Chemical Data Assimilation and Air Quality Forecasting using CMAQ

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Introduction

- Assimilating real-time observations is essential in weather forecasting
- AIRNOW observations are available in near real time. It has potential to be applied operationally for air quality forecasting
- Optimal interpolation (OI) is simple to apply and computation overhead is minimal
- In data assimilation, background error covariance (B) is important
  - Determines the weighting between observations and a priori background
  - Determines the spread of the increment in space and between variables

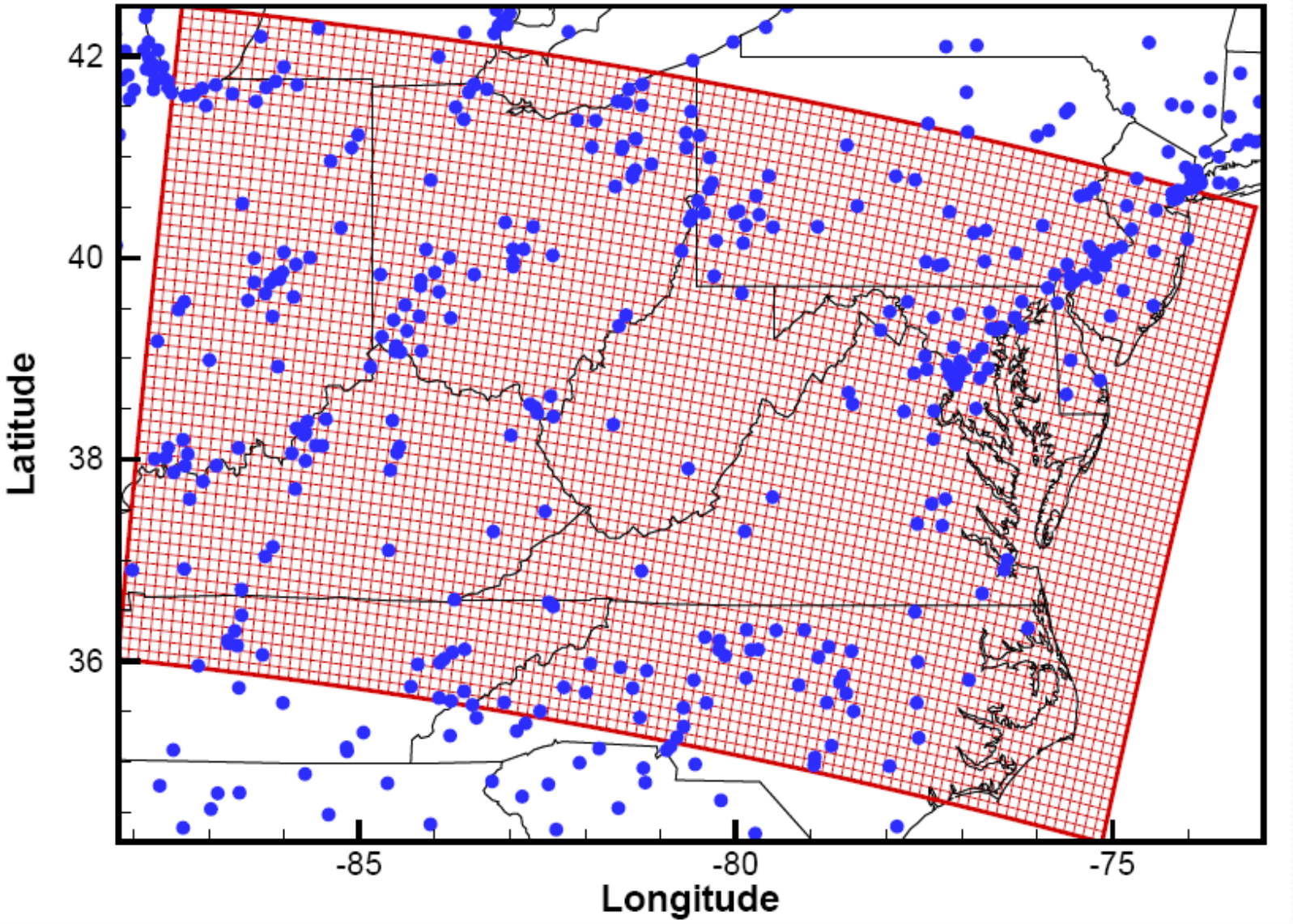
Optimal Interpolation (OI)

- OI is a sequential data assimilation method. At each time step, we solve an analysis problem

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

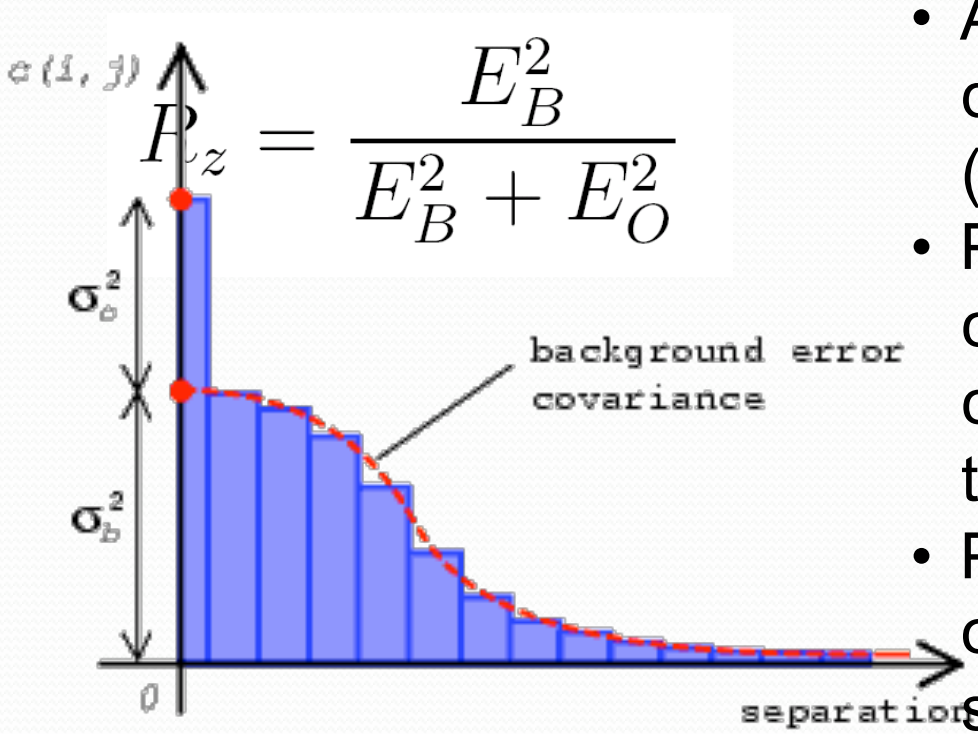
- We assume observations far away (beyond 1.5 background error correlation length scale) have no effect in the analysis
- In the current study, the analysis is solved in two steps: first in horizontal direction, then vertical

Domain, Grid (100x60), and AIRNOW Stations



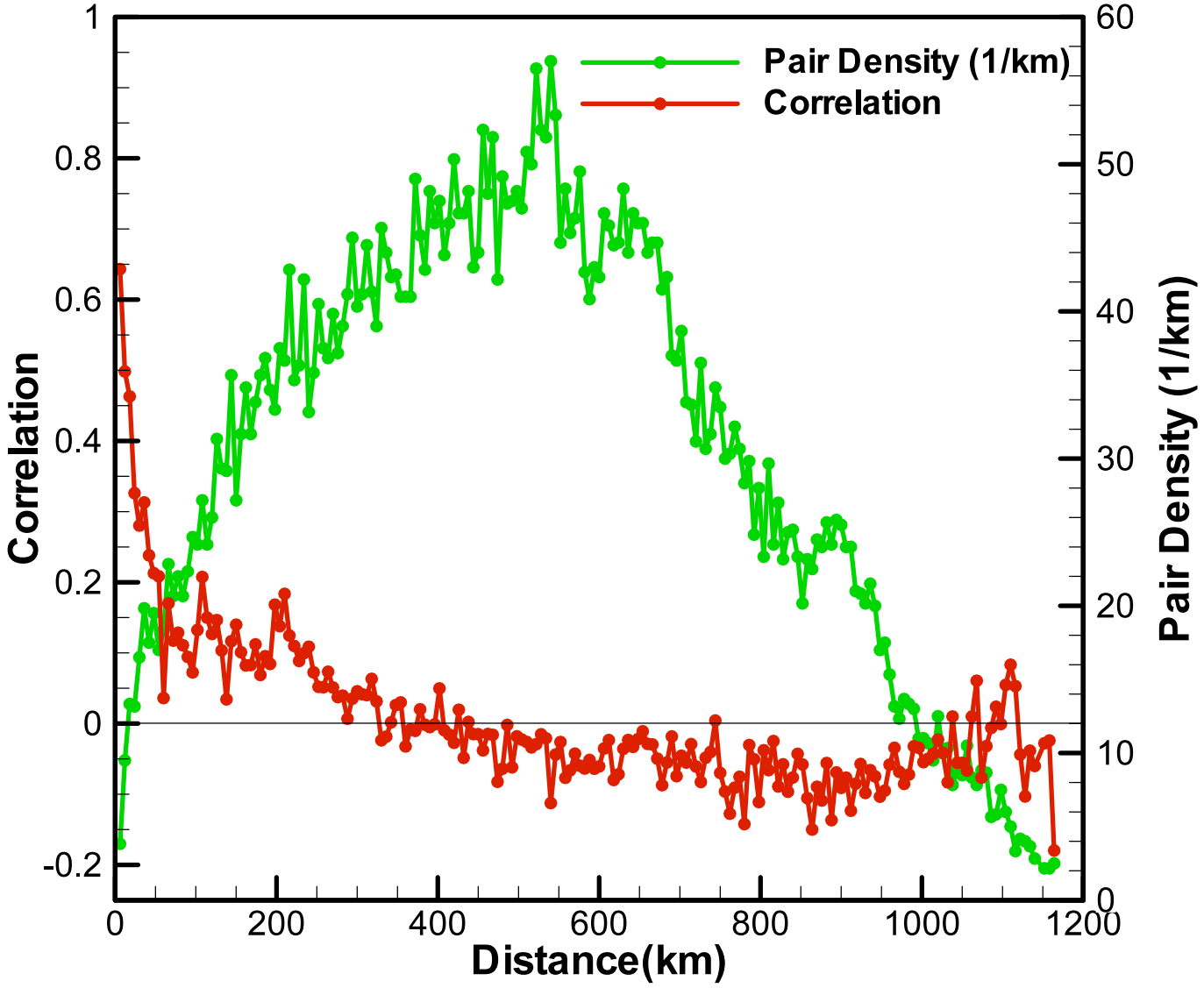
Estimate Model Error Statistics with Hollingsworth-Lönnberg Method

$$P_z = \frac{E_B^2}{E_B^2 + E_O^2}$$



- At each station, calculate differences between forecasts (B) and observations (O)
- Pair up AIRNOW stations, and calculate the correlation coefficients between the two time series at the paired stations
- Plot the correlation as a function of the distance between the two stations,

Horizontal Error Statistics



E_B ~

14.2 ppbv

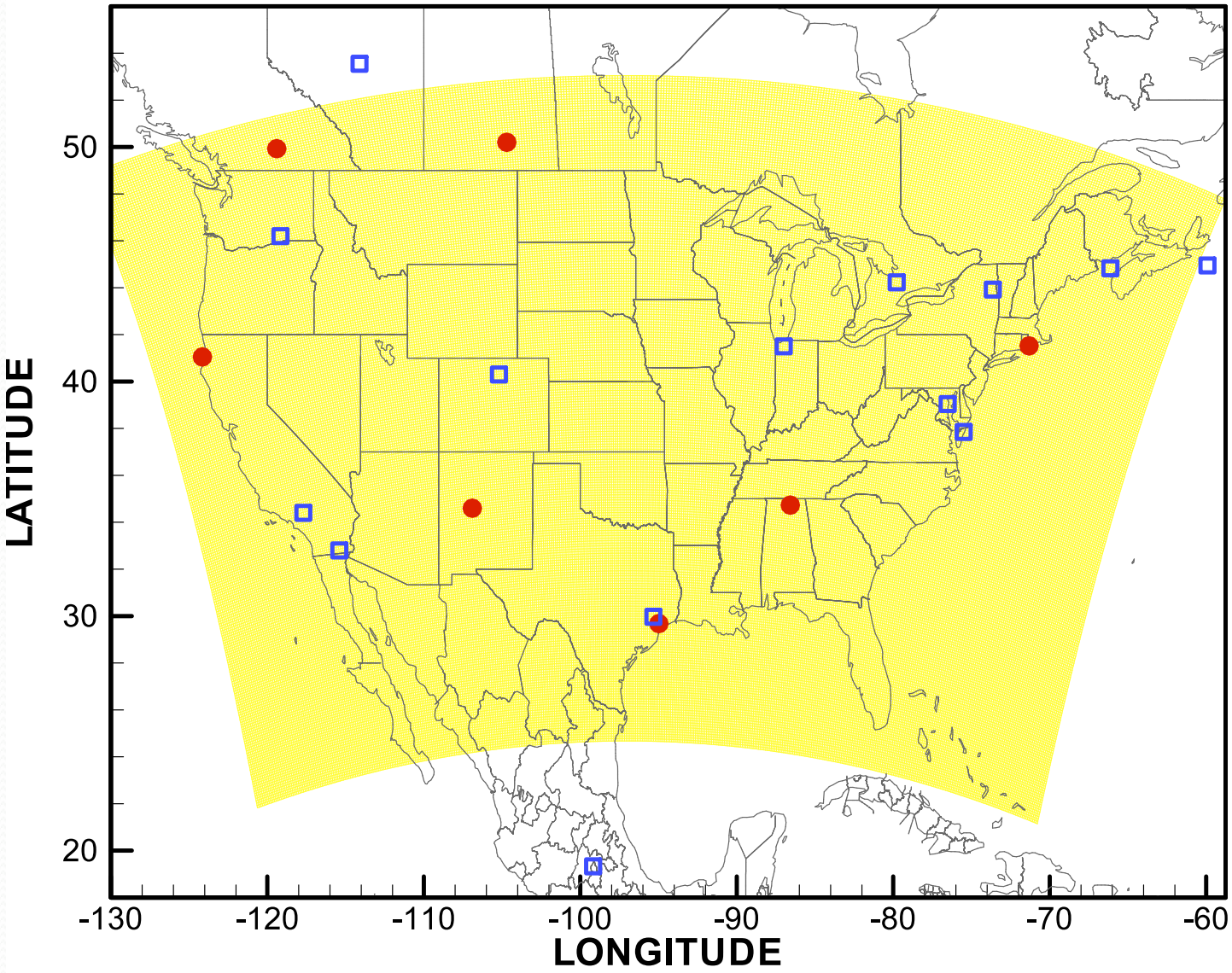
E_O ~

3.3 ppbv

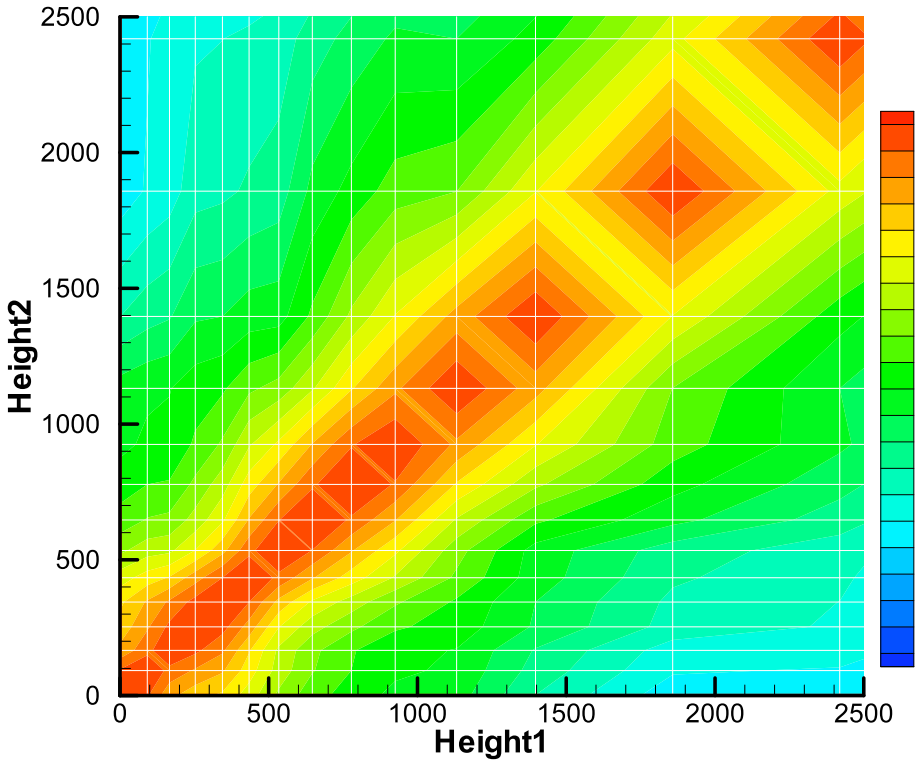
Correlation length:

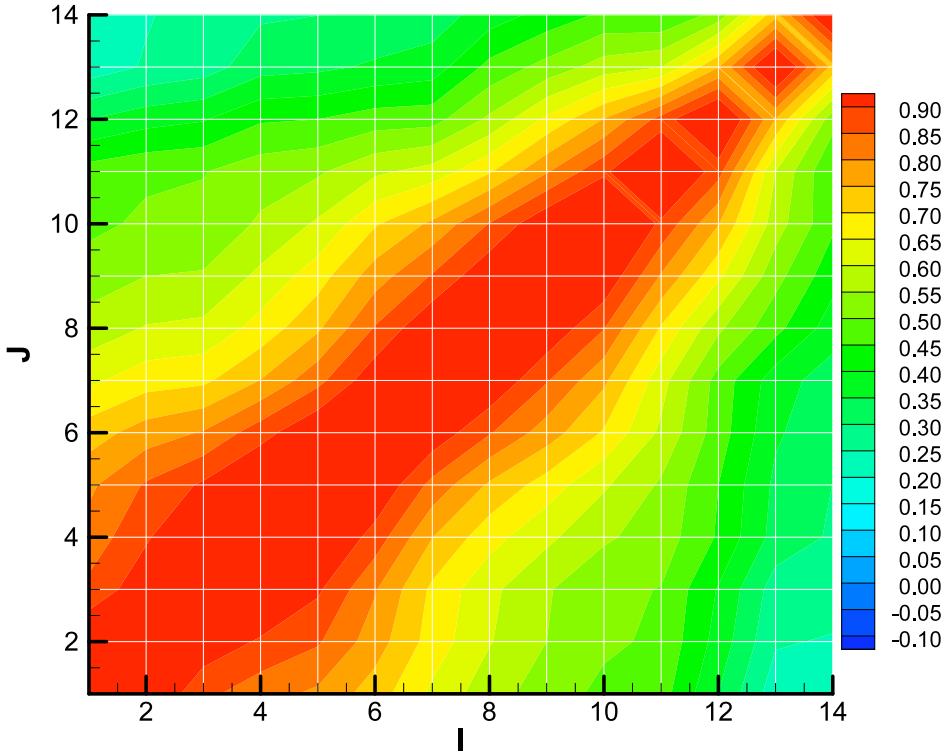
60 km

Ozonesonde: Vertical Error Statistics



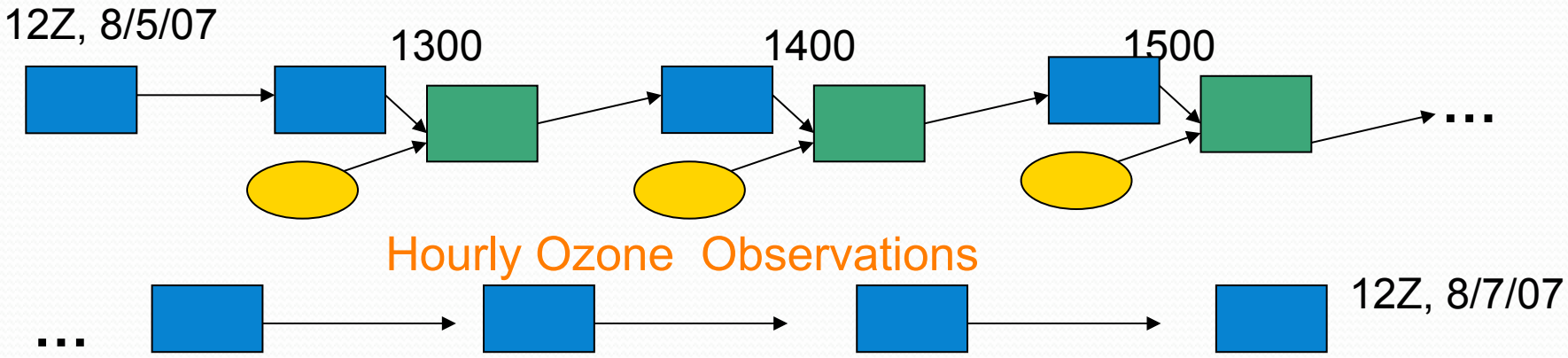
Vertical Correlation



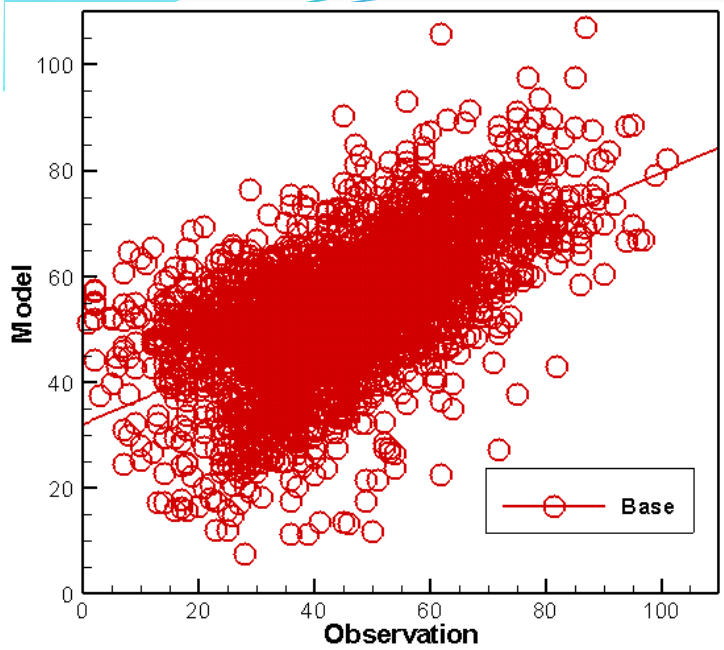


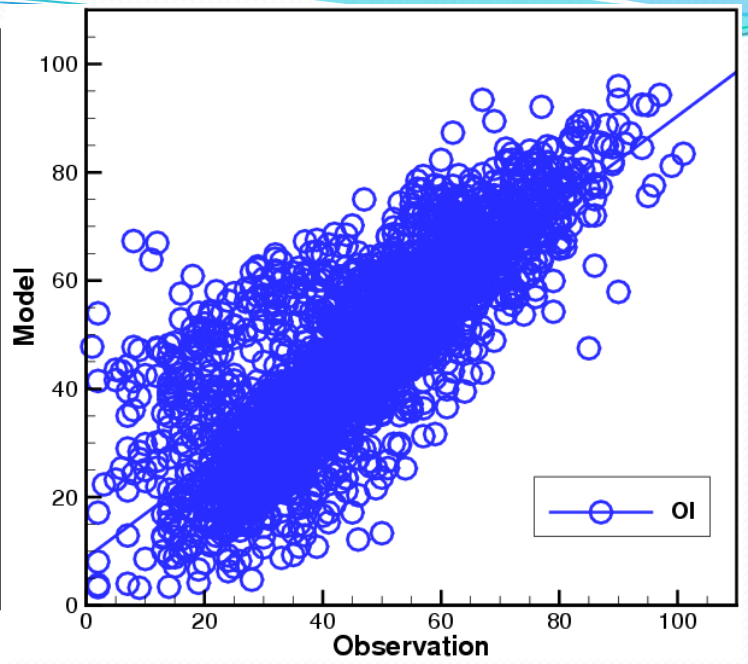
Setup of OI Assimilation Tests

- CMAQ 4.6, Model starts at 12Z, 8/5/07
- Hourly AIRNOW observations assimilated in first day
- Model continues to run another day without observations



Observation-Prediction (in ppbv)

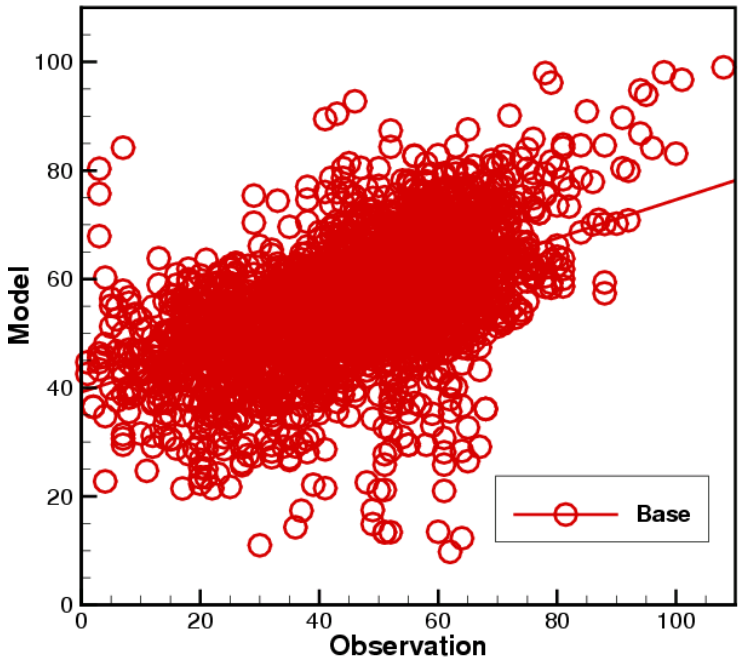


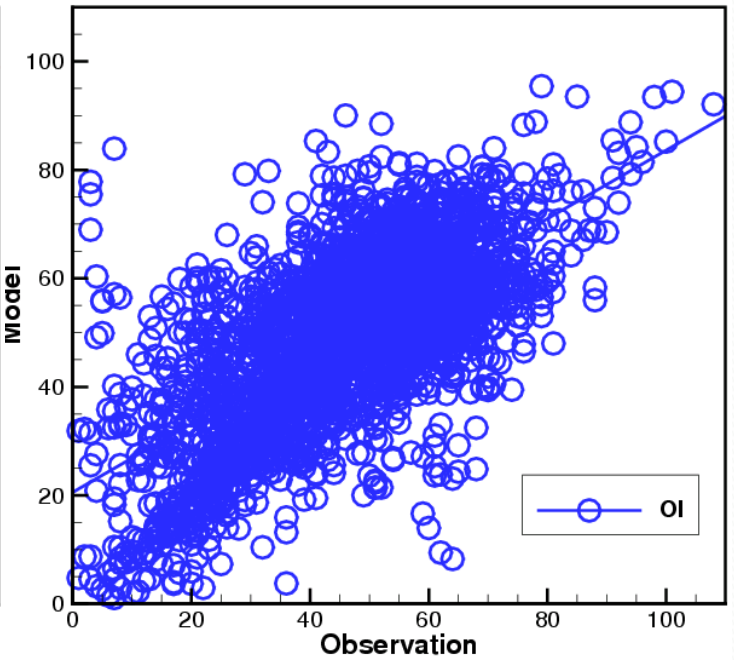


Day 1

R=0.59 R=0.81

1300 - 2400 Z



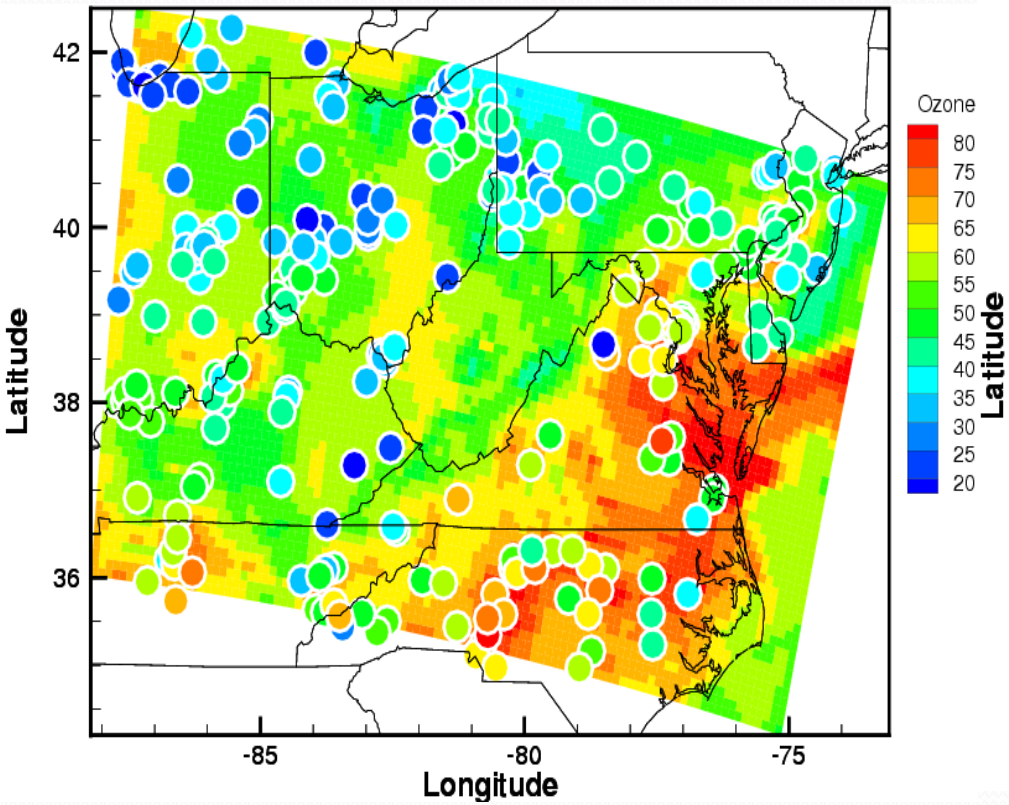


R=0.56 R=0.68

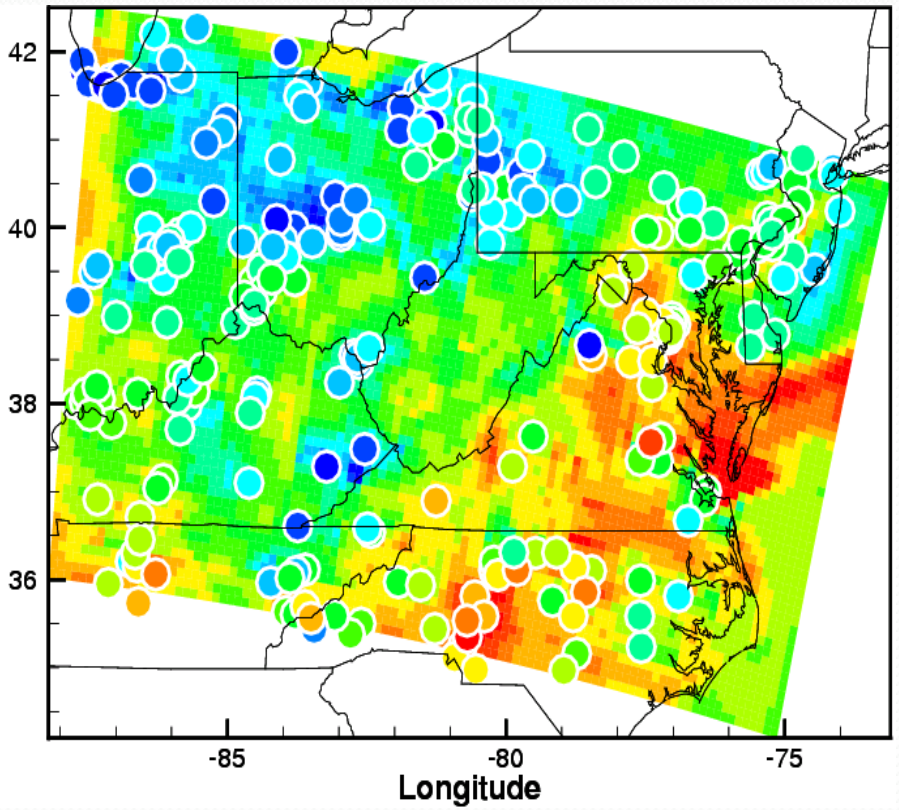
Day 2

Surface O_3 at 1800Z, 8/5/07

Base Case

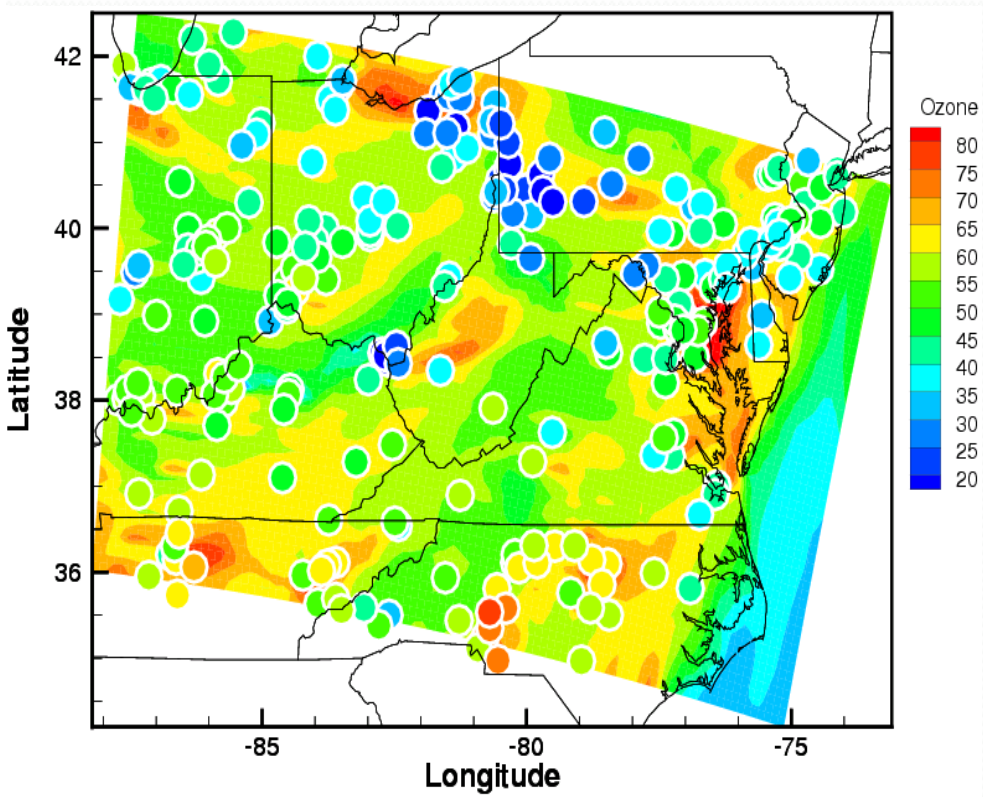


OI (Analysis)

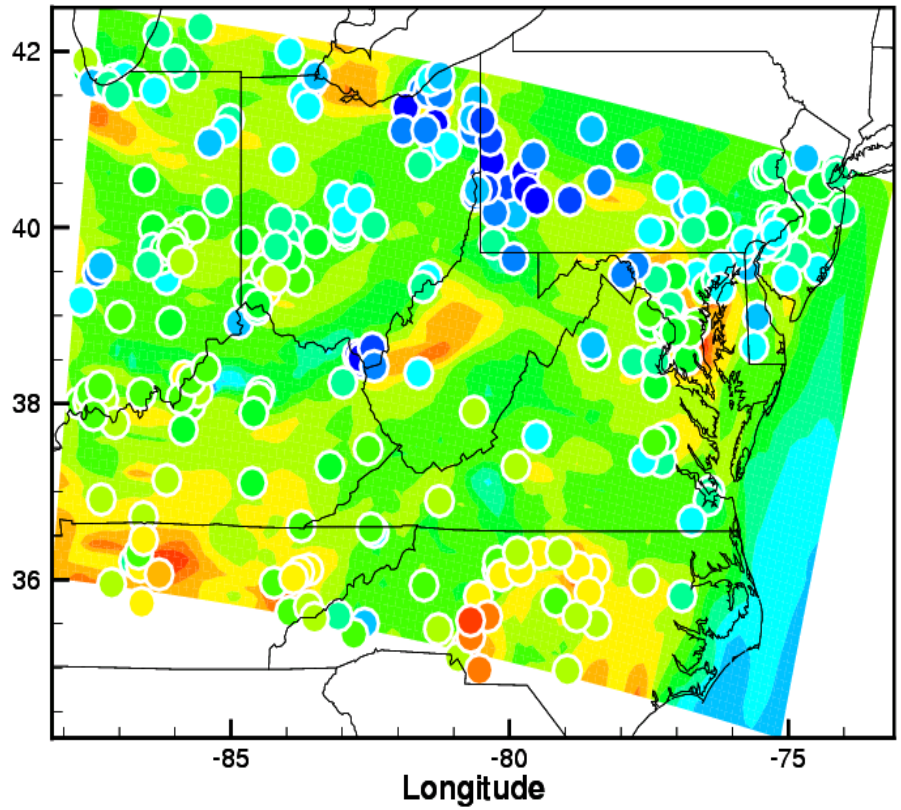


Surface O_3 at 1800Z, 8/6/07 (6 hours after OI)

Base Case



OI (Forecast)



4D-Var Data Assimilation

1. CMAQ 4.5 Adjoint was developed by A. Sandu *et al* (adjoint available for transport and chemistry)
2. Assimilation time window is reduced to 15 hours
3. Only initial O_3 are adjusted to minimize the cost functional (using L-BFGS-B routine)

$$J = \frac{1}{2}\left[c_0 - c_b\right]^T B^{-1}\left[c_0 - c_b\right] + \frac{1}{2}\left[y - h(c)\right]^T O^{-1}\left[y - h(c)\right]$$

4D-Var .vs. OI

	DA method	**B**	Bias (Day1)	RMS (Day1)	Bias (Day2)	RMS (Day2)
1	n/a	n/a	*8.3*	*15.9*	*8.7*	*16.3*
2	4D-Var	Diagonal	*-0.8*	*11.0*	*7.6*	*15.6*
3	OI	Diagonal	*2.6*	*12.7*	*7.5*	*15.8*
4	OI	H⊗V	*-1.3*	*13.2*	*3.1*	*12.8*
5	4D-Var	H⊗V	*?*	*?*	*?*	*?*

Biases and RMS errors are calculated at day time (8am-8pm LT) . Units : ppbv.

1. 4D-Var (V4.5) gives slightly better results than OI (V4.6)
2. "⊗" denotes Kronecker product and "TSVD" method is used for the inverse of B matrix (Chai, *et al* , Four dimensional data assimilation experiments with ICARTT ozone measurements, JGR, 2007)

Summary

- CMAQ model error statistics has been estimated using Hollingsworth-Lönnberg method in both horizontal and vertical directions
- Assimilating AIRNOW observations into CMAQ model using Optimal Interpolation proves to be beneficial for the next-day ozone forecasting
- A 4D-Var data assimilation test shows slightly better results than OI with same diagonal B
- Model error covariance results are utilized to assimilate AIRNOW observations with OI approach (B=H[illegible]V, implemented using TSVD method), it shows significant improvement over OI with diagonal B