The Decoupled Direct Method for atmospheric sensitivity analysis

Daniel Cohan
Georgia Dept. of Natural Resources,
Environmental Protection Division

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Concept: Brute force and DDM sensitivity analysis

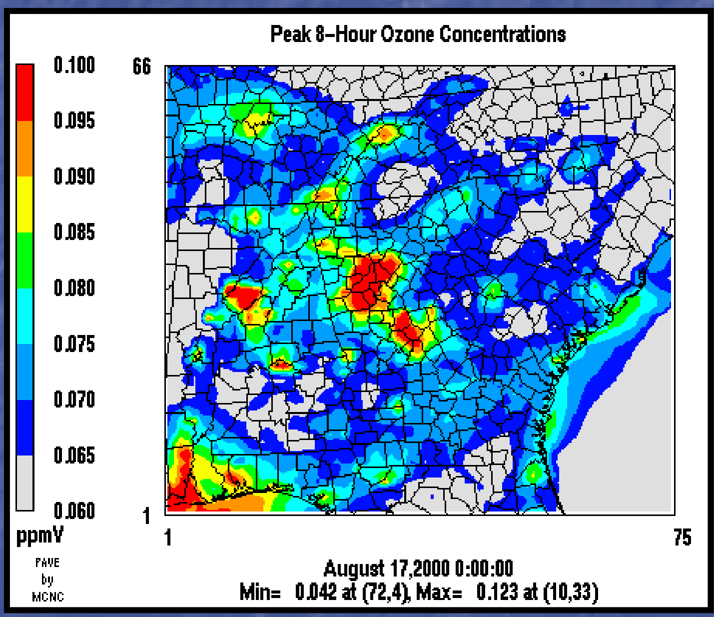
Emissions, Initial Conditions, Boundary Conditions, etc.

↓

Air Quality Model

↓

Concentrations



Check scientific understanding
Extend beyond observations
Forecasting and prediction

Δ (e.g., Atlanta Emissions)

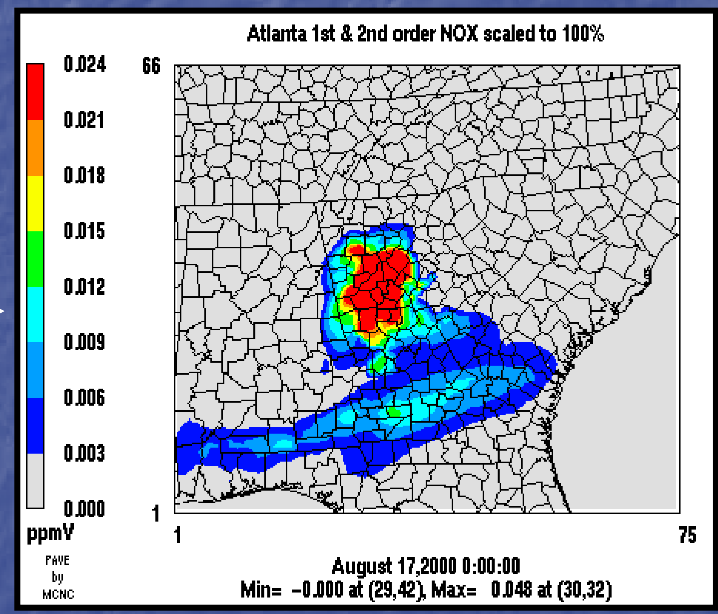
↓

Air Quality Model

↓

Sensitivities

Δ →



Atmospheric response
Control strategies
Source apportionment

Brute force and DDM

- **Brute-Force Method:**
  Run CMAQ separately for each of N perturbations, and finite difference from "base case"
- **Decoupled Direct Method:**
  Solve for local sensitivities decoupled from concentrations, using the same numerical routines

1st order

$$S_n^{(1)} = \frac{C_n - C_0}{\Delta\varepsilon_n}$$

$$S_n^{(1)} = \frac{\partial C}{\partial \varepsilon_n}$$

2nd order

$$S_n^{(2)} = \frac{C_{+n} - 2C_0 + C_{-n}}{(\Delta\varepsilon_n)^2}$$

$$S_n^{(2)} = \frac{\partial^2 C}{\partial \varepsilon_n^2}$$

Solving the atmospheric diffusion equation

Concentrations

$$\frac{\partial C}{\partial t} = -\nabla(uC) + \nabla(K\nabla C) + R + E$$

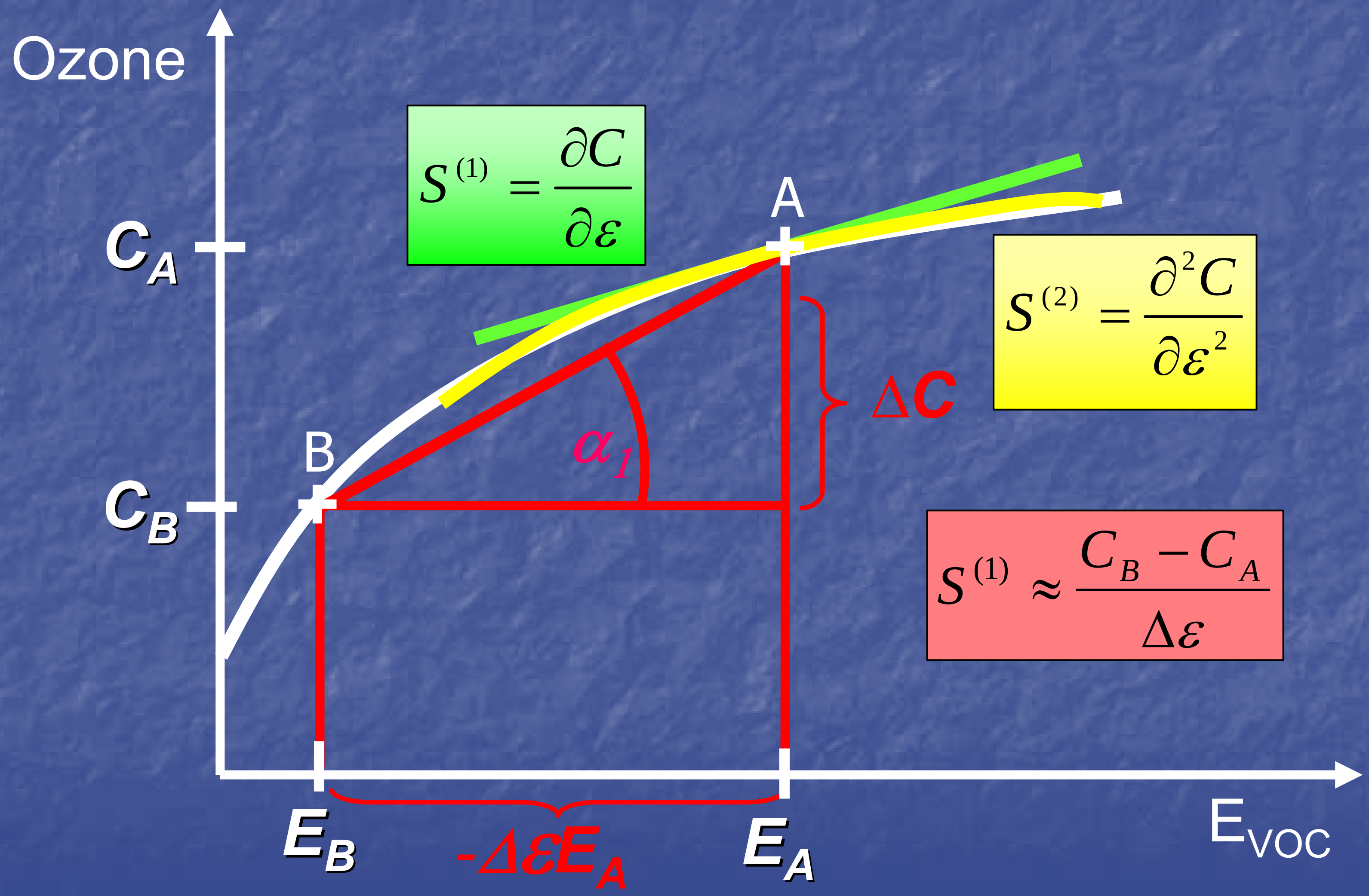
↑ Advection ↑ Diffusion ↑ Chem. ↑ Emis.

↓ ↓ ↓ ↓

Sensitivities

$$\frac{\partial S}{\partial t} = -\nabla(uS) + \nabla(K\nabla S) + JS + \tilde{E}$$

Brute Force and HDDM-3D

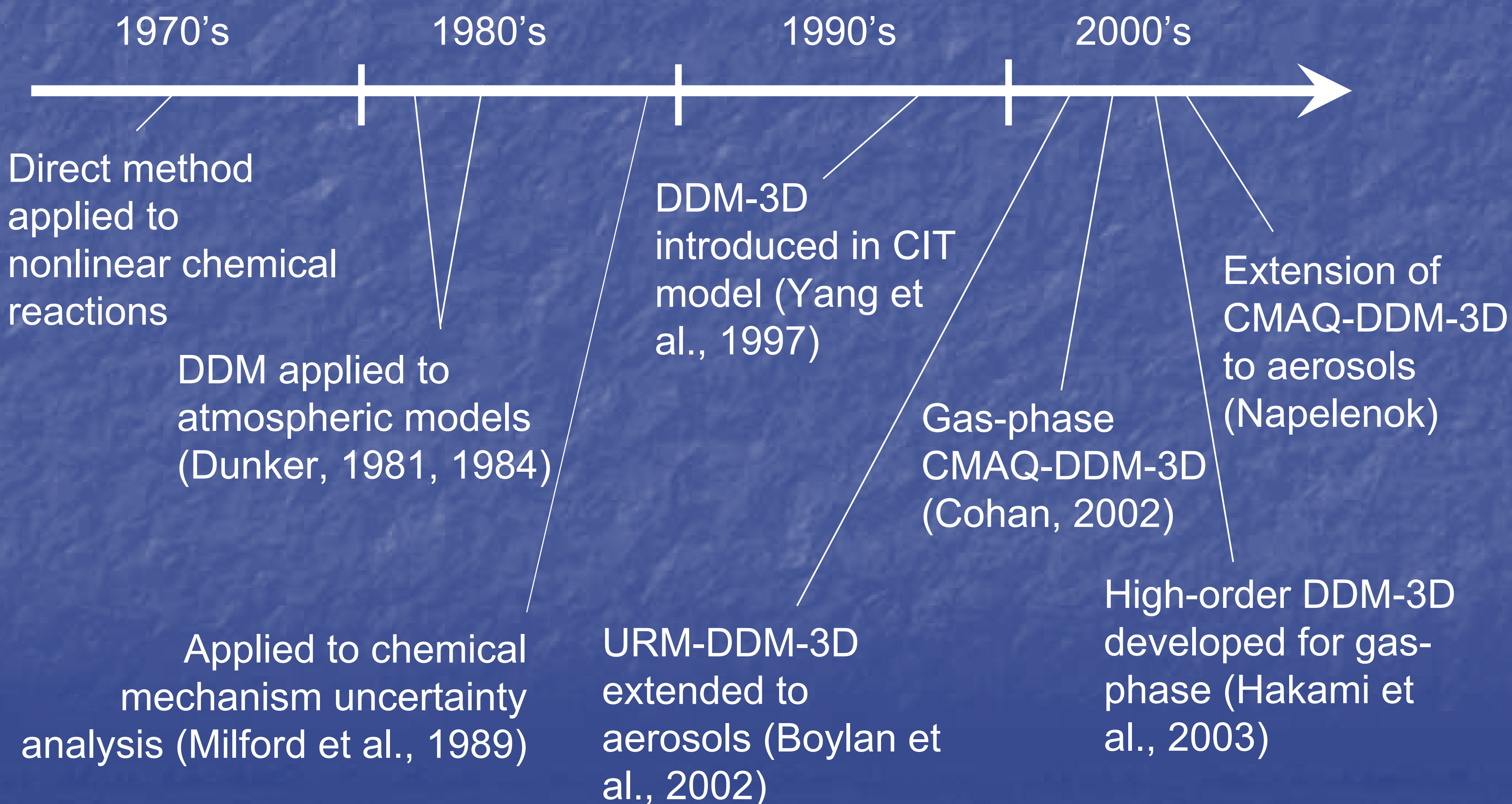


DDM Pro & Con

- ✓ Computational and space efficiency
  - ✓ In CMAQ, speed-up is only ~1/3 because chemistry is fast
- ✓ Very accurate, avoids numerical error for small Δ (local slope)
- ✓ Examine nonlinearity with HDDM

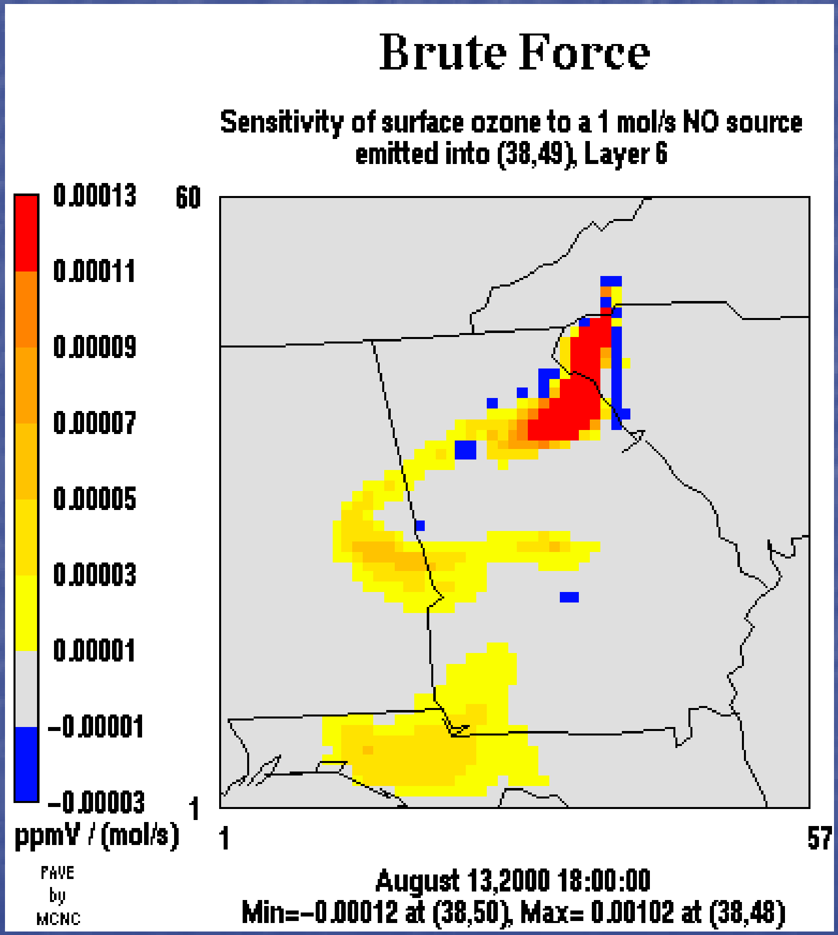
- ✗ Complex to install
  - ✗ Aqueous & aerosol especially difficult
  - ✗ Must update each time model changes
- ✗ Inaccurate for large Δ
  - ✓ May be addressed with high-order coefficients

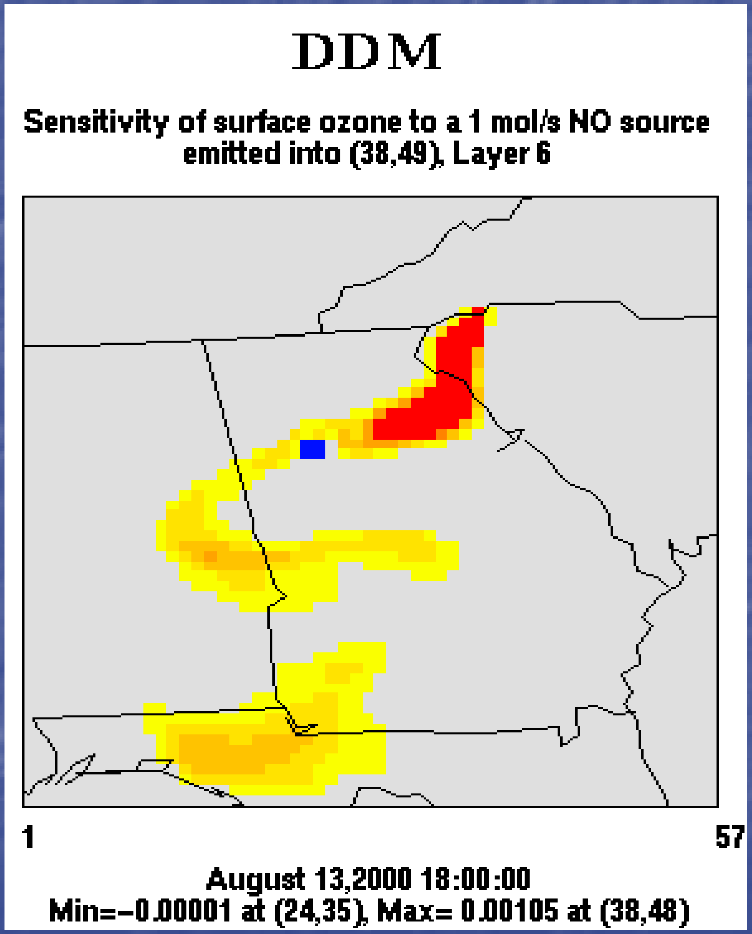
DDM timeline



Performance: CMAQ-HDDM-3D

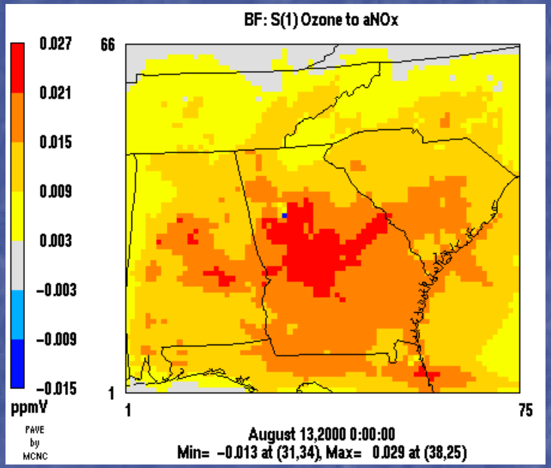
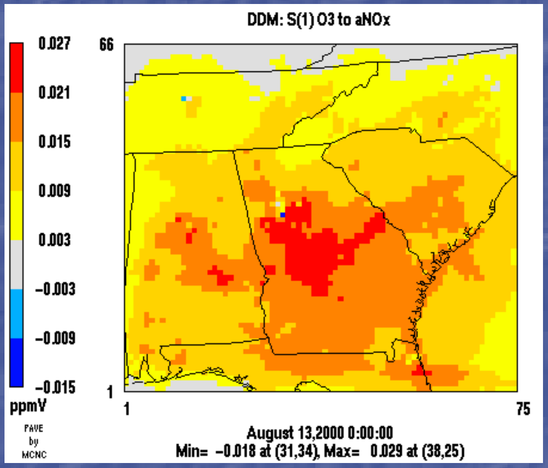
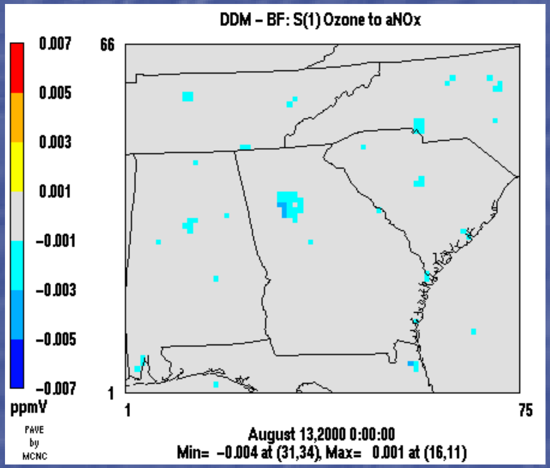
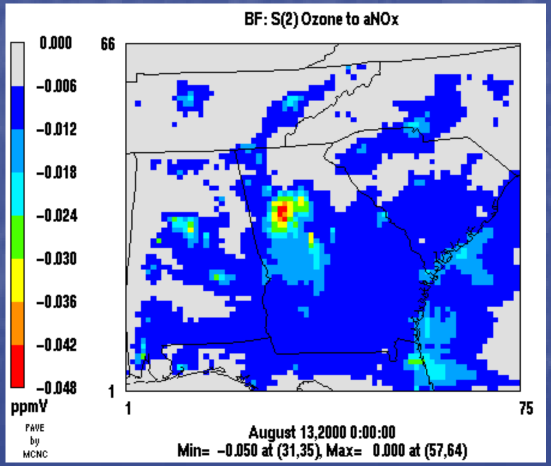
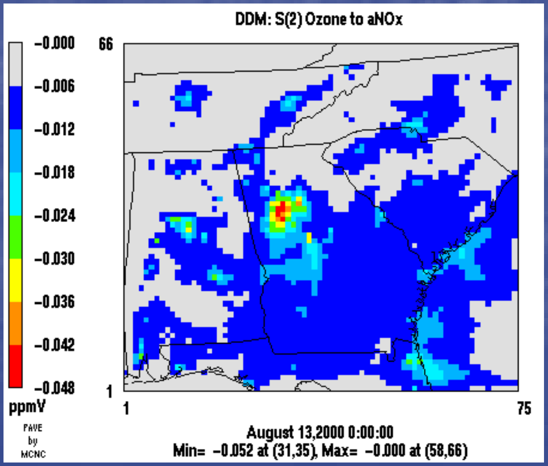
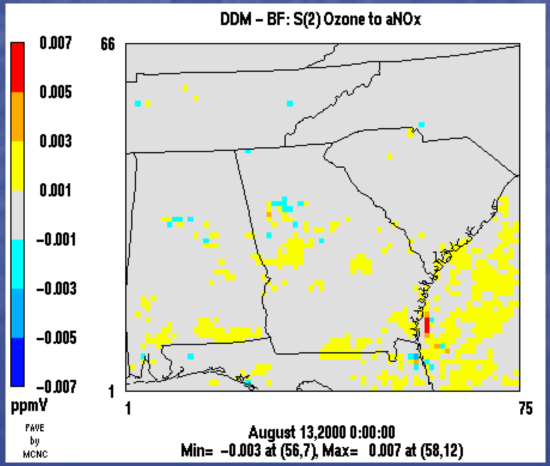
Advantage DDM: Averting numerical error





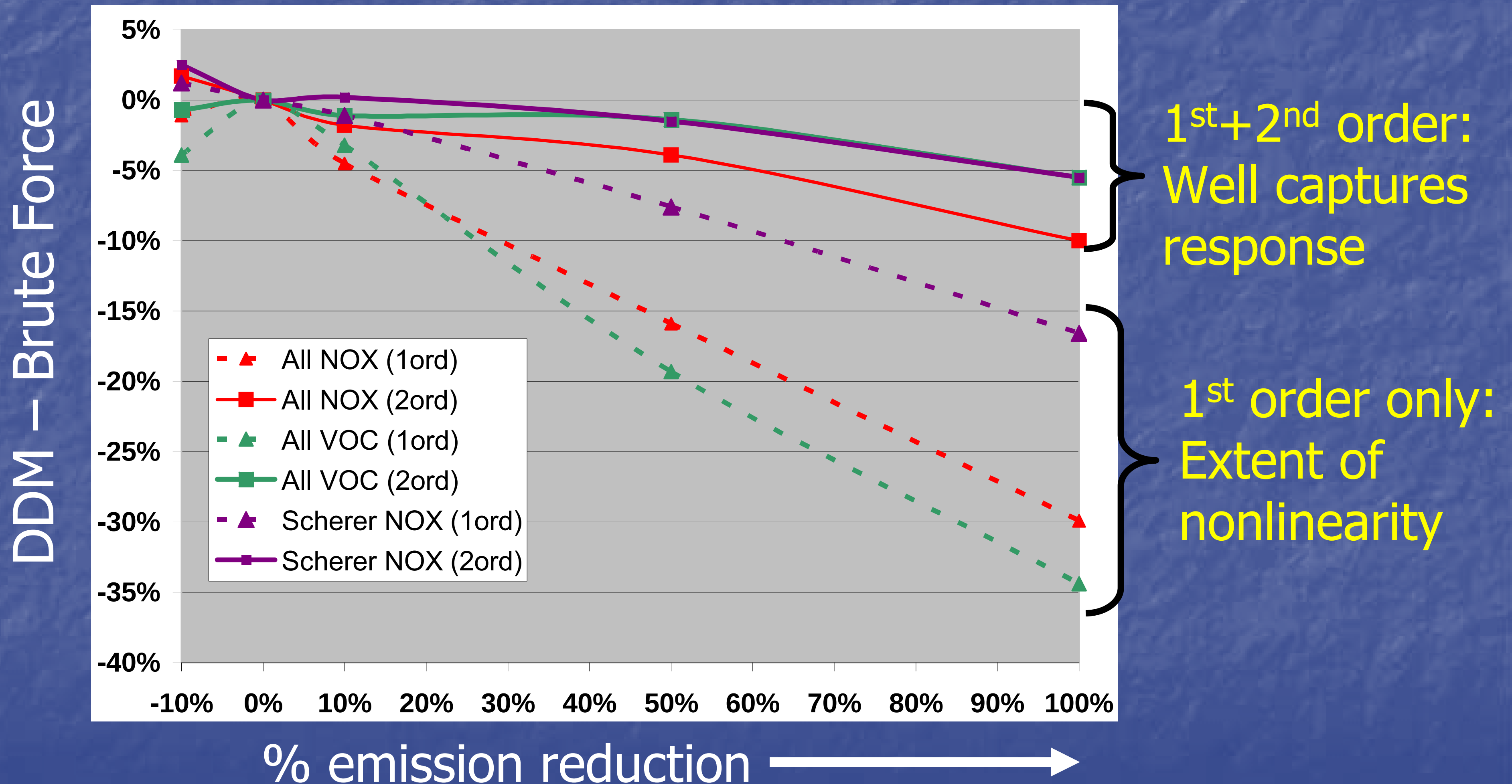
Note: Bott advection scheme

Sensitivity to domain-wide aNOx

	Brute Force	DDM	DDM - BF
$S^{(1)}$ O3 to NOx			
$S^{(2)}$ O3 to NOx			

Episode-average 8-hour ozone, 2007 emissions

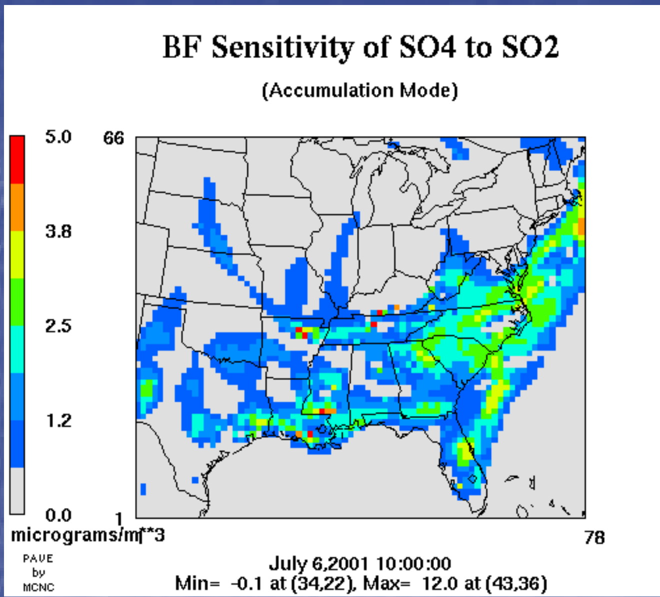
HDDM performance & nonlinearity

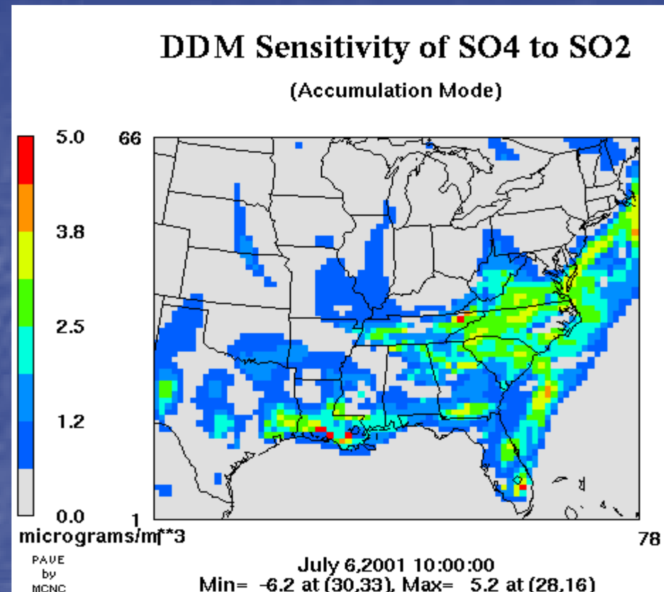


For 8-hr ozone, averaged over 12-km domain, Aug. 13-19, 2000 (2007 emissions)

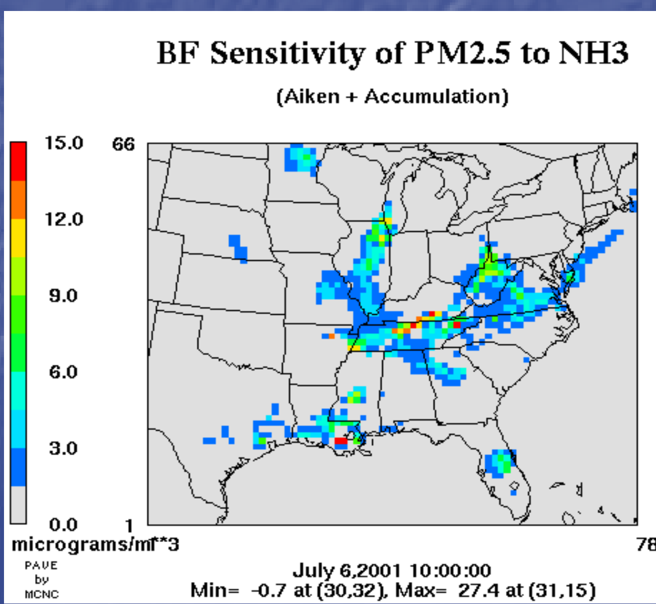
Brute Force

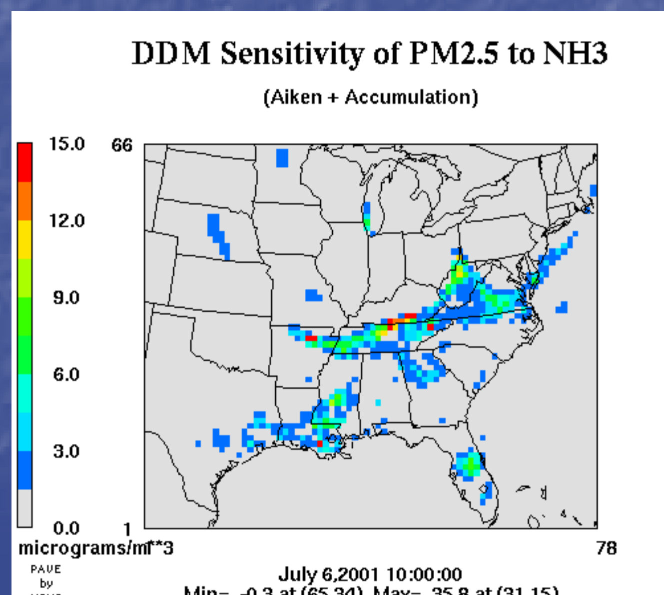
CMAQ-DDM-AERO





SO_4 to SO_2:
Good





$PM_{2.5}$ to NH_3:
Fair

S. Napelenok, GA Tech

DDM-AERO v. BF performance*

ug/m³	Conc.	SO_2	NO_x	NH_3	Xylene	Terpene
Sulfate	7.0	4.0	3.0	4.0	0.1	0.1
Nitrate	5.0	-2.0	7.0	6.0	0.5	-0.7
Ammonium	3.0	1.5	2.0	4.0	0.3	-0.1
Anth. SOA	0.3	-0.1	-0.2	~0.0	0.2	0.02
Biog. SOA	7.0	-0.1	0.6	-0.01	0.01	7.0
PM2.5	20.0	4.0	8.0	12.0	0.5	7.0

GOOD	FAIR	POOR	SMALL

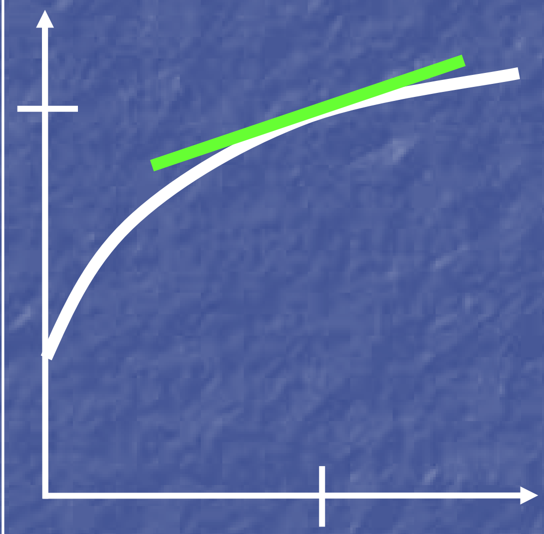
*Table shows typical sensitivities of aerosols to domain-wide emissions of selected gases

S. Napelenok, GA Tech

Applications of DDM

Applications: Taylor Expansions of HDDM-3D

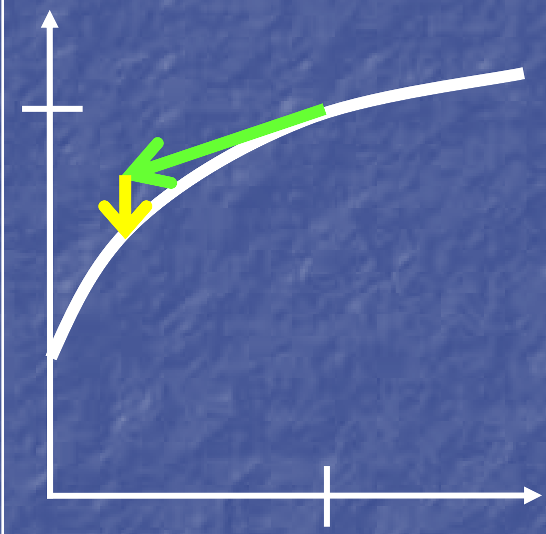
Incremental sensitivity



First-order sensitivity

$S^{(1)} = \partial C / \partial \varepsilon$

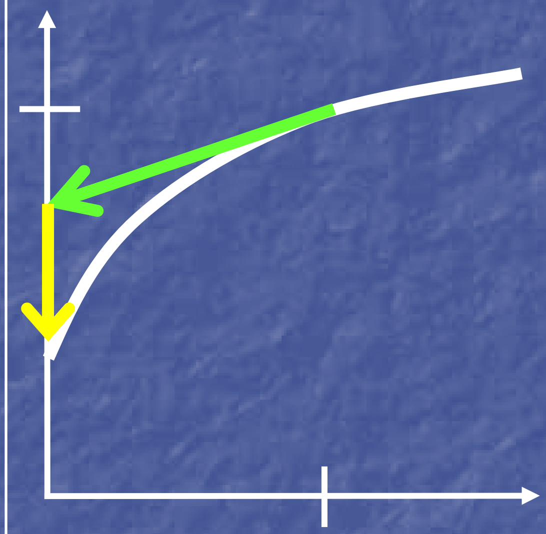
Control strategy



Taylor expansion ($\varepsilon < 0$)

$C \approx C_0 + \varepsilon S^{(1)} + 0.5\varepsilon^2 S^{(2)}$

Source apportionment

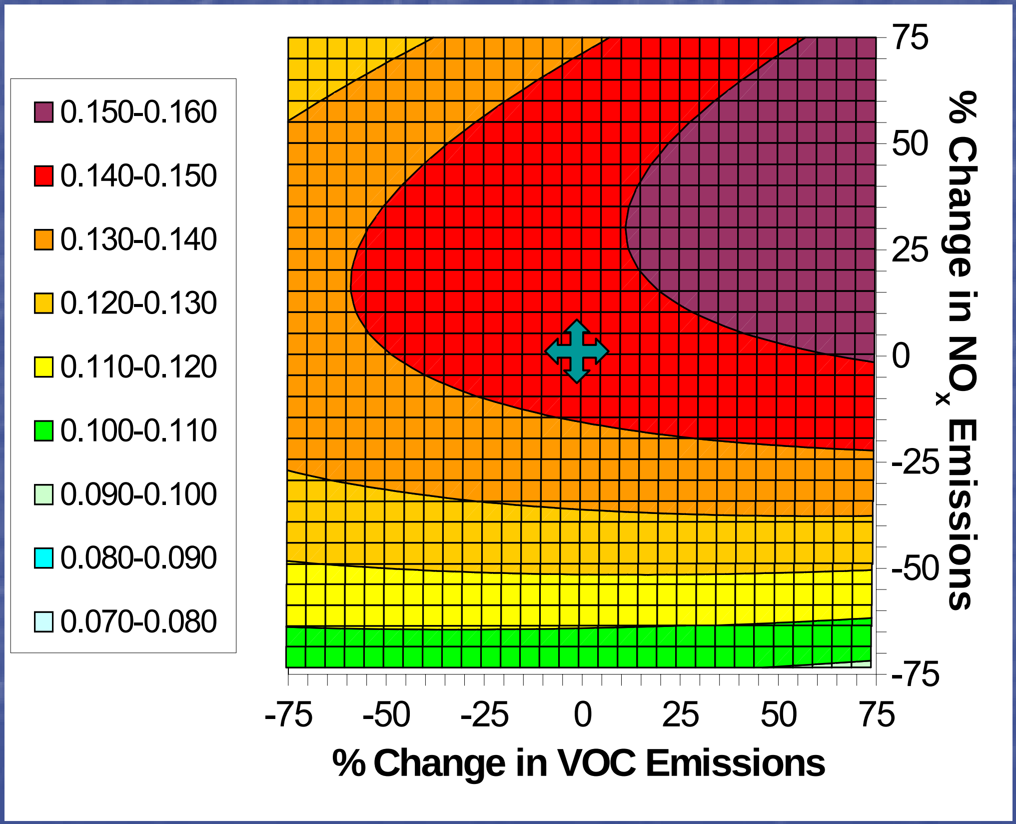


Taylor expansion ($\varepsilon = -1$)

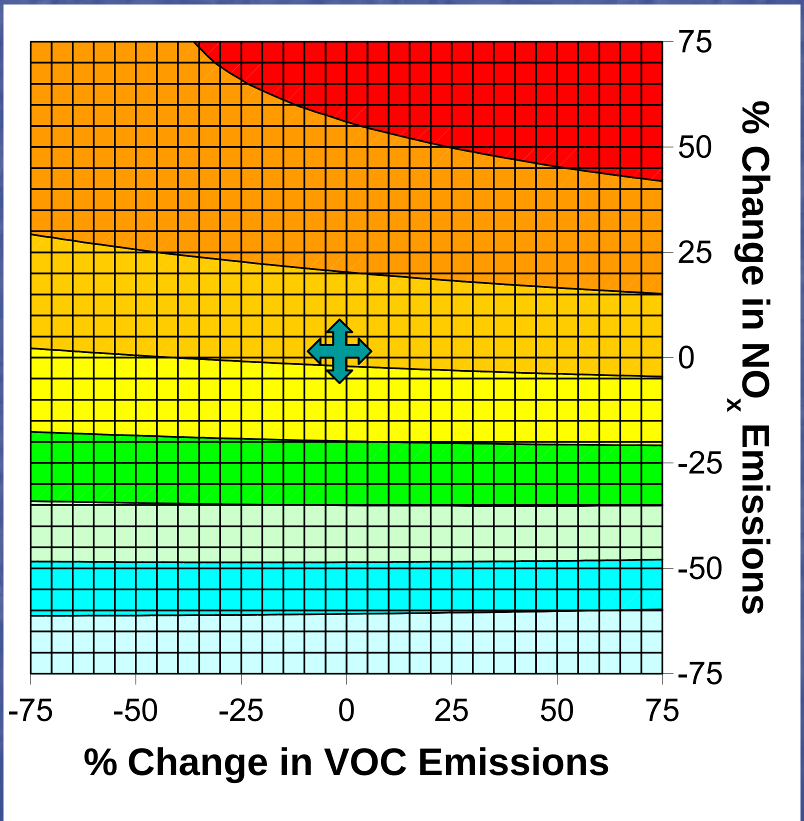
$S.C. \approx S^{(1)} - 0.5 \cdot S^{(2)}$

Ozone isopleths

Atlanta



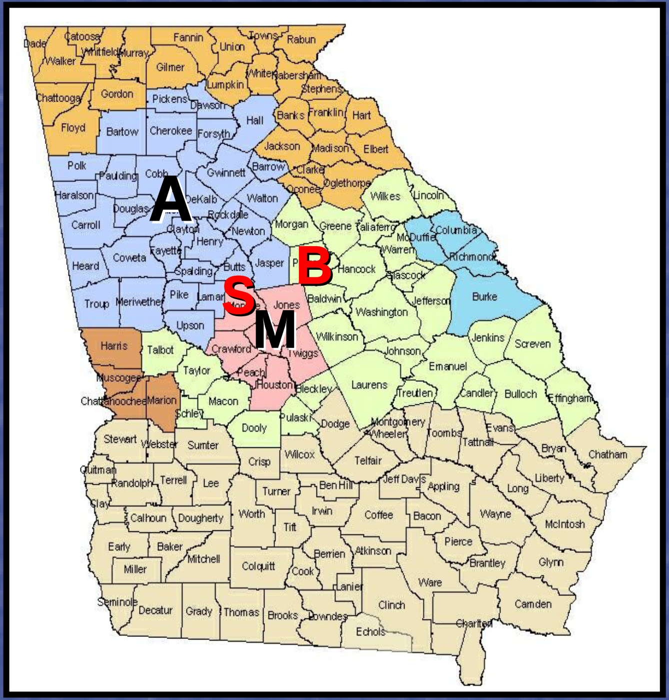
Macon

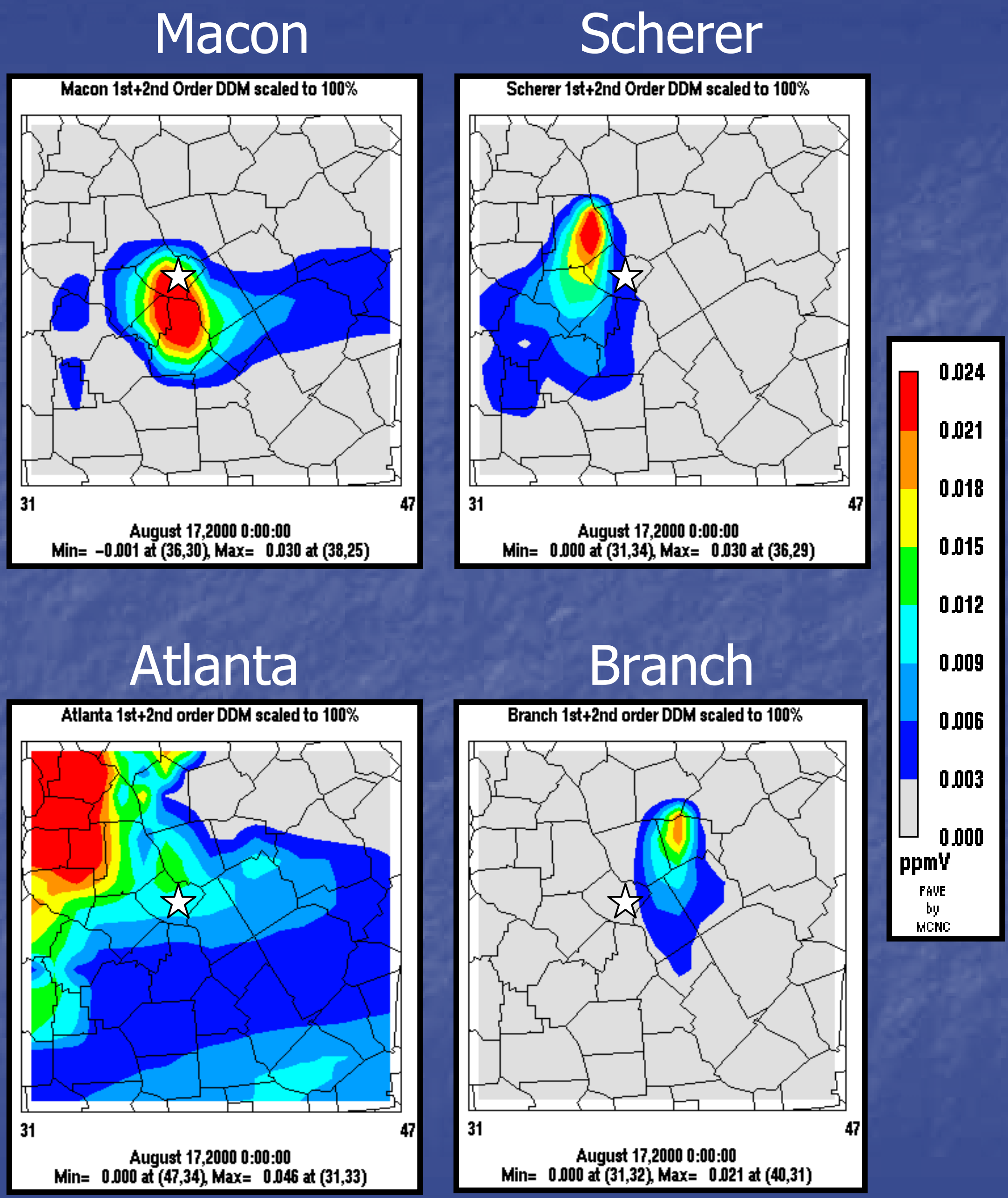


August 17, 2000, for domain-wide
Year 2000 emissions

(from the method of Hakami *et al.*, 2003)

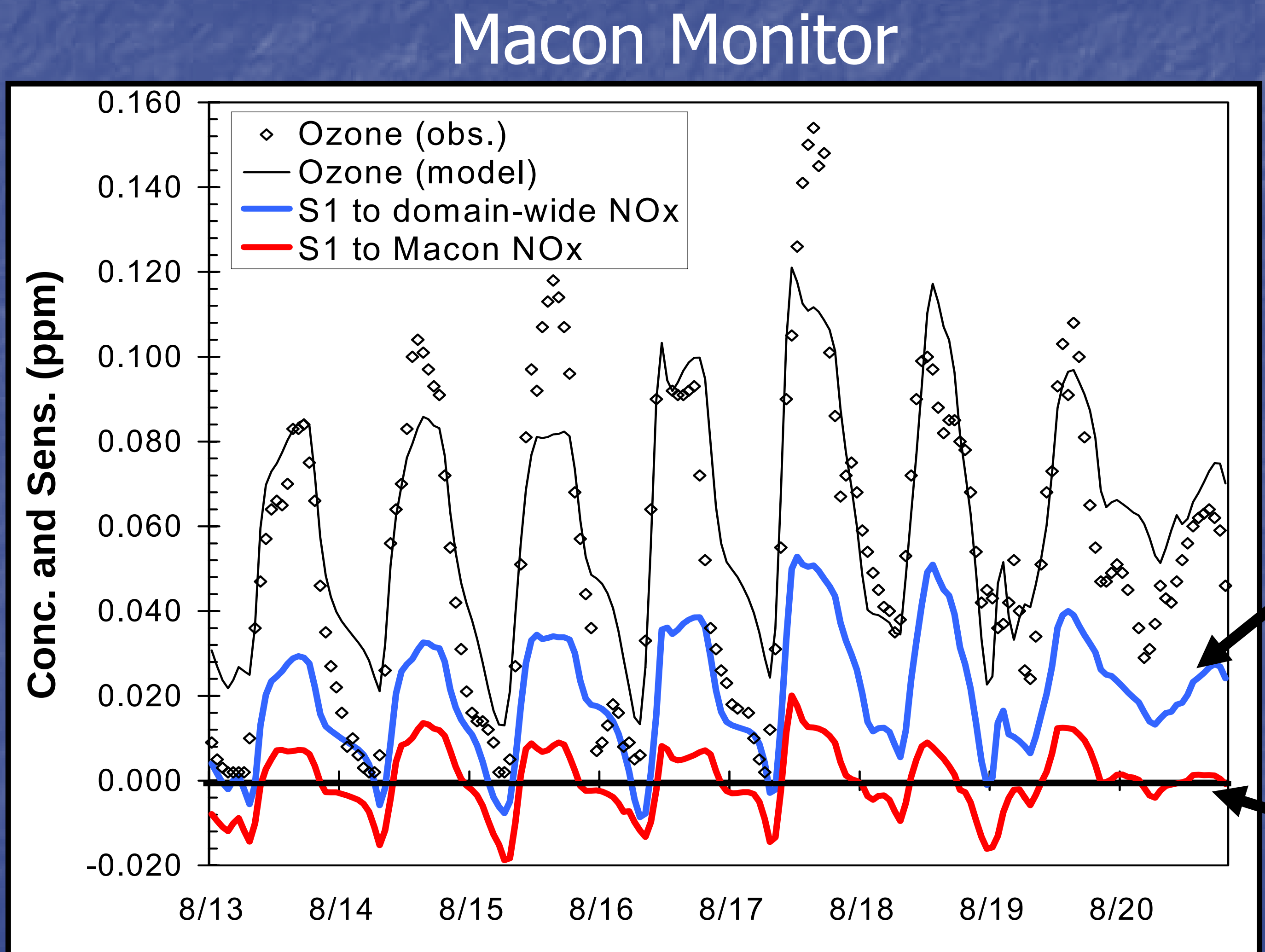
Sources of Macon ozone





8-hr ozone, Aug. 17, 2000
(2007 emissions)

Domain-wide v. local



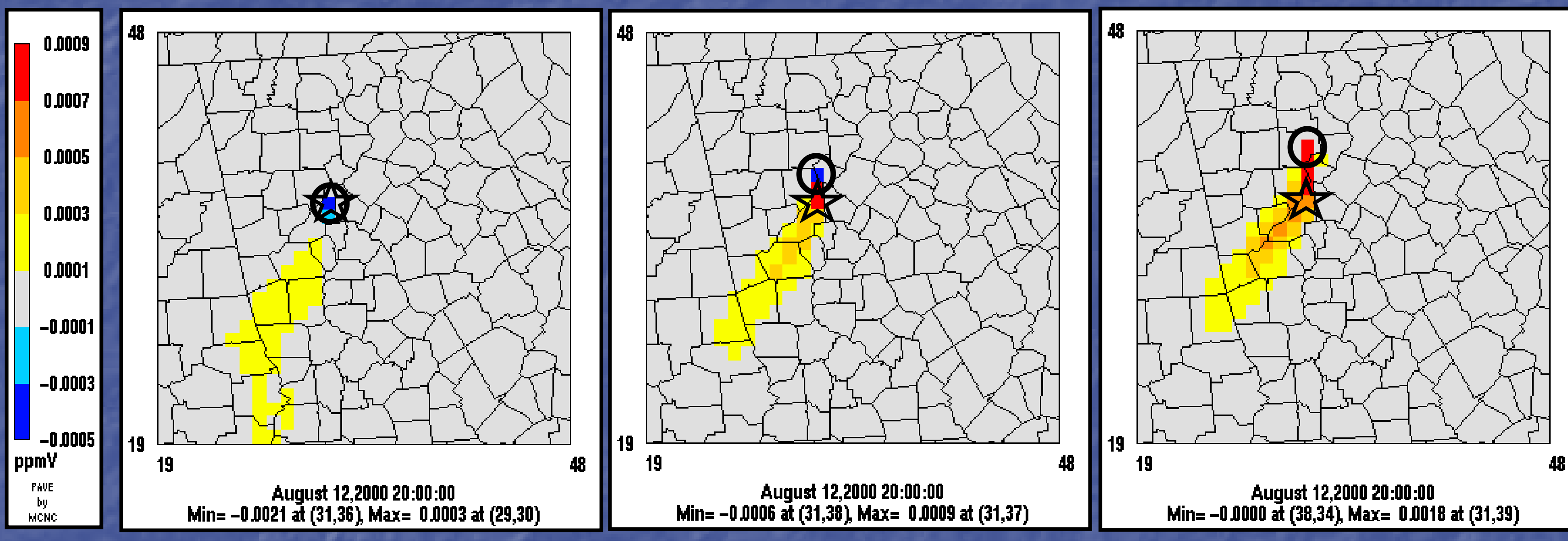
$S^{(1)}$ to dwide NO_x

$S^{(1)}$ to Macon NO_x

August 2000 episode; Year 2000 emissions

Impact of ground-level NO_x emitted from…

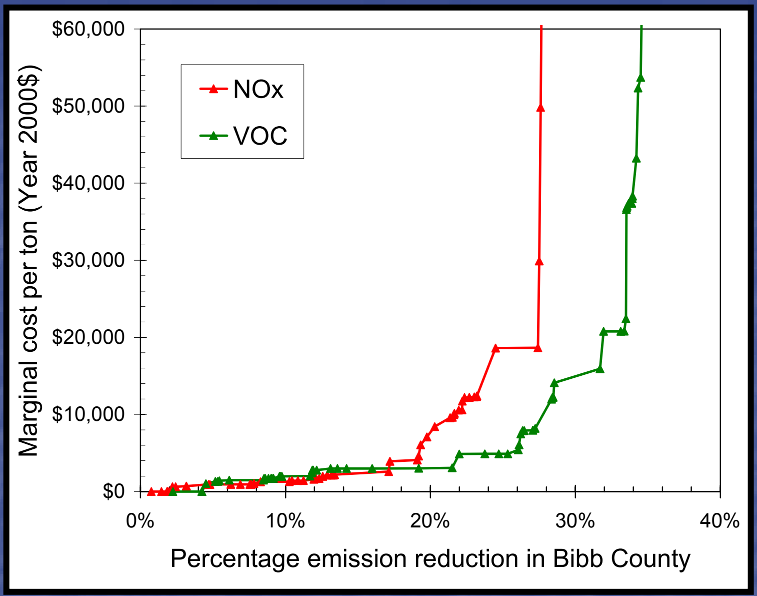
Atlanta Center | 24km north | 48 km north

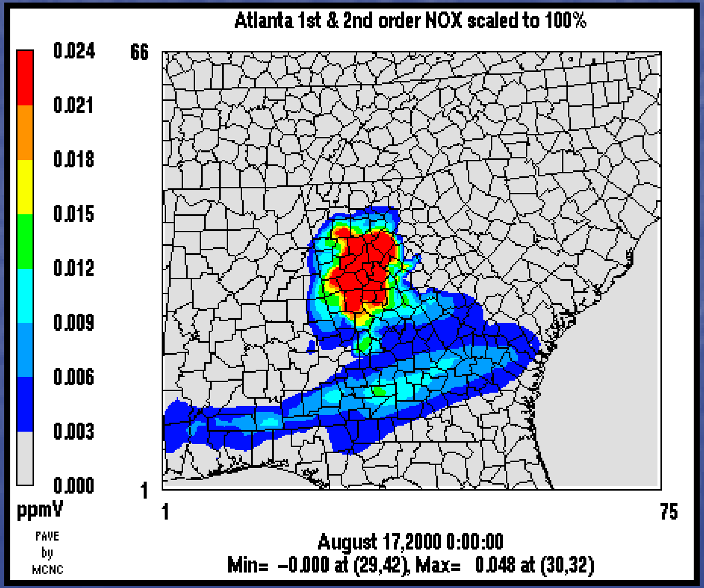


Max	0.3 ppb	0.9 ppb	1.8 ppb
Min	-2.1 ppb	-0.6 ppb	-0.0 ppb

Time-varying Layer 1 emission averaging 1 mol/s;
Ground-level ozone impact at 4 p.m. EDT, 8/12/2000

Marginal Abatement Costs by Region





Source-Receptor Response

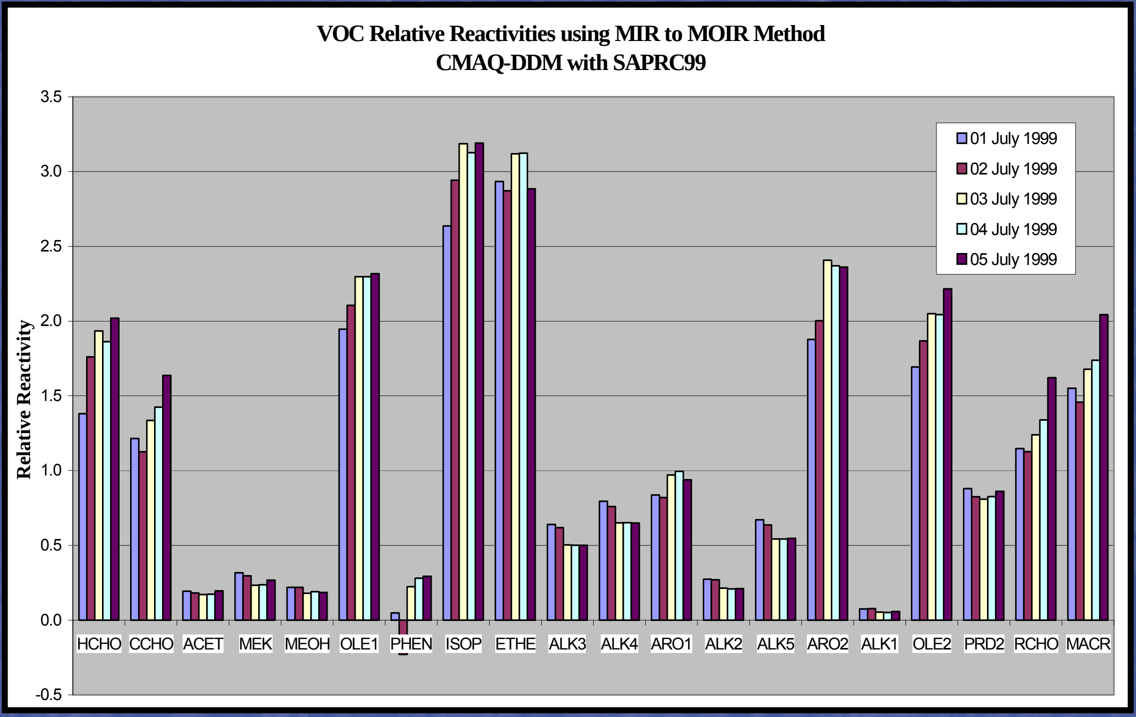
Cost

Impact

Cost-optimization:
Choose options with lowest marginal cost per impact until goal is attained or budget constraint reached

CMAQ-DDM: Community of users

- Georgia Tech
- U.S. EPA
  - Reactivity study
  - CMAQ development
- U.C. Berkeley
- NESCAUM
- Argonne National Laboratory
- CMAS (Carolina Environmental Program)
- University of Houston



(courtesy of Dr. Michelle Mebust)

For more information:

Daniel Cohan
Georgia Environmental Protection Division
(404) 362-4569
Dan_Cohan@dnr.state.ga.us

Key literature about DDM:

Dunker (1984). The decoupled direct method for calculating sensitivity coefficients in chemical kinetics. *J. Chem. Phys. 81*, 2385-2393.

Yang et al. (1997). Fast, direct sensitivity analysis of multidimensional photochemical models. *Environ. Sci. Technol. 31*, 2859-2868.

Hakami et al. (2003). High-order, direct sensitivity analysis of multidimensional air quality models. *Environ. Sci. Technol. 37*, 2442-2452.