Constraining Aerosol Health Impacts with Sensitivity Analysis using the Adjoint of CMAQ

Comprehensive Exam Proposal Presentation

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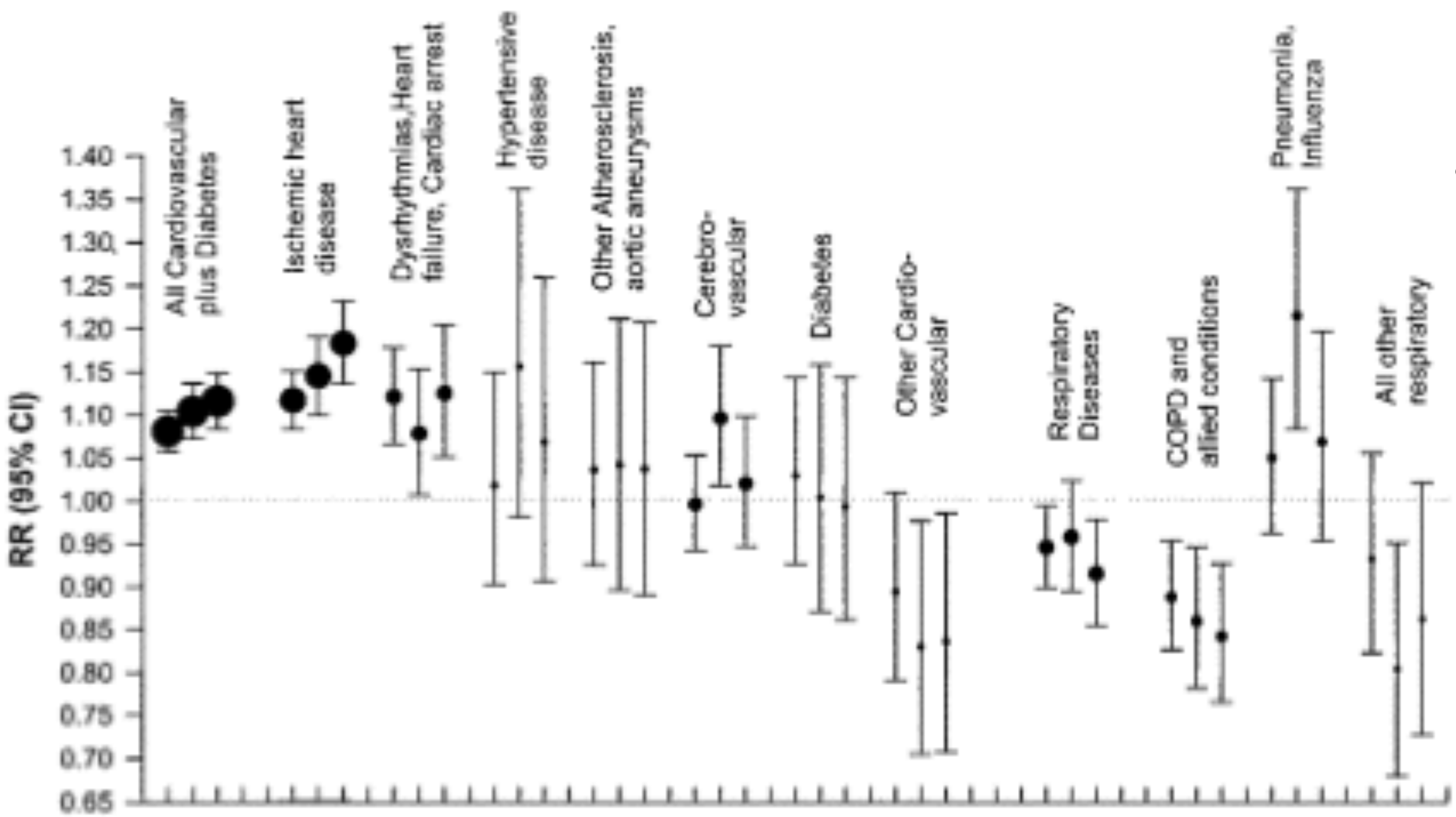
Outline

- Background
  - PM
  - Health Effects
  - Climate Effects
- Objectives
- Methods
  - CMAQ
  - Adjoint modeling
- Adjoint Validation
- Results
- Future Work

Particulate Matter (PM)

- PM is divided into three modes:
  - Coarse:
    - diameter between 2.5μm and 10μm
    - short lifetime - minutes to hours
  - Accumulation:
    - diameter between 0.1μm and 2.5μm
    - long lifetime - days to weeks
  - Nucleation:
    - diameter below 0.1μm
    - short-lived

Health Impacts of Long-term Exposure to Aerosols

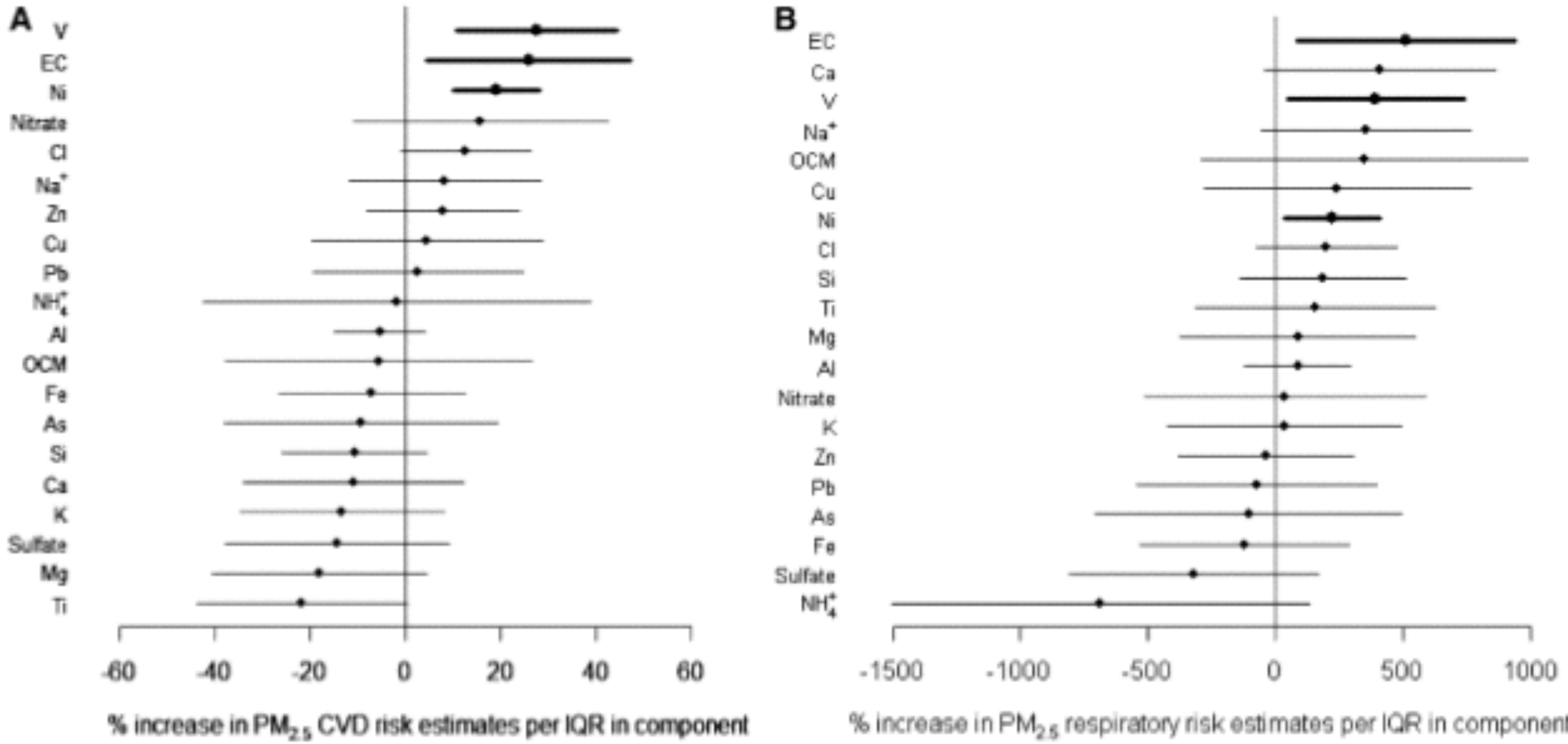


- Relative Risk ratios for cardiovascular and respiratory mortalities (Pope et al., 2004)

Cause of death/stratum-specific estimates according to characteristics at enrollment	*n* participants (*n* person-years)	RR (95% CI) for 10-μg/m^3 increase in $PM_{2.5}$
All-cause	8,096 (212,067)	1.14 (1.07, 1.22)
Cardiovascular	7,961 (195,941)	1.26 (1.14, 1.40)
Lung cancer	7,961 (195,941)	1.37 (1.07, 1.75)
COPD	7,805 (180,106)	1.17 (0.85, 1.62)

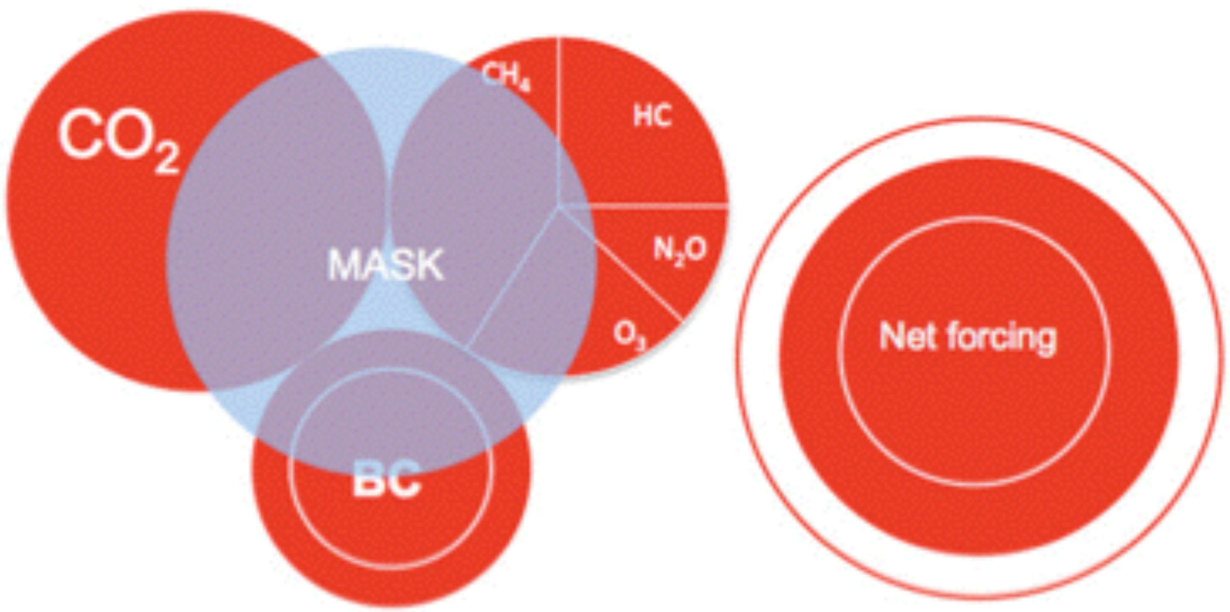
- Association between $PM_{2.5}$ and mortality (Lepeule et al., 2012)

Component-Specific Health Impacts



Percent increase in health effects estimates for cardiovascular hospitalizations (A) and respiratory hospitalizations (B) (Bell et al., 2009)

Aerosol Effects on Climate Change



Ramanathan and Xu, 2010

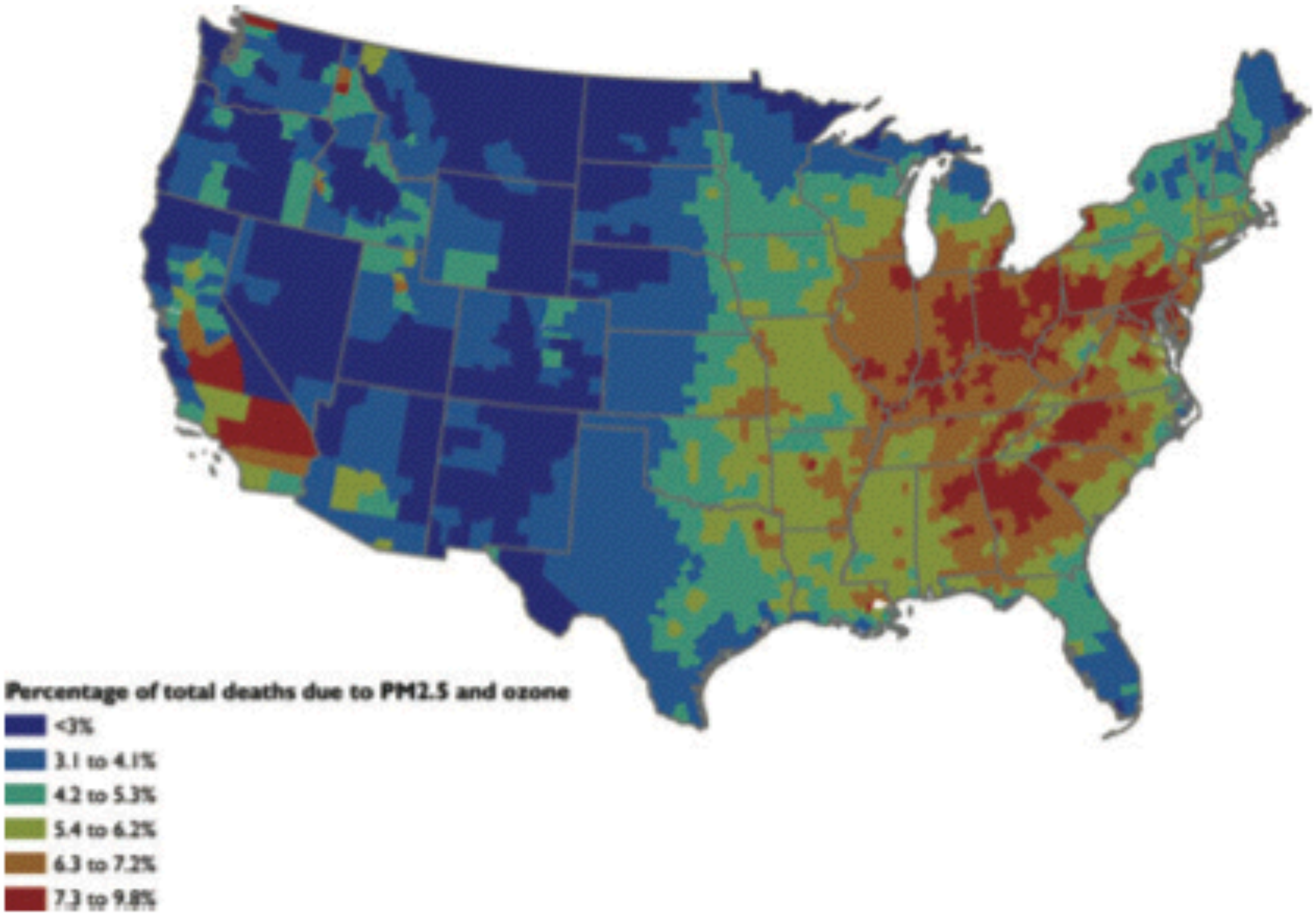
- Aerosols have direct, indirect, and semi-direct effects
- GHG have added 3Wm^{-2} of radiant energy
- BC adds 0.5-0.9 Wm^{-2}
- Other aerosols reflect radiation back to space (-2.1 Wm^{-2})

Arctic Climate Effects of BC

- BC deposited on snow and ice
  - High contrast in albedo results in enhanced absorption
  - Global mean surface temperature warming from BC on snow is 3 times more than equal CO_2 forcing (Flanner et al., 2007).
  - Arctic more susceptible to regional forcings than other locations.

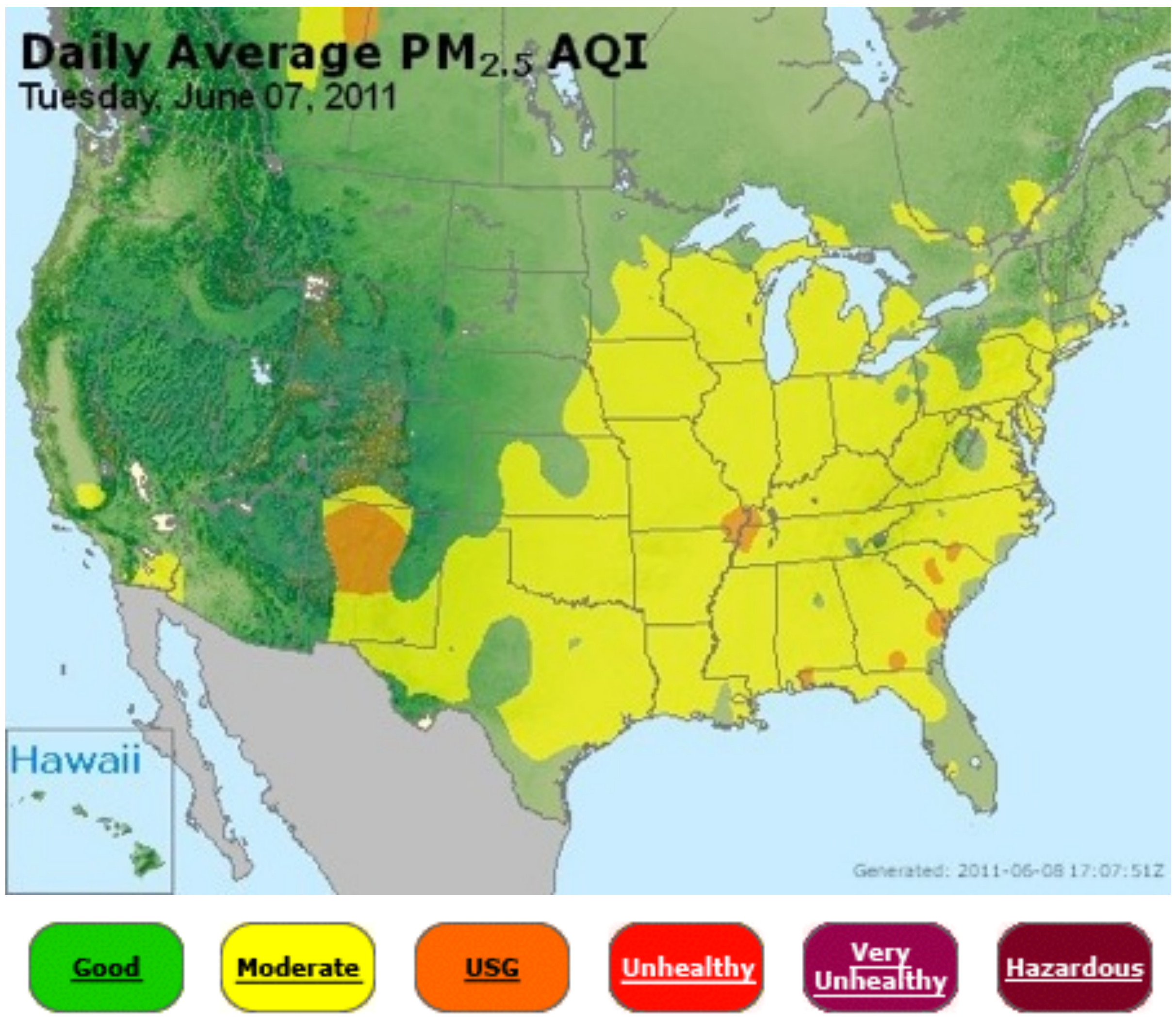
Schematic representation of BC effect on Arctic melting (UNEP, 2011)

Health Burden of PM Exposure

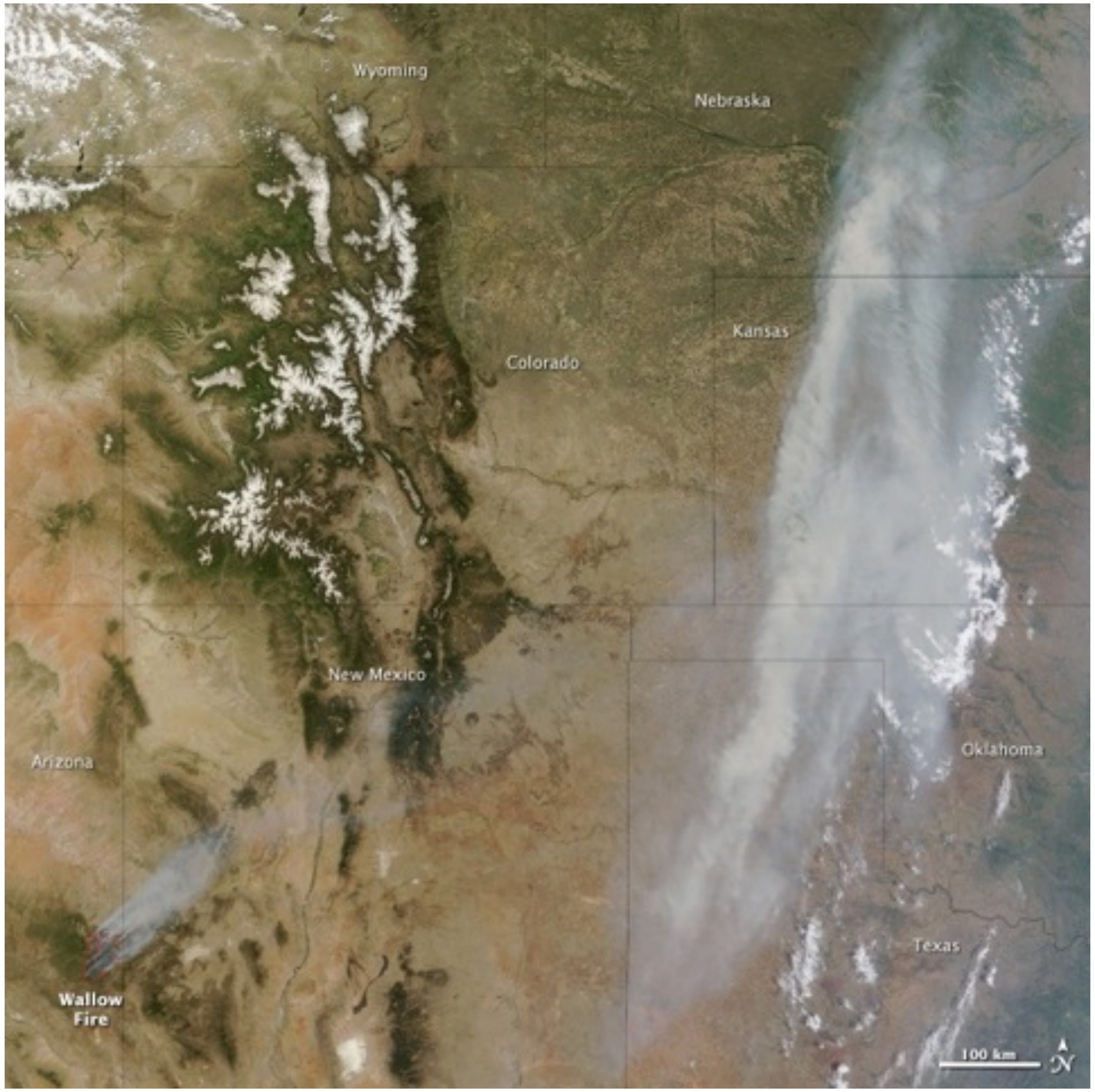


- Percentage of premature deaths attributable to 2005 $PM_{2.5}$ and ozone air quality (Fann et al., 2012)

Where is it Coming From?



EPA AIRNow
June 07, 2011



MODIS
June 07, 2011

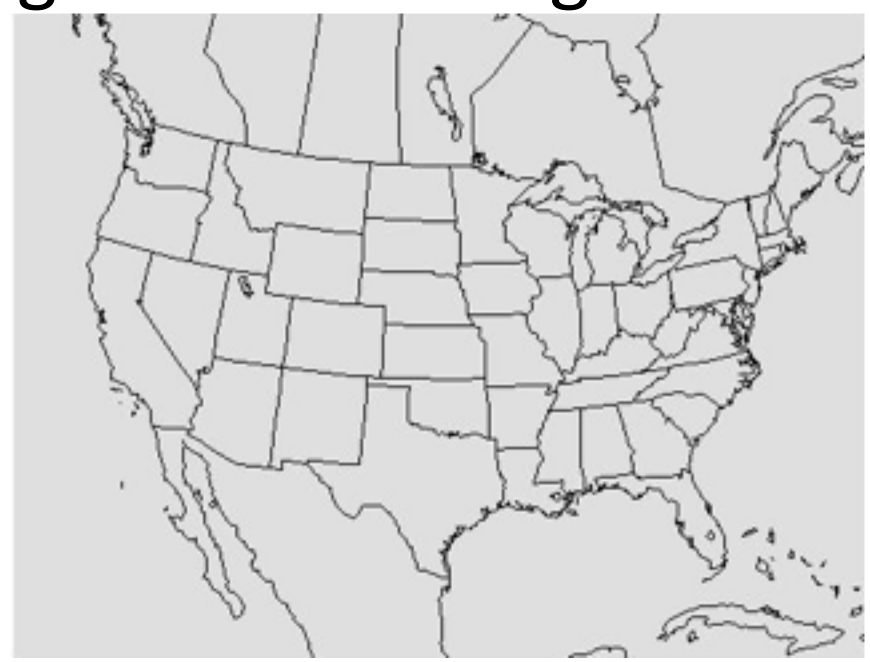
Objectives

- Use adjoint sensitivity analysis to attribute health impacts to emissions from specific locations, species, and sectors to facilitate more effective control strategies.
  - Develop the adjoint of aerosol microphysics for the CMAQ adjoint model.
- Accurately estimate regional radiative and air quality impacts of aerosols by constraining emissions through the use of inverse modeling.

CMAQ Model

Solve 3D chemical continuity equations on regional Eulerian grid

Modules
- Emissions
- Aerosols
- Chemistry
- Transport
- Deposition



12-km resolution:

396 × 246 grid cells

24 vertical layers

Input Data
- Emissions - 2008 NEI v2, Canada's 2006 Inventory, Mexico's Phase III 2008 inventory, BEIS3.14, SMARTFIRE2
- Meteorological Data - WRF v3.1: hourly-varying wind, temperature, moisture, vertical diffusion rates, rainfall rates
- Boundary Conditions - GEOS-Chem v8.02.03, 3 hour interval

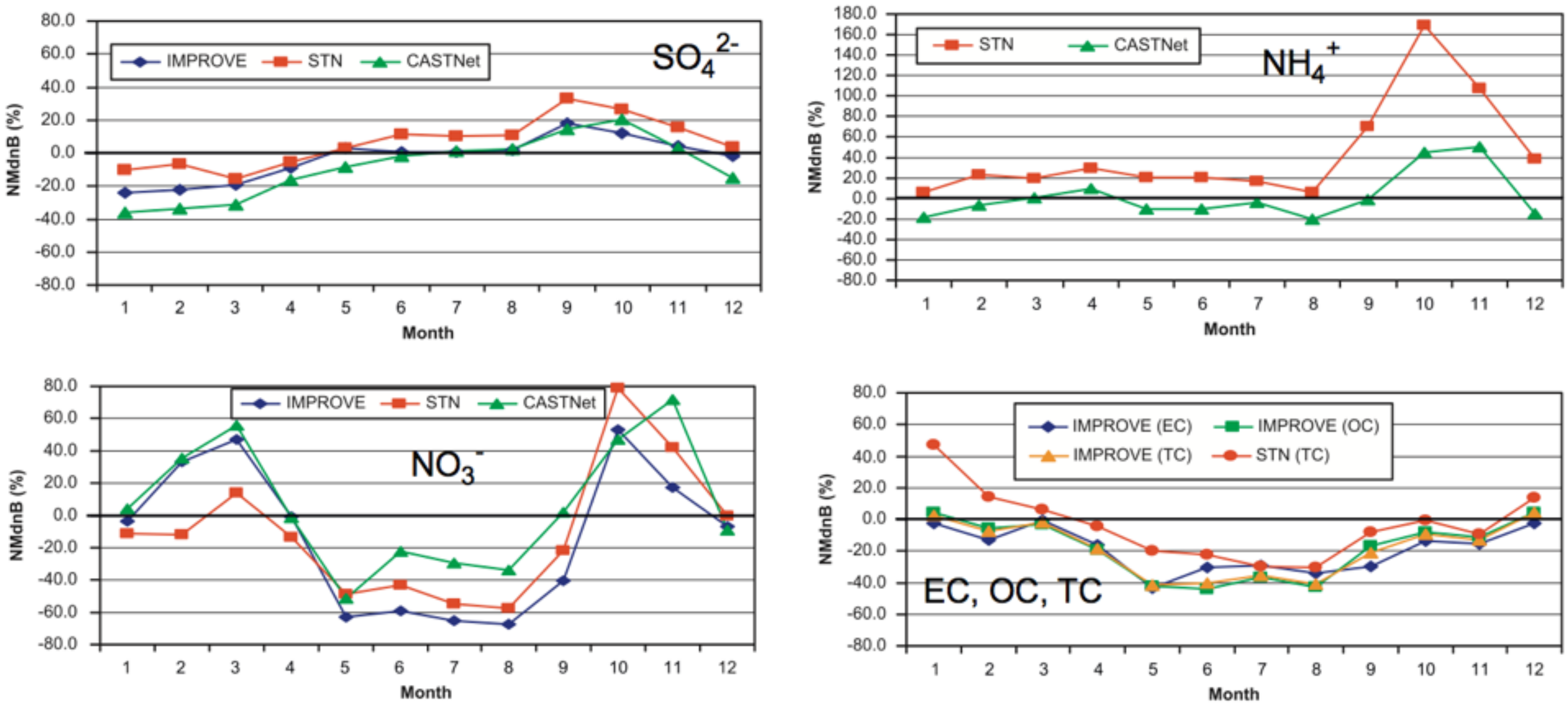
Aerosol Dynamics

$$\frac{\partial}{\partial t} n(v,t) = \frac{1}{2}\int_0^v K(v-q,q)n(v-q,t)n(q,t)dq$$
$$- n(v,t)\int_0^\infty K(q,v)n(q,t)dq$$
$$- \frac{\partial}{\partial v}(I(v)n(v,t)) + J_0(v)\delta(v-vo) + S(v) + R(v)$$

CMAQ Aerosol Module

- Particle size distribution is represented as superposition of three lognormal sub-distributions
- Processes:
  - Coagulation - intermodal and intramodal
  - SOA - Calculates SOA formation.
  - Heterogeneous Chemistry - Heterogenous conversion of N2O5 to HNO3
  - VOLINORG - Calculates partitioning of inorganic components between aerosol and gas phase. Includes condensational growth, nucleation of H2O and H2SO4. Dynamic mass transfer of species to/from coarse mode is also calculated. Includes ISORROPIA II
  - Mode Merging - If the Aitken mode mass is growing faster than accumulation mode mass and the Aitken mode number concentration exceeds accumulation mode number concentration, then modes are merged

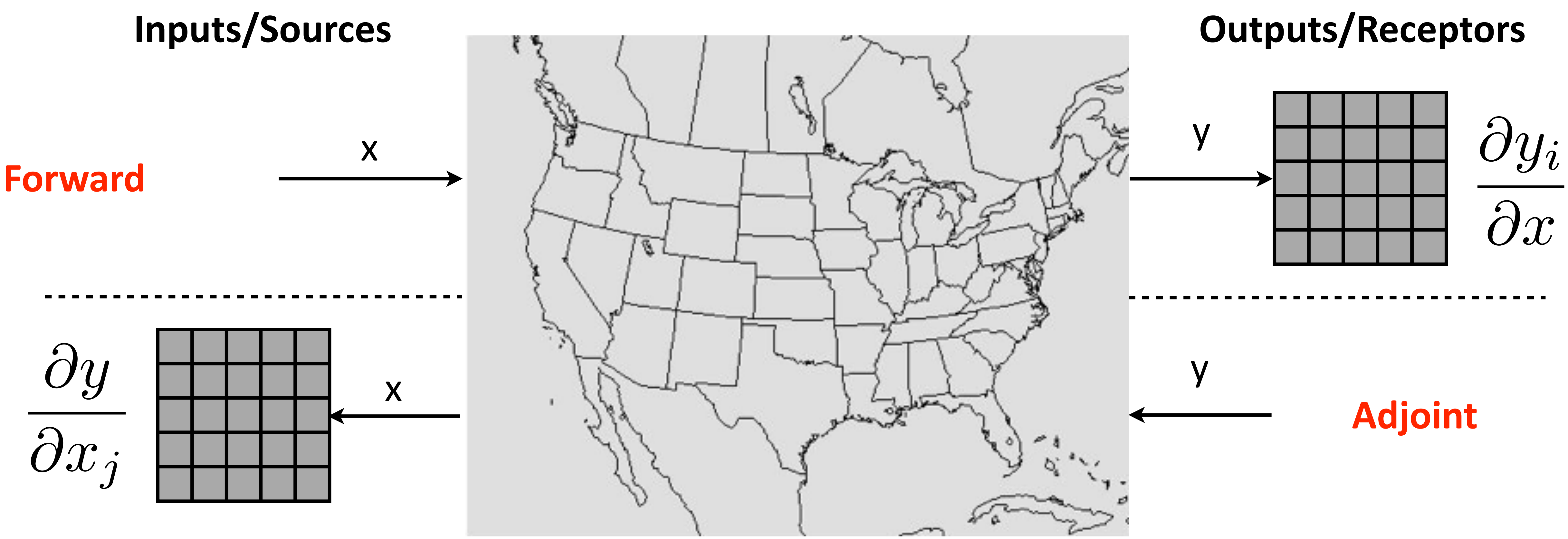
CMAQ $PM_{2.5}$ Evaluation



Monthly normalized median bias (NMdnB) for SO_4^{2-}, NH_4^+, BC and NO_3^- (Appel et al., 2008)

Adjoint Models

- Forward sensitivity analysis are source-based
- Adjoint method provides receptor-based sensitivities
- Main advantage of adjoint method over FD:
  - Quickly calculate sensitivities with respect to all model parameters (sources) at the same time.



CMAQ Adjoint Development

- CMAQ v4.5 gas-phase adjoint developed by Hakami et al., 2007.
- Transport - Peter Percell
- Gas-phase chemistry - Amir Hakami
- Aqueous chemistry - Amir Hakami group @ Carleton University
- Checkpointing - Jaroslav Resler
- Aerosols - Matt Turner and Shunliu Zhao
  - SOA - Shunliu Zhao
  - Driver - Shunliu Zhao
  - Mode Merging - Shunliu Zhao
  - Heterogenous chemistry - Matt Turner
  - Coagulation - Matt Turner
  - Volatile Inorganics - Matt Turner
  - Aerosol Thermodynamics - Shannon Capps (Capps et al., 2011)

Adjoint Validation

- Adjoint validation performed by comparing adjoint sensitivities to FD and CVM sensitivities.
- Aerosol module validated for many species
- Sensitivities with respect to emissions have been implemented and validated.
- Current model configuration validated for BC processes.
- Validation of simulations that combine gas-phase chemistry and aerosols yet to be completed.

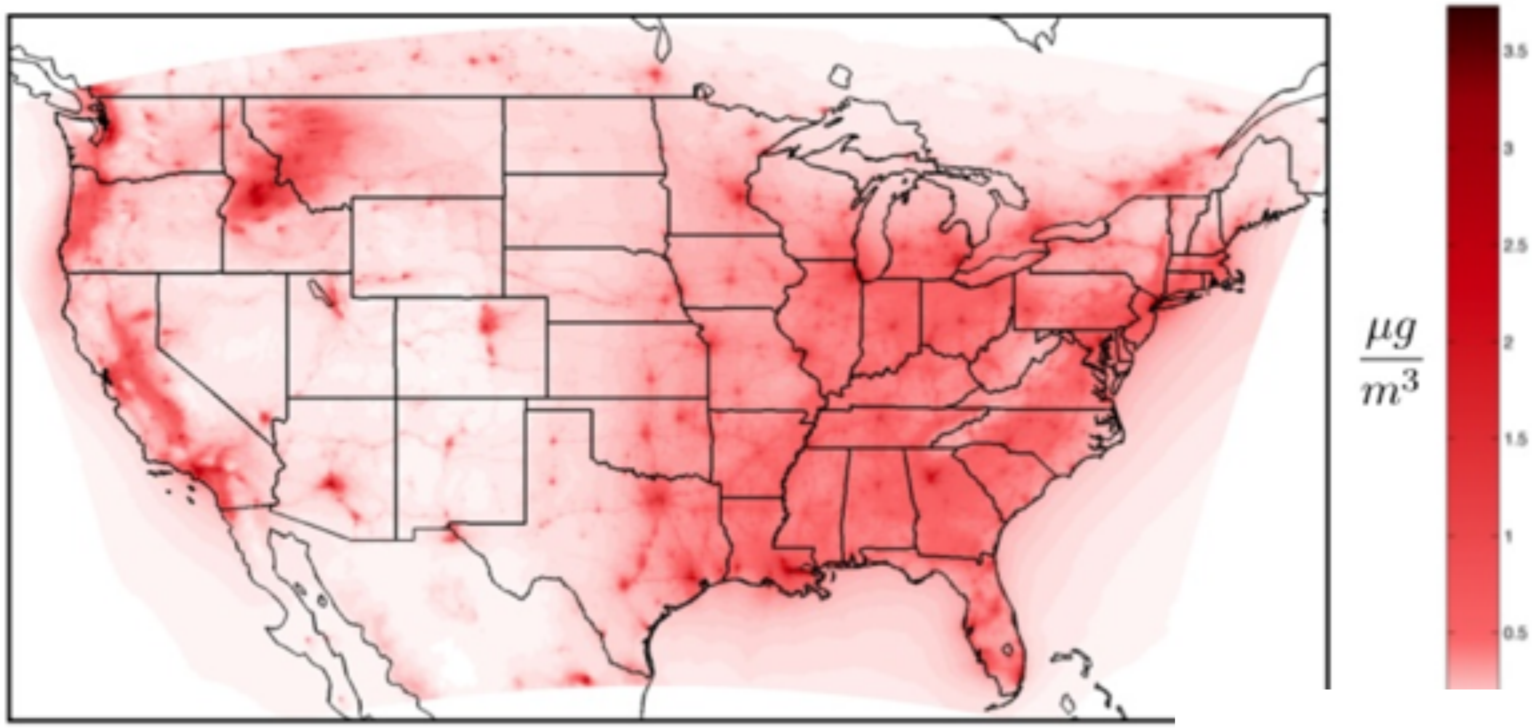
Cost Function for National Mortalities

$$J = \sum_{i=1}^{N} Mort_i * (1 - exp^{-\beta * C_{av,i}})$$

$$\frac{\partial J}{\partial C_{i,t}} = \frac{Mort_i}{T} * \beta * exp^{-\beta * C_{av,i}}$$

- $Mort$ = gridded annual mortalities in the US
- C_{av} = gridded annual average concentration
- T = number of timesteps in a year
- i = grid cell index
- N = total number of grid cells for which cost function is calculated
- β = concentration response factor, 0.005827 (Krewski et al., 2009)
- t = timestep index

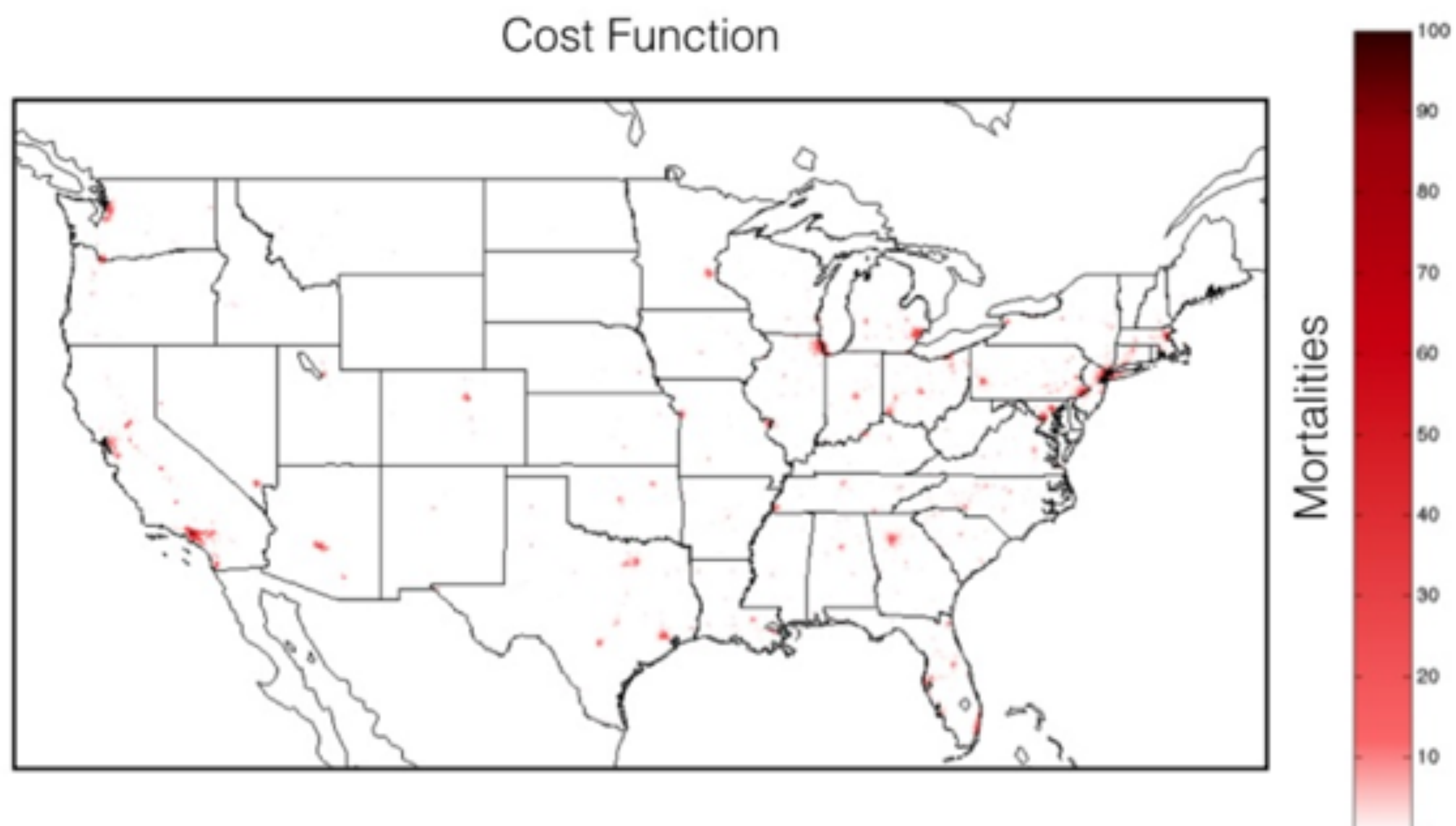
Forward Model Simulations



Forward simulations run from Dec. 21, 2006 to Dec. 31, 2007

↑ Annual average BC concentration

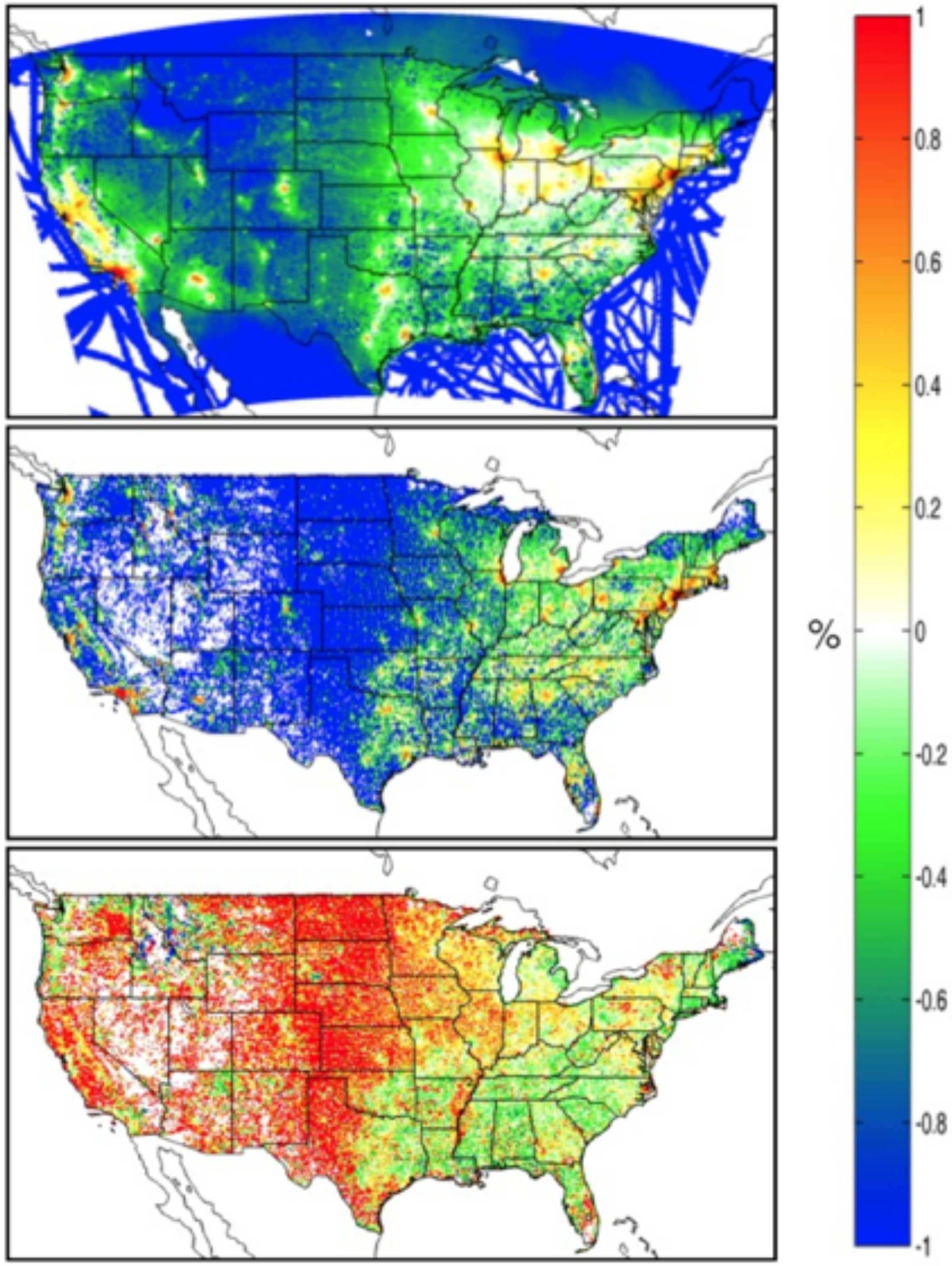
Gridded annual premature mortalities associated with exposure to BC →



Sensitivity of BC Health Impacts - Definitions

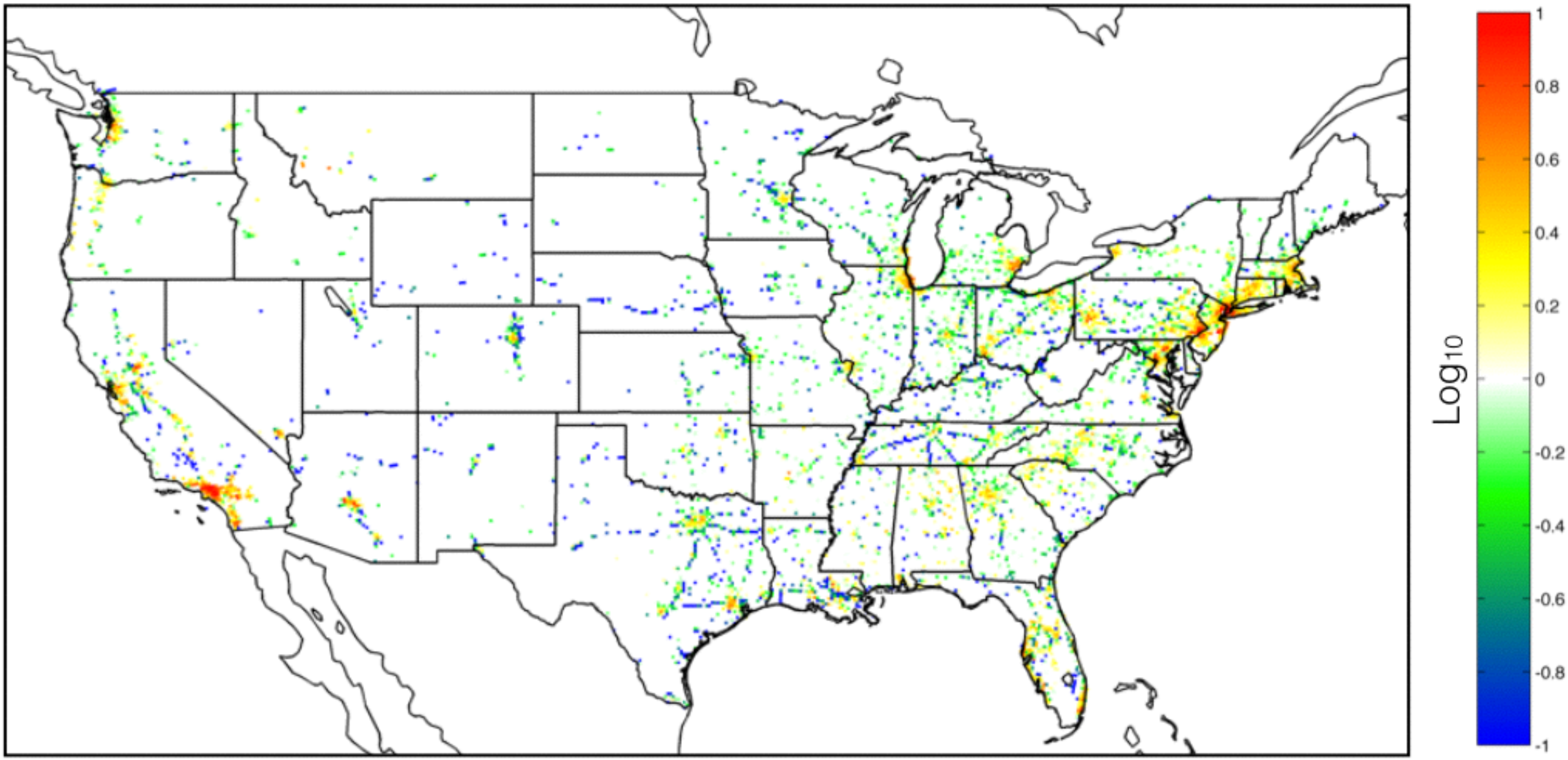
- 12 1-week adjoint simulations performed for the first week of each month
  - $\frac{\partial J}{\partial E_{i,k}}$ = Resulting sensitivities averaged and scaled to yearly
- $\frac{\partial J}{\partial E_{i,k}} * E_{i,k}$ = Contributions: semi-normalized sensitivities with respect to emissions scaling factors
- $\frac{\partial J}{\partial E_{i,k}} * \frac{E_{i,k}}{J} * 100\%$ = Contribution percentage: fraction of contribution from sectoral emissions in a single grid cell to sum of sectoral contributions
- $\frac{E_{i,k}}{\sum E_{i,k}} * 100\%$ = Emission percentage: fraction of sectoral emissions in a single grid cell to sum of sectoral emissions.

Sensitivity of BC Health Impacts

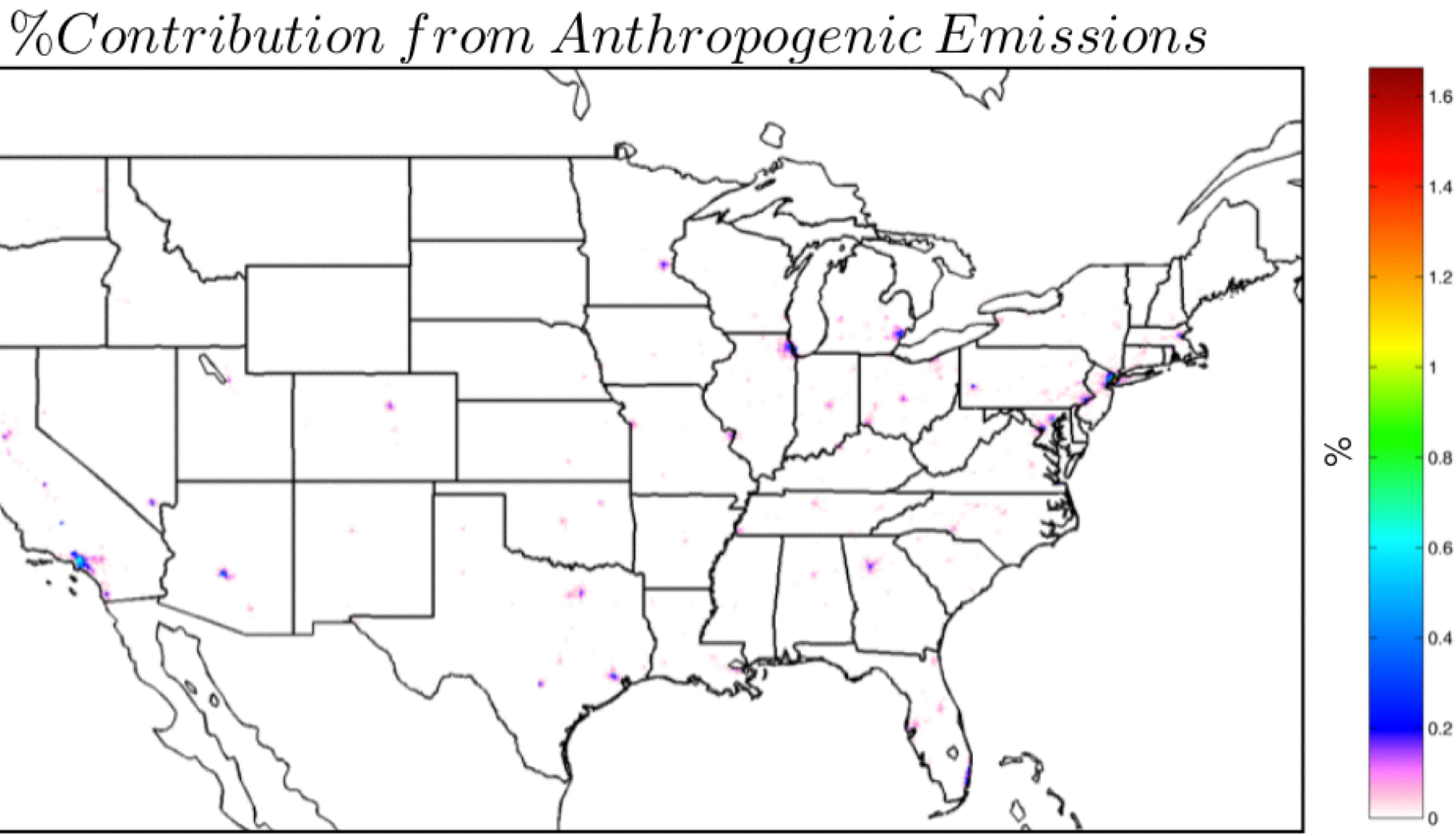


- Data from approximately 10% of grid cells plotted.
  - Emphasize locations with larger values
- This figure includes all data.
- Grid cell in eastern Montana:
  - $\frac{\%Contribution}{\%Mortality} = 273$
  - Contribution = 0.003
  - Mortality = 0.0013

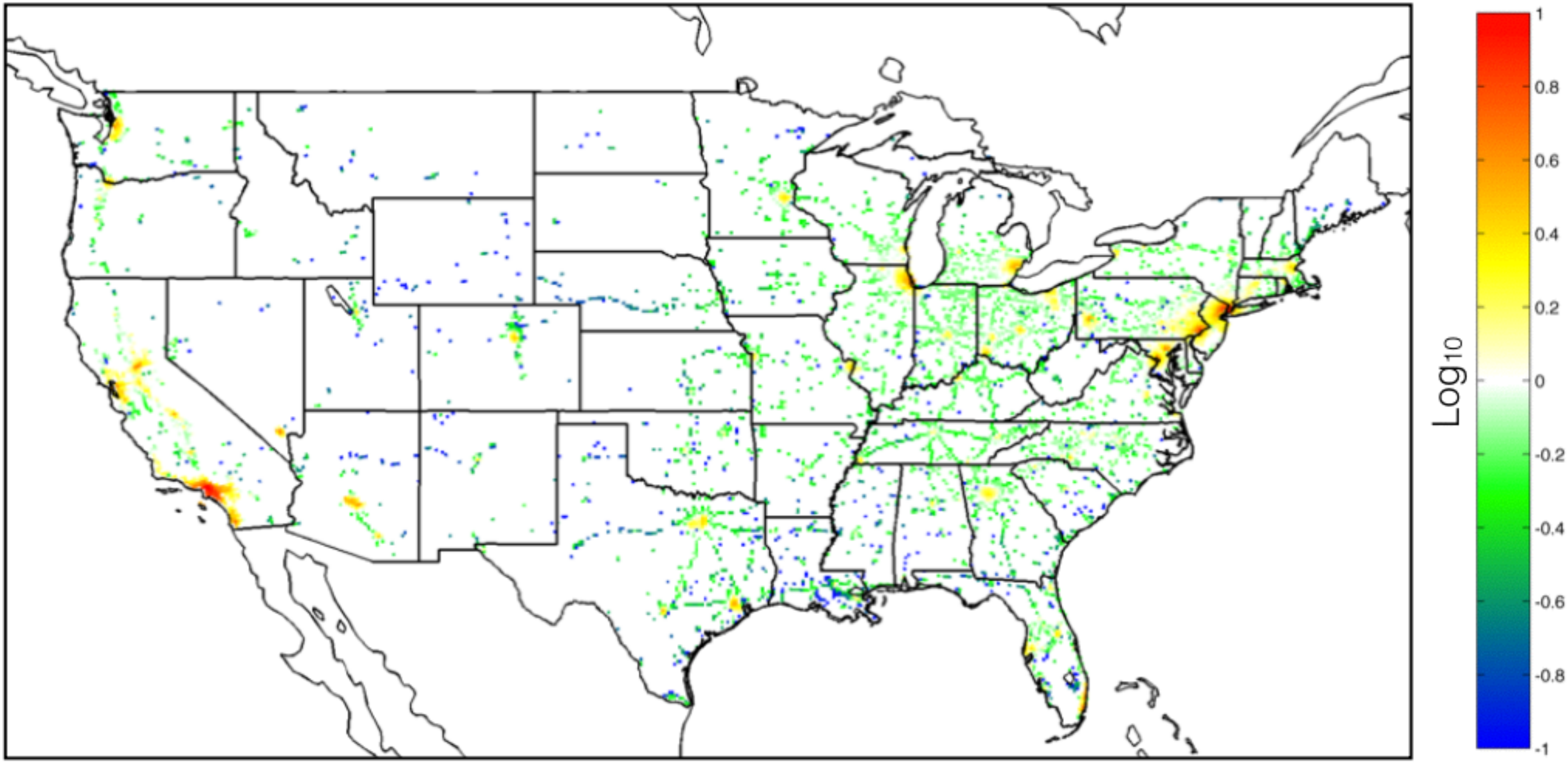
$$\frac{\%Mortality}{\%Emis_{anthropogenic}}$$



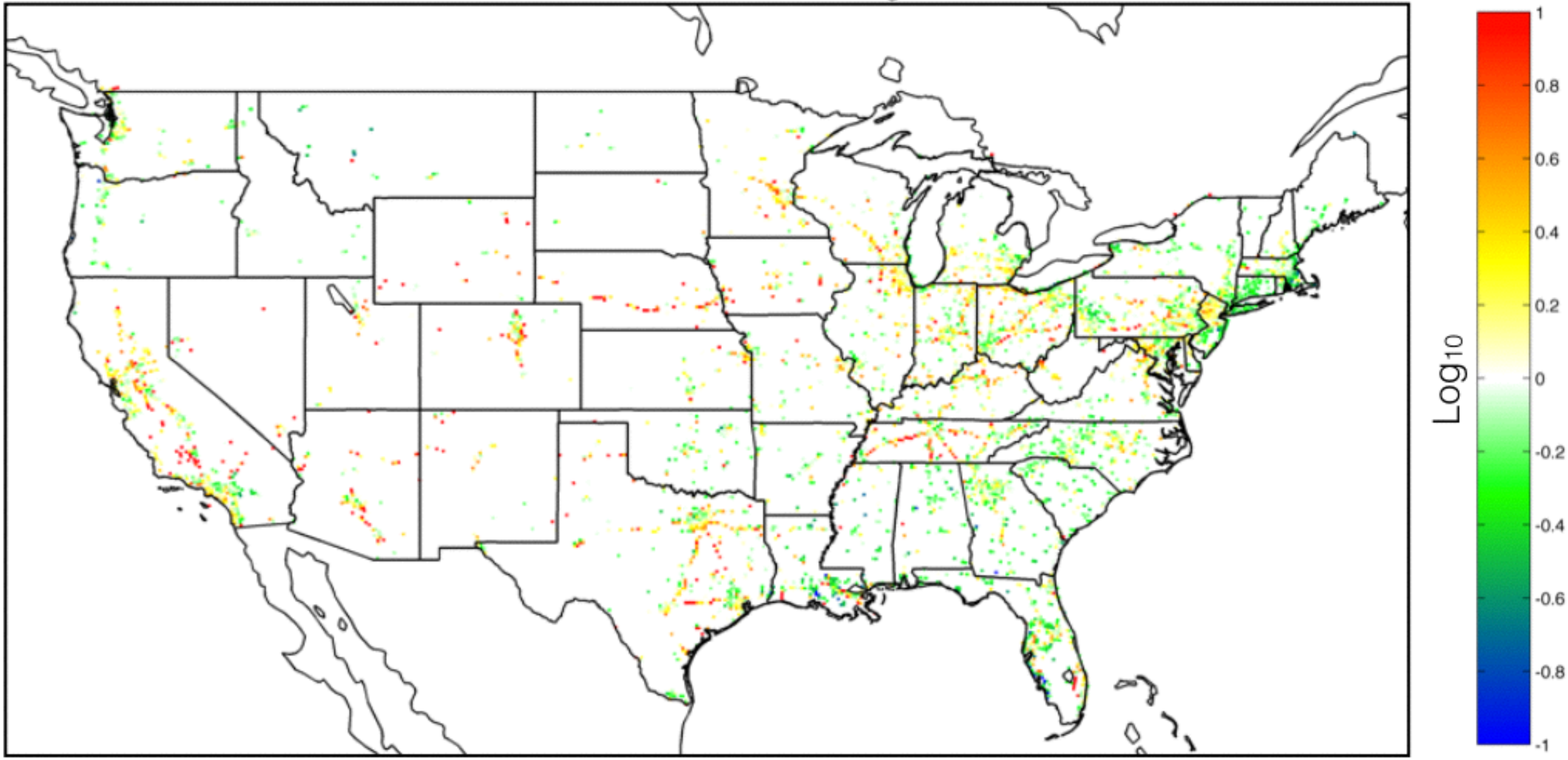
Sensitivity to Anthropogenic Emissions



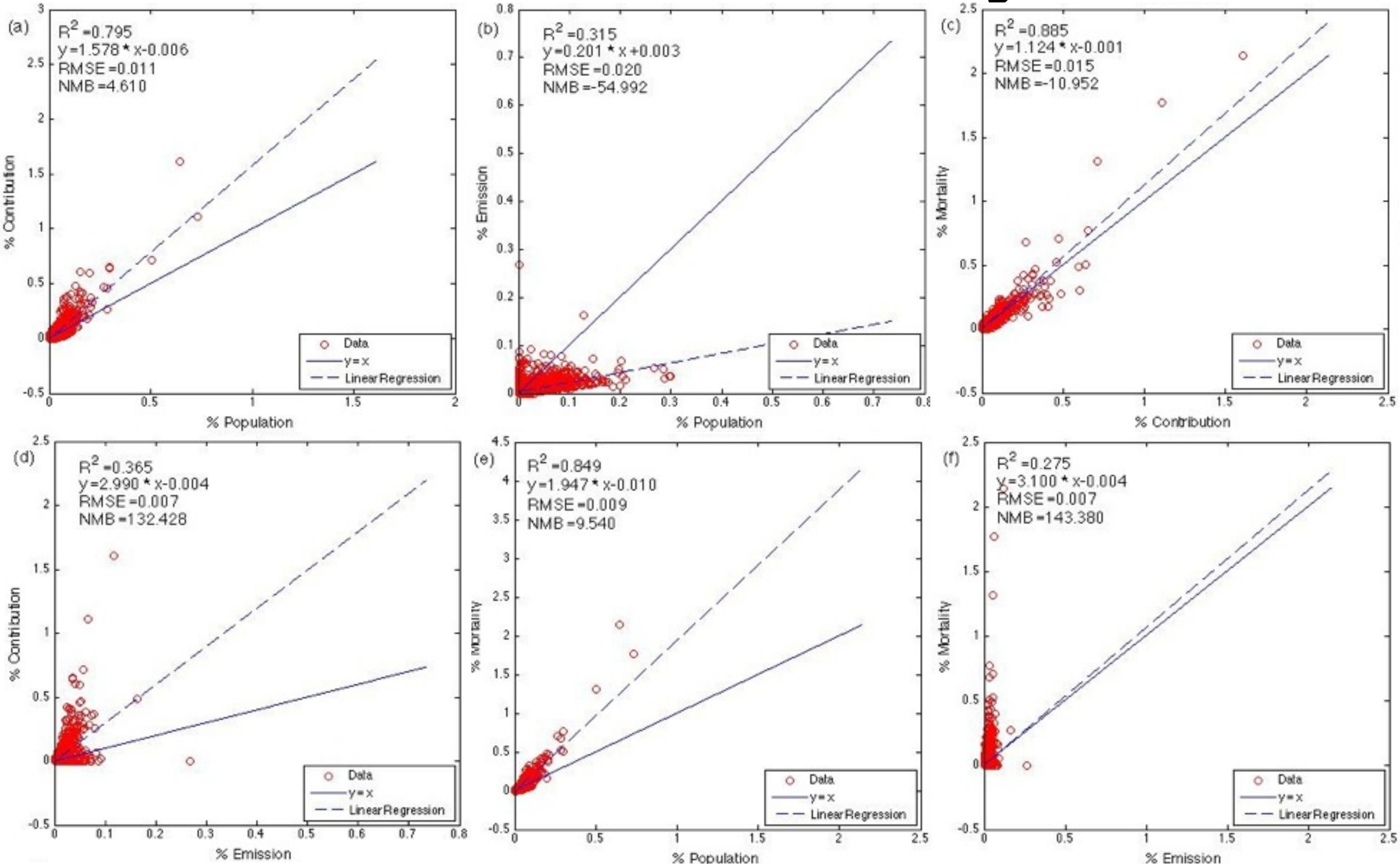
$$\frac{\%Contribution_{Anthropogenic}}{\%Emis_{Anthropogenic}}$$



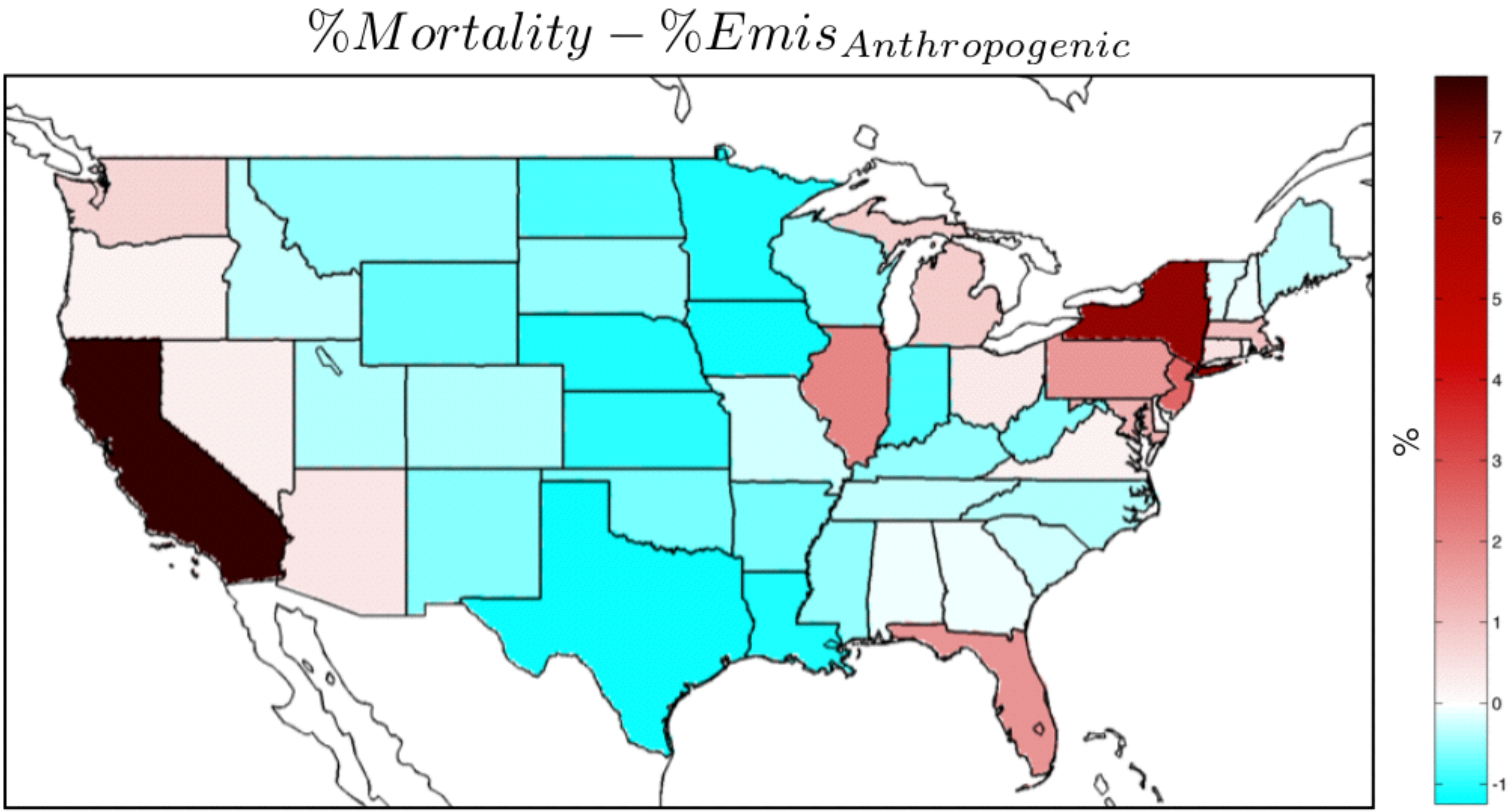
$$\frac{\%Contribution_{Anthropogenic}}{\%Mortality}$$



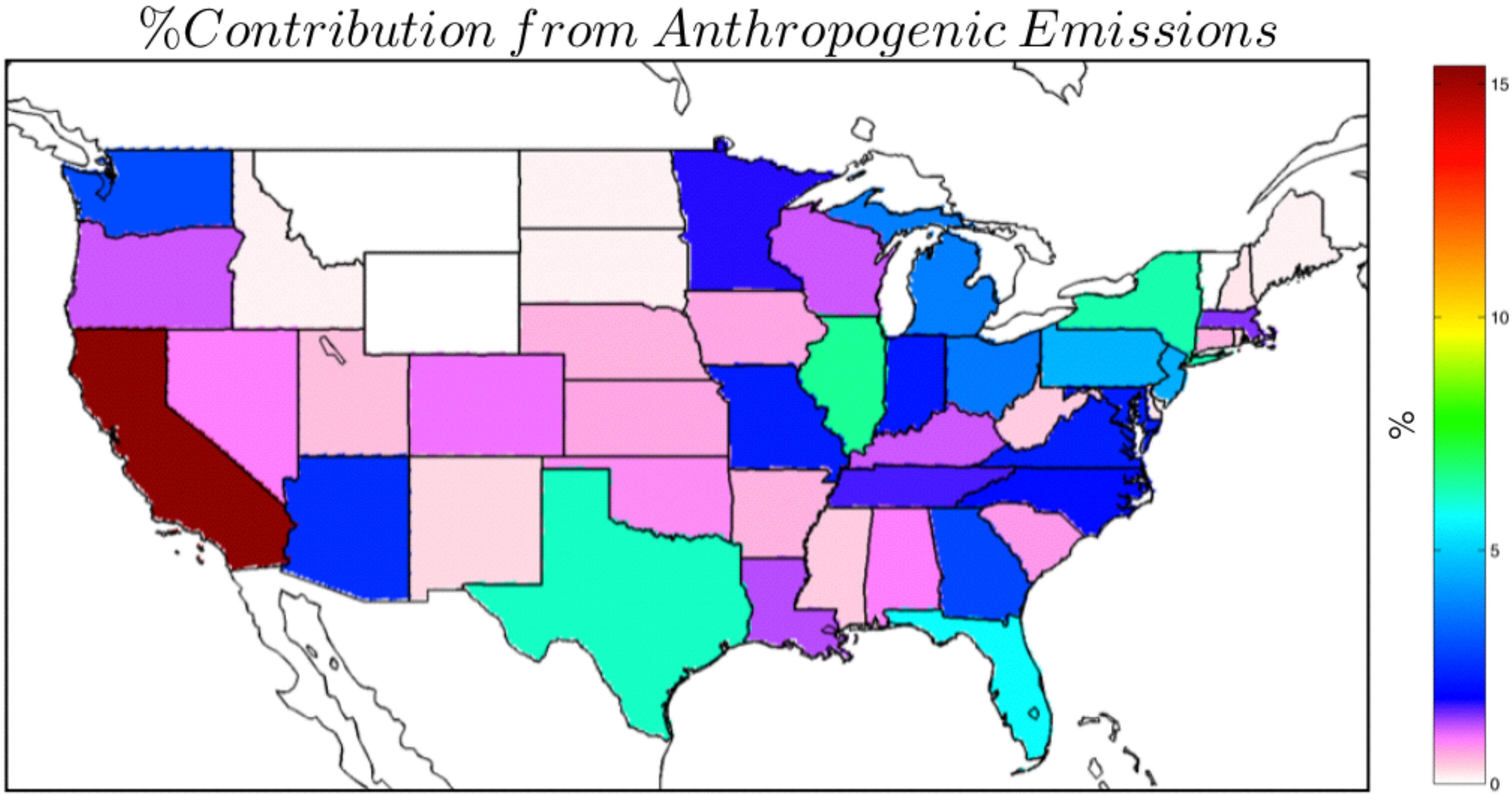
Statistical Analysis



Sensitivity to Anthropogenic Emissions, Summed by State

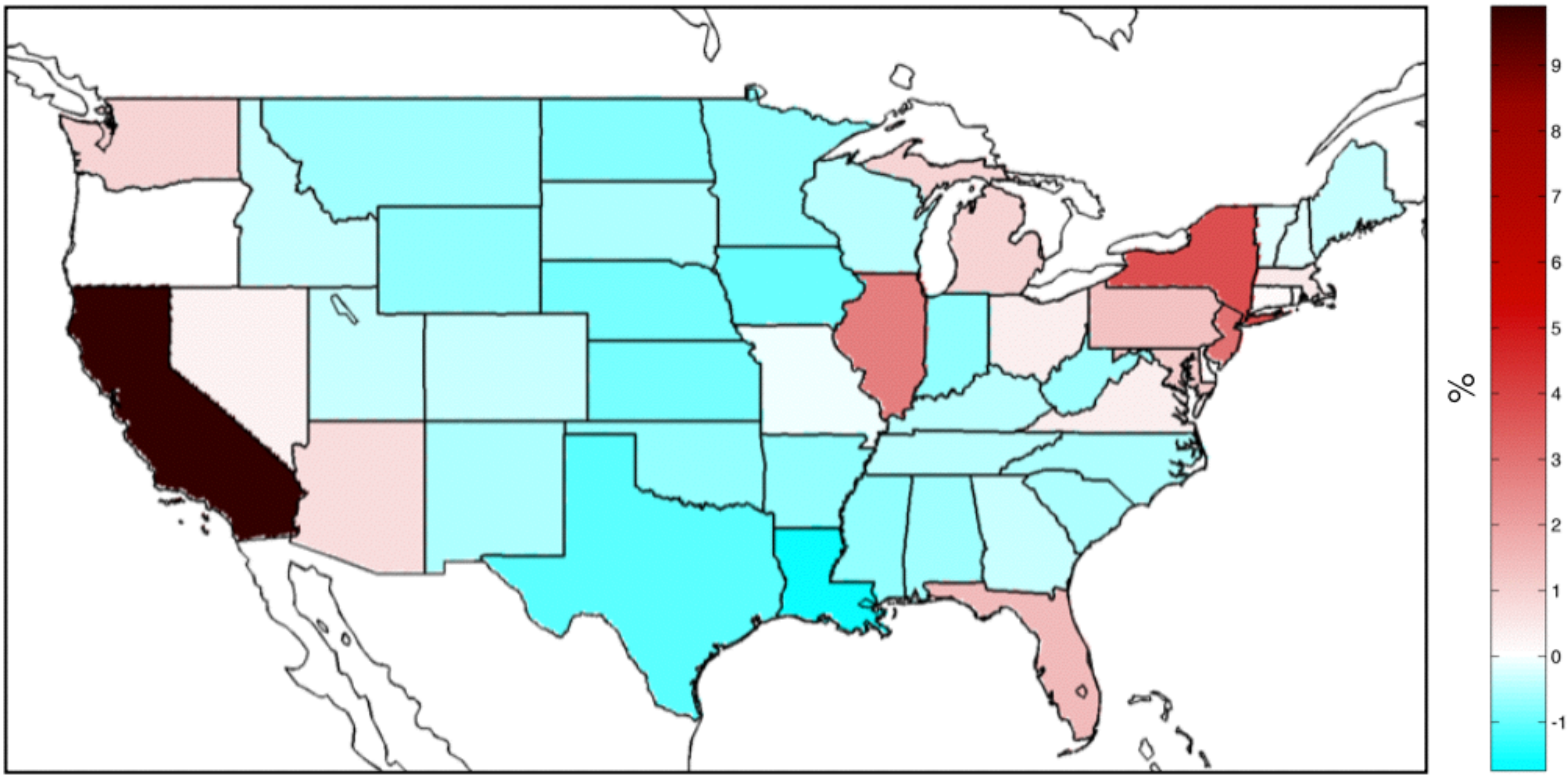


Sensitivity to Anthropogenic Emissions, Summed by State



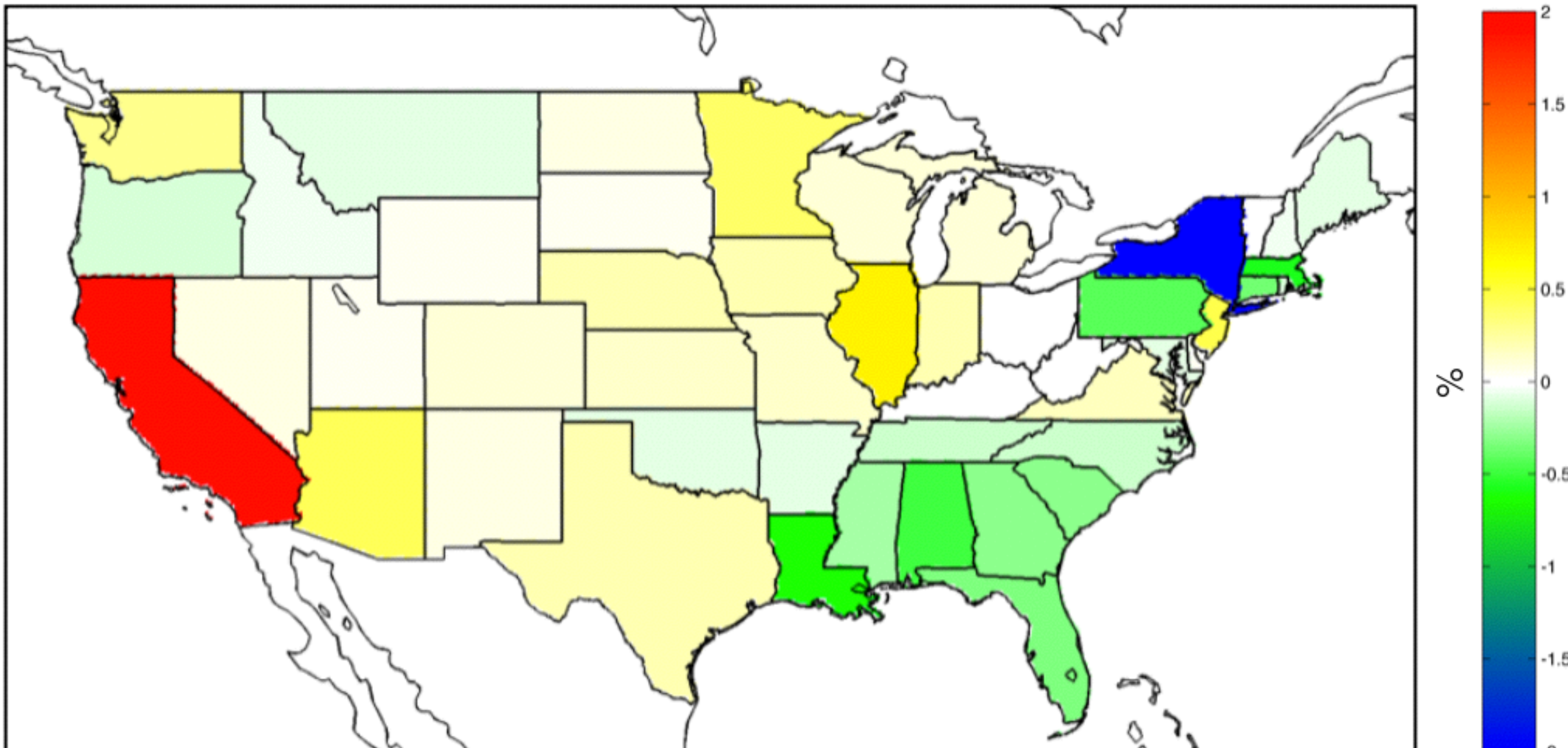
Sensitivity to Anthropogenic Emissions, Summed by State

$$\%Contribution_{Anthropogenic} - \%Emis_{Anthropogenic}$$

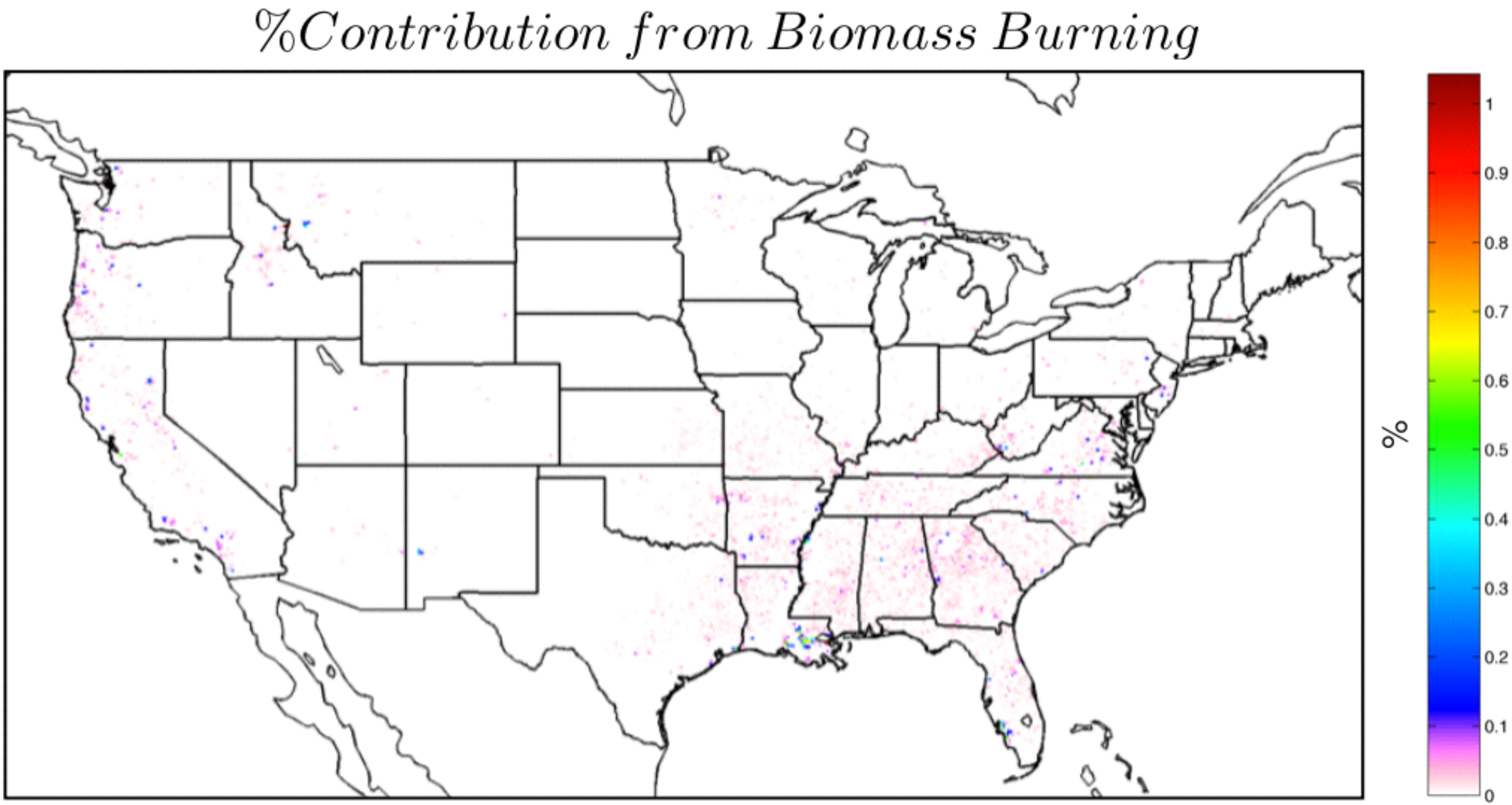


Sensitivity to Anthropogenic Emissions, Summed by State

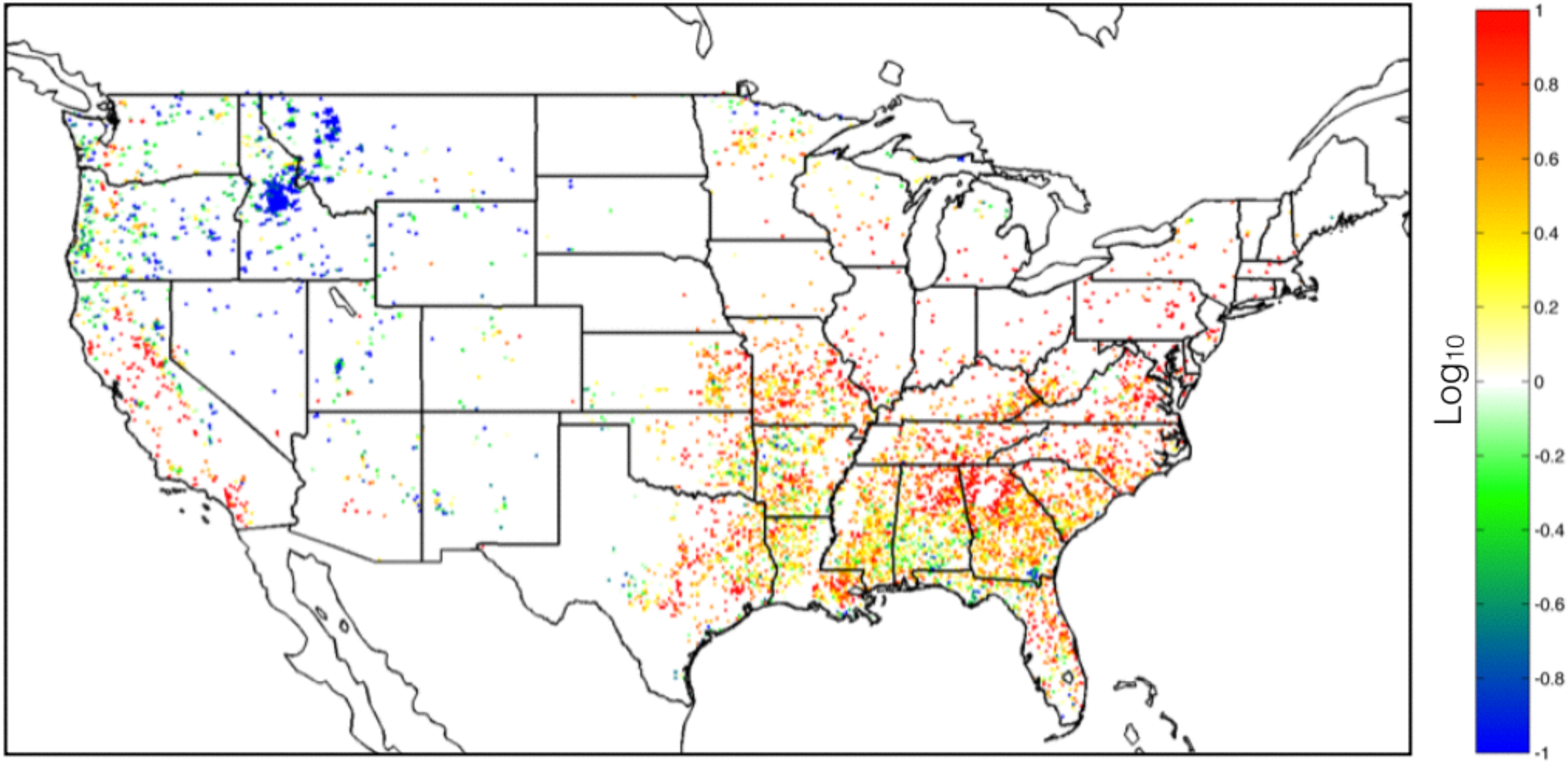
$$\%Contribution_{Anthropogenic} - \%Mortality$$



Sensitivity to Biomass Burning Emissions



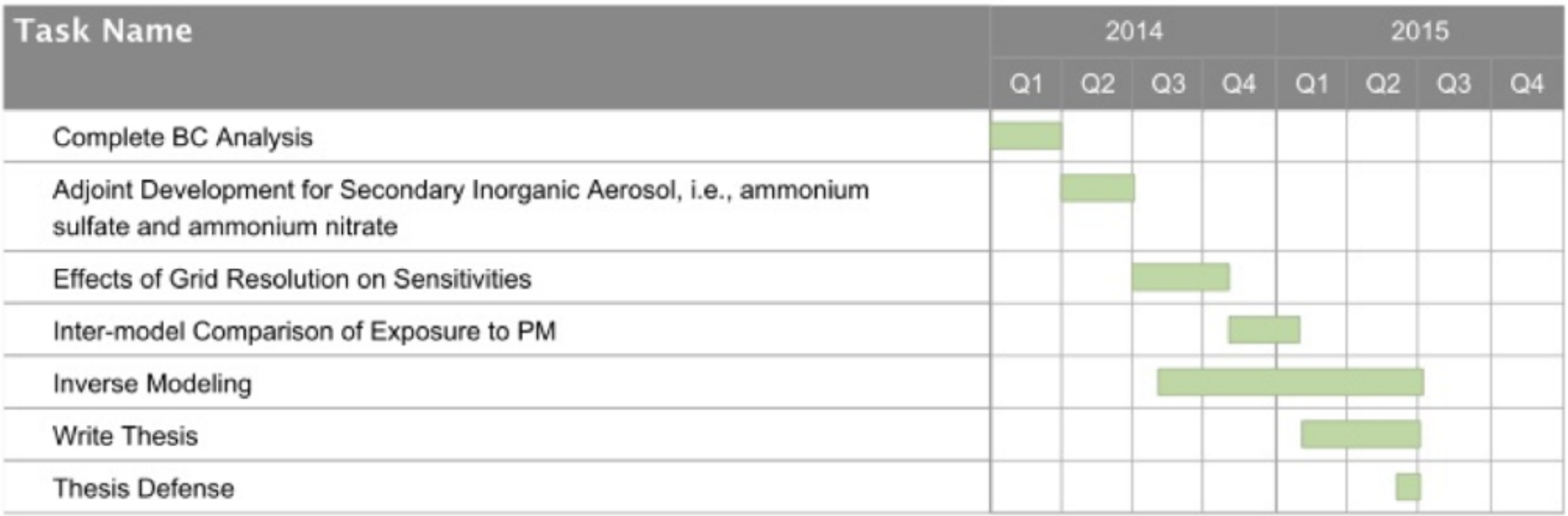
$$\frac{\%Contribution_{Biomass}}{\%Emis_{Biomass}}$$



Summary

- Adjoint of aerosol microphysics has been developed and validated.
  - Model has been shown to accurately calculate BC sensitivities
- Using the CMAQ adjoint model, we estimated sensitivities of mortality attributed to exposure to BC with respect to emissions at a highly resolved spatial and sectoral level of specificity.
- Showed that transport plays an important role for source-attribution studies of short-lived species.
- Additional regulations to the highest emission locations would not be the most effective means of reducing mortalities to BC exposure.
  - Stricter controls on nonattainment areas would be most effective.
- Emissions in areas upwind of highly populated areas contribute to more mortalities than there are mortalities in those locations.

Future Work


Task Name
2014
2015
Q1
Q2
Q3
Q4
Q1
Q2
Q3
Q4
Complete BC Analysis
Adjoint Development for Secondary Inorganic Aerosol, i.e., ammonium sulfate and ammonium nitrate
Effects of Grid Resolution on Sensitivities
Inter-model Comparison of Exposure to PM
Inverse Modeling
Write Thesis
Thesis Defense

Questions?