Improved Forecasting of Next Day Ozone Concentrations in the Eastern U.S.

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Modeling Goals

- For U.S. EPA AIRNow real-time operational system, provide a forecast spatial map of next day daily 8-hr maximum O_3 concentrations
  - Using gridded numerical model output and point air monitoring data
- Map needed soon after last hourly O_3 measurement of previous day (i.e. 11pm)
- What we have done:
  - Using a small test data set (Aug 2-14, 2005), have developed several forecast maps and validation statistics
  - Evaluated several models based on comparative fits
  - Results appear to be encouraging

Modeling Overview

- Bayesian space-time model uses point monitoring data and gridded eta-CMAQ forecast data in a regression structure avoiding:
  - avoids change of support problem of some fusion approaches; does not require integration of the observed point level monitoring process to the grid level one
  - avoids modeling ALL eta-CMAQ data and overwhelming information in monitoring data;
- Solve ‘change of support’ problem by inferring on spatial process at a point level given information at both the areal and point level

Ozone (O_3) Pollution

- Ground level O_3: adverse health effects, can cause respiratory problems
- O_3 is a secondary pollutant
- Sunlight + VOC + $NO_x \rightarrow O_3$
- Interested in daily 8-hr maximum O_3 levels:
  - Maximum of averages formed by 8 successive hourly O_3 levels in a day

Sources of Spatial Data

O_3 Monitoring Data:

- Hourly data from 390 real-time monitoring sites in the eastern U.S.
  - Calculate maximum of all 8-hr avg's within a day
- Use data from 350 sites for modeling (estimation and forecasting)
- Set aside data from 40 sites for validation
- Test data for 15 days, August 2-14, 2005
- Some missing data

Eta CMAQ Hourly O_3 Forecast Output:

- High resolution 12 km gridded output over the eastern U.S. (~10,000 grid cells)
  - Calculate daily 8-hr maximum
- Includes next day forecast

Use of Data in Model

- Model the daily 8-hr maximum data for a running window of 7 consecutive days during the two weeks

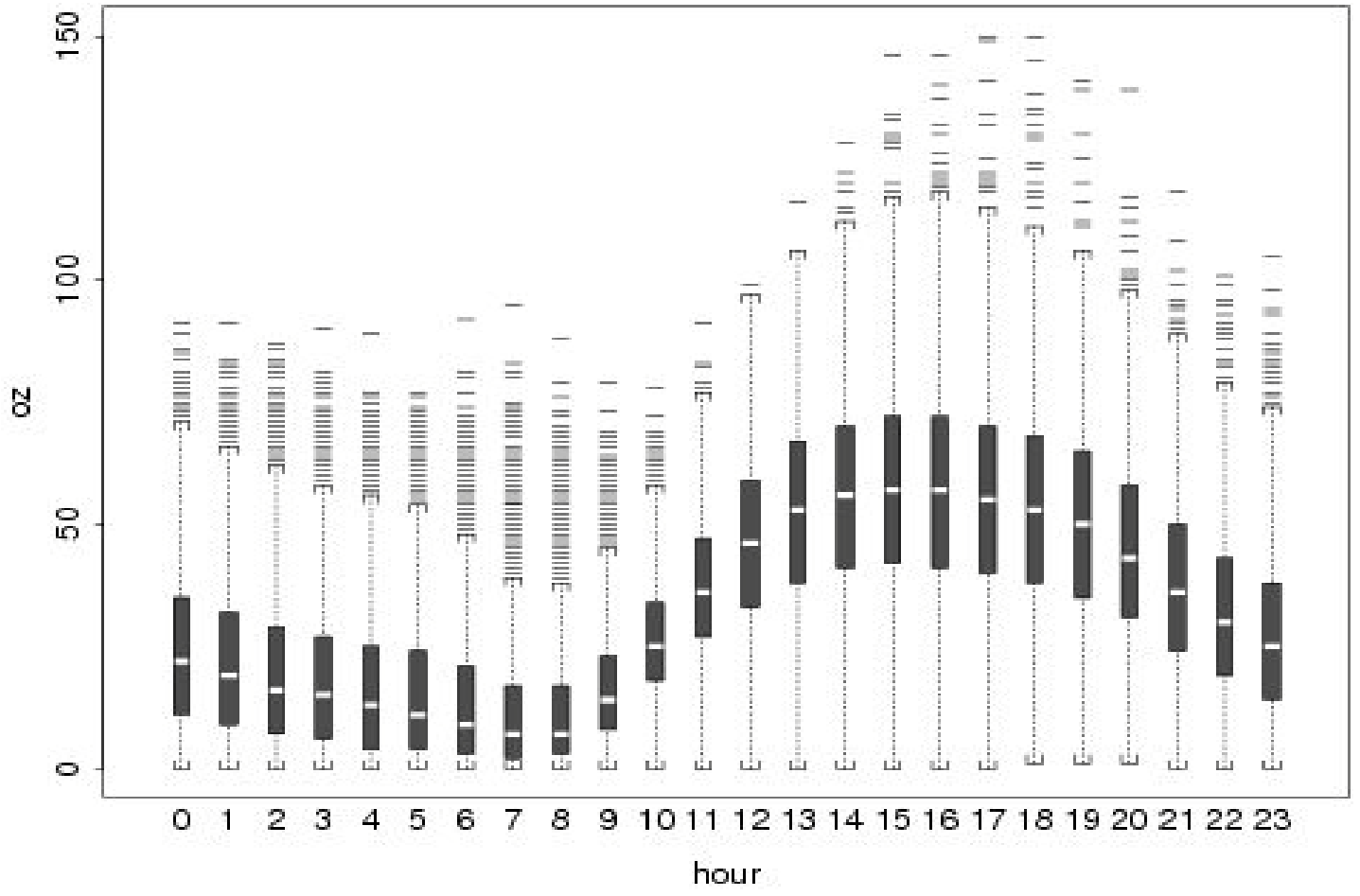
  - weekly cycle arbitrarily chosen, could include more distant data, but initial modeling results show no improvement in forecasts

- Forecast next days spatial pattern of maximum 8-hr average concentrations

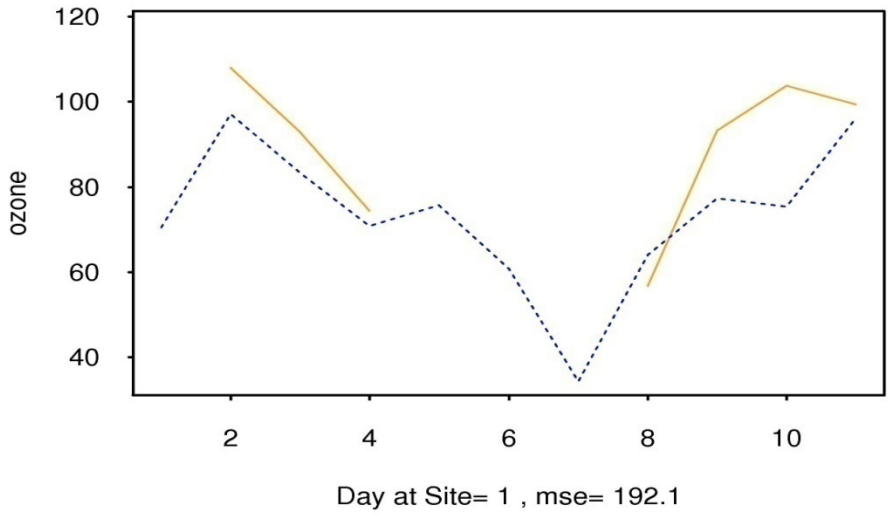
- For each monitoring site, we find the nearest eta CMAQ grid cell centroid to use as a covariate

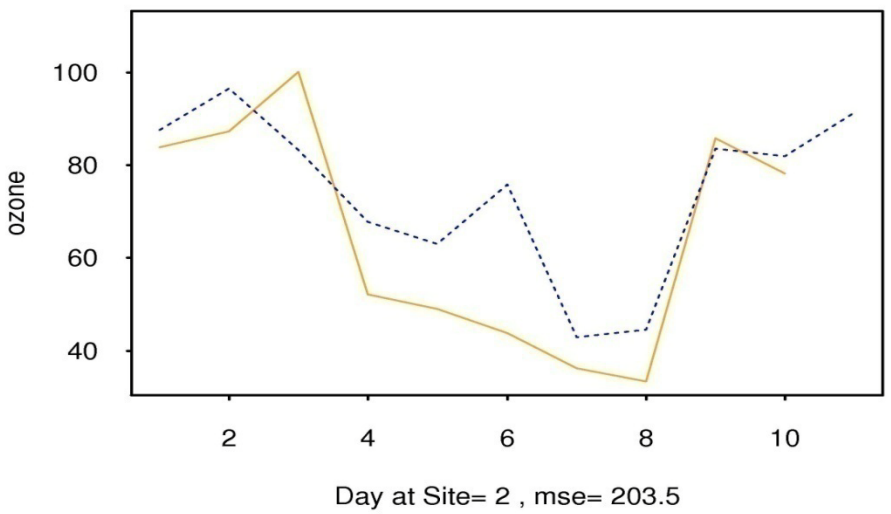
- Finally, randomly sample 3000 CMAQ grid locations to use as a predictive grid; just illustrative for now

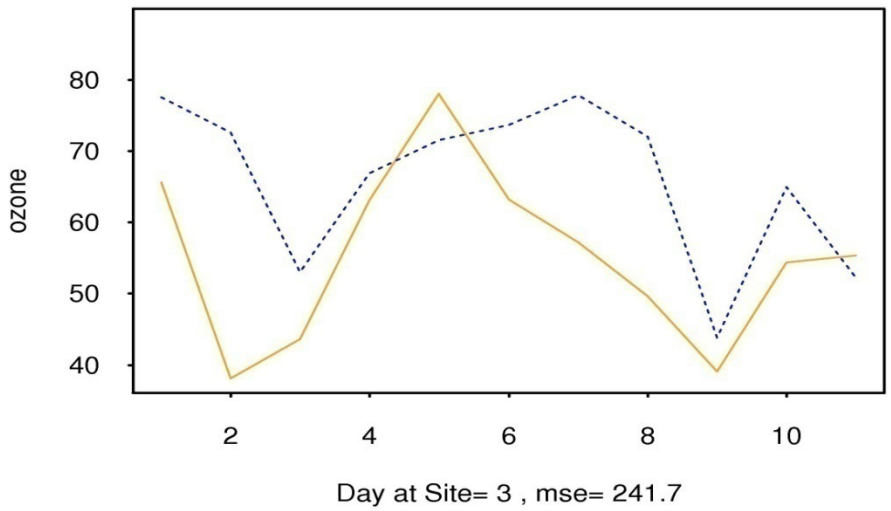
Diurnal Pattern

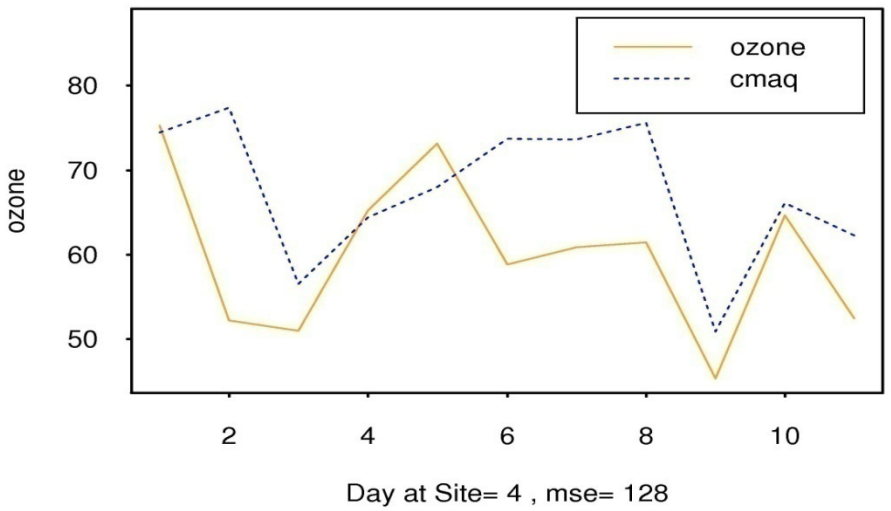


Observed O_3 (tan) vs. Eta-CMAQ O_3 (blue)

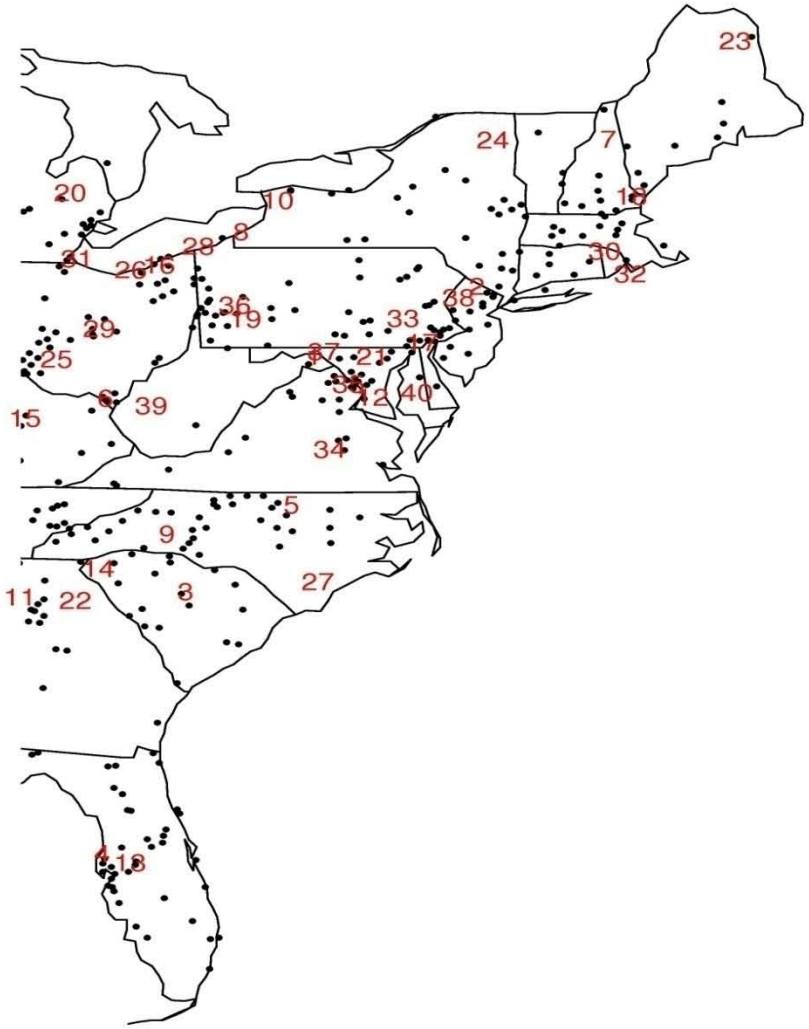


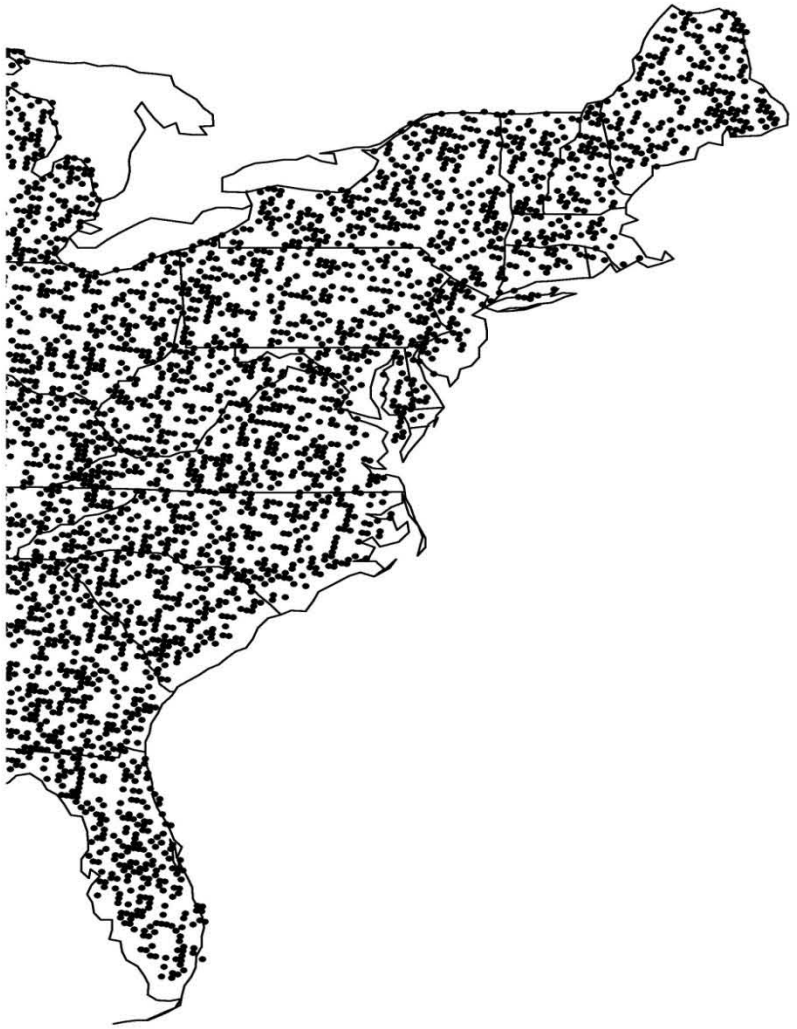






Locations of Model Fitting and Validation sites (left), Predictive grid (right)





Modeling Details

- Model developed here is motivated by Sahu, Gelfand, and Holland (2007), J. American Stat. Assoc., 107, 1221-34.

Square-Root O_3:

- Observed = $Z(\mathbf{s},t)$ at location **s** and time *t*.
- Develop model for n sites denoted by $\mathbf{s}_1,\ldots,\mathbf{s}_n$ for a running window of *t*=1,…,T=7 days
- True square-root O_3 = $O(\mathbf{s},t)$.

Measurement Error Model: Data represent true concentration plus random measurement error

$$Z(\mathbf{s},t) = O(\mathbf{s},t) + \varepsilon(\mathbf{s},t)$$

$$\varepsilon(\mathbf{s},t) \sim N(0,\sigma_\varepsilon^2).$$

for $i = 1,\ldots n;\ \ t = 1,\ldots,T$

$\varepsilon_l(\mathbf{s},t)$ is a white noise process capturing the 'nugget' effect with variance σ_ε^2.

Forecast Model

$$O(\mathbf{s}_i,t) = \xi + \rho O(\mathbf{s}_i,t-1) + \left(\beta_0 + \beta(\mathbf{s}_i^*)\right) x(\mathbf{s}_i^*,t) + \eta(\mathbf{s}_i,t)$$

- ξ is a constant mean across space and time
- $\rho O(\mathbf{s}_i, t\text{-}1)$ is autoregressive ($0 < \rho < 1$)
- $\left(\beta_0 + \beta(\mathbf{s}_i^*)\right)\mathrm{x}(\mathbf{s}_i^*,t)$ spatially varying regression term using Eta-CMAQ as a covariate; $\mathbf{s}_i^*$ denotes CMAQ grid cell containing $\mathbf{s_i}$
  - $\beta \sim N(\mathbf{0}, \Sigma_\beta)$, where $\Sigma_\beta(i,j) = \sigma_\beta^2 \rho_\beta(\mathbf{s}_i - \mathbf{s}_j; \phi_\beta)$
- $\eta(\mathbf{s}_i,t)$ is a spatially correlated, but independent in time error term.
  - $\eta \sim N(\mathbf{0}, \Sigma_\eta)$, where $\Sigma_\eta(i,j) = \sigma_\eta^2 \rho_\eta(\mathbf{s}_i - \mathbf{s}_j; \phi_\eta)$
- Use cross-validation method to decide on including $\beta(\mathbf{s}_i^*)$

Inference Using the Posterior

Using vector notation, e.g. $\mathbf{O}_t = (O(\mathbf{s}_1,t),...,O(\mathbf{s}_n,t))'$

Let $\vartheta_t = \xi\mathbf{1} + \rho\mathbf{O}_{t-1} + \beta_0\mathbf{x}_t + \mathrm{X}_t\boldsymbol{\beta}$ for t=1,…,T, $\boldsymbol{\theta} = \{\beta_0, \boldsymbol{\beta}, \rho, \sigma_\varepsilon^2, \sigma_\eta^2, \sigma_\beta^2, \xi\}$

w denote all unknowns: $\mathbf{O}_t$, missing data $z^*(\mathbf{s}_i,t)$, and non-missing data $z(\mathbf{s}_i,t)$

Then, the log of the posterior distribution, $\log\pi(\boldsymbol{\theta},\mathbf{w}\,|\,\mathbf{z})$, is

$$-\frac{nT}{2}\log(\sigma_\varepsilon^2) - \frac{1}{2\sigma_\varepsilon^2}\sum_{t=1}^{T}(\mathbf{Z}_t - \mathbf{O}_t)'(\mathbf{Z}_t - \mathbf{O}_t) - \frac{nT}{2}\log(\sigma_\beta^2)$$

$$-\frac{1}{2\sigma_\eta^2}\sum_{t=1}^{T}(\mathbf{O}_t - \vartheta_t)'S_\eta^{-1}(\mathbf{O}_t - \vartheta_t) - \frac{nT}{2}\mathrm{lo}\ (\sigma_\beta^2) - \frac{1}{2\sigma_\beta^2}\boldsymbol{\beta}'S_\beta^{-1}\boldsymbol{\beta} + \log(\pi(\boldsymbol{\theta}))$$

ξ, β_0 are independently $N(0,10^4)$, $\rho \sim \mathrm{N}(0,10^4)\mathrm{I}(0<\rho<1)$

$1/\sigma_\varepsilon^2, 1/\sigma_\eta^2, 1/\sigma_\beta^2$ are independently $G(2,1)$ to have a proper prior

Prediction Details

- First predict at any new locations in $t = 1, \ldots, T$
- From measurement error model:

$$Z(\boldsymbol{s}',t) \sim N\left(O(\boldsymbol{s}',\mathrm{t}),\sigma_{\varepsilon}^{2}\right)$$

  - $O(\mathbf{s}',t+1?)$ can only be sequentially determined using previous $O(\mathbf{s}',t)$ up to time t.

- Posterior predictive distribution of $Z(\mathbf{s}',t)$ is obtained by Integrating over all unknown quantities:

$$\pi\left(Z(\mathbf{s}',t)\,|\,\mathbf{z}\right) = \int \pi\left(Z(\mathbf{s}',t)\,|\,O(\mathbf{s}',[t],\sigma_{\varepsilon}^{2}\right)\pi\left(O(\mathbf{s}',[t]\,|\,\beta(\mathbf{s}'),\boldsymbol{\theta},\mathbf{w}\right)$$

$$\times\pi\left(\beta(\mathbf{s}')\,|\,\boldsymbol{\theta}\right)\,dO(\mathbf{s}',[t])\,d\beta(\mathbf{s}')\,d\boldsymbol{\theta}\,d\mathbf{w}$$

Prediction (cont.)

- MCMC methods are used to sample the posterior
- Draws from the posterior distribution $\pi(\boldsymbol{\theta} \mid \mathbf{z}, \mathbf{w})$ and the conditional distribution $\pi(\beta(\mathbf{s}') \mid \boldsymbol{\theta})$ facilitate evaluating the integral in the joint posterior

- In summary, we implement the following algorithm to predict $Z(\mathbf{s}', t), t = 1, ..., T.$

1. Draw a sample $\boldsymbol{\theta}^{(j)}, \mathbf{w}^{(j)}$, $j \geq 1$ from the posterior
2. Draw $\beta^{(j)}(\mathbf{s}')$ using $\beta(\boldsymbol{s}' \mid \boldsymbol{\theta})$
3. Draw $\mathbf{O}^{(j)}(\mathbf{s}', [t])$ sequentially using $\mathbf{O}(\mathbf{s}', t) \mid \beta(\mathbf{s}'), \mathbf{O}_t, \boldsymbol{\theta}, \mathbf{w}$

   - Note that the initial value $O^{(j)}(\mathbf{s}', 0)$ is a constant for all $\mathbf{s}'$

Prediction (cont.)

4. Finally draw $Z^{(j)}(\mathbf{s}',t)$ from $N\left(O^{(j)}(\mathbf{s}',t),\sigma_{\varepsilon}^{2(j)}\right)$

Median is used as a summary measure to preserve 1:1 relationship between O, Z and O^2, Z^2.

Analysis/Results

- Under weak prior assumptions, cannot estimate all covariance parameters, $\sigma_\varepsilon^2, \sigma_\eta^2, \sigma_\beta^2, \phi_\eta, \phi_\beta$, consistently:
  - hence, we use set-aside data to select decay parameters ϕ_η, ϕ_β
  - use a 2-dimensional grid of reasonable ϕ_η, ϕ_β values to optimize MSE
- Only a few $\beta(\mathbf{s}_i)$ were significant:
  - Based on Bayesian model selection criterion of Gelfand and Ghosh (1998), we decided to exclude this term
  - any sort of local lack-of-fit may be compensated by $\eta(\mathbf{s}_i, t)$
- Does not mean that eta-CMAQ has no spatial-temporal bias; if *goal is to estimate bias*, consider eliminating $\rho O(\mathbf{s}_i, t-1)$ from model

Mean-square errors

Validation Days	Eta CMAQ	$\beta(\mathbf{s})\neq 0$	$\beta(\mathbf{s})=0$
Aug 2-9	229.6	84.4	50.5
Aug 3-10	246.4	58	50
Aug 4-11	260.5	77.8	64.5
Aug 5-12	253.4	99.1	62.1
Aug 6-13	240.6	72.5	45.4

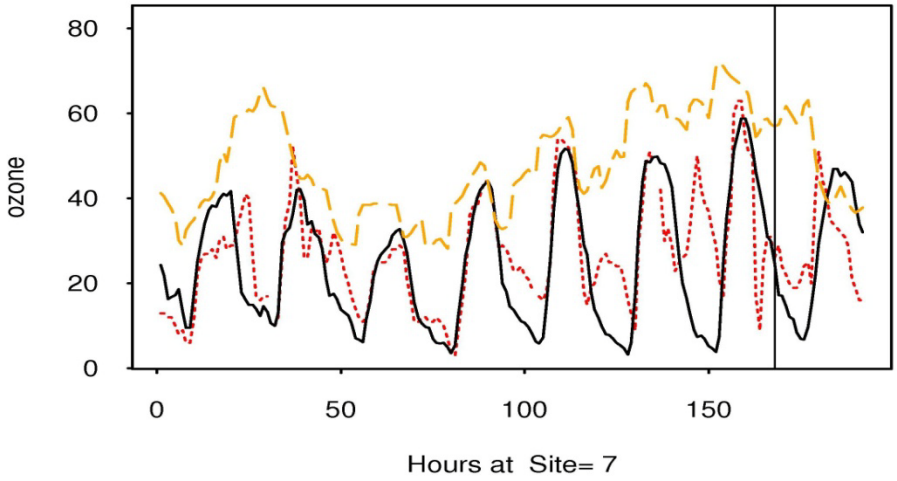
Hit and False Alarm Rates

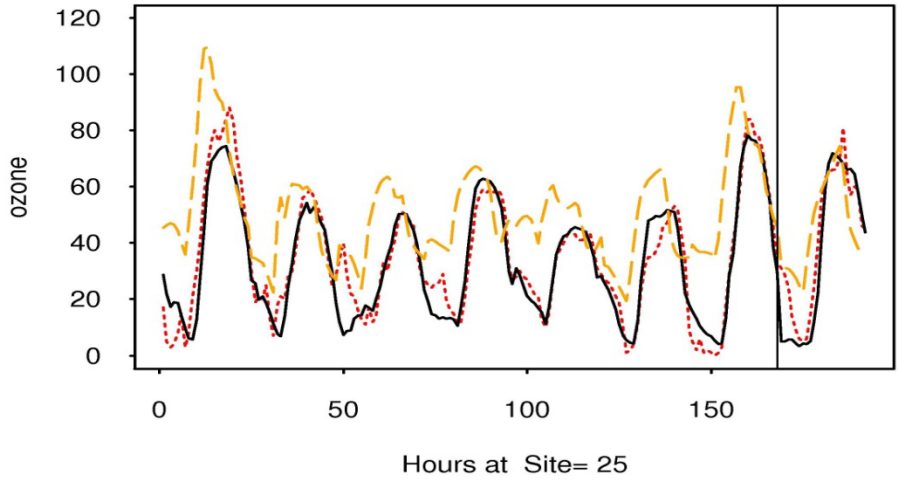
- Hit: defined as event where both the validation observation and forecast are either greater or less than 75 *ppb*
- False Alarm: observation is less than 75 *ppb*, but forecast is greater than 75 *ppb*

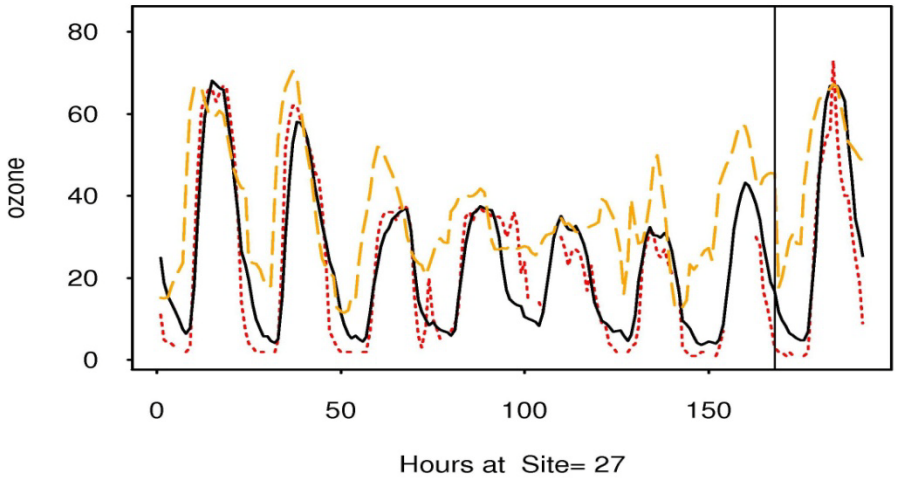
Hit and False Alarm percentages for O_3 exceeding 75 *ppb*

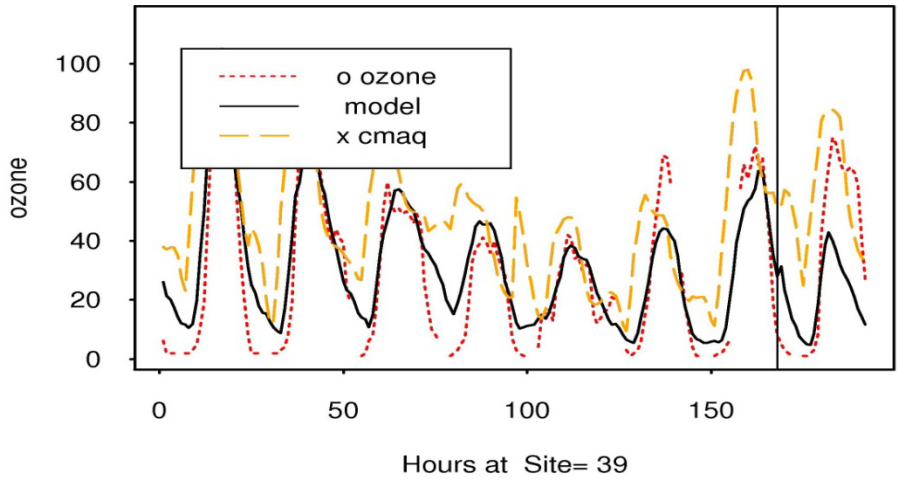
	Eta-CMAQ		Model: $\beta(\mathbf{s}) = 0$	
	Hit	False Alarm	Hit	False Alarm
Aug 2-9	81.7	17.1	90.9	4.9
Aug 3-10	79.6	19.4	92.7	3.7
Aug 4-11	78.9	20.0	93.9	2.6
Aug 5-12	80.7	18.8	93.4	1.5
Aug 6-13	79.9	19.6	93.0	2.5

Hourly Validation, Aug 11
obs data (red), Eta-CMAQ (tan), Forecast (black)









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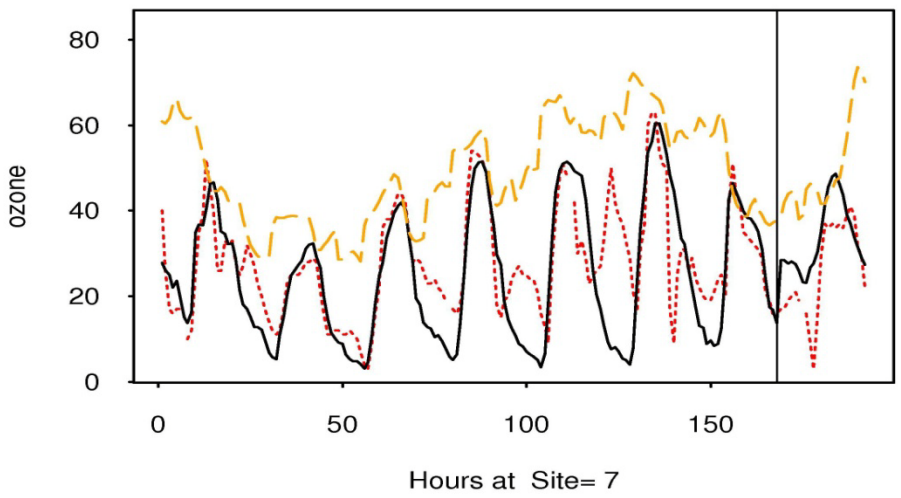
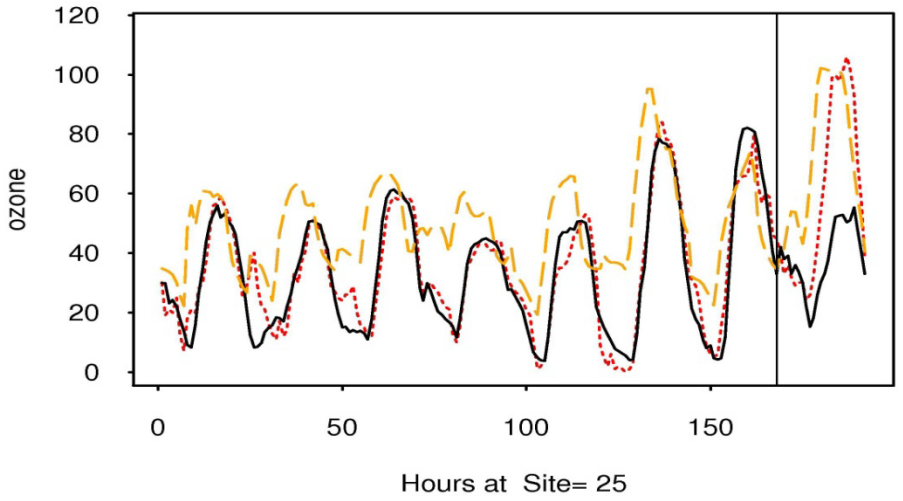
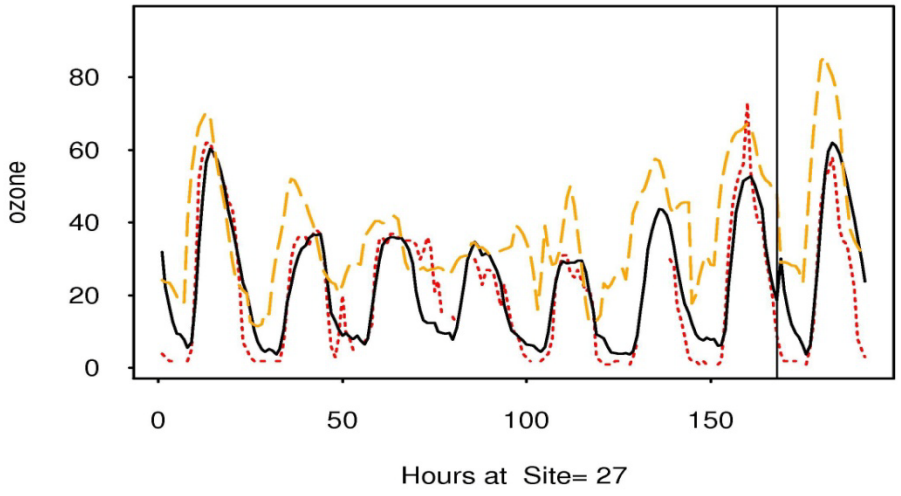
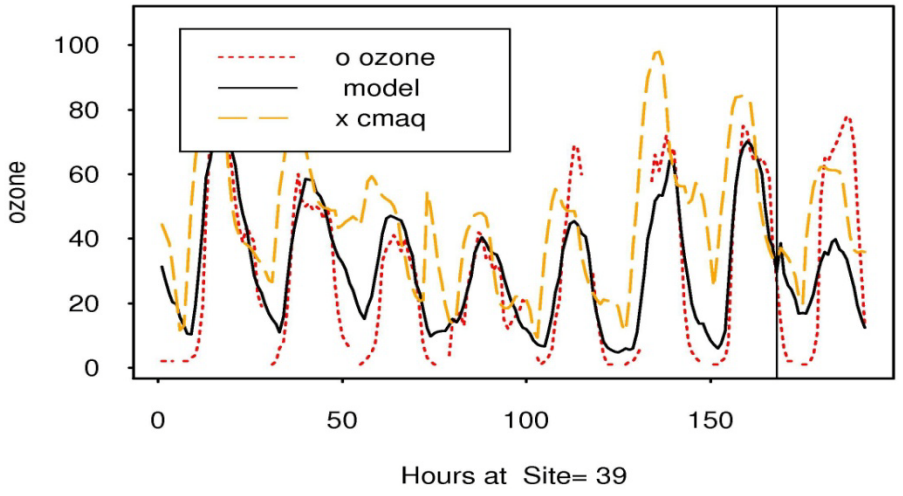
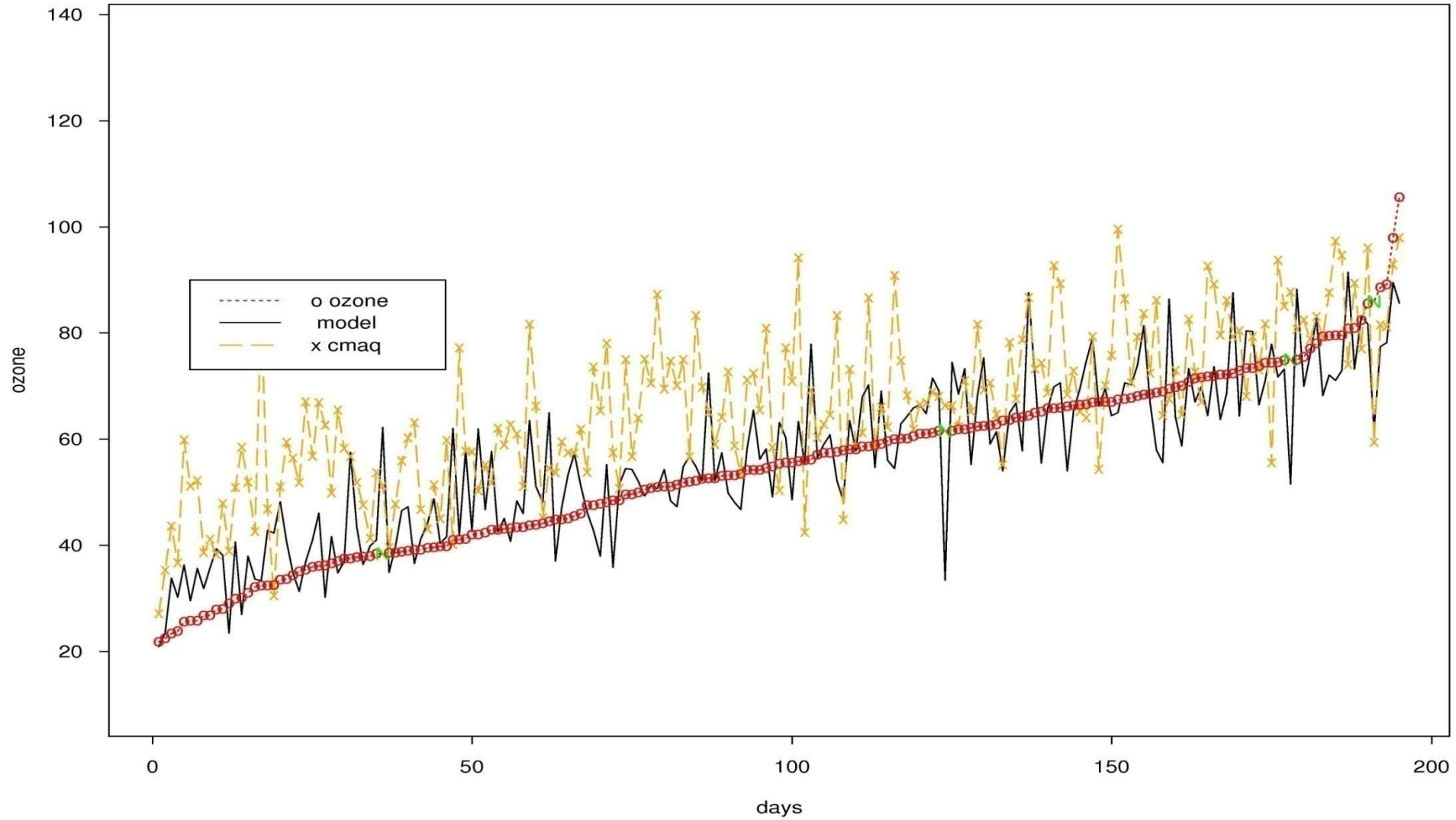




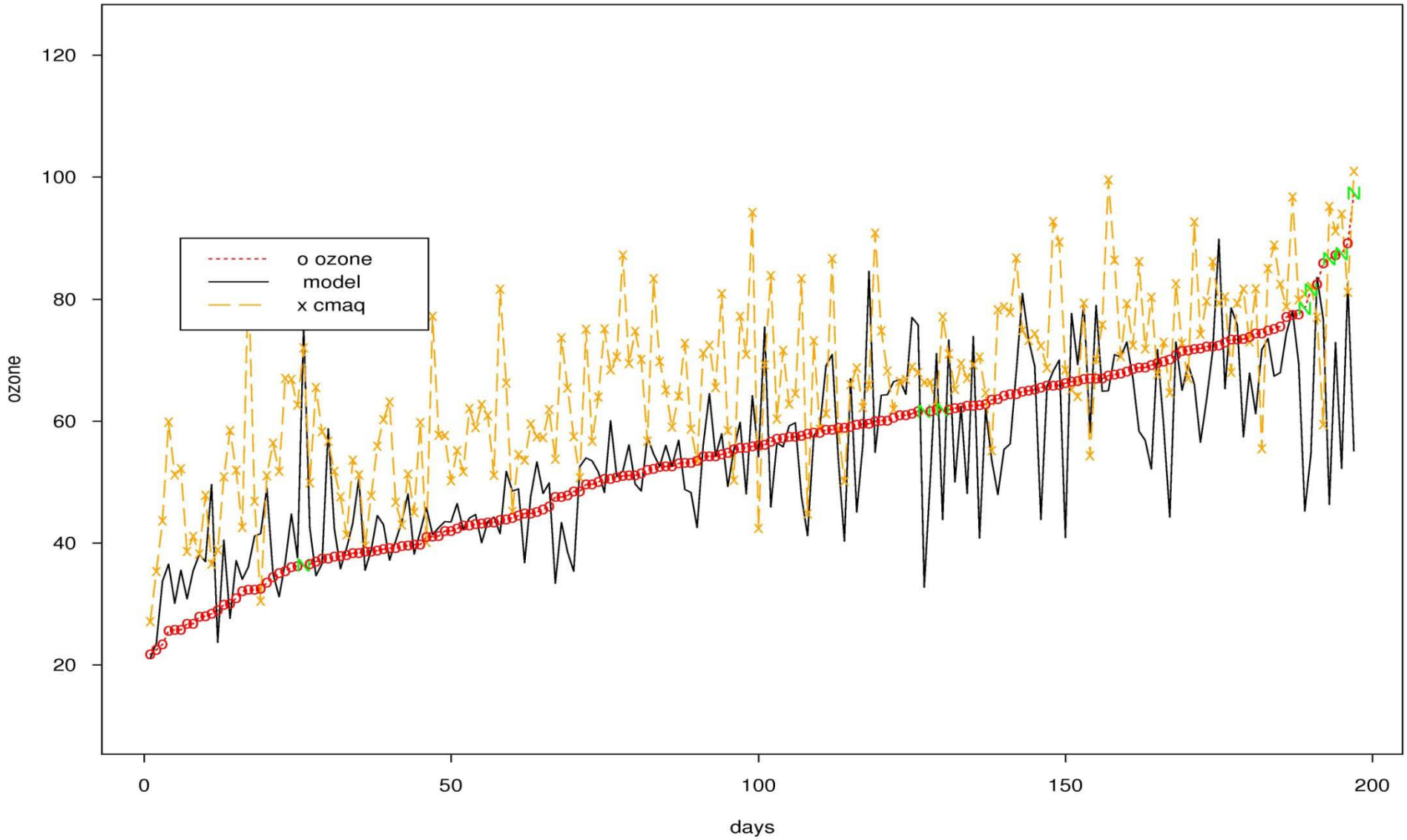




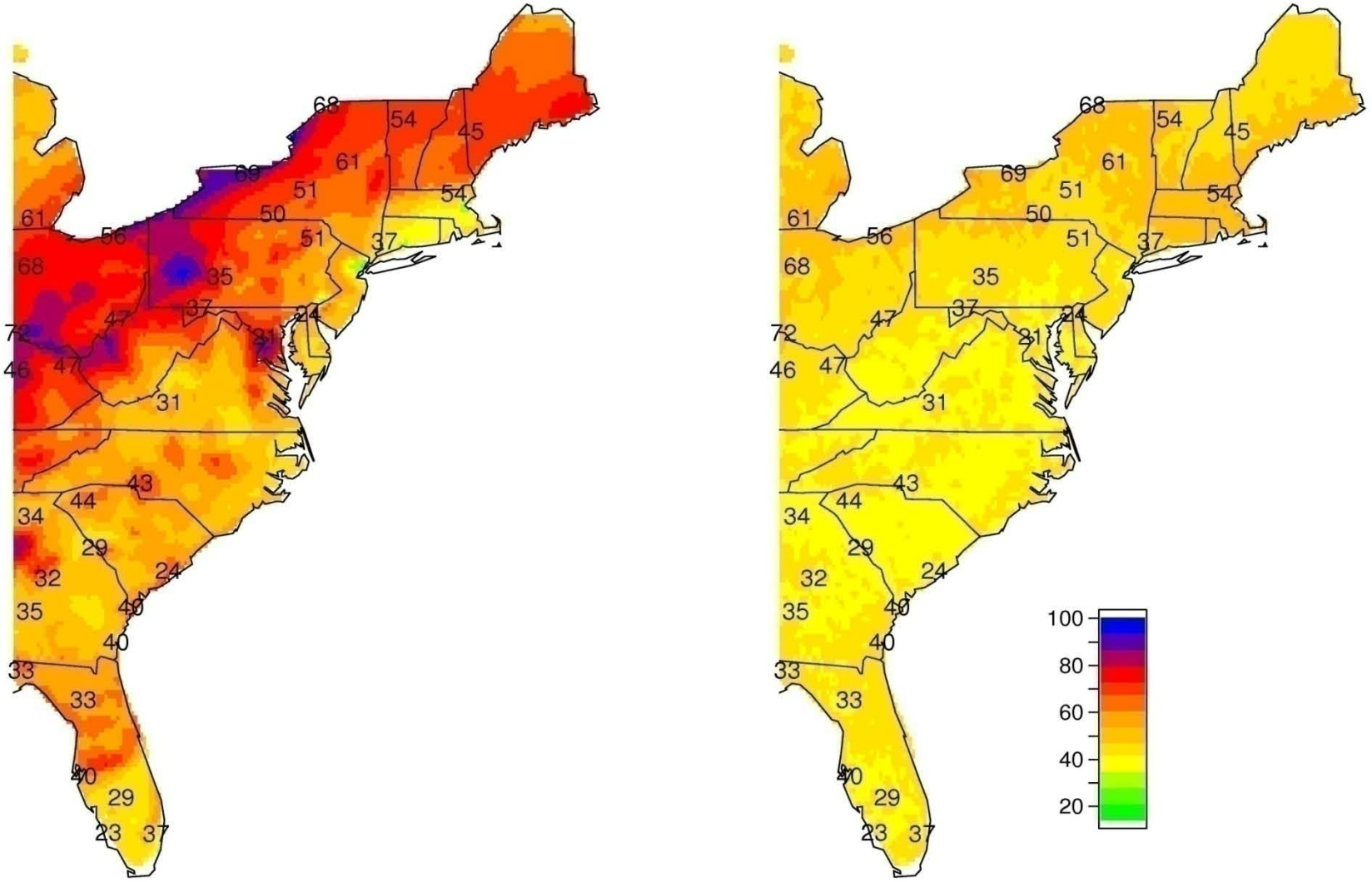
Validation: daily to Aug 11
data (red), Eta-CMAQ (tan), Forecast (black)



Validation: daily to Aug 12
data (red), Eta-CMAQ (tan), Forecast (black)



Forecast Maps for August 9
Eta-CMAQ (left), Forecast model $\beta(s)=0$ (right)



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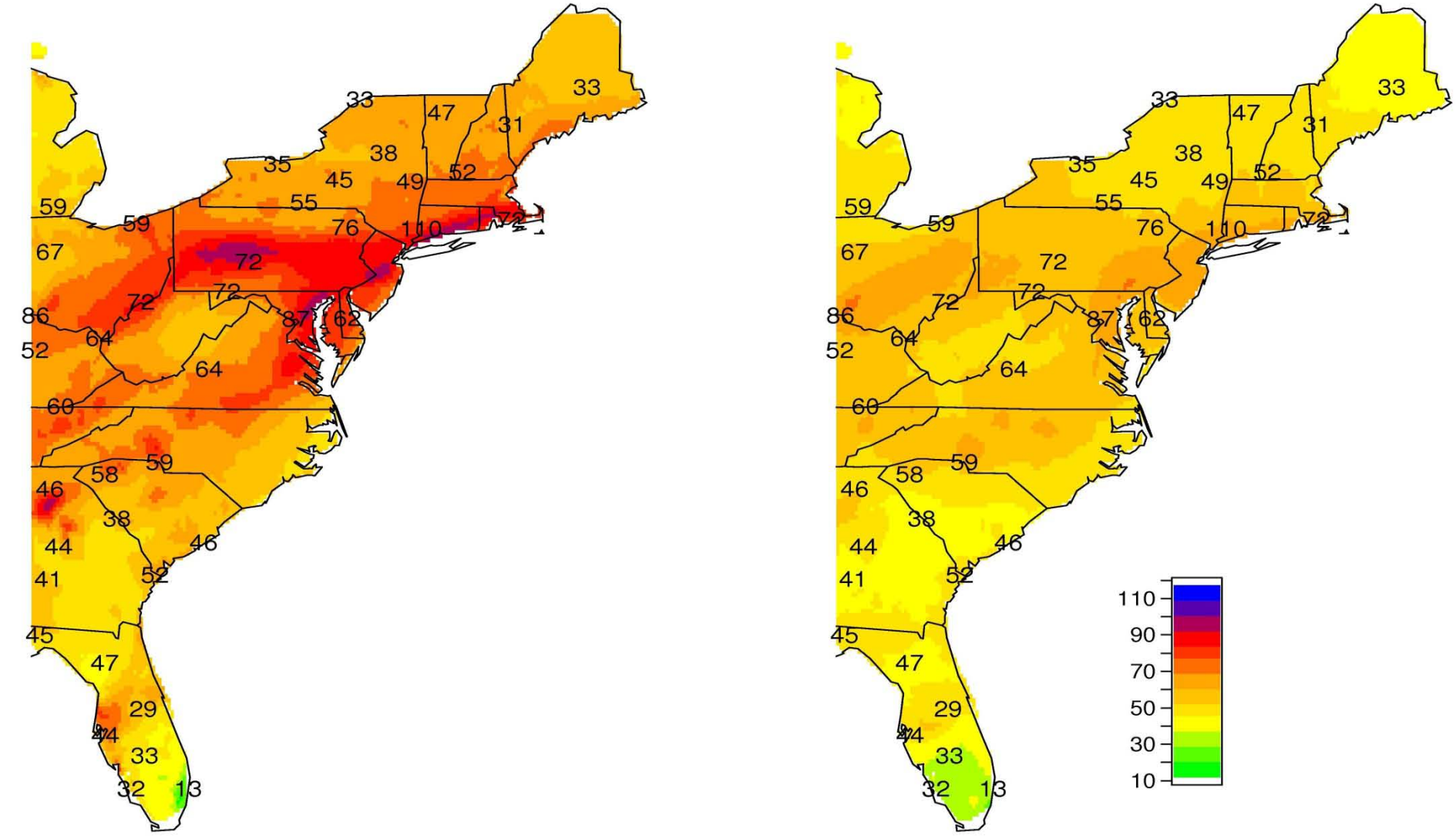
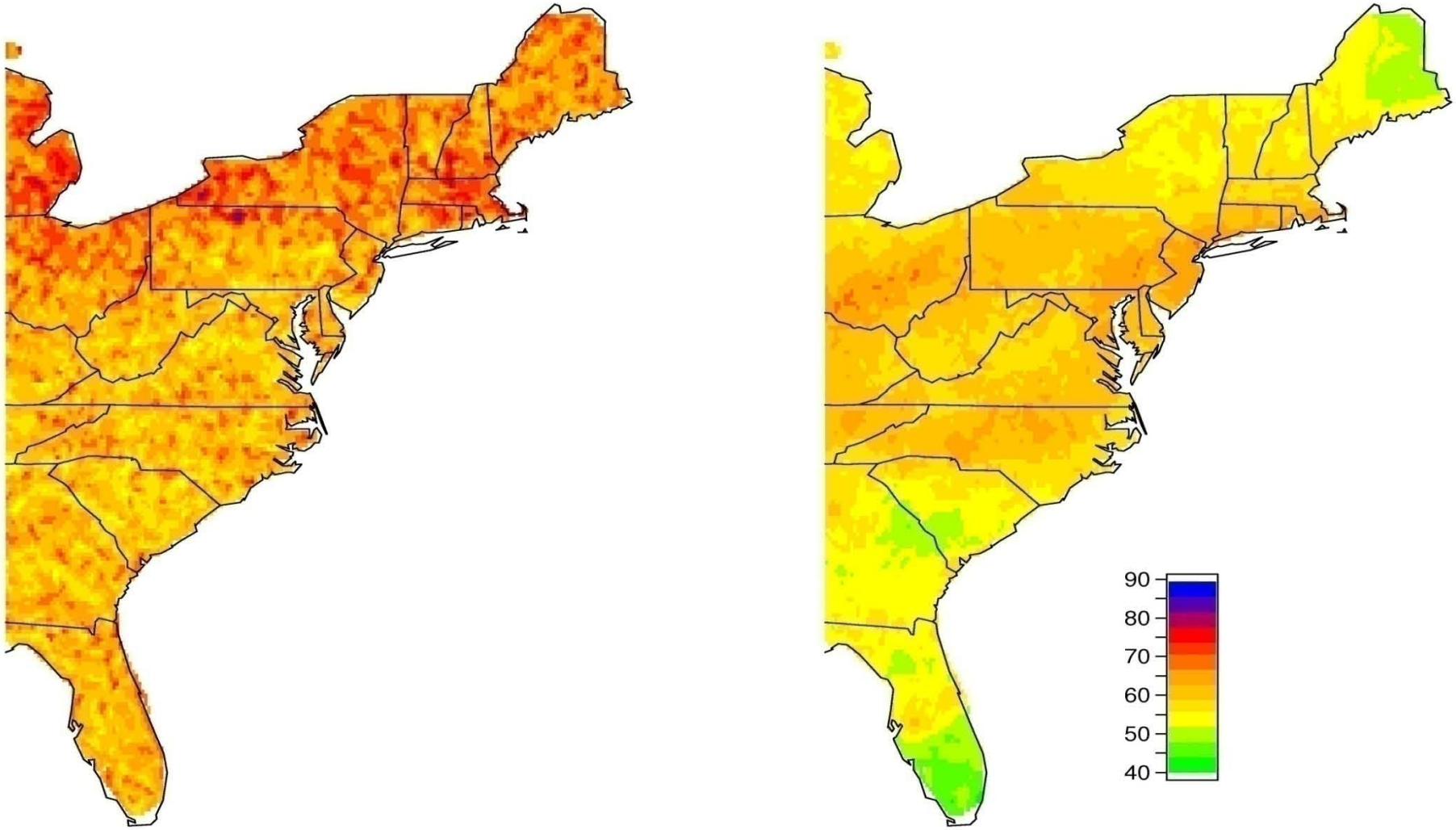


Lengths of 95% Confidence intervals for forecasts on Aug 9 (left) and Aug 12 (right)



Conclusions/Future Directions

- Model improves upon forecast results from Eta-CMAQ output
- High resolution model seems adequate for fast EPA AirNow implemention
- Can attach prediction uncertainties to forecasts
- In process of developing a real-time forecast system using this model
- Companion effort, predict current 8-hr average O3 levels based on predictions for each of the 4 previous hours, current hour, and for the next 3 hours