Air Quality Modeling and Advanced Nesting Techniques

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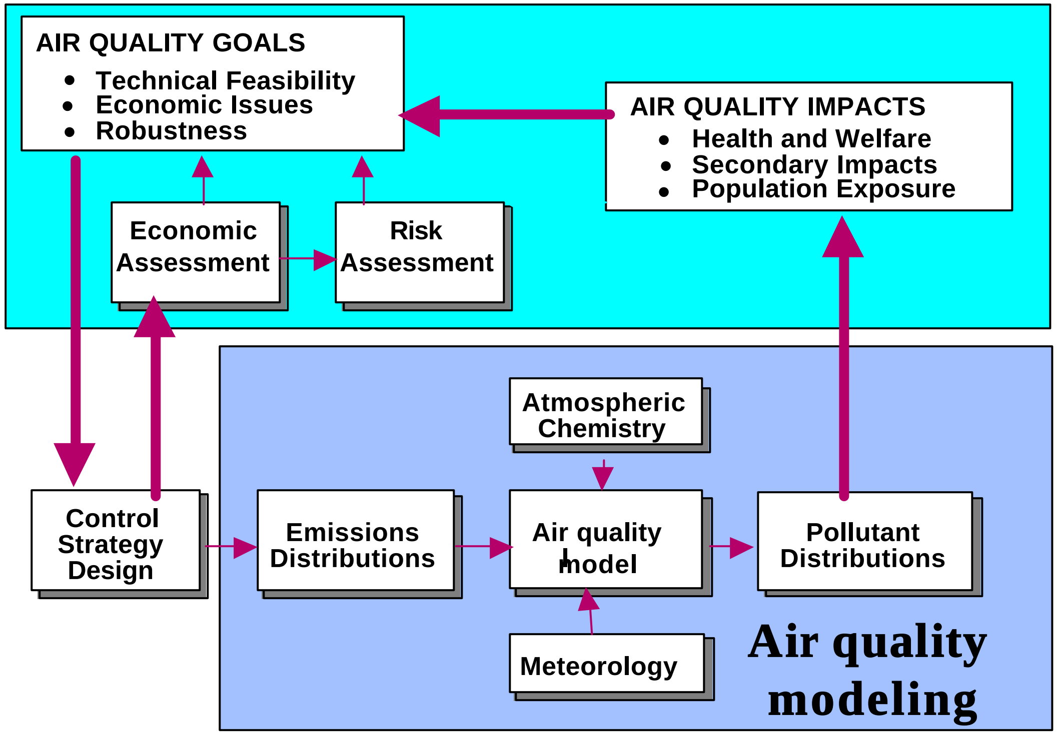
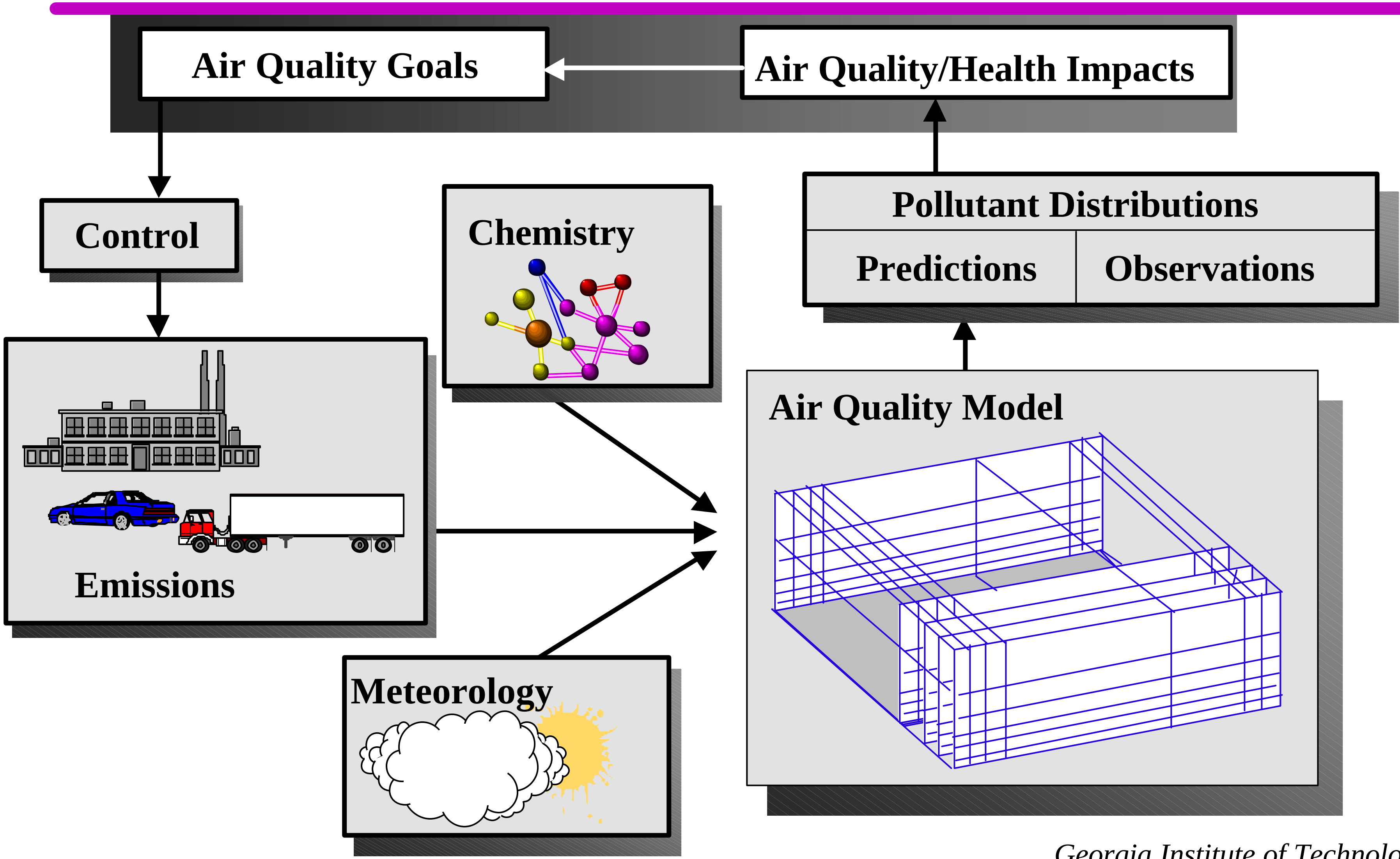
Issues

- Much of the world’s population lives in areas with “poor” air quality
  - Virtually every major city!
  - Ozone and particulate matter major concerns
- About $100 billion / year spent on controls worldwide
  - “Clean” air will cost even more
- Demand for identifying optimal controls
  - Need for effective tools
    - System is highly non-linear

Role of Air Quality Models in Air Quality Management

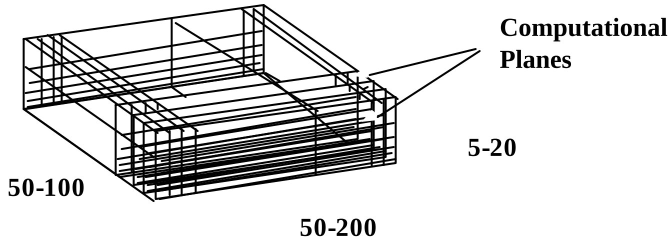


Air Quality Modeling



Air Quality Model

- Representation of physical and chemical processes
  - Numerical integration routines
- Scientifically most sound method to link future emissions changes to air quality



Air Quality Model

$$\frac{\partial c_i}{\partial t} = -\nabla(\mathrm{u}c_i) + \nabla(\mathrm{K}\nabla c_i) + R_i + S_i$$

Atmospheric Diffusion Equation

↓ Discretize

$$\frac{\partial \mathrm{c}}{\partial \mathrm{t}} + \mathrm{L}(\mathbf{x},\mathrm{t})\mathrm{c} = \mathrm{f}(\mathbf{x},\mathrm{t})$$

↓ Operator splitting

$$\mathrm{c}(\mathrm{t}+2\Delta\mathrm{t}) = \mathrm{L}_x(\Delta\mathrm{t})\ \mathrm{L}_y\ (\Delta\mathrm{t})\ \mathrm{L}_{cz}(2\Delta\mathrm{t})\ \mathrm{L}_y(\Delta\mathrm{t})\ \mathrm{L}_x(\Delta\mathrm{t})\ \mathrm{c}(\mathrm{t})$$

200 species x 5000 hor. grids x 20 layers= 20 million coupled, stiff non-linear differential equations

Atmospheric Diffusion Equation (ADE)

$$\frac{\partial c_i}{\partial t} = -\nabla(\mathrm{u}c_i) + \nabla(\mathrm{K}\nabla c_i) + R_i + S_i$$

I.C.: $c_i(t_o) = c_i^b$

B.C.:

(1) $\mathrm{u}c_i - \mathrm{K}\nabla c_i = \mathrm{u}c_i^b$ inflow

(2) $-\nabla c_i = 0$ *outflow*

(3) $v_g^i c_i - \mathrm{K}_{zz}\frac{\partial c_i}{\partial z} = E_i$ $z = 0$

(4) $-\frac{\partial c_i}{\partial z} = 0$ $z = H$

Solutions of the ADE using Operator Splitting

$$c_i(t + Dt) = L_H\left(\frac{Dt}{2}\right) L_V(Dt) L_{RS}(Dt) L_H\left(\frac{Dt}{2}\right) c_i(t)$$

where

$$\textit{Horizontal transport operator}: \; L_H(c_i) = -\nabla_H(u c_i) + \nabla_H(K \nabla_H c_i)$$

$$\textit{Vertical transport operator}: \; L_V(c_i) = -\nabla_V(u_z c_i) + \nabla_V(K \nabla_V c_i)$$

$$\textit{Chemistry and emissions operator}: \; L_{RS}(c_i) = R_i + S_i$$

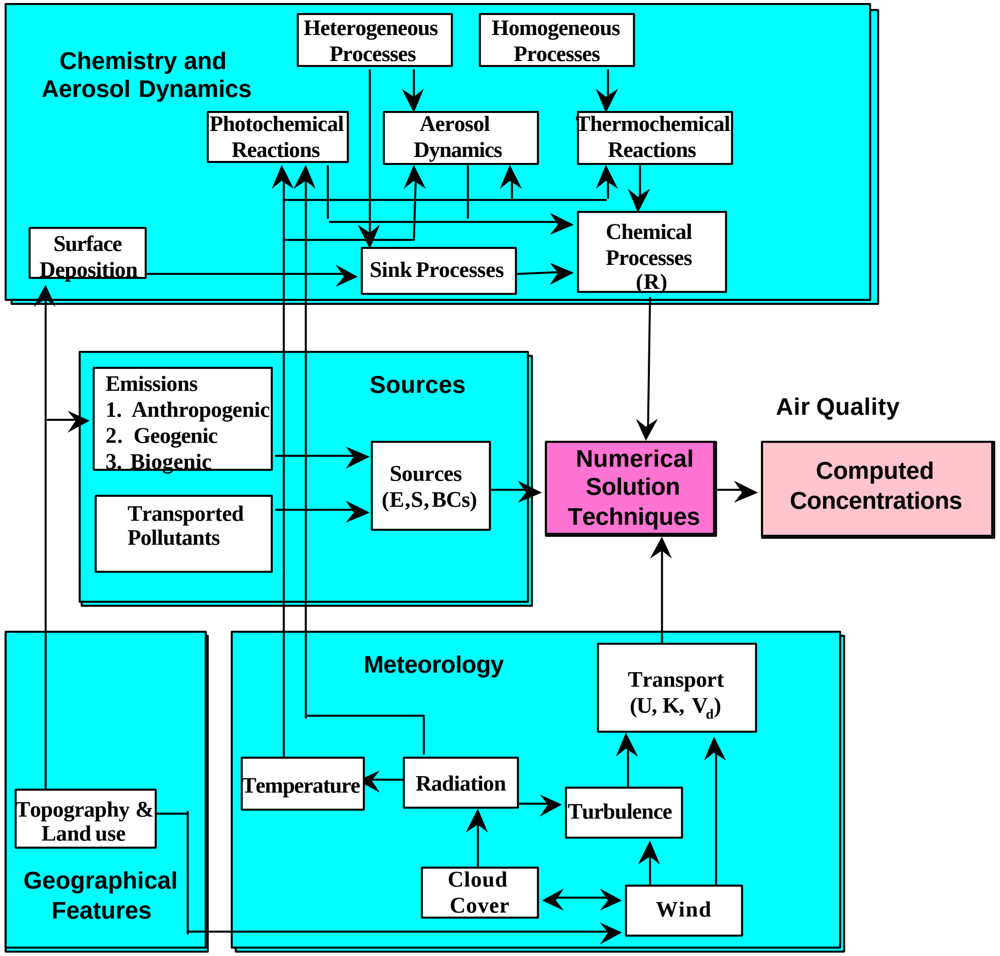
Operator Splitting

- Efficiency
  - Can use fast solution techniques
    - Chemical dynamics solution 85% of time
- Accuracy
  - Specialized, accurate techniques developed for
    - **Horizontal transport (hyperbolic)**
      - ✓ **Probably the most difficult**
      - ✓ **Where major advances can be made**
    - Chemistry (stiff, first order)
    - Vertical transport (parabolic)
- More readily updated

Other Model Components

- Chemical Mechanism
  - Describes important chemical reactions
    - 100-200 species 150-400 reactions
    - Gas and condensed phase
- Aerosol dynamics solver
  - Allows following the transport, formation and growth of aerosols
- Meteorology and land use sub-models
  - Transforms meteorological and land use inputs to parameters used by the model
- Emissions processor
- Advanced diagnostic techniques
  - Sensitivity analysis

Air Quality Model

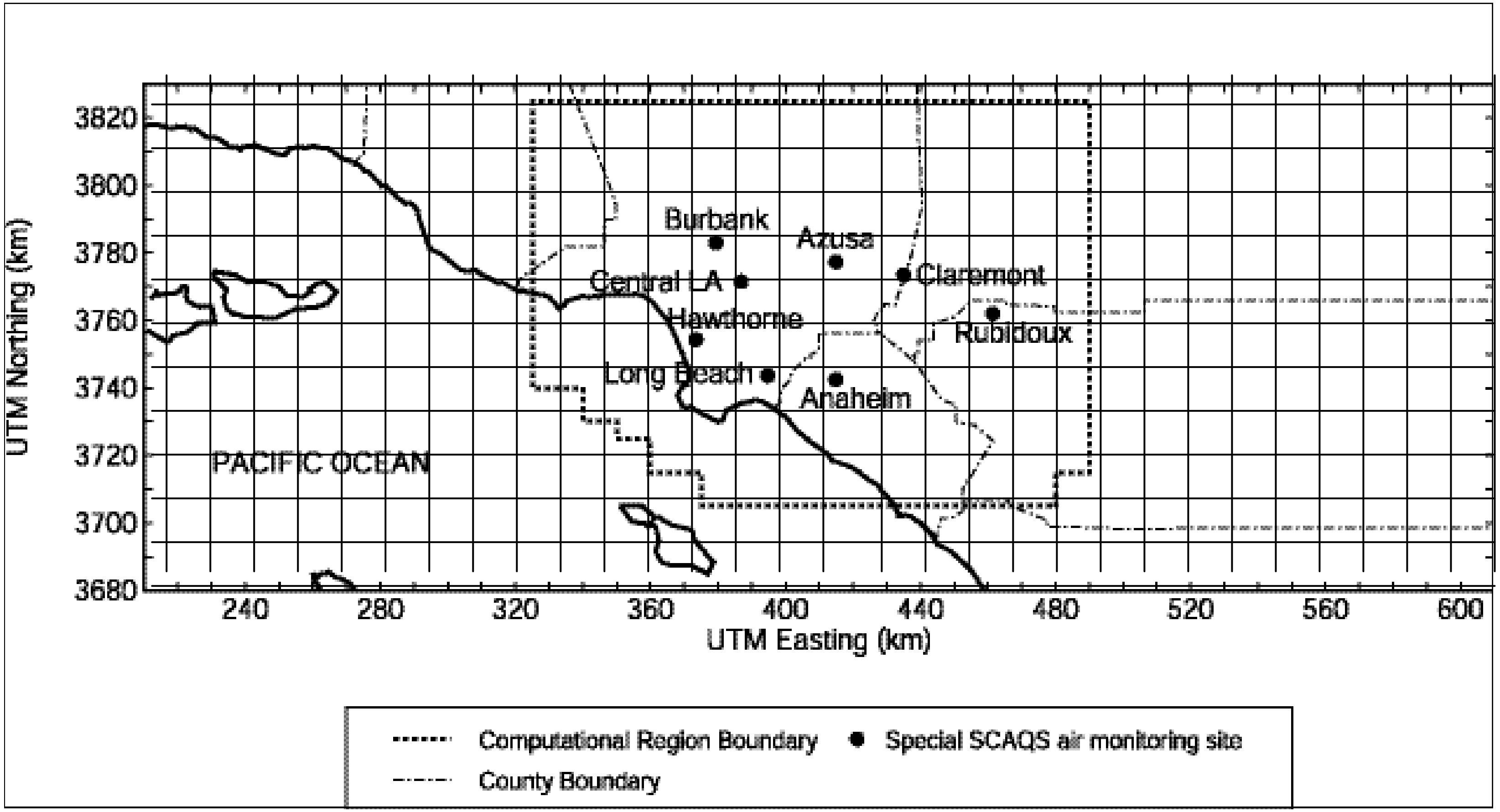


Horizontal Transport Solvers: Nesting/Multiscale/Adaptive Grid Techniques

Horizontal Transport Schemes

- Need to accurately describe the horizontal advection of pollutants
- Various techniques developed
  - Monoscale grid (oldest)
  - Nested grids (monoscale grid in a monoscale grid)
    - One and two-way nesting
  - Multiscale (similar to used in CFM)
  - Adaptive grids (wave of the future?)

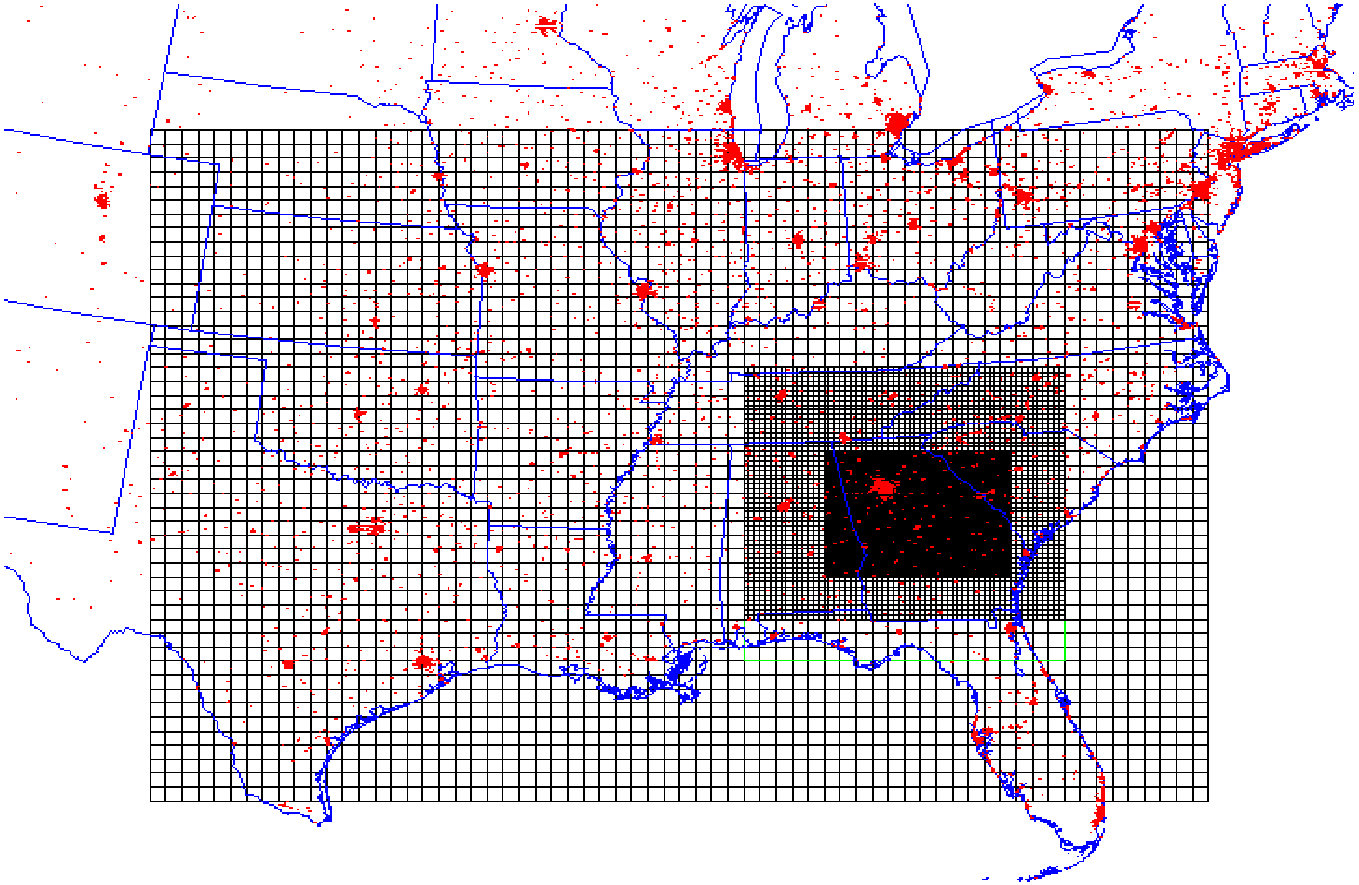
Monoscale Grid



Monoscale Grid

- Strengths
  - Simple and fast
- Weaknesses
  - Ineffective for treating regional domains
    - Need fine resolution in urban areas
      - ✓ Requires too many computational nodes
    - Coarse resolution o.k. for rural areas
      - ✓ But does a poor job in urban areas

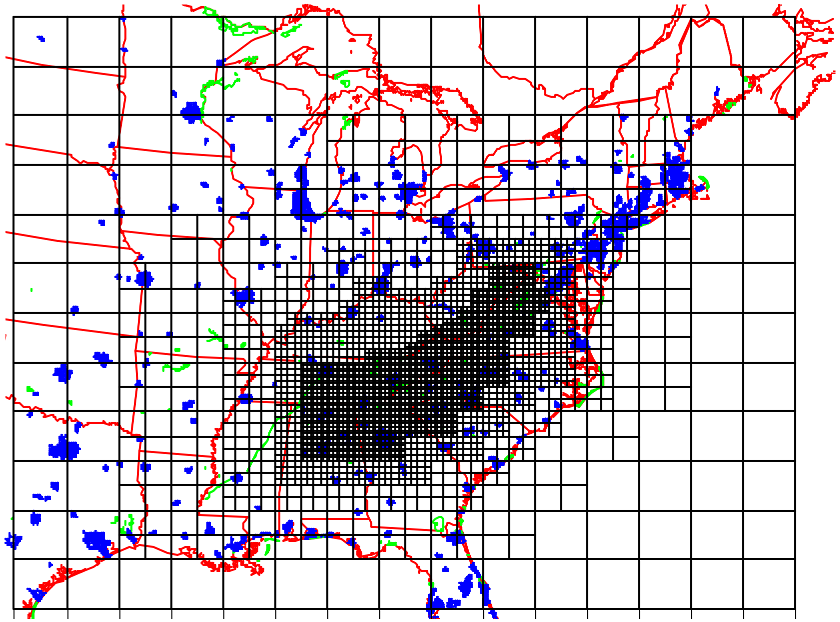
Nested Grid

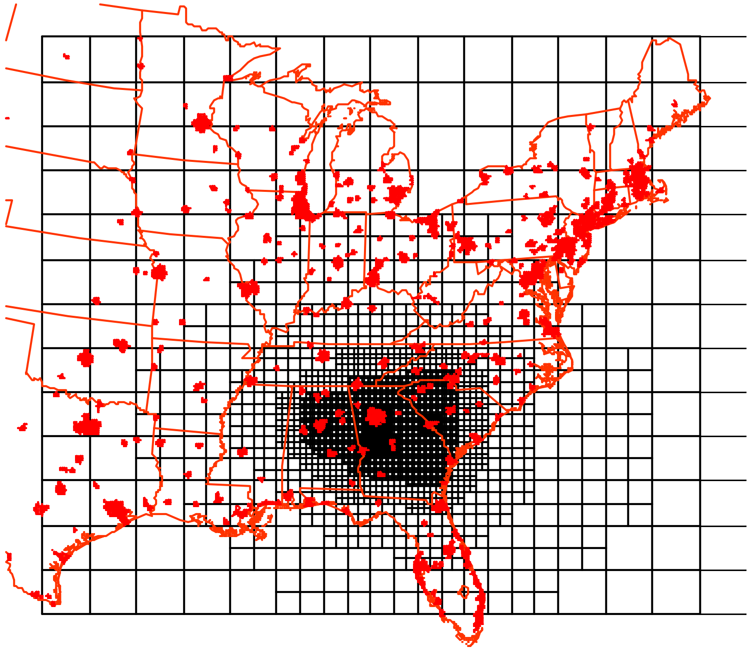


Nested Grids

- Strengths
  - Can have varying scale grid resolution
    - Fine grids over urban areas
    - Coarse grids over rural areas
    - Computationally more efficient than monoscale grids
  - Relatively simple
- Weaknesses
  - Must decide on grid pattern before application
  - Grid pattern does not adapt
  - usually limited to rectangular nests
    - Inefficient
  - Must do chemical calculations twice in some regions

Multiscale Grids

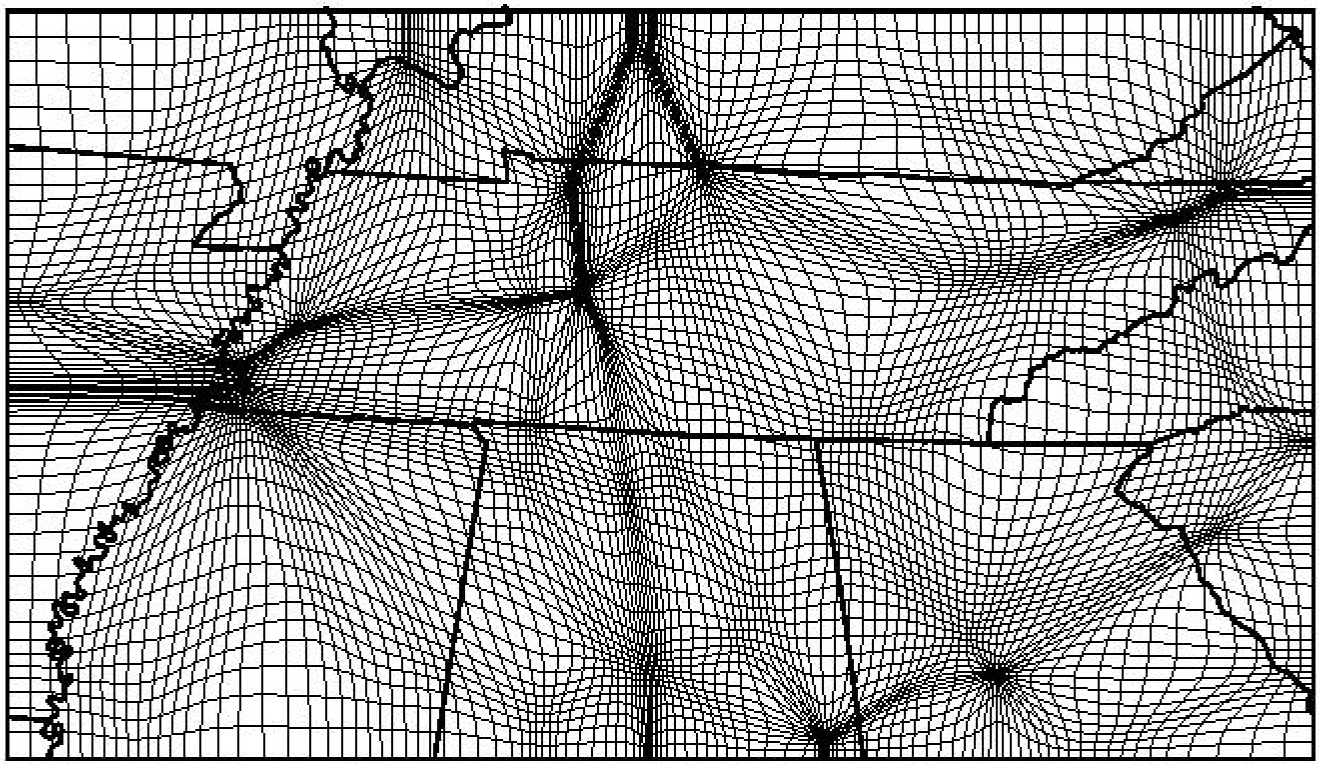




Multiscale Grids

- Strengths
  - Allows appropriate resolution over various areas
  - Need not have rectangular nests
  - Computationally very efficient
- Weaknesses
  - Must decide on grid structure before application
  - Grid is static
  - Some noise

Adaptive Grids



Motivation for Adaptive Grids

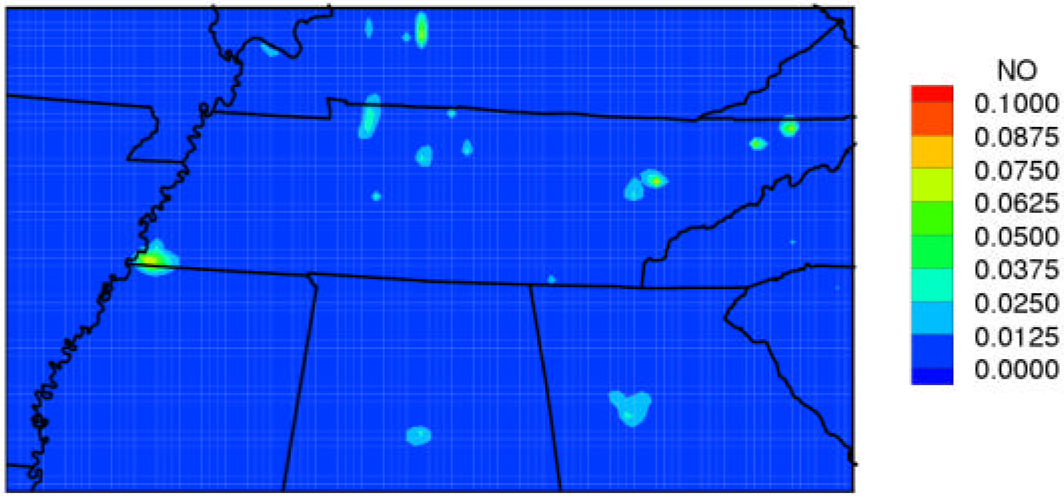
- Fixed grids (nested and multiscale) have limitations:
  - Assumptions are made in placing finer grid resolution,
  - Some accuracy is lost due to grid interface problems,
  - Fixed grids cannot adjust to dynamic changes in solution requirements.
- Adaptive grids offer an effective and potentially more efficient alternative.
  - Interactions of urban and point source plumes with the surrounding atmosphere can be better resolved.
  - No need to spend time determining grid structure

Adaptive Grid Methodology

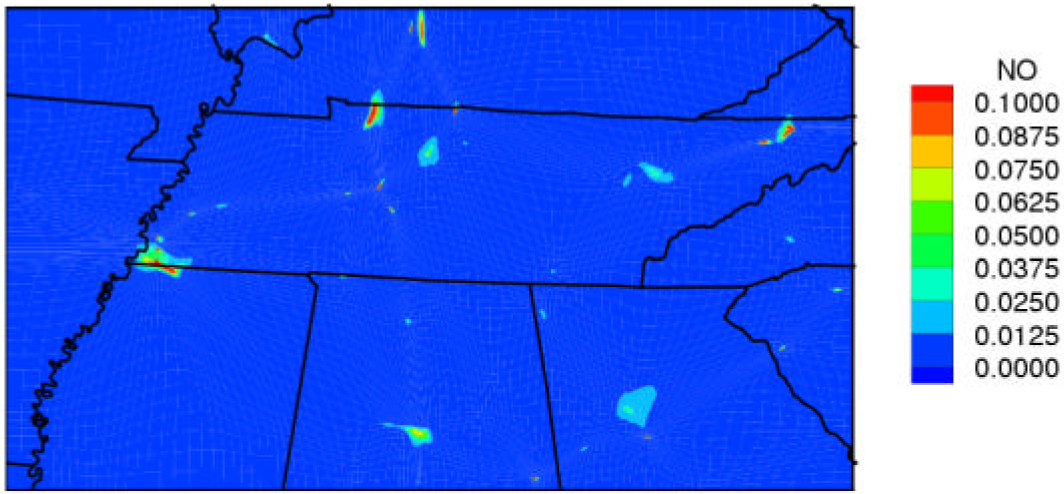
- The number of grid nodes is constant
  - The domain is divided into *NxM* quadrilateral grid cells
- Grid node movement criteria
  - A user defined function (weight function) controls the grid node movement. Defines the grid resolution requirements
- Grid nodes move throughout the simulation
  - Grid cells are automatically refined / coarsened to reduce error in variables
  - The <u>structure</u> of the grid is maintained

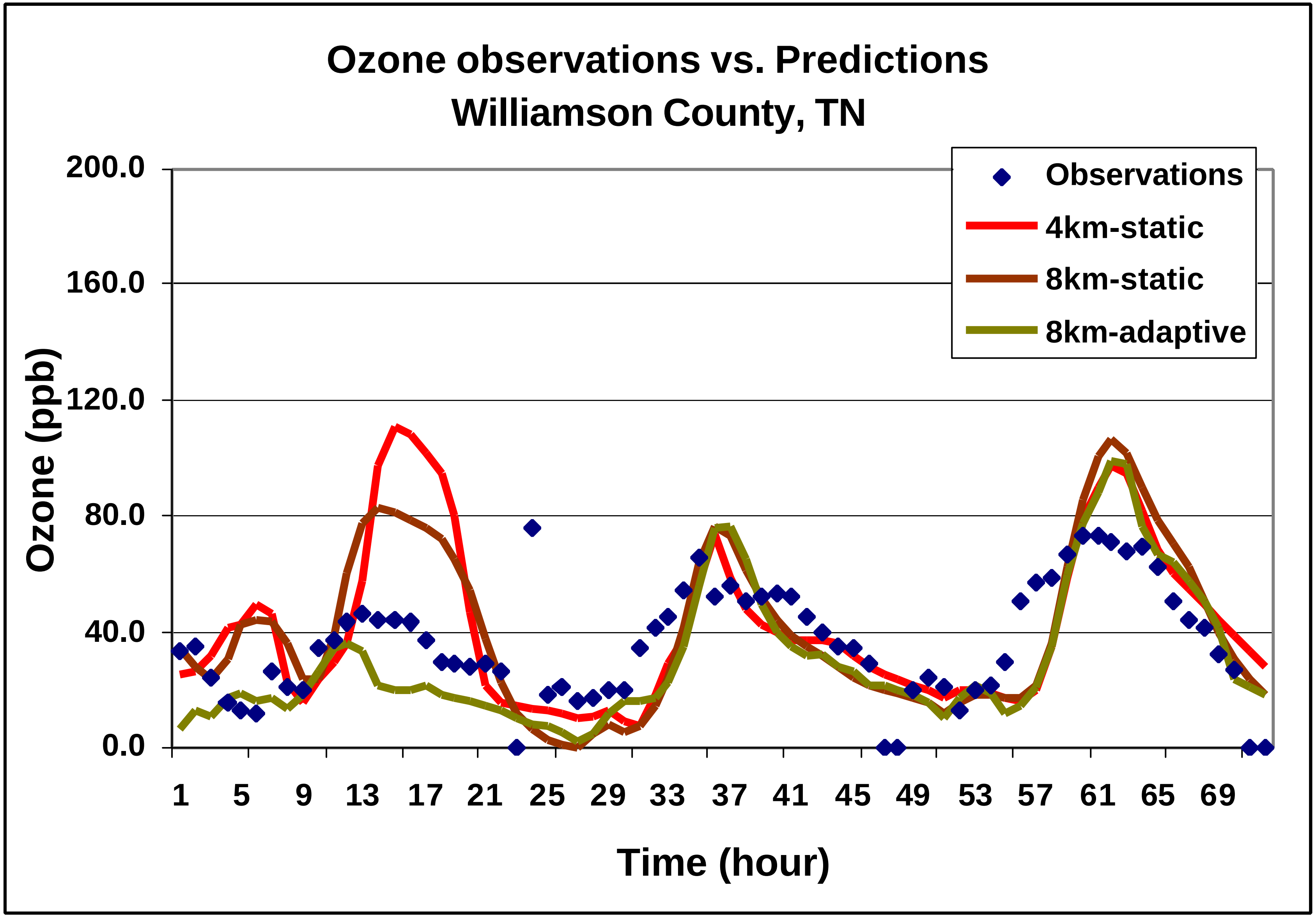
NO levels (ppm): 11:00 EST July 9, 1995

Fixed Grid
8x8km



Adaptive Grid





Ozone observations vs. Predictions
Williamson County, TN
Ozone (ppb)
200.0
160.0
120.0
80.0
40.0
0.0
1
5
9
13
17
21
25
29
33
37
41
45
49
53
57
61
65
69
Time (hour)
Observations
4km-static
8km-static
8km-adaptive

Nesting Techniques Summary

- Currently, multiscale techniques more powerful
  - Computationally efficient
  - Grid flexibility
- Adaptive grids promise to be wave of the future
  - More accurately follows plumes
  - Less personnel resource intensive
    - Optimal grid determined on the fly

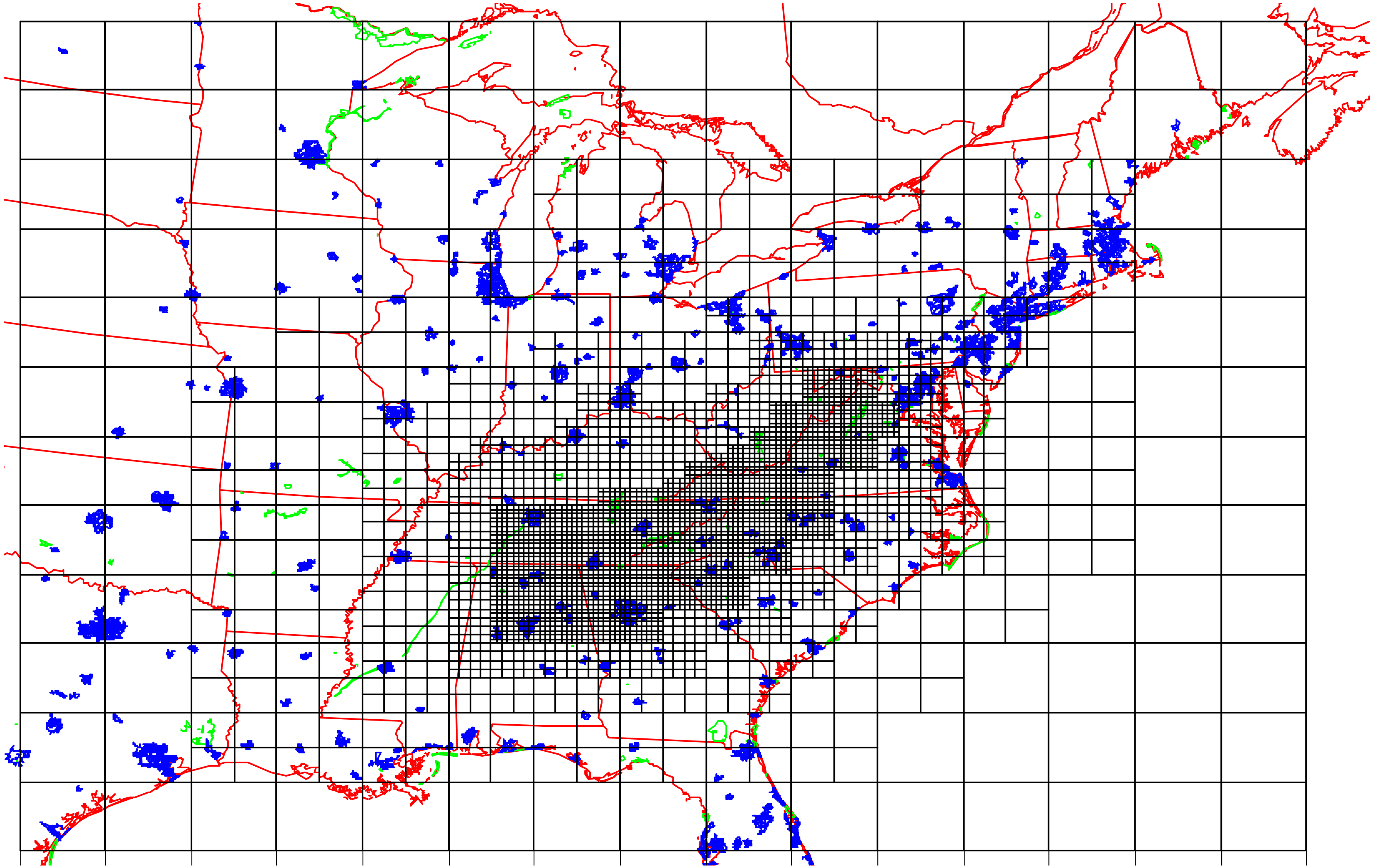
Multiscale Grid Model Application Example: SAMI

- Southern Appalachians Mountains Initiative (SAMI)
  - Stakeholder process to develop regional strategy to deal with:
    - Ozone (Sum06), PM, haze, acid deposition
    - Single model applied to suite of 5, 10 day episodes
      - ✓ Episodes chosen to represent typical year

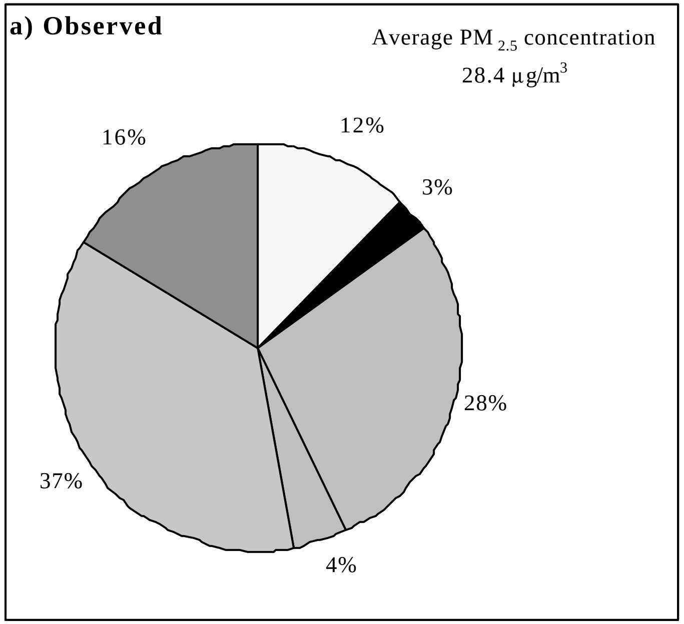
Urban-to-Regional Multiscale (URM) Model

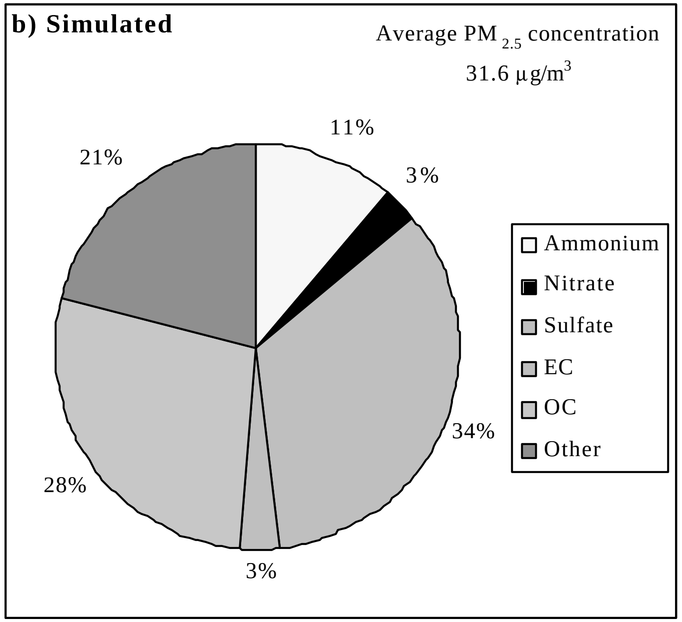
- Three-dimensional Eulerian photochemical model
  - Finite element, multiscale transport scheme (Odman & Russell, 1991)
  - Gas-phase chemistry
    - SAPRC mechanism (Carter, 1994)
  - Aerosol dynamics
    - Sectional approach
    - ISORROPIA thermodynamic equilibrium (Nenes, *et al*., 1998)
    - Organic aerosol yields (Pandis, *et al*., 1992)
  - Acid Deposition
    - Wet: Reactive Scavenging Module (Berkowitz, *et al*., 1989)
    - Dry: three-resistance approach
  - Sensitivity analysis
    - Direct decoupled method (Yang, *et al*., 1997)
- "One atmosphere" modeling approach

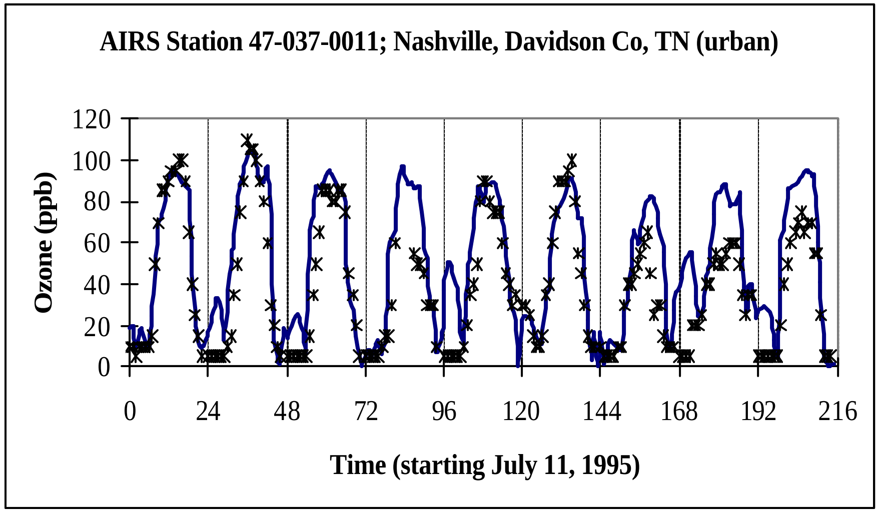
Multiscale Model Grid for SAMI

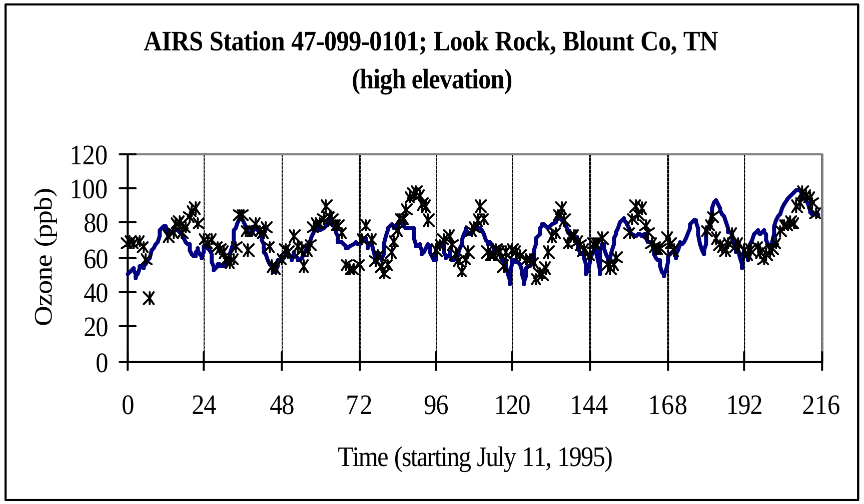


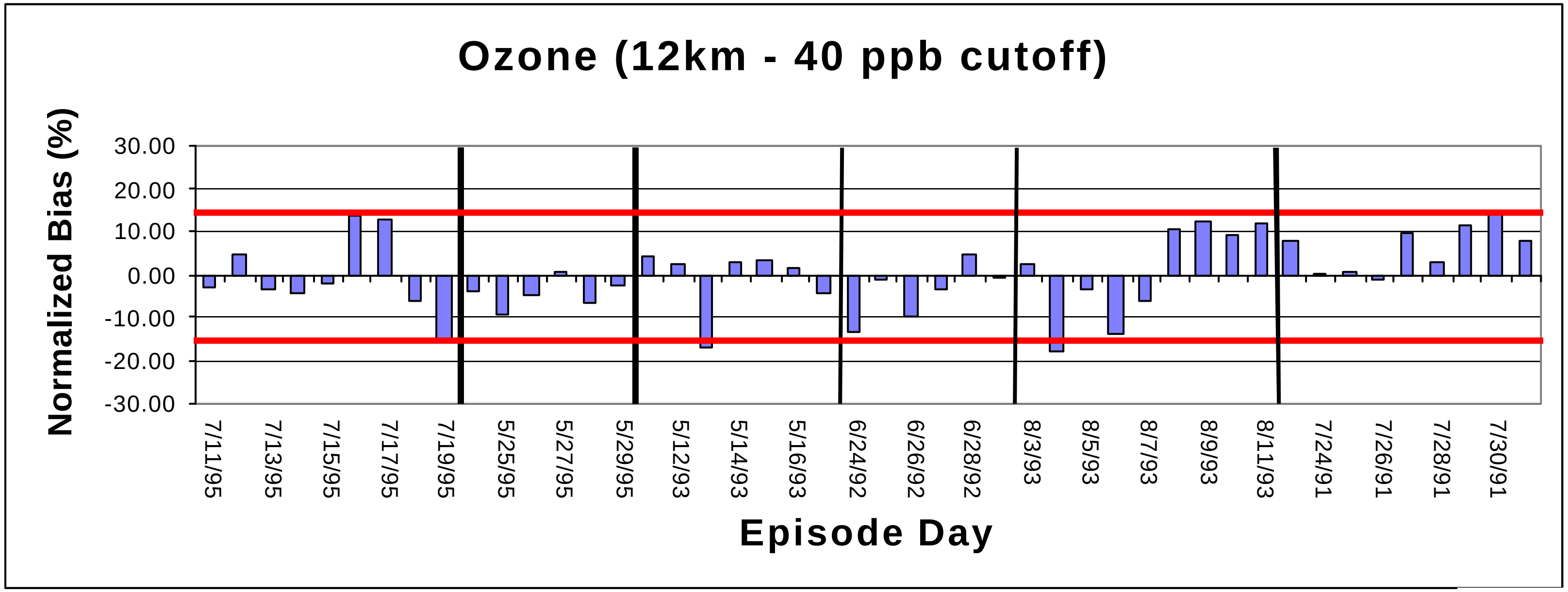
Model Performance



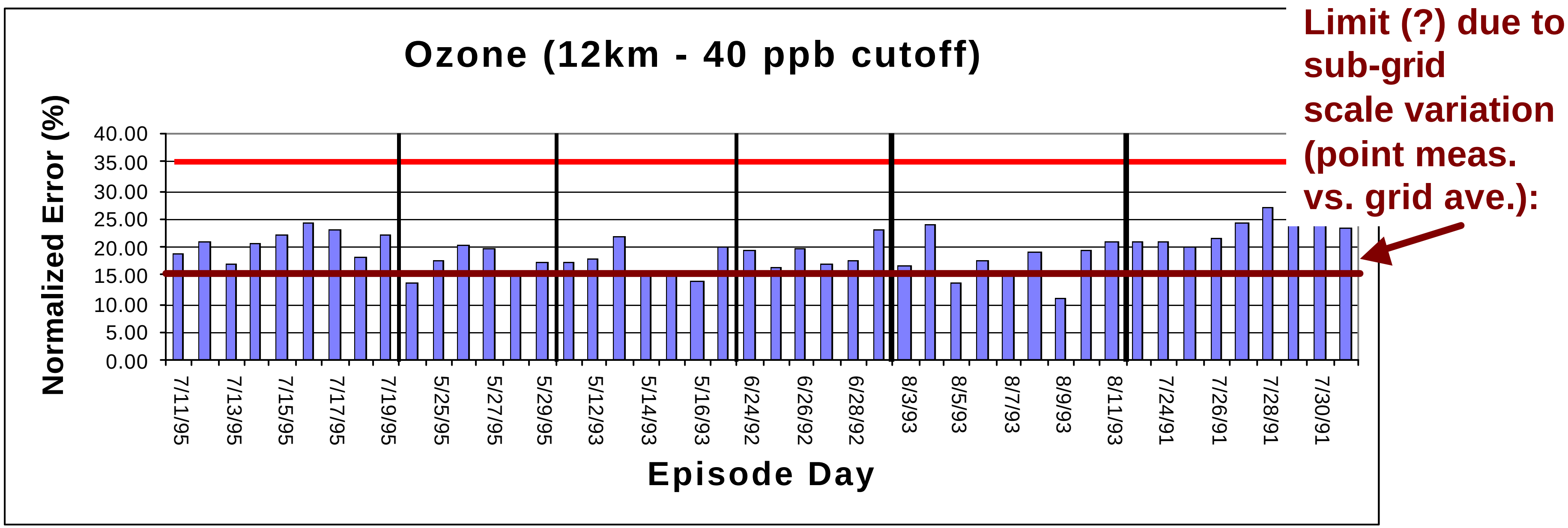








Ozone (12km - 40 ppb cutoff)
Normalized Bias (%)
30.00
20.00
10.00
0.00
-10.00
-20.00
-30.00
7/11/95
7/13/95
7/15/95
7/17/95
7/19/95
5/25/95
5/27/95
5/29/95
5/12/93
5/14/93
5/16/93
6/24/92
6/26/92
6/28/92
8/3/93
8/5/93
8/7/93
8/9/93
8/11/93
7/24/91
7/26/91
7/28/91
7/30/91
Episode Day

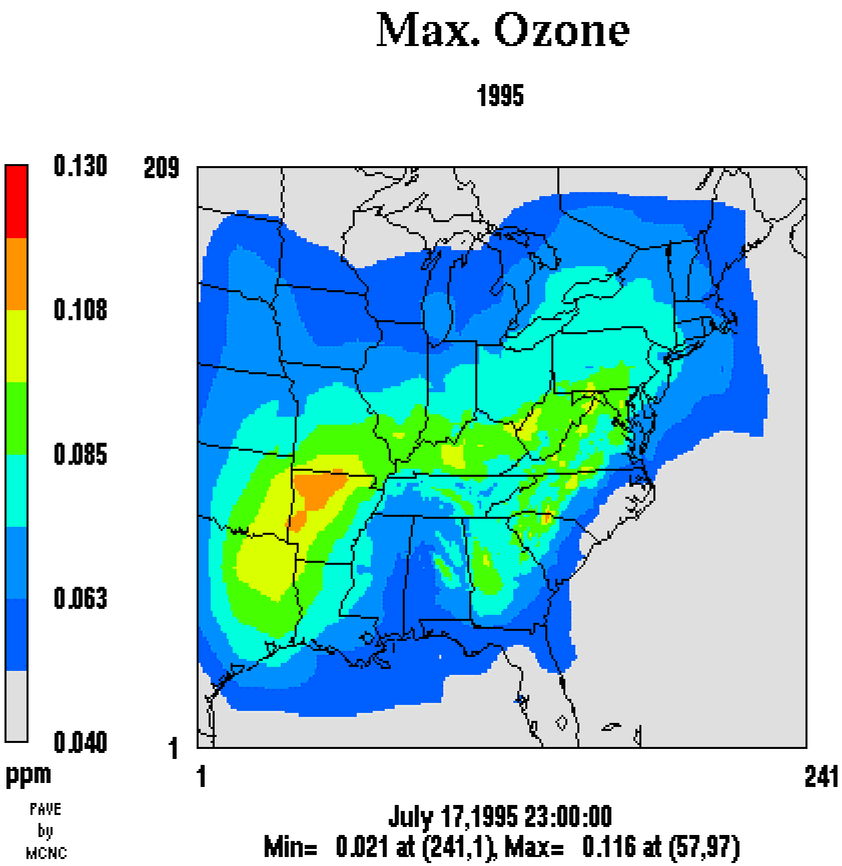


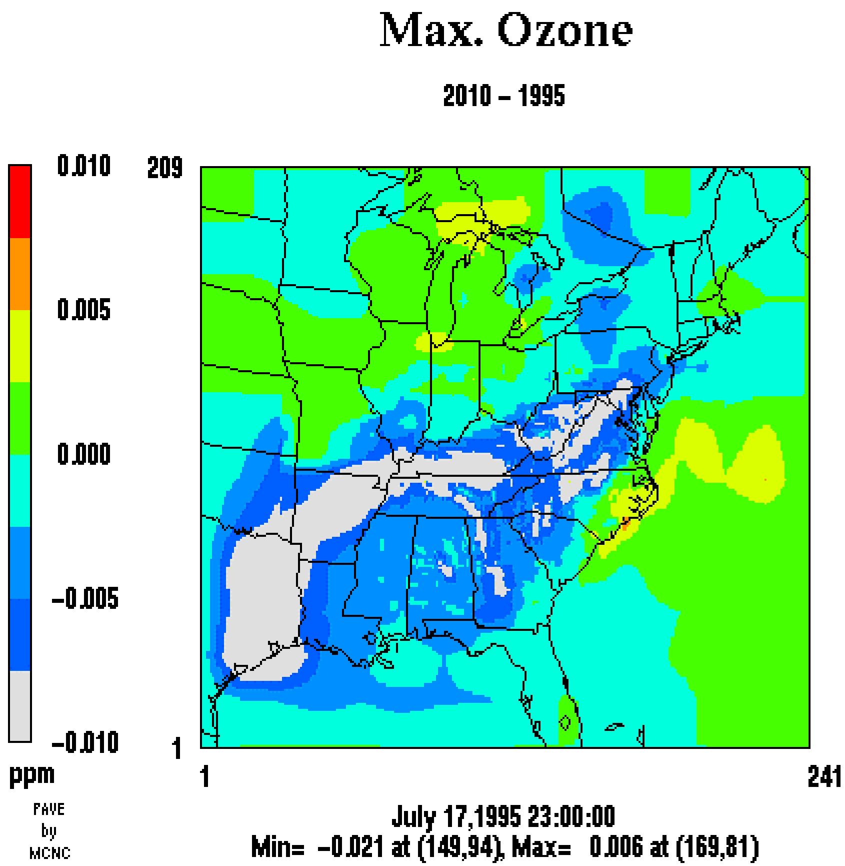
Ozone (12km - 40 ppb cutoff)
Normalized Error (%)
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
7/11/95
7/13/95
7/15/95
7/17/95
7/19/95
5/25/95
5/27/95
5/29/95
5/12/93
5/14/93
5/16/93
6/24/92
6/26/92
6/28/92
8/3/93
8/5/93
8/7/93
8/9/93
8/11/93
7/24/91
7/26/91
7/28/91
7/30/91
Episode Day
Limit (?) due to sub-grid scale variation (point meas. vs. grid ave.):

Assess Impact of Emissions Controls

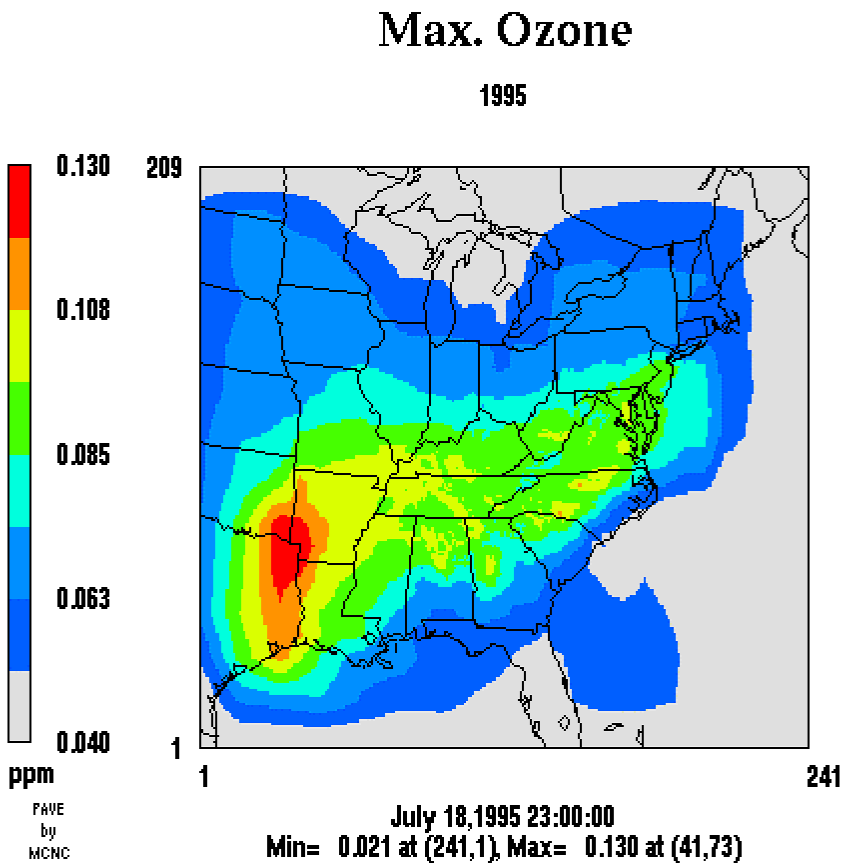
- Applied Urban-to-Regional Multiscale Model to 11 day episode
  - Evaluated using 1995 data
- Assessed impact of expected emissions changes between 1995 and 2010
- Calculated sensitivity to various controls
  - NOx

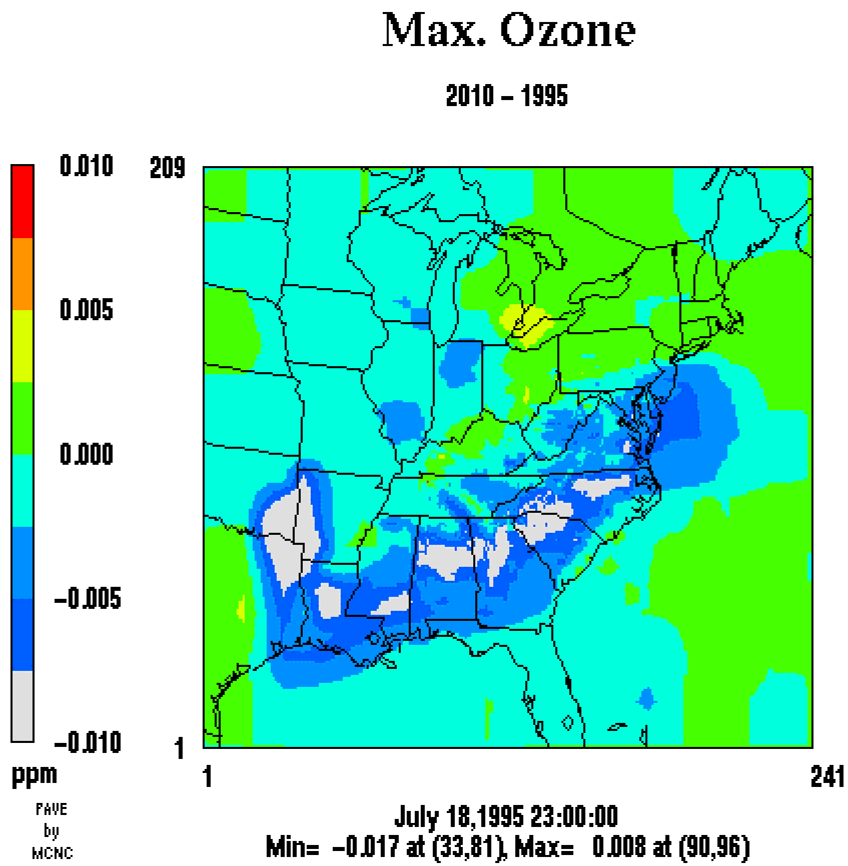
Max. Ozone - July 17





Max. Ozone - July 18





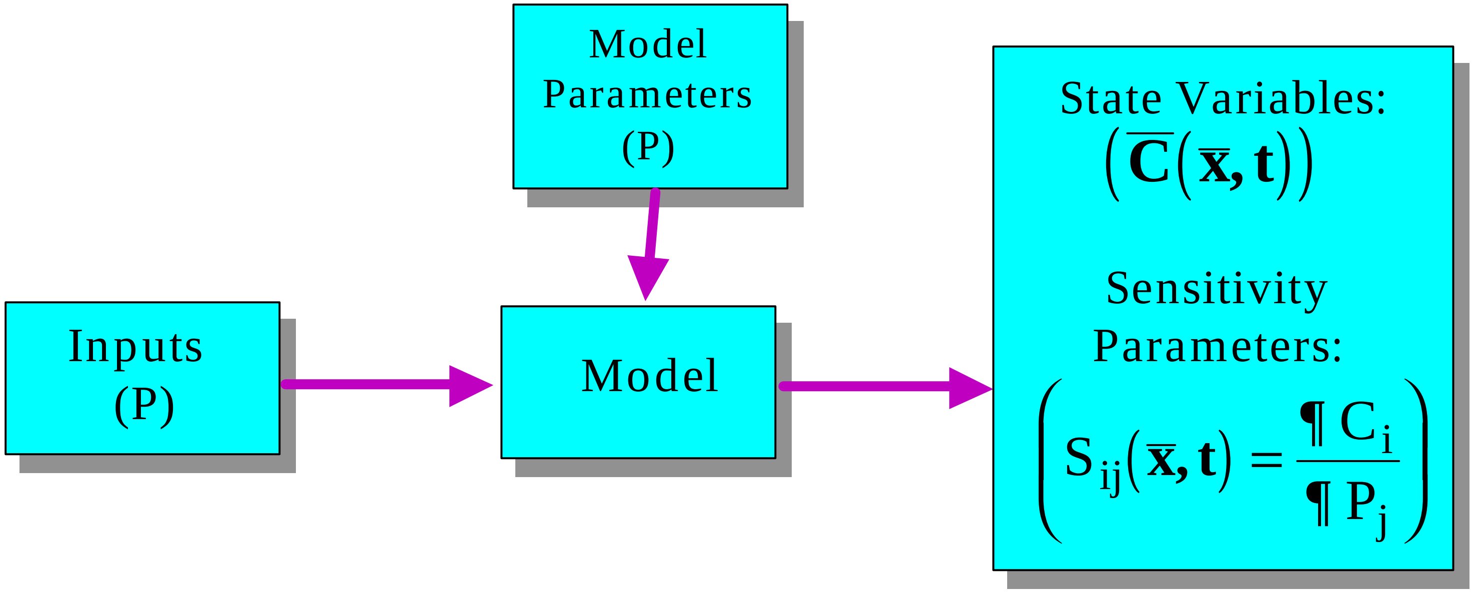
Direct Sensitivity Analysis

Role of Sensitivity Analysis

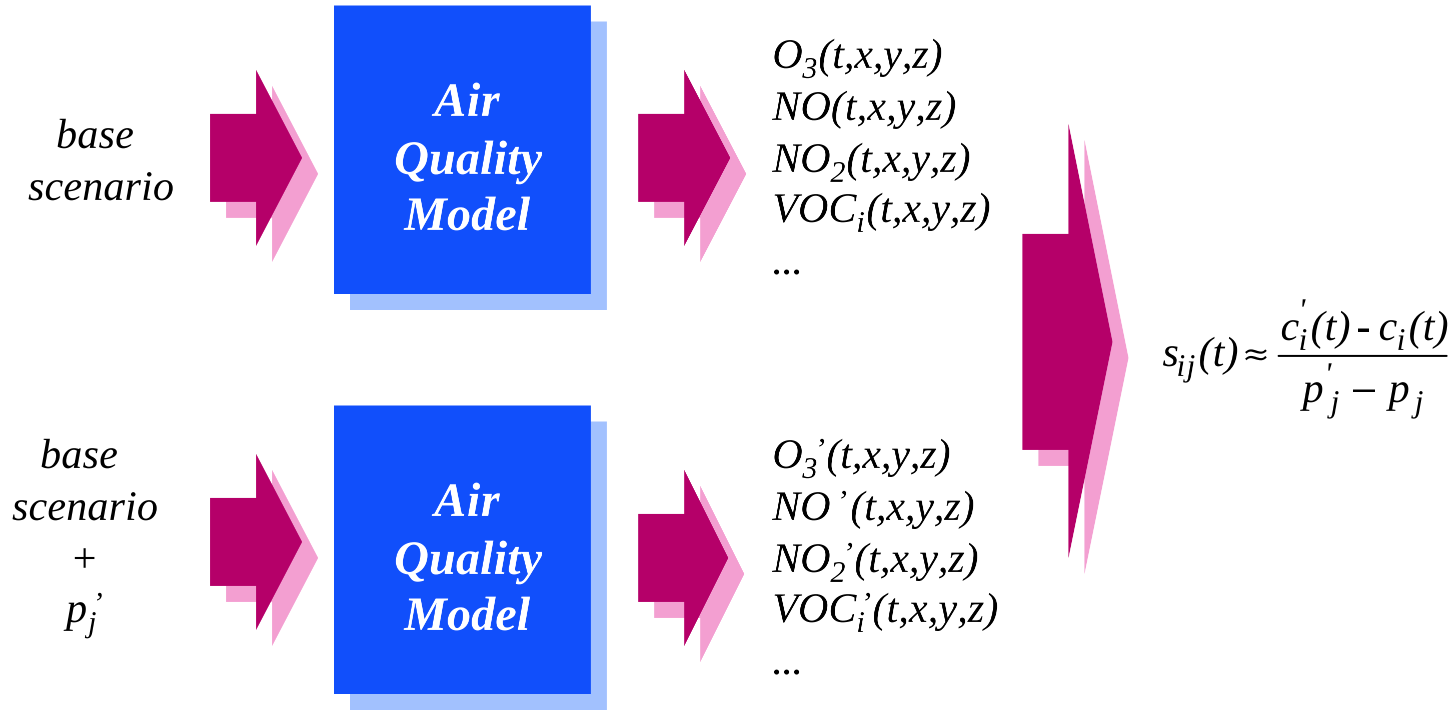
- Air quality model uses
  - Assess response of species concentrations to controls
  - Understand role of specific physical and chemical processes in species dynamics
- Knowledge of how system responds to changes in model inputs and parameters provides answers and understanding
  - Sensitivity analysis

Sensitivity analysis

- Given a system, find how the state (concentrations) responds to incremental changes in the input and model parameters:



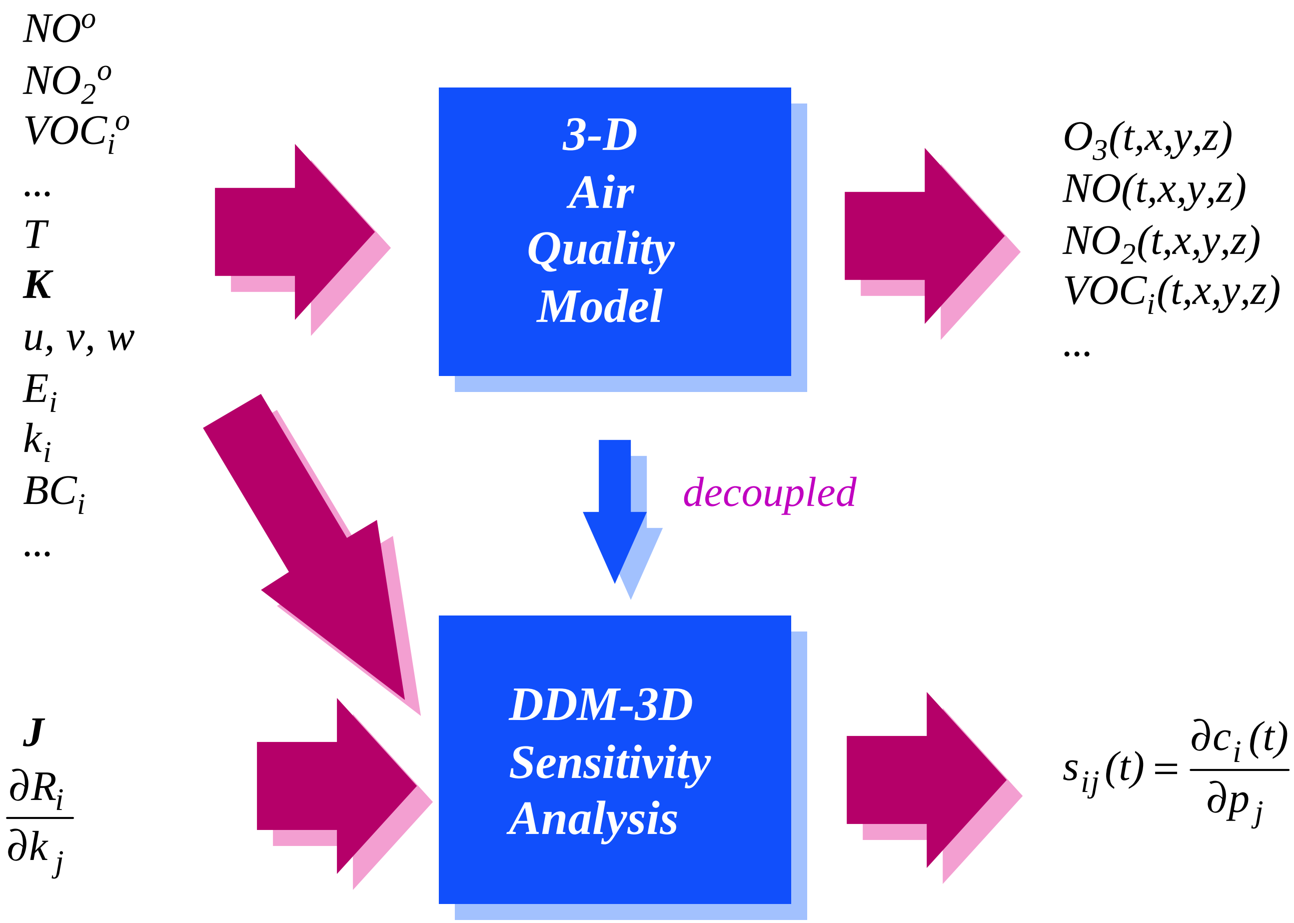
Brute-Force Sensitivity Analysis



Brute Force

- Strengths
  - Easily implemented
  - Efficient for few parameters
- Weaknesses
  - Inefficient for many parameters
  - Inaccurate for small responses

DDM-3D


NO^o
$NO_2{}^o$
$VOC_i{}^o$
...
T
$\mathbf{K}$
u, v, w
E_i
k_i
BC_i
...
3-D Air Quality Model
$O_3(t,x,y,z)$
$NO(t,x,y,z)$
$NO_2(t,x,y,z)$
$VOC_i(t,x,y,z)$
...
decoupled
$\mathbf{J}$
$\frac{\partial R_i}{\partial k_j}$
DDM-3D Sensitivity Analysis
$s_{ij}(t) = \frac{\partial c_i(t)}{\partial p_j}$

Fast Solution

- Sensitivity equations have same structure as ADE
  - Calculation re-use
- Long time step viable for integration of sensitivity equations
  - Implicit approach
  - Concentrations known
  - Decoupled approach gains stability

Relative Execution Time of Sensitivity Analysis

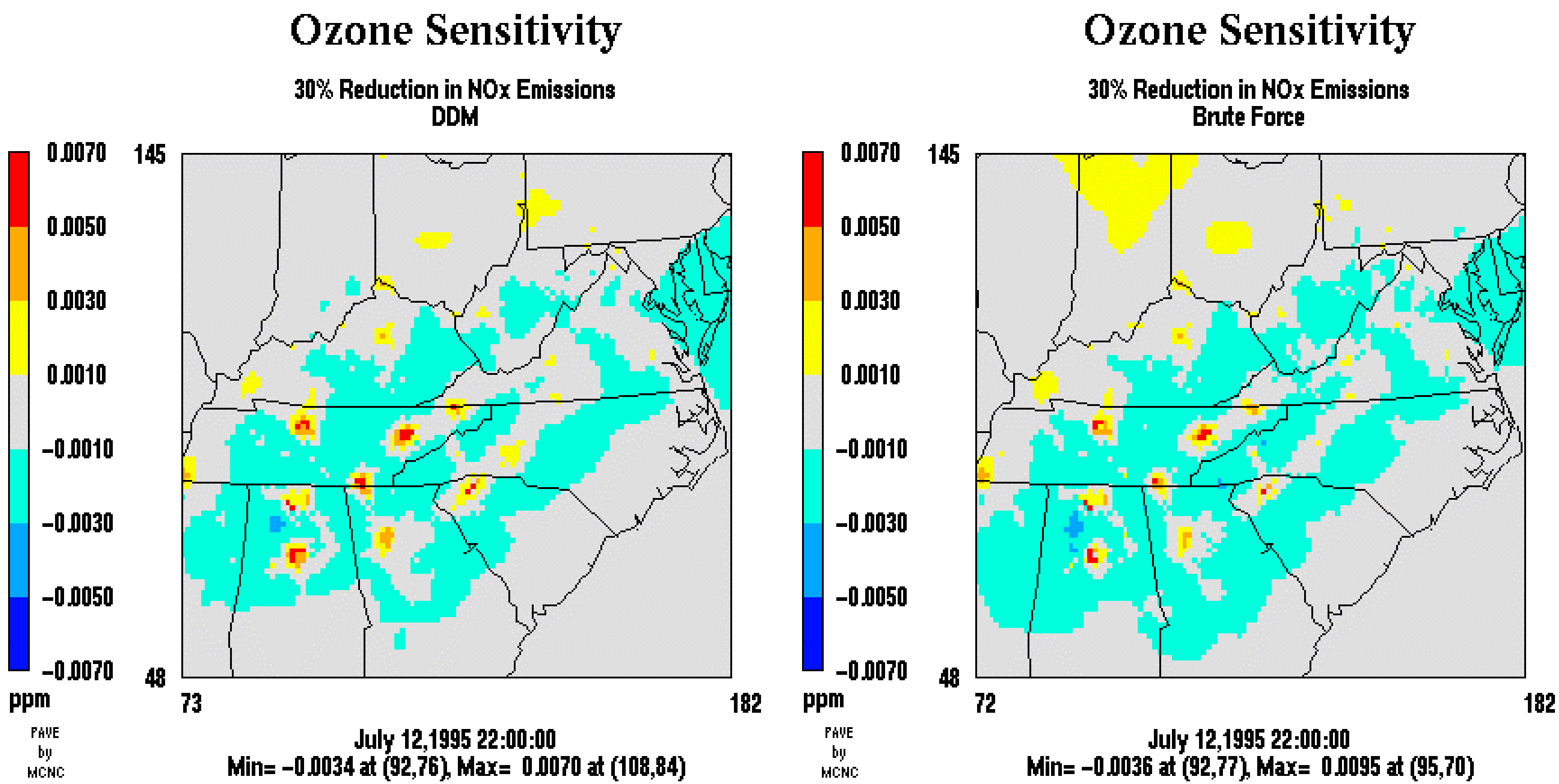
Relative execution time for sensitivity analysis[a]	
Concentrations alone (base case simulation)	1.0
Sensitivity coefficients to one parameters[b,c]	1.30
Sensitivity coefficients to ten parameters[b,d]	1.52
Sensitivity coefficients to twenty parameters[b,e]	1.81

[a] A set of sensitivity coefficients represent all compound sensitivities to a given parameter or input.
[b] Includes time needed to calculate concentrations.
[c] Ozone initial concentration.
[d] Five initial conditions and five rate constants.
[e] Five initial conditions and fifteen rate constants.

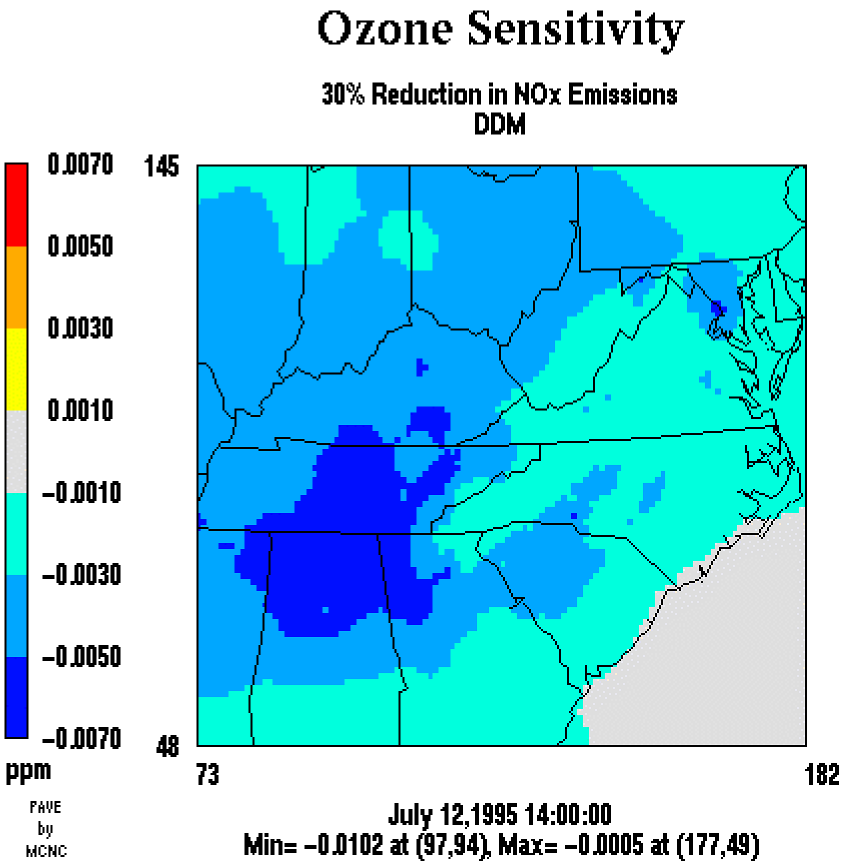
Direct Sensitivity Analysis

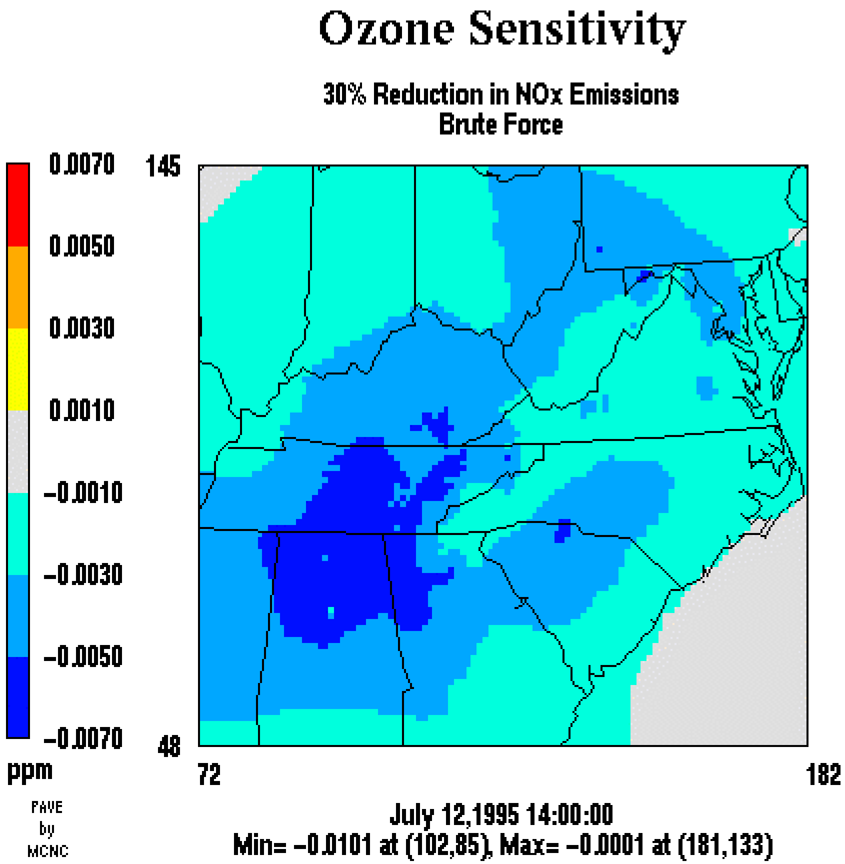
- Tests
  - Compare against brute force @ +/- 10%, 30% changes in emissions
    - Same general results without numerical noise (which dominates at 10%)
    - Response to NO_x & VOC emissions changes ~linear up to > 30%
    - Works for aerosols, though dealing with equilibriums adds complexity
- Applications
  - Uncertainty analysis of chemical mechanism
  - Reactivity analysis
    - VOC impact on ozone by species
  - Long range transport for “small” emission changes
    - Individual sources too small to detect accurately using traditional approach
  - Source-receptor Quantification
  - Inverse modeling for emissions assessment

Test of DDM & Nonlinearities

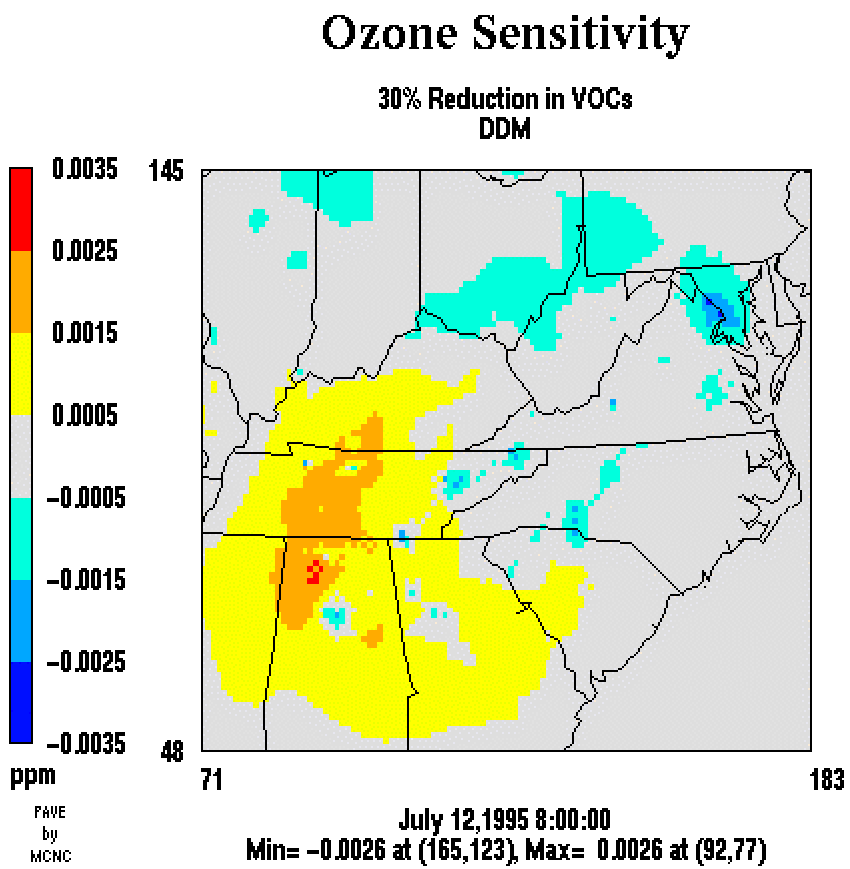


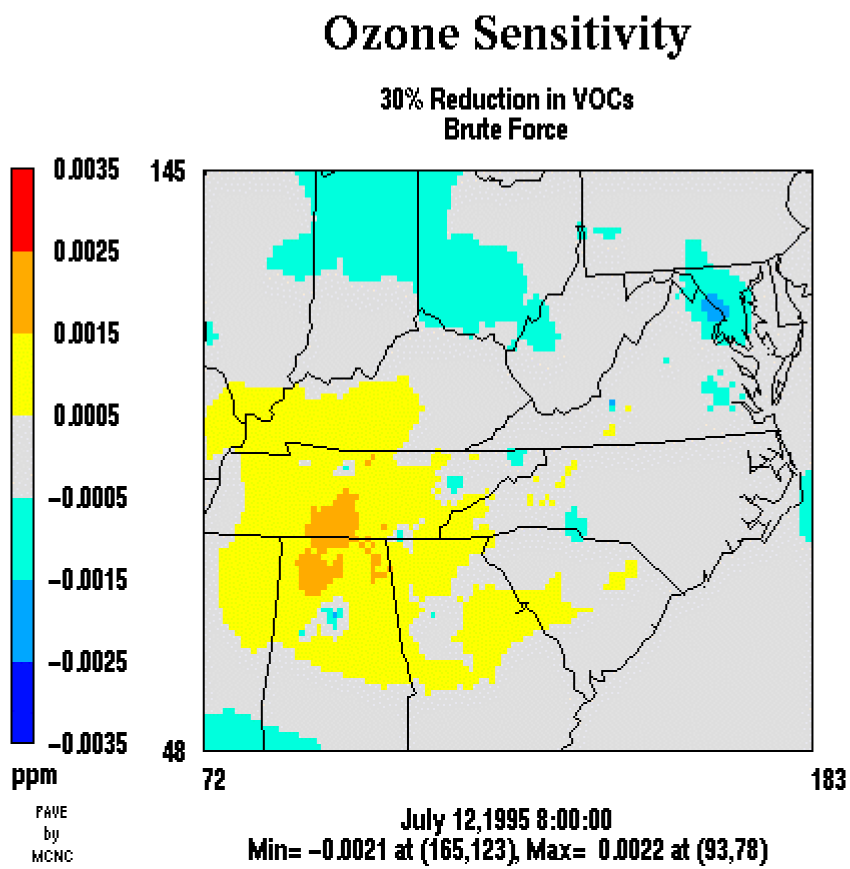
Test of DDM & Nonlinearities





Test of DDM & Nonlinearities



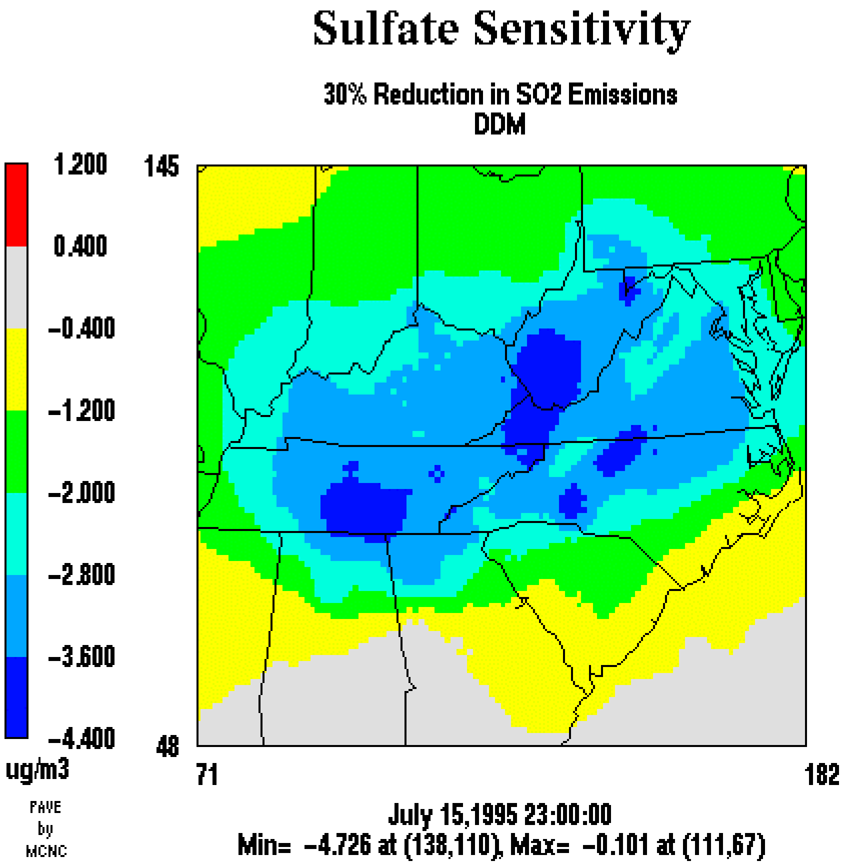


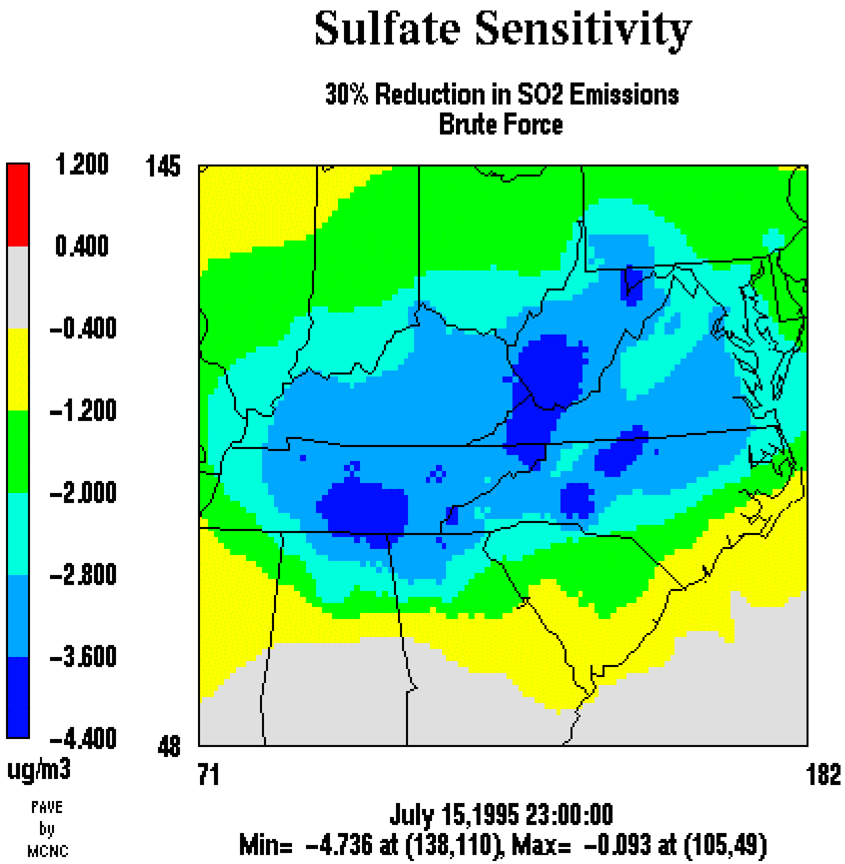
DDM had ~15% greater dynamic response

Application of DDM-3D

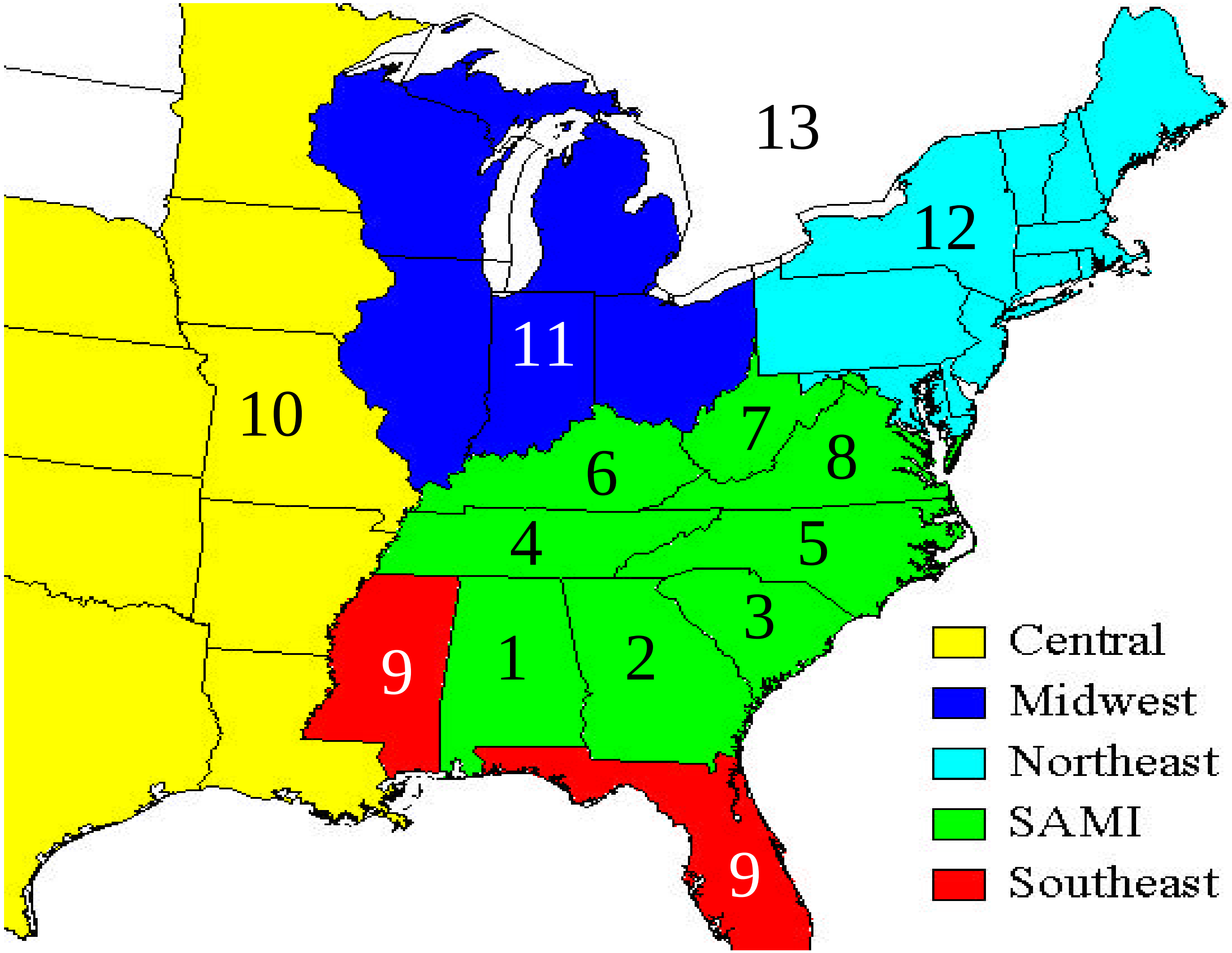
- Implemented in CIT, URM, MAQSIP and CMAQ photochemical AQMs
- Initial application to Los Angeles
  - Examine sensitivity of model results to:
    - Rate constants
    - Emissions
    - Deposition velocities
    - I.C.s and B.C.s
  - Results used for "Area of Influence" method demonstration, uncertainty analysis, etc.
- Applied to U.S.-Mexico Border, eastern US, elsewhere
- Example: Application in URM to SAMI

Sulfate Sensitivity to SO_2 Emissions

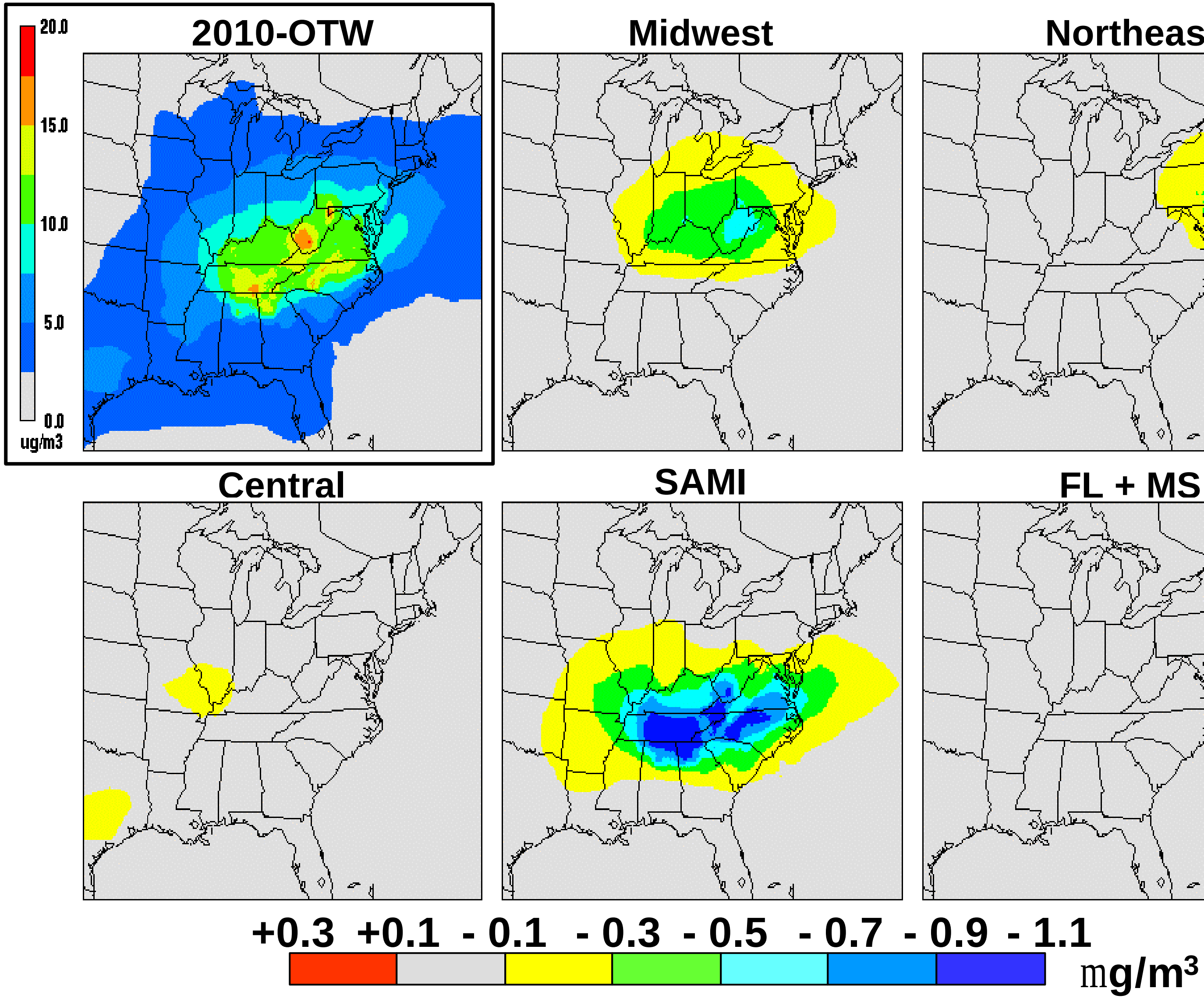




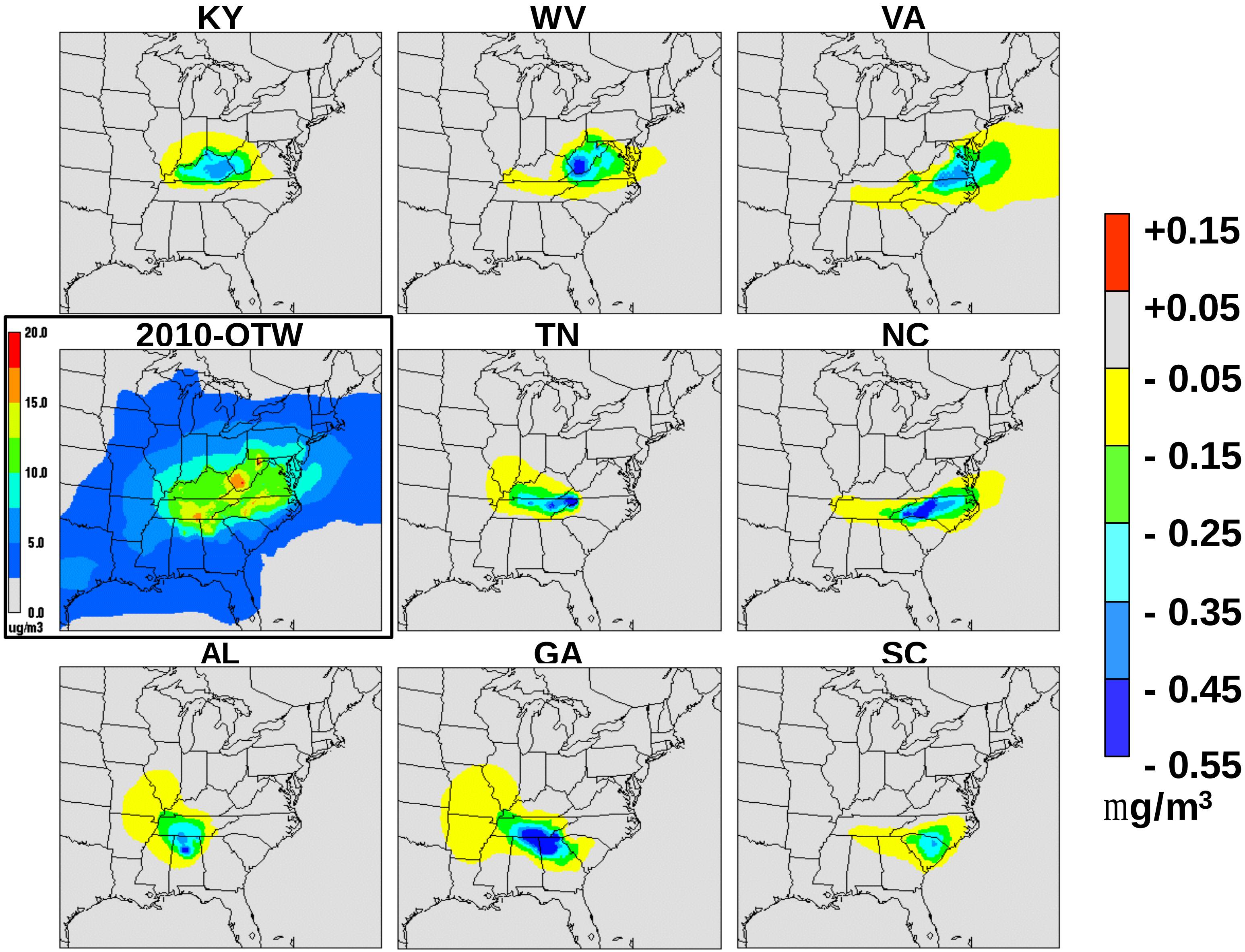
Geographic Sensitivity Regions



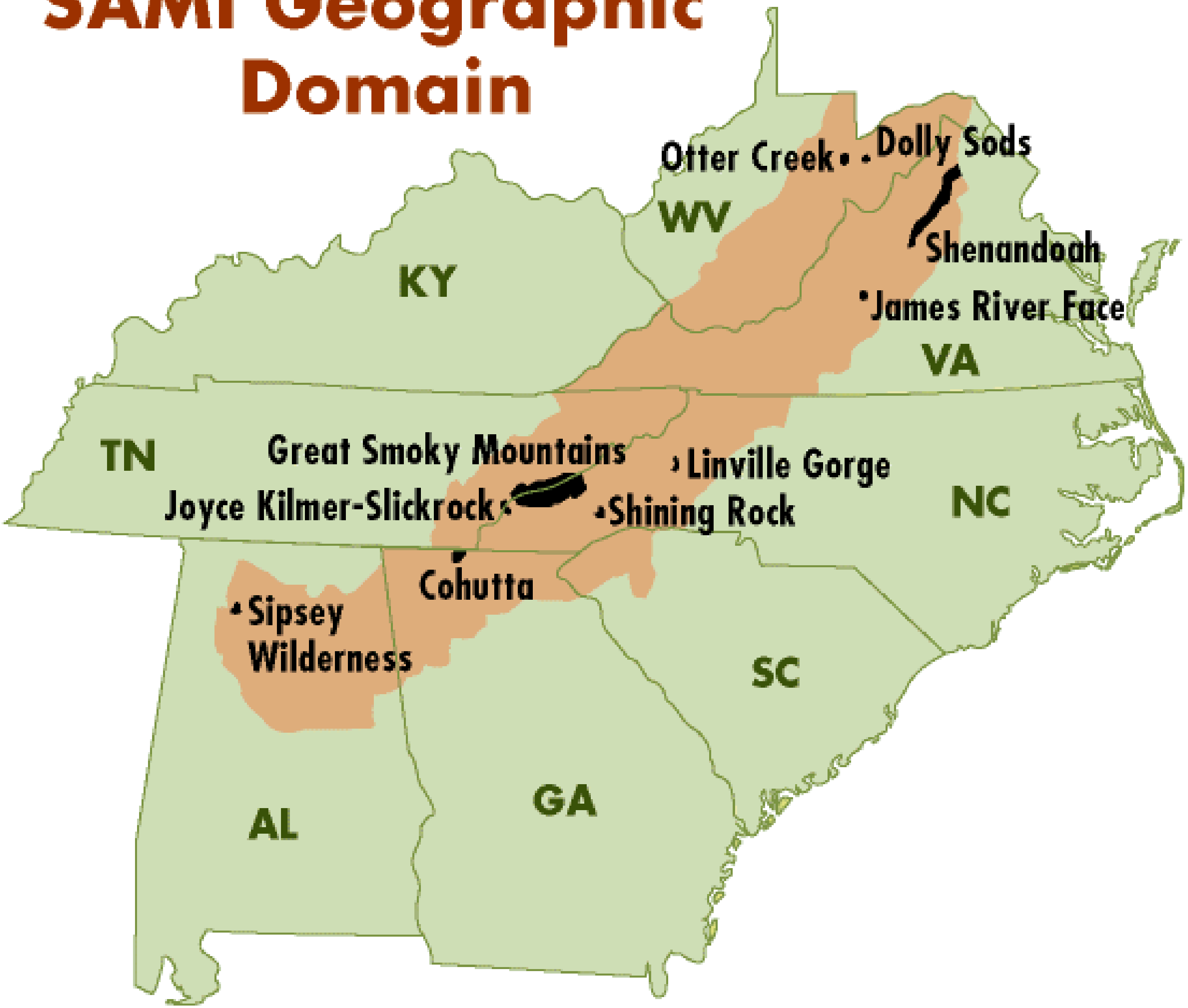
SO_4 & its Change on July 15, 1995 for a 10% Reduction of 2010-OTW SO_2 Emissions from Different Regions

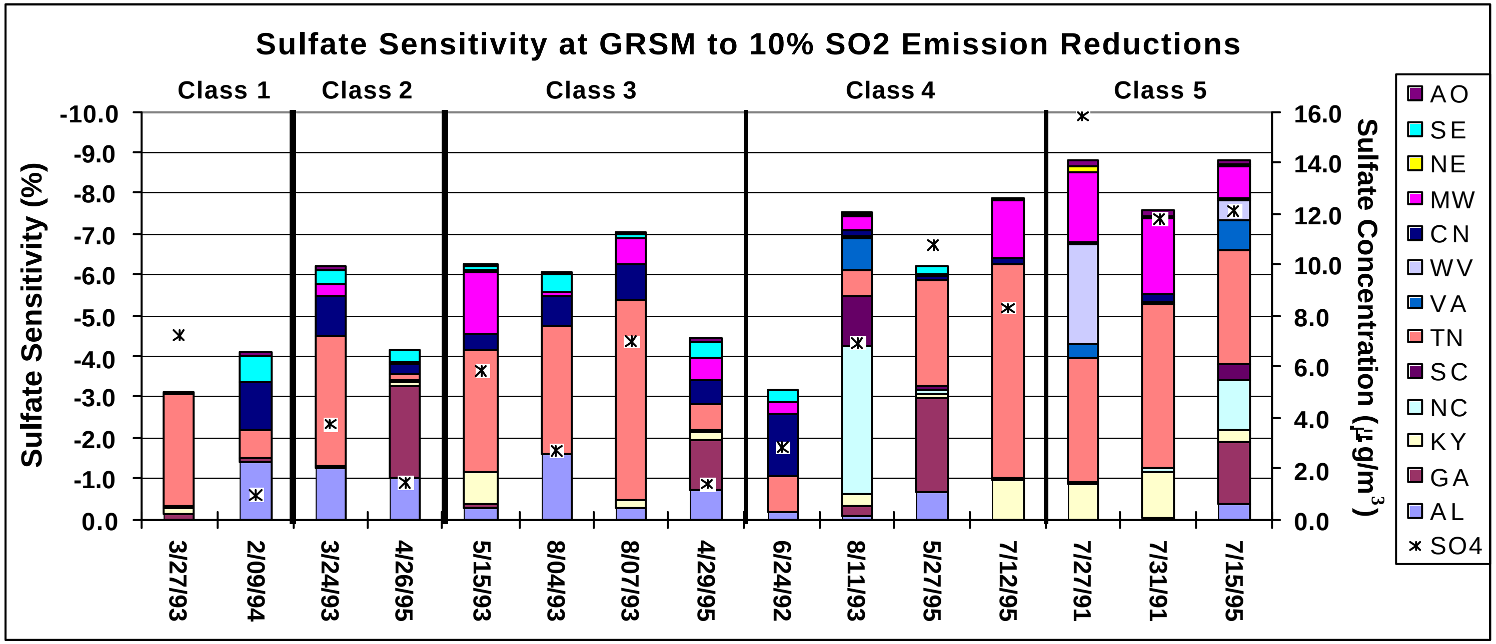
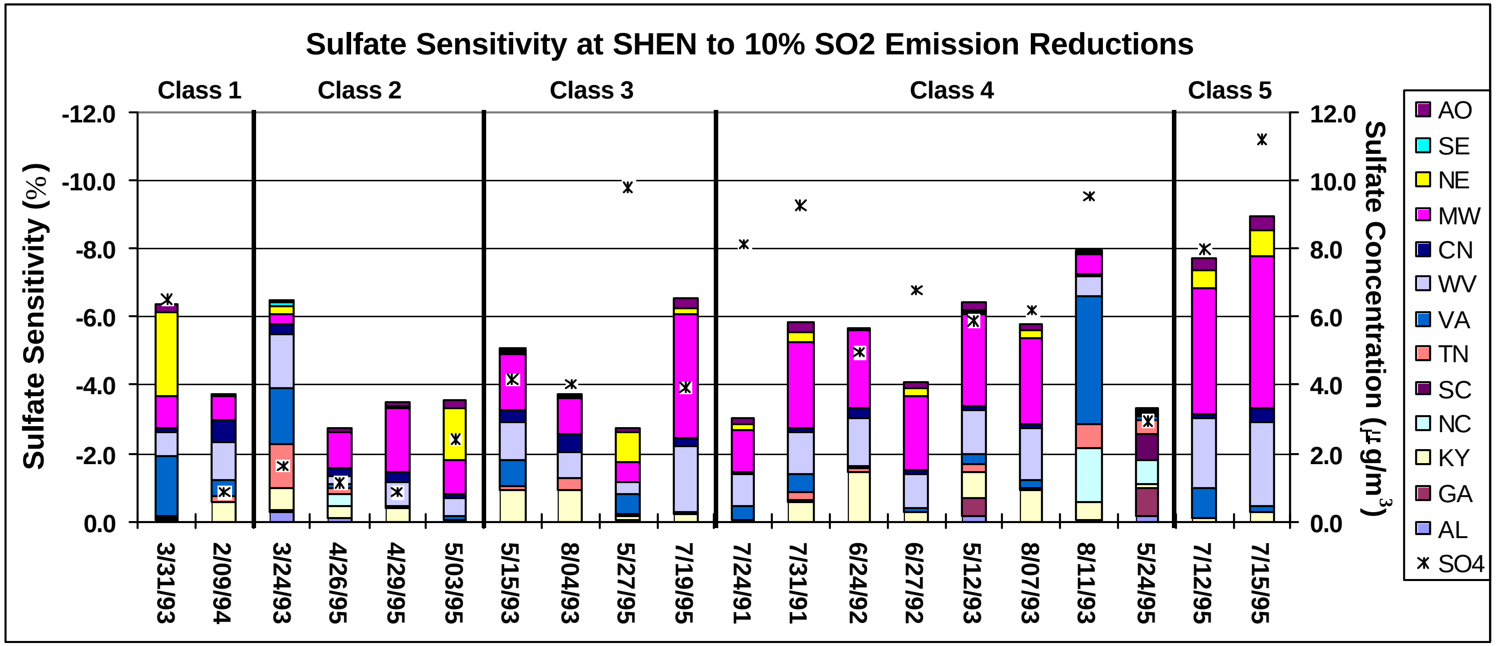


SO_4 & its Change on July 15, 1995 for a 10% Reduction of 2010-OTW SO_2 Emissions from SAMI States

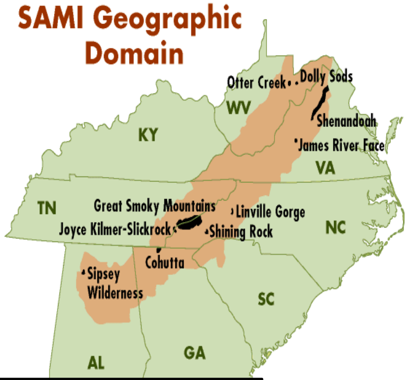


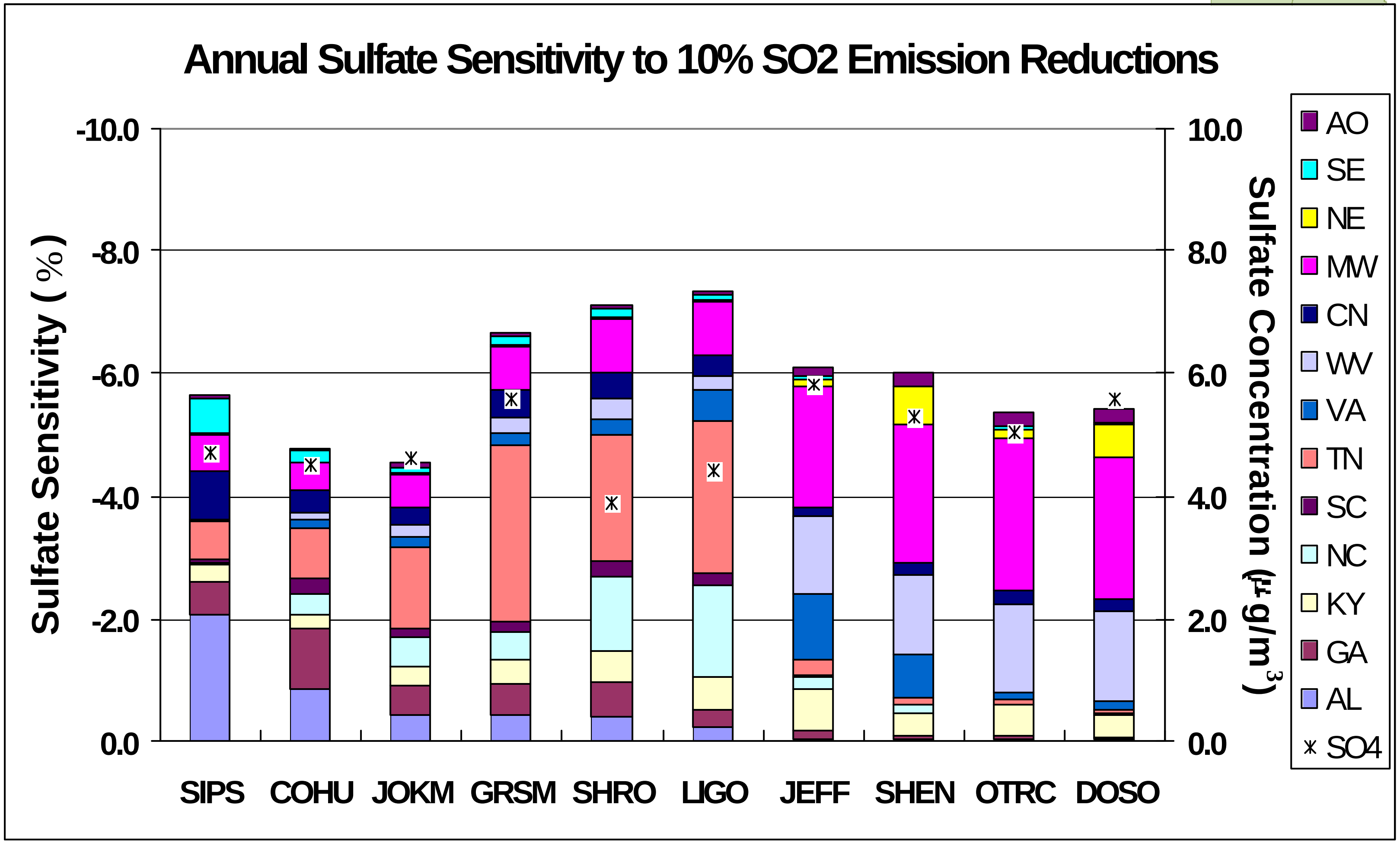
SAMI Geographic Domain




Sulfate Sensitivity at GRSM to 10% SO2 Emission Reductions
Class 1
Class 2
Class 3
Class 4
Class 5
Sulfate Sensitivity (%)
Sulfate Concentration (µg/m3)
-10.0 -9.0 -8.0 -7.0 -6.0 -5.0 -4.0 -3.0 -2.0 -1.0 0.0
16.0 14.0 12.0 10.0 8.0 6.0 4.0 2.0 0.0
3/27/93 2/09/94 3/24/93 4/26/95 5/15/93 8/04/93 8/07/93 4/29/95 6/24/92 8/11/93 5/27/95 7/12/95 7/27/91 7/31/91 7/15/95
AO SE NE MW CN WV VA TN SC NC KY GA AL SO4

Sulfate Sensitivity at SHEN to 10% SO2 Emission Reductions
Class 1
Class 2
Class 3
Class 4
Class 5
Sulfate Sensitivity (%)
Sulfate Concentration (µg/m3)
-12.0 -10.0 -8.0 -6.0 -4.0 -2.0 0.0
12.0 10.0 8.0 6.0 4.0 2.0 0.0
3/31/93 2/09/94 3/24/93 4/26/95 4/29/95 5/03/95 5/15/93 8/04/93 5/27/95 7/19/95 7/24/91 7/31/91 6/24/92 6/27/92 5/12/93 8/07/93 8/11/93 5/24/95 7/12/95 7/15/95
AO SE NE MW CN WV VA TN SC NC KY GA AL SO4

Annual Sulfate Sensitivity





Summary

- Advanced “Nesting” Techniques
  - Multiscale methods currently most advanced
  - Adaptive grids on the horizon
- Advanced modeling techniques
  - Sensitivity analysis provides detailed knowledge about model responses
- Model performance is very good
  - Ozone simulated well
  - PM still has uncertainties