONS

Updated isoprene OA Mechanism

- Comparison of CMAQ-simulated SOA from isoprene to observations from AMS factors led to updates
  - Assimilated PBL measurements
  - Improved IEPOX physics and chemistry:
    - Dry deposition resistance reduced
    - Updated reaction rate constants
    - Modified Henry's law for IEPOX