Aerosols Processes in the CMAQ Adjoint

International Aerosol Modeling Algorithms Conference, 2011

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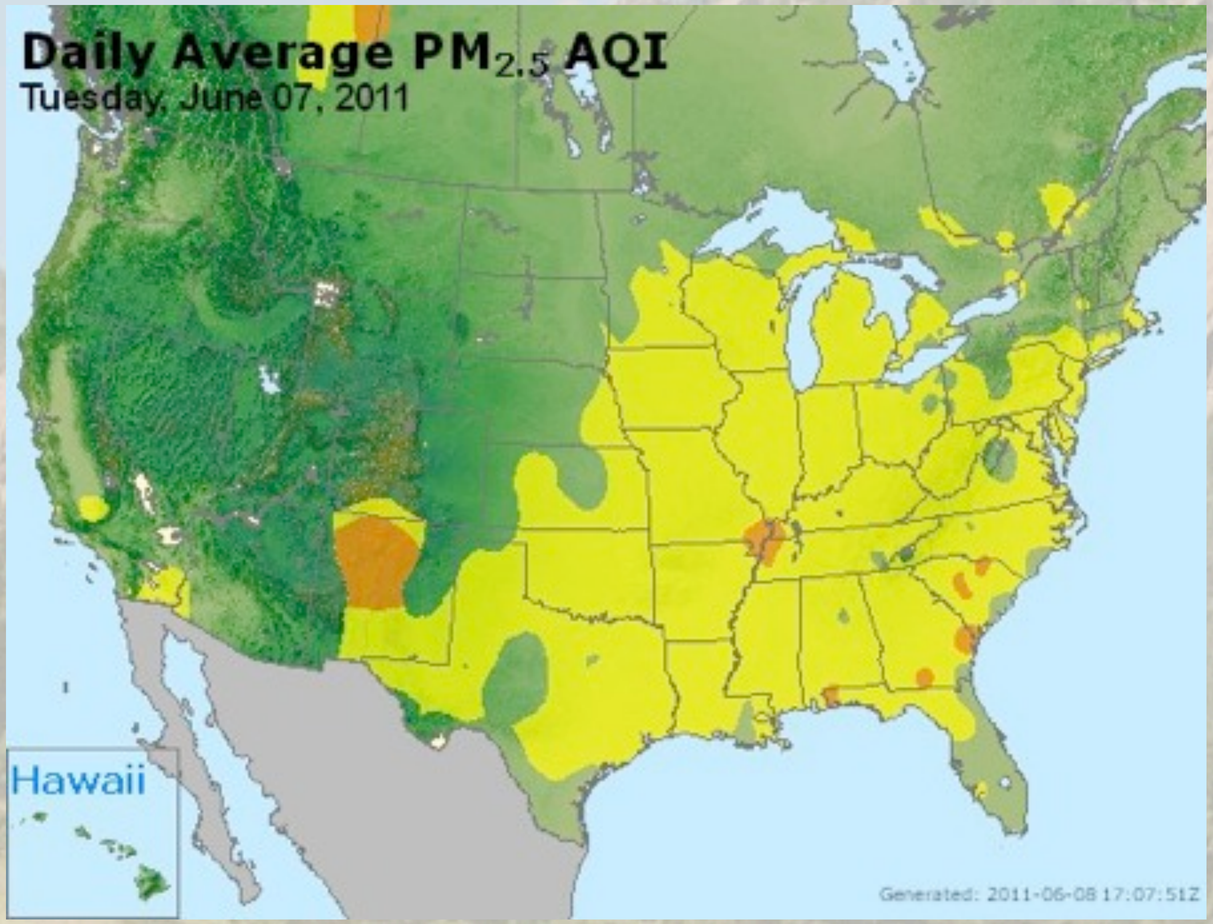
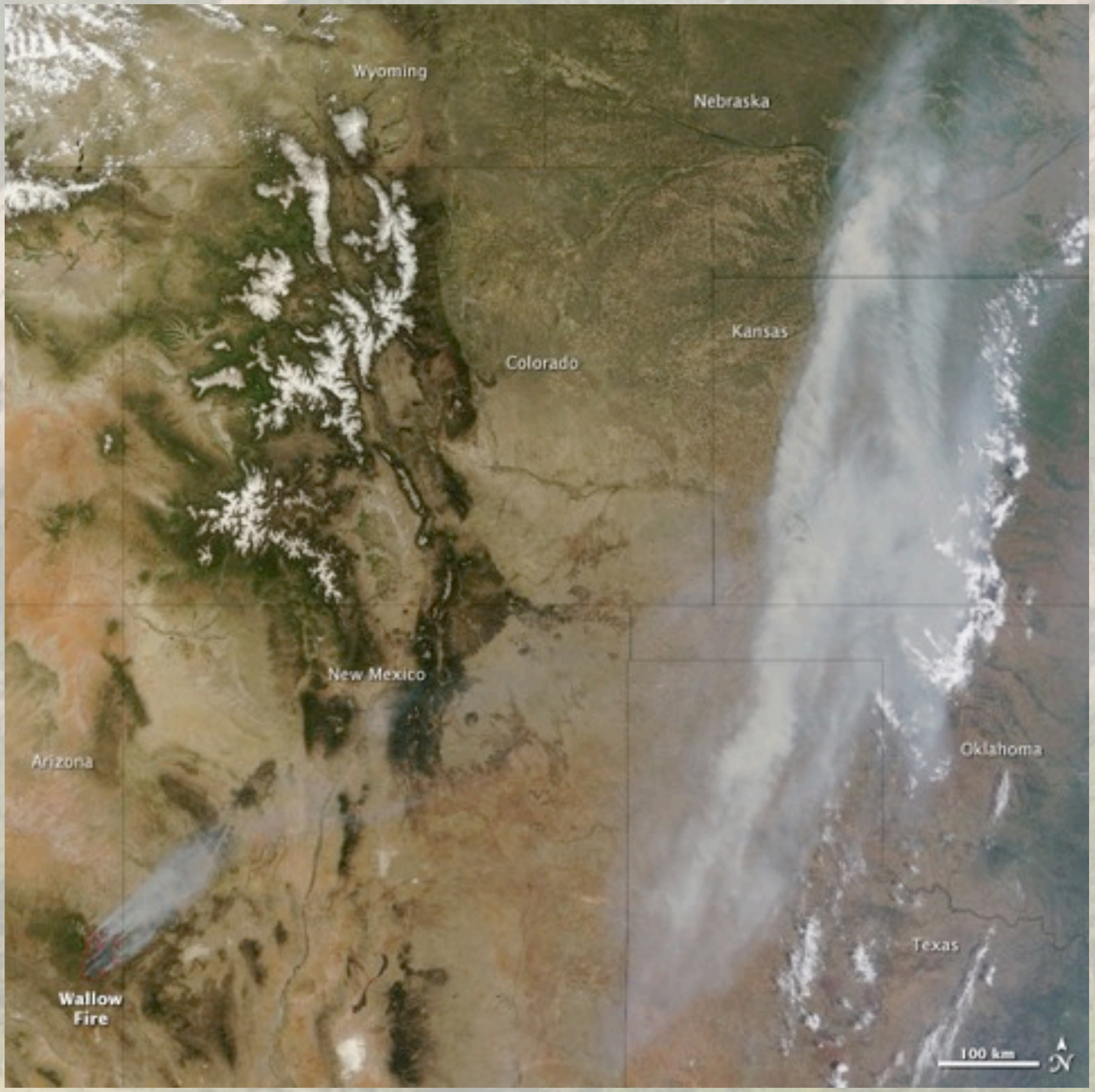
Where is it Coming From?



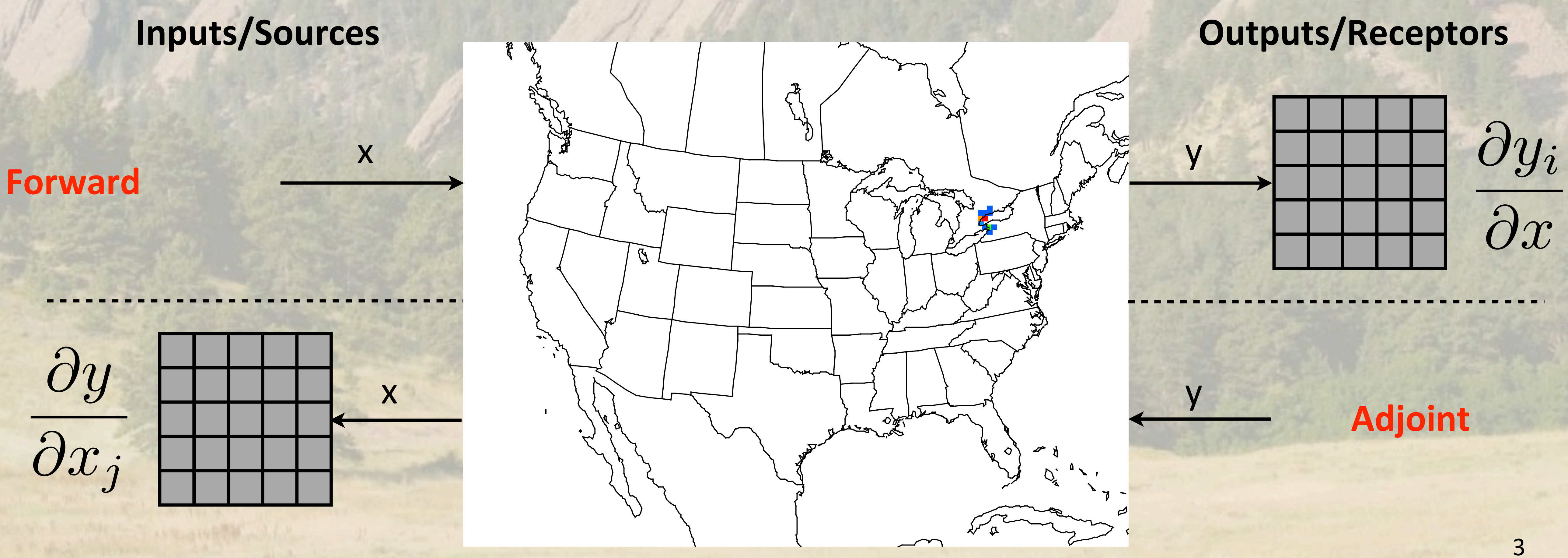
EPA AIRNow
June 07, 2011



MODIS
June 07, 2011

Adjoint Models

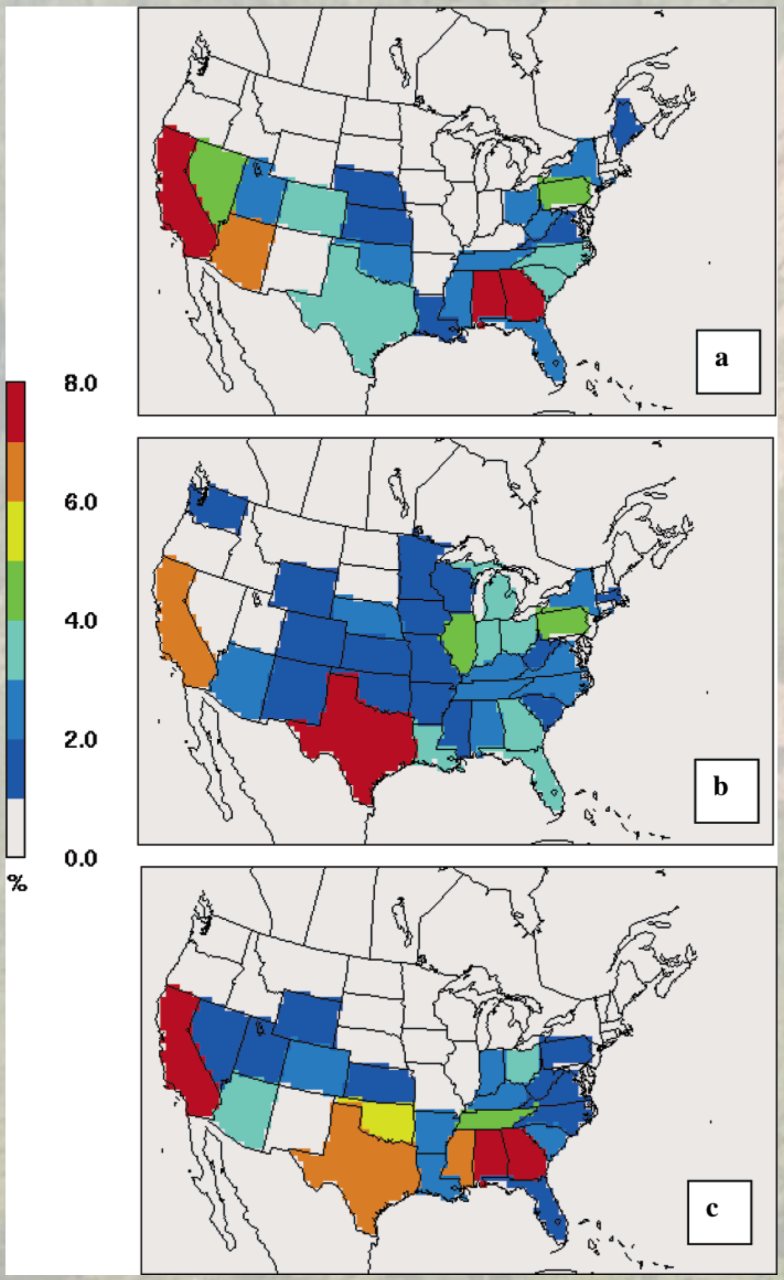
- Forward sensitivity analysis are source-based
- Adjoint method provides receptor-based sensitivities
- Adjoint method has 2 main advantages over FD:
  - Quickly calculate sensitivities with respect to all model parameters (sources) at the same time.
  - Don’t need multiple forward runs
  - Computed gradient is exact



Applications of Adjoints

- Data Assimilation:
  - Hakami et al. 2005: Adjoint Inverse Modeling of Black Carbon
  - Zhang et al. 2008: AOD Data Assimilation over Global Oceans
  - Henze et al. 2009: Inverse Modeling of inorganic $PM_{2.5}$ emissions
- Sensitivity Analysis:
  - Hakami et al. 2006: Adjoint Sensitivity Analysis of Ozone Nonattainment
  - Martien et al. 2006: Adjoint Sensitivity Analysis for a 3D Photochemical Model

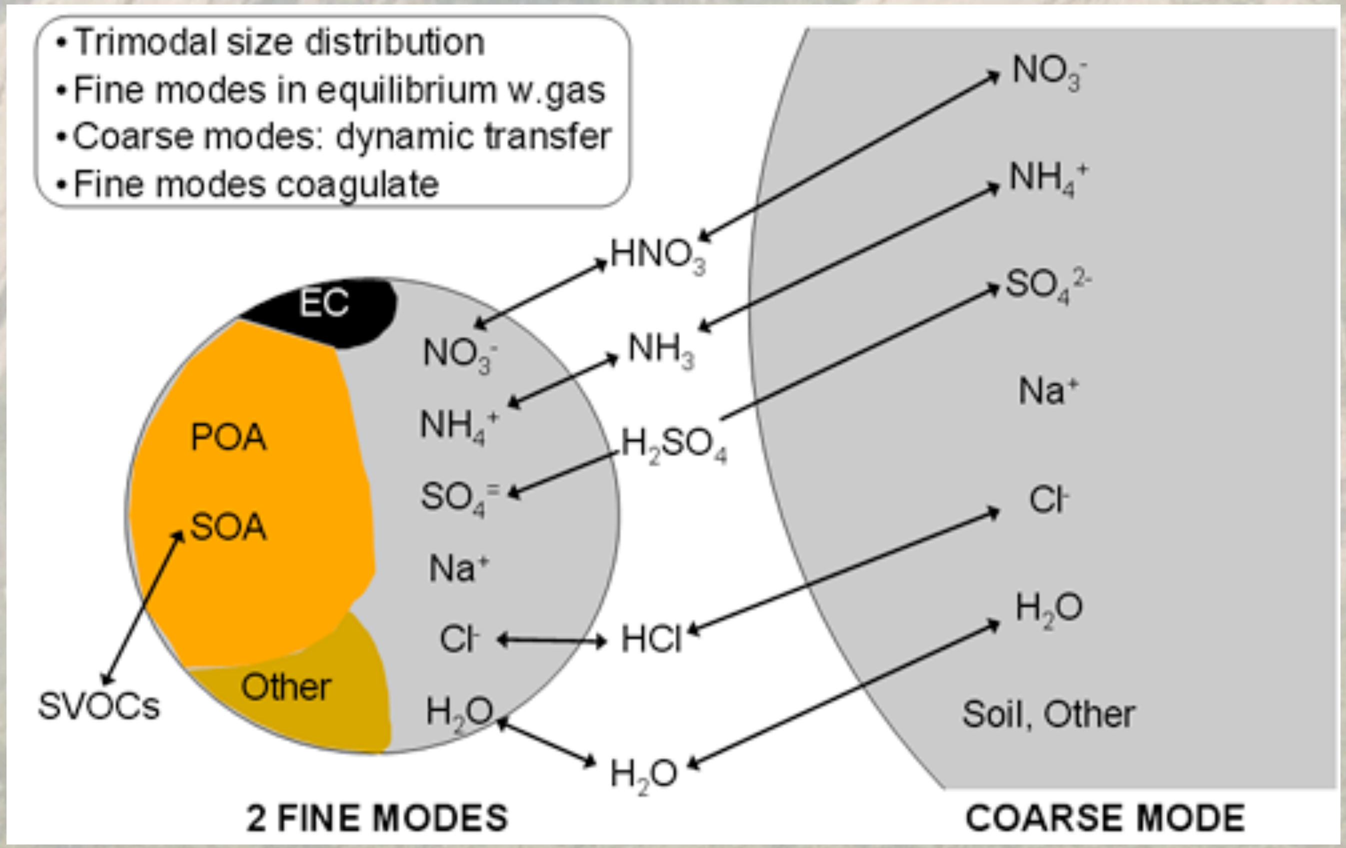
Currently no regional adjoint includes aerosols



State shares (%) in nationwide (a) nonattainment (b) NO_x emissions, and (c) nonattainment sensitivities. **Hakami et al. 2006**

CMAQ Aerosol Module

- Modal approach with 3 modes
  - Aitken: fresh particles either from nucleation or direct emission
  - Accumulation: aged particles
  - Coarse
- Aerosol Module contains:
  - Aerosol Dynamics
  - Nucleation
  - Primary Emissions
  - Mode Merging
  - Dry Deposition
  - Cloud Processing of Aerosols
  - Aerosol Chemistry
  - SOA
  - Visual Range (diagnostic)



Representation of PM size and composition (EPA Atmospheric Modeling and Analysis Division)

Note: Image for CMAQ 4.7.1

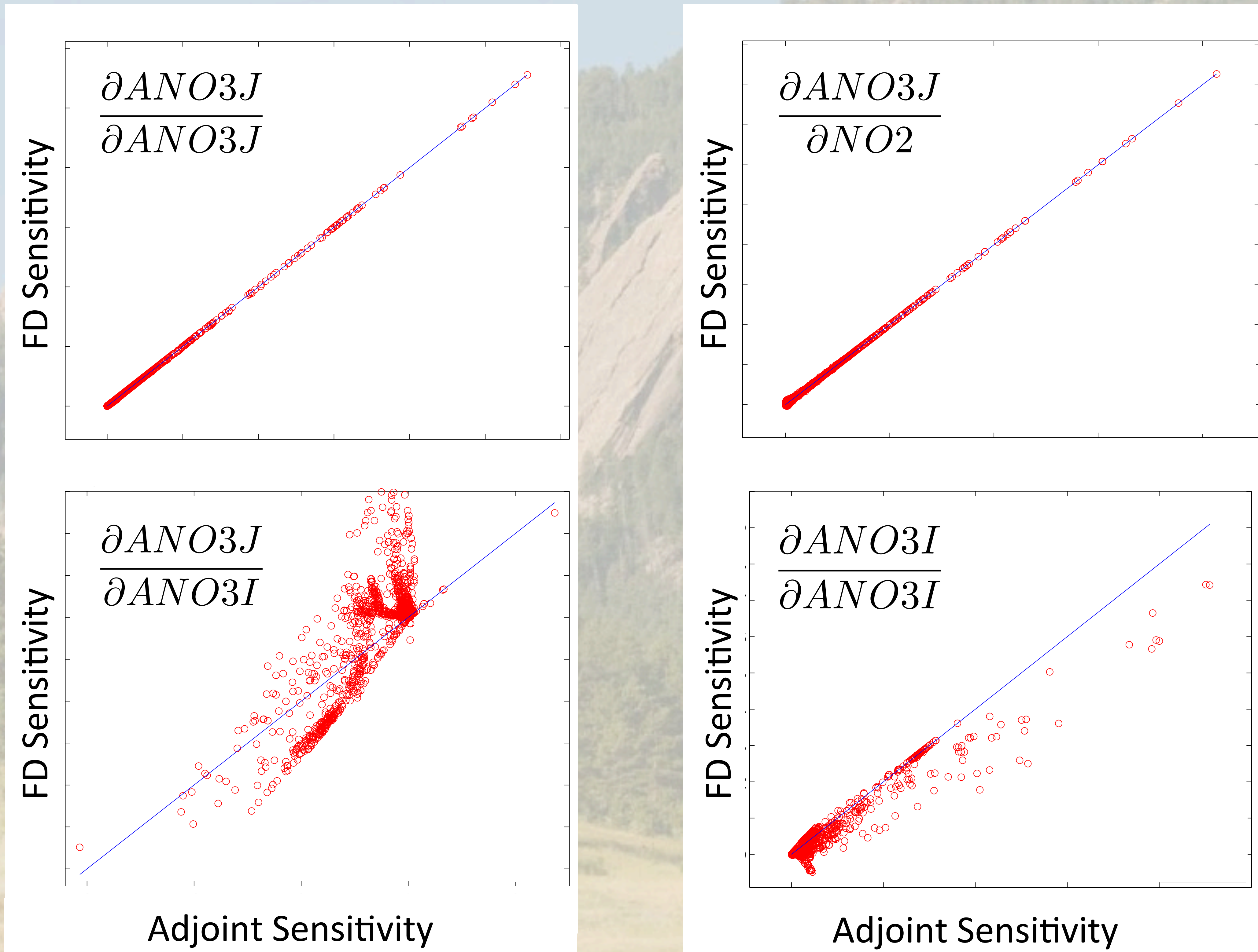
Adjoint Validation

- Validate adjoint by comparing Finite Difference sensitivities to Adjoint sensitivities.
- Finite Difference:
  - Run simulation --> store output values
  - Run simulation after perturbing parameter --> store output values
  - FD = (Perturbed output - base output) / perturbation
- Adjoint:
  - Specify adjoint forcing (what drives adjoint model)
  - Run simulation

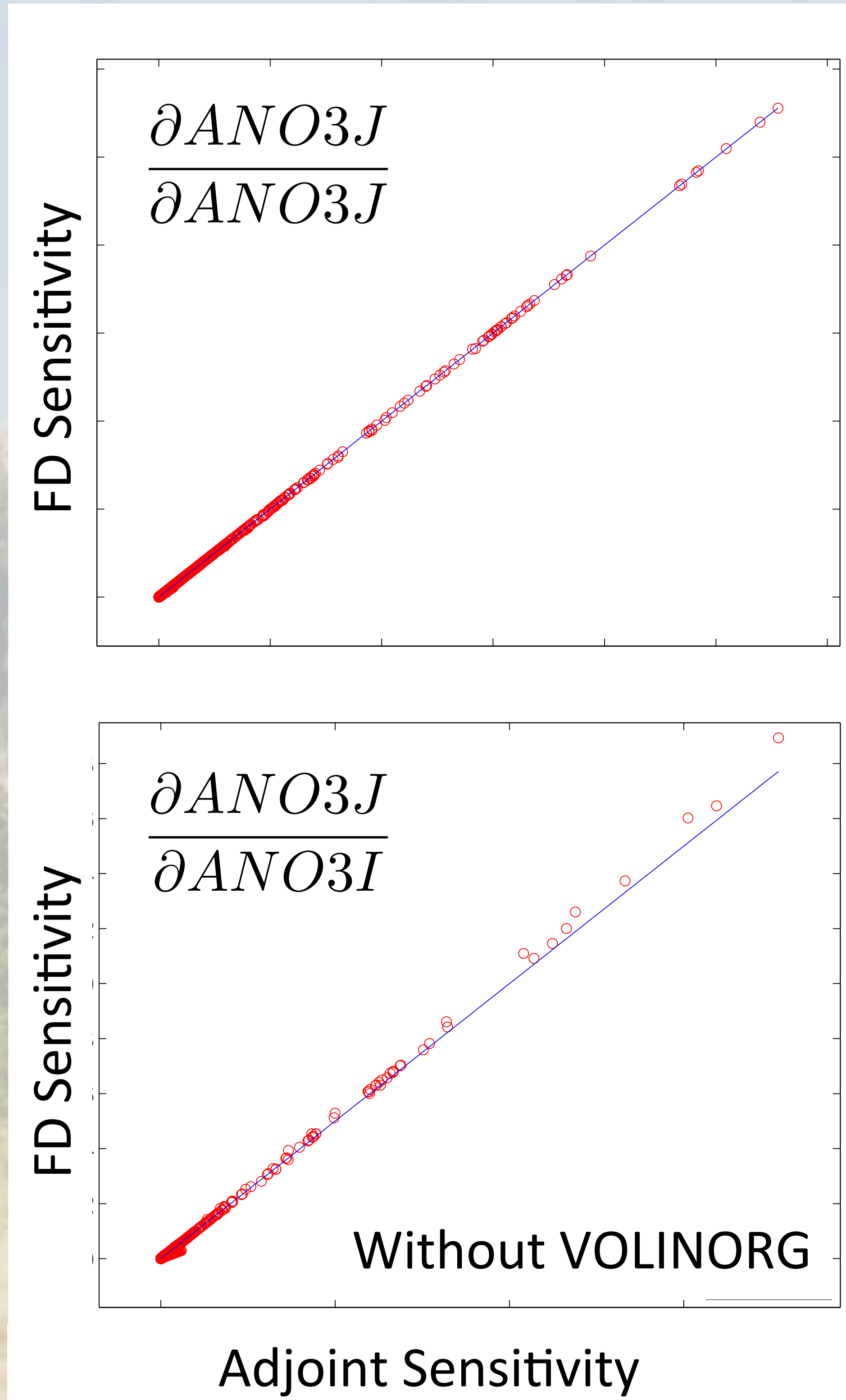
Aerosol Dynamics Validation

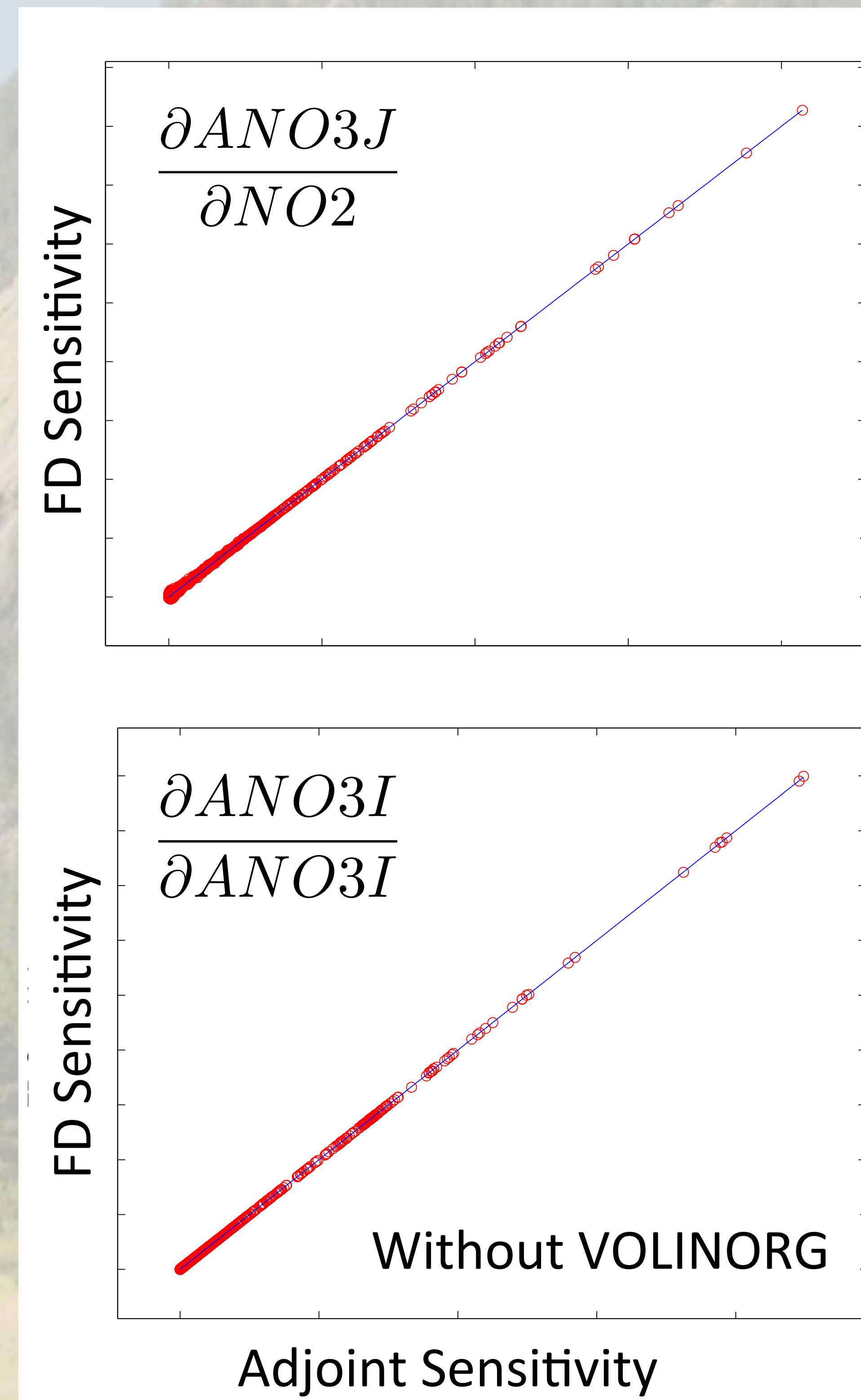
File	Validated in Full Model?	Process Info
hetchem	*Yes*	Heterogeneous conversion of N2O5 to HNO3
n2o5prob	*Yes*	N2O5 heterogeneous reaction probability
getcoags	*Yes*	Coagulation rates using approximate algorithm for 2nd moment. 0th and 3rd moments calculated by analytic expressions
volinorg	*Yes*	Partitioning of inorganic components between aerosol and gas phase
calc_h2o	*Yes*	Water content of aerosol
hcond3	*Yes*	Calculates size-dependent term in condensational growth rate expression for 2nd and 3rd moments using harmonic mean method
compute_flux	*No*	Evaporative/condensational flux of volatile inorganic species to aerosol modes
newpart3	*Yes*	Calculates new particle production rate due to binary nucleation of H2SO4 and H2O vapor
getpar	*Yes*	Calculates 3rd moments, masses, aerosol densities, and geometric mean diameters of all 3 modes

Aerosol Adjoint Validation: Full Model

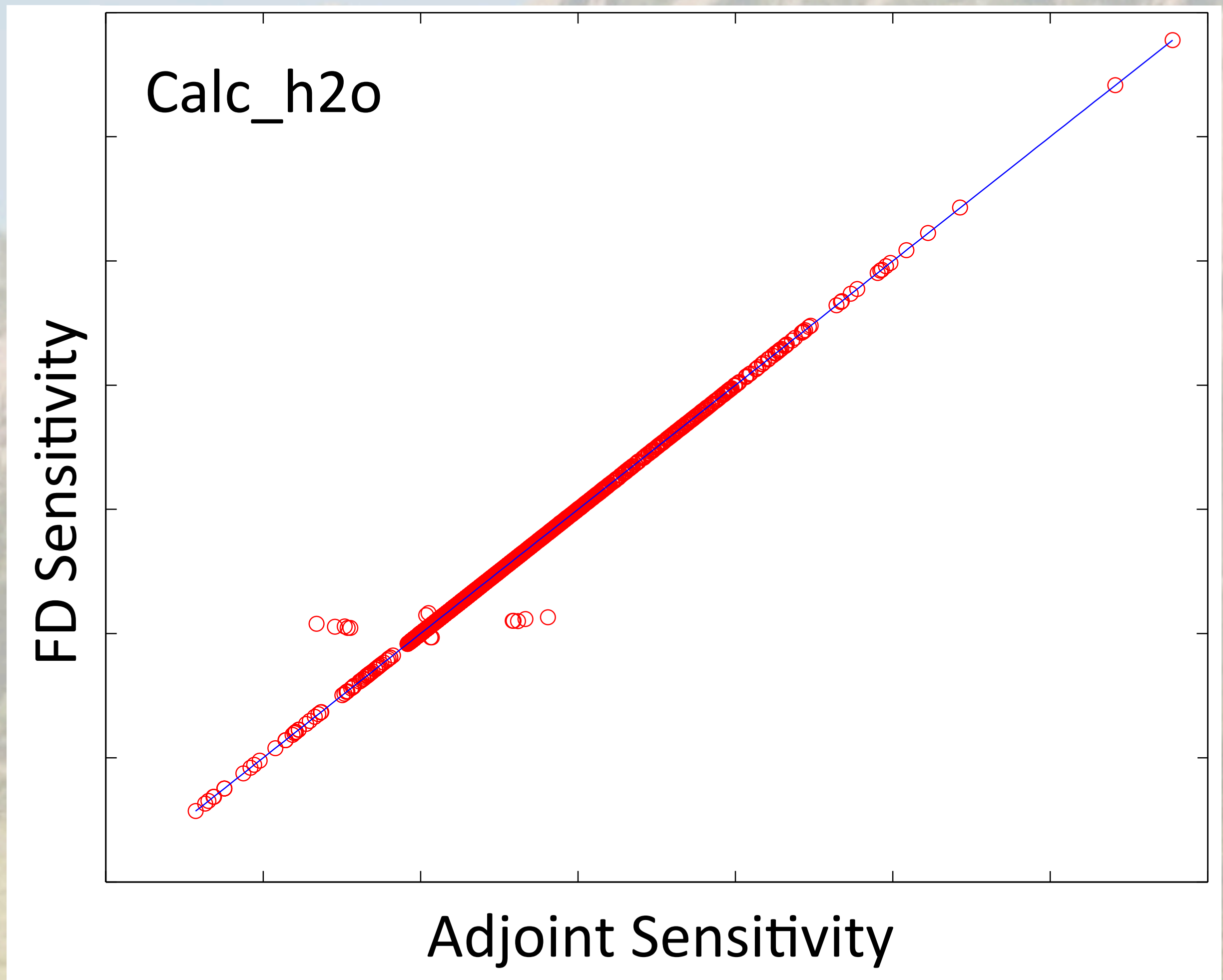


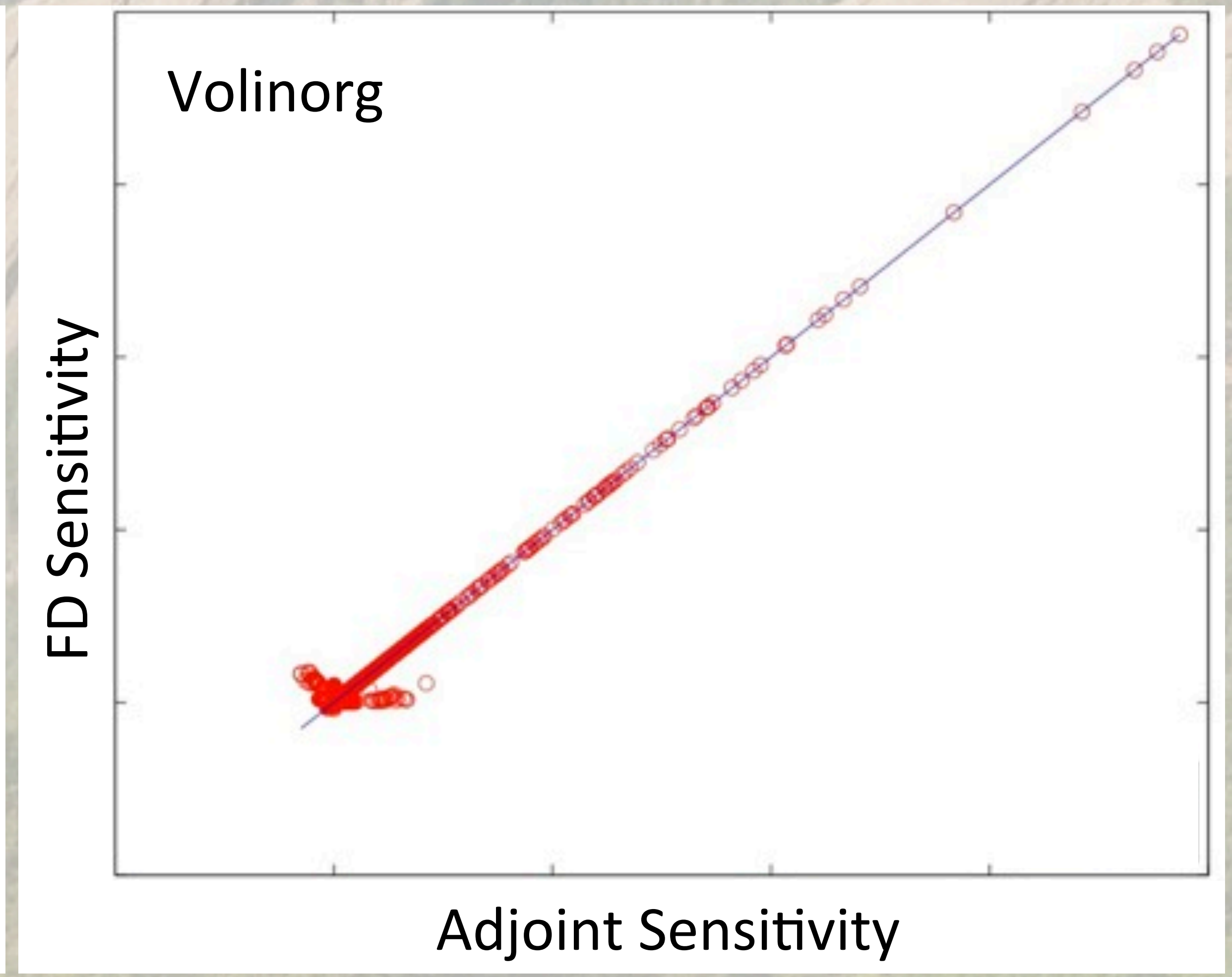
Aerosol Adjoint Validation: Full Model



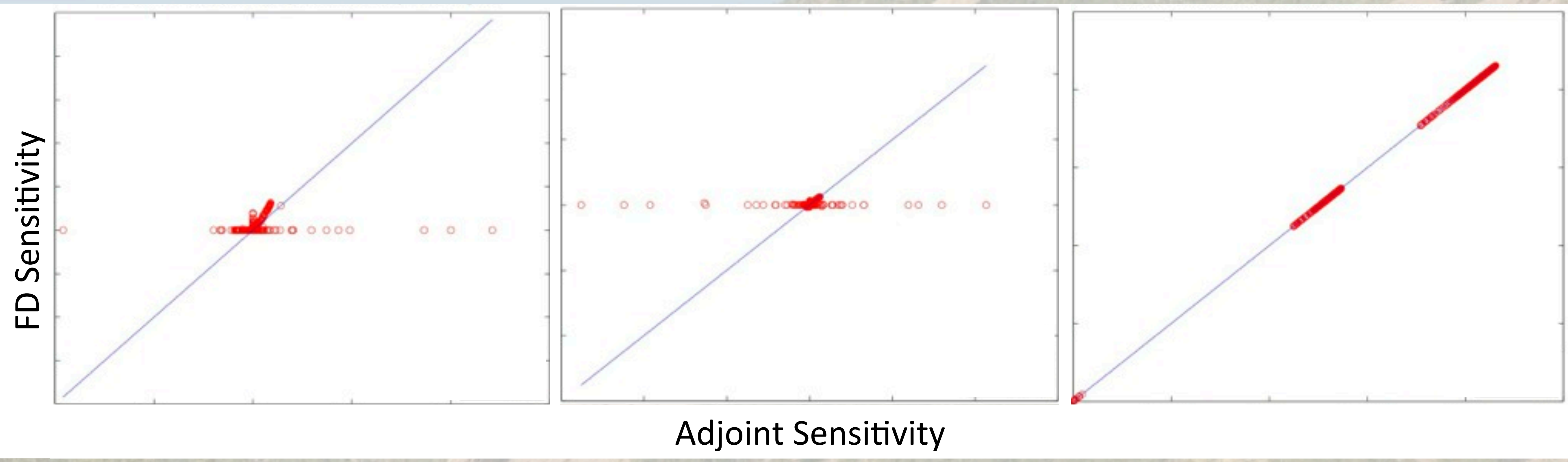


Process level adjoint validation





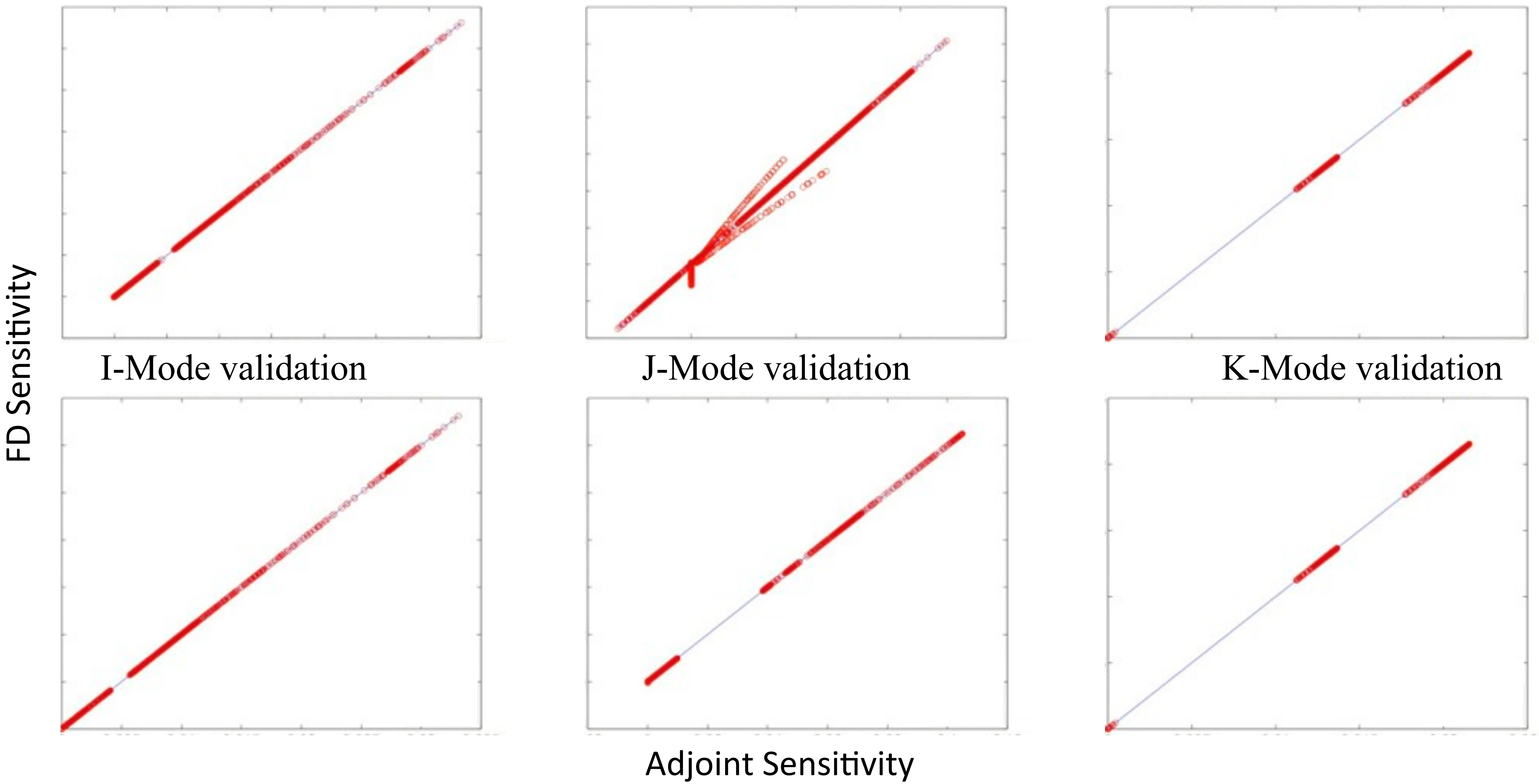
Process level adjoint validation: condensation (VOLINORG)



I-Mode validation J-Mode validation K-Mode validation

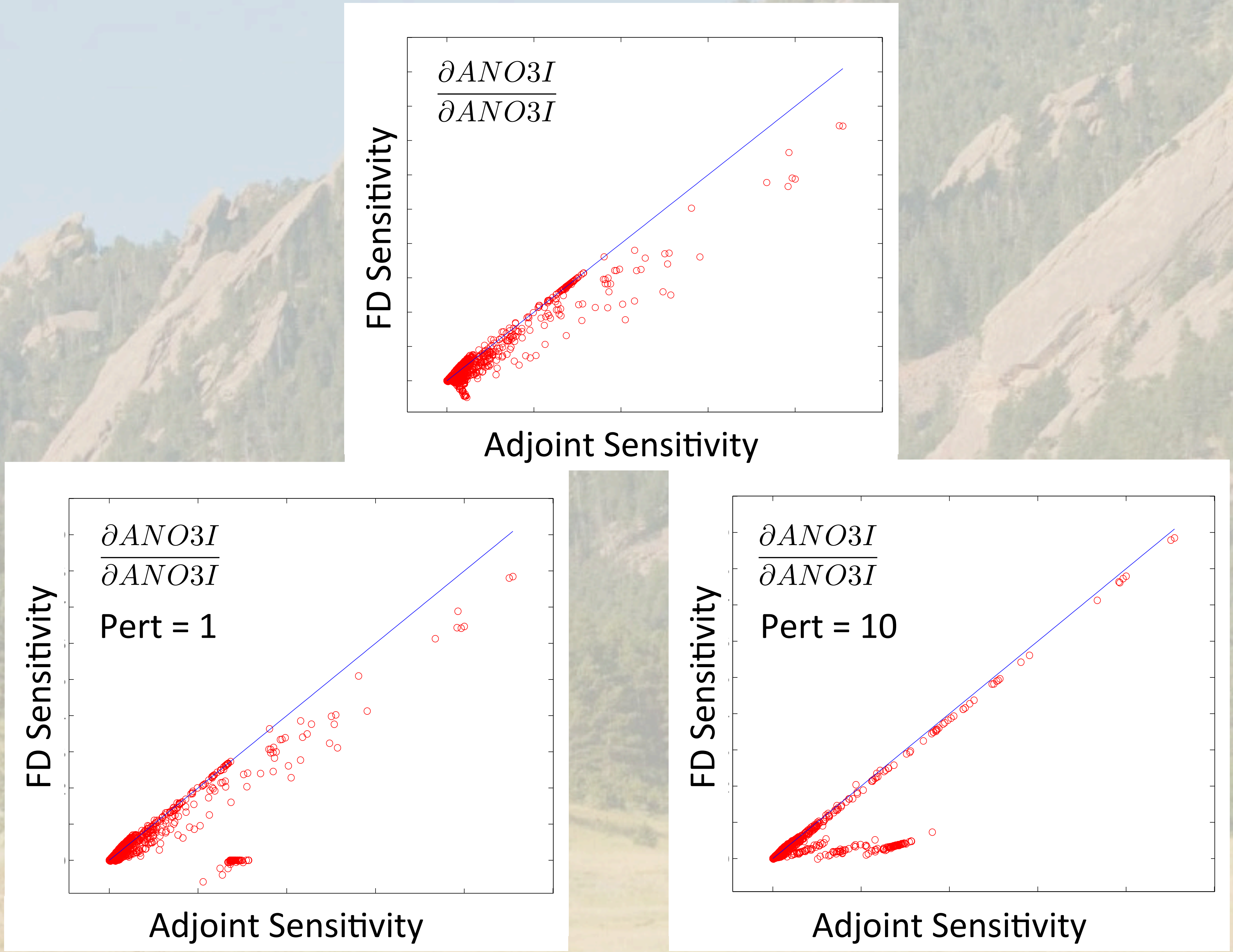
- VOLINORG contains calls to many other subroutines.
- Discrepancies only for:
  – Sulfate, Ammonium, Nitrate, Sodium, Chloride

VOLINORG w/o ISORROPIA



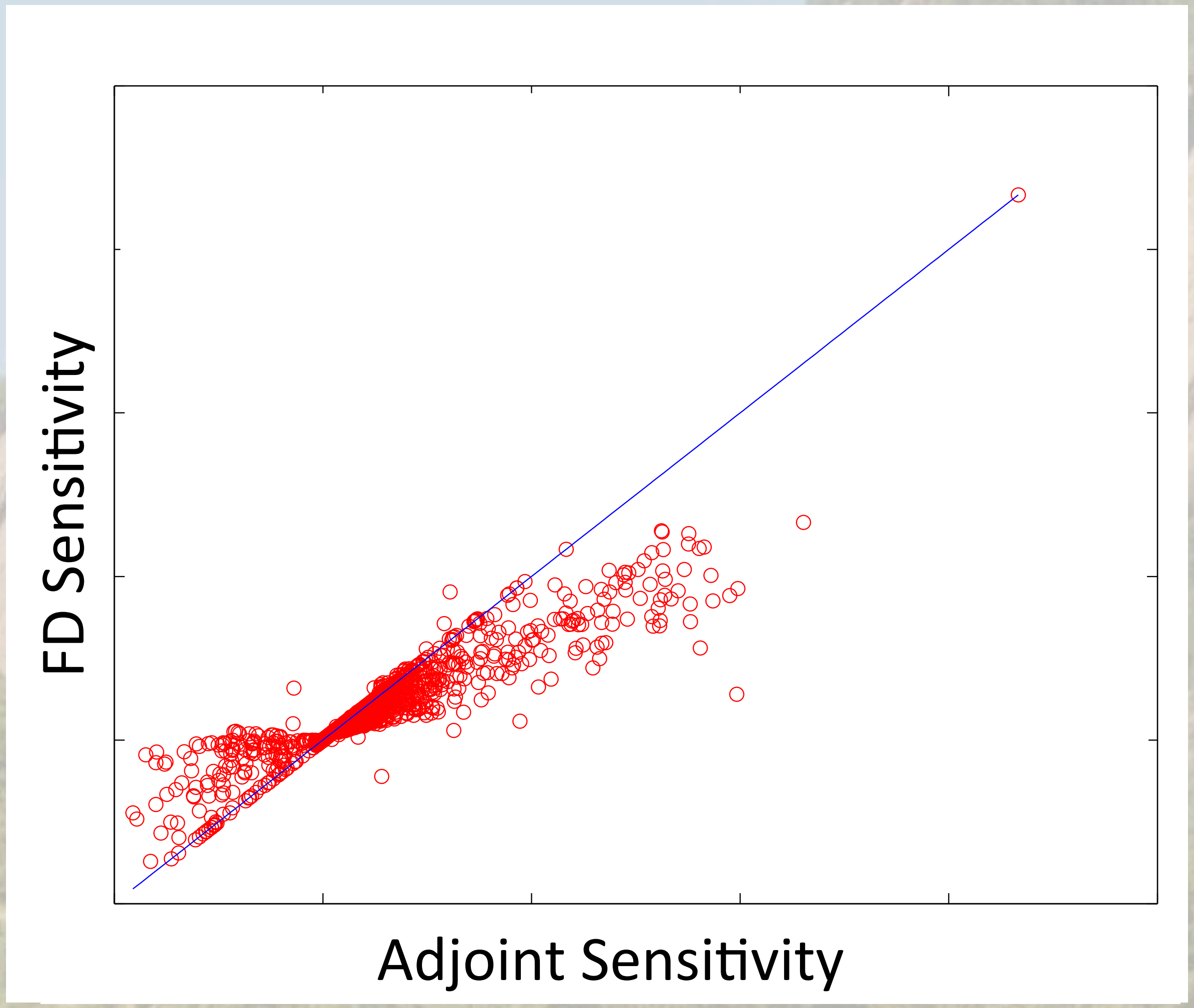
Validation of VOLINORG. Top 3 plots are Volinorg w/o ISORROPIA.
Bottom 3 plots are Volinorg w/o ISORROPIA or Calc_h2o

Aerosol Dynamics - Box Model

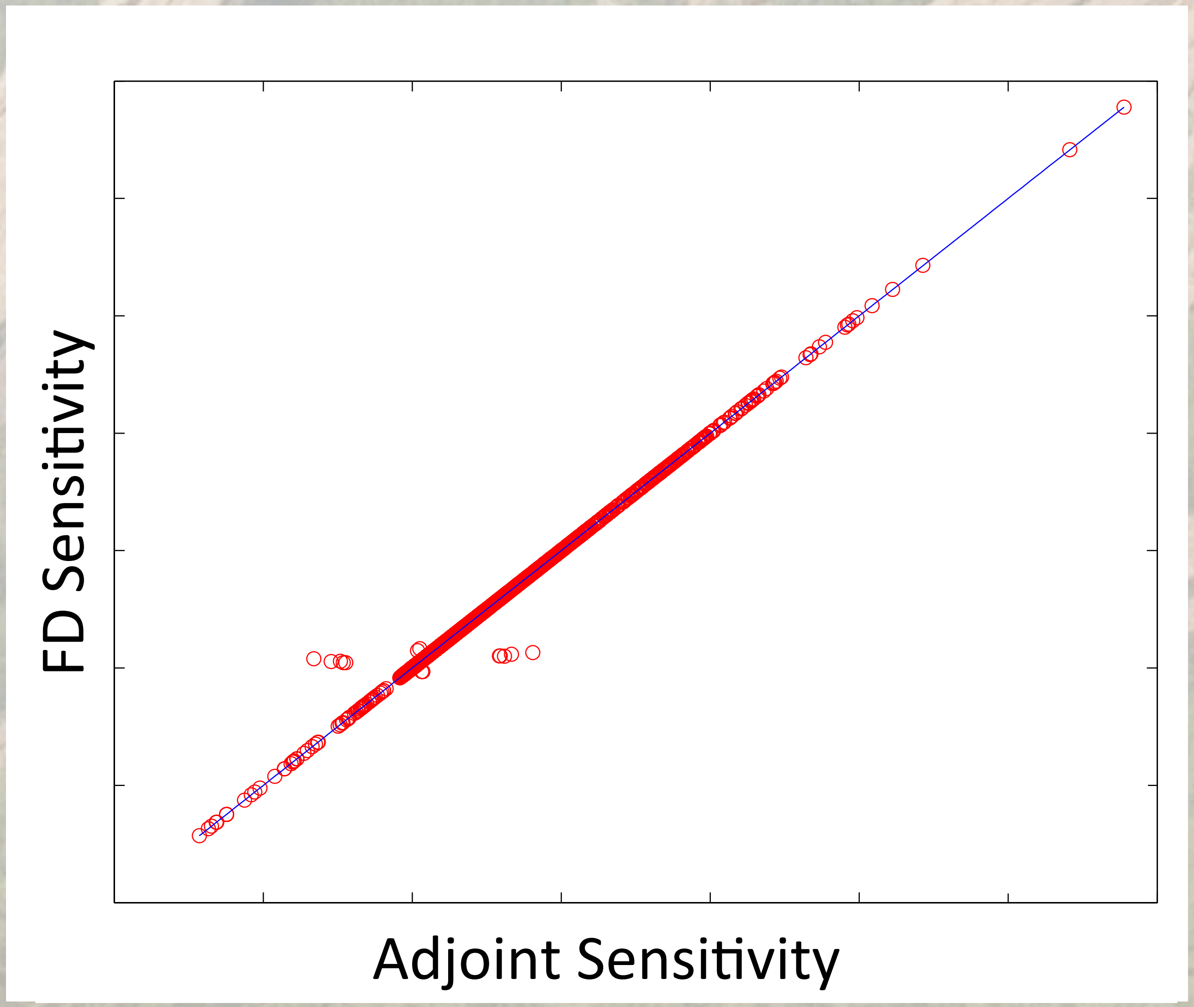


Validation using Finite Difference

Finite difference sensitivities depend upon the perturbation size:



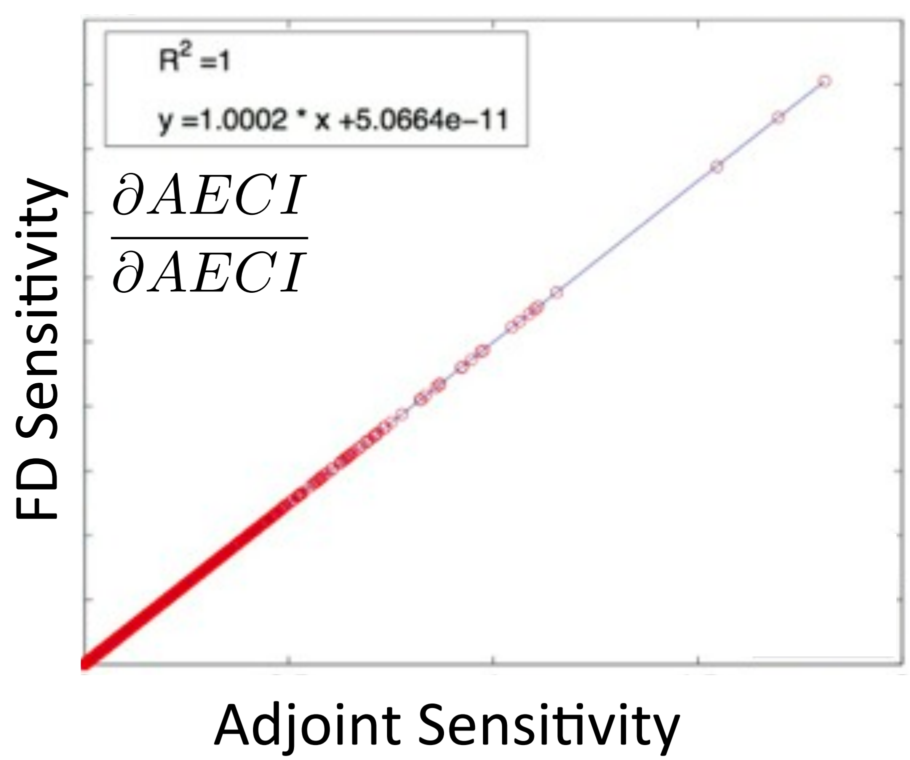
Validation of Calc_H2O Subroutine.
Finite Difference perturbation of 0.1

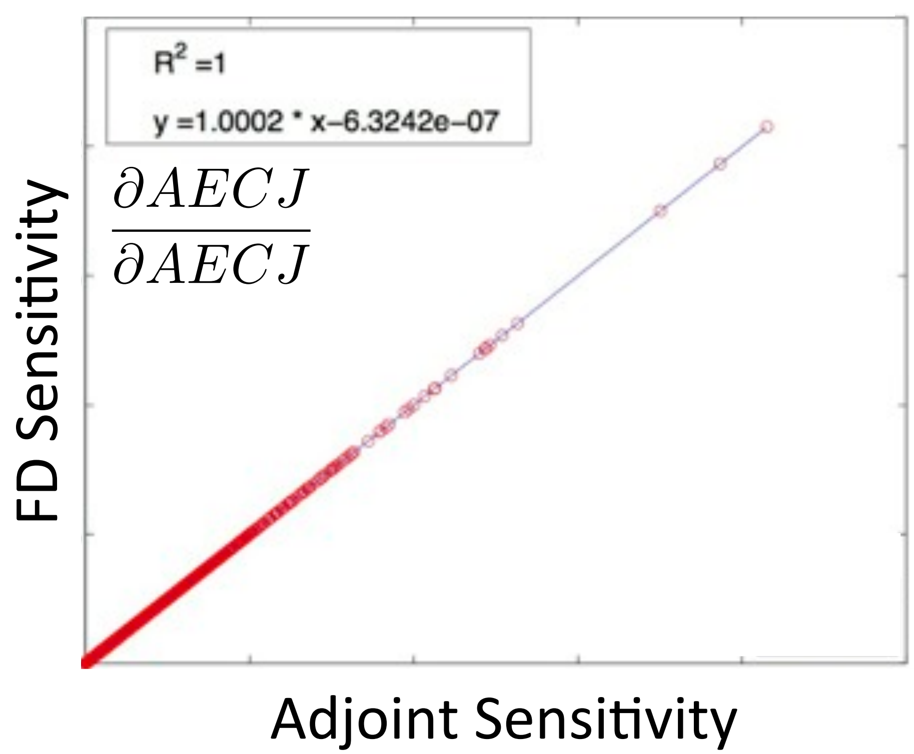


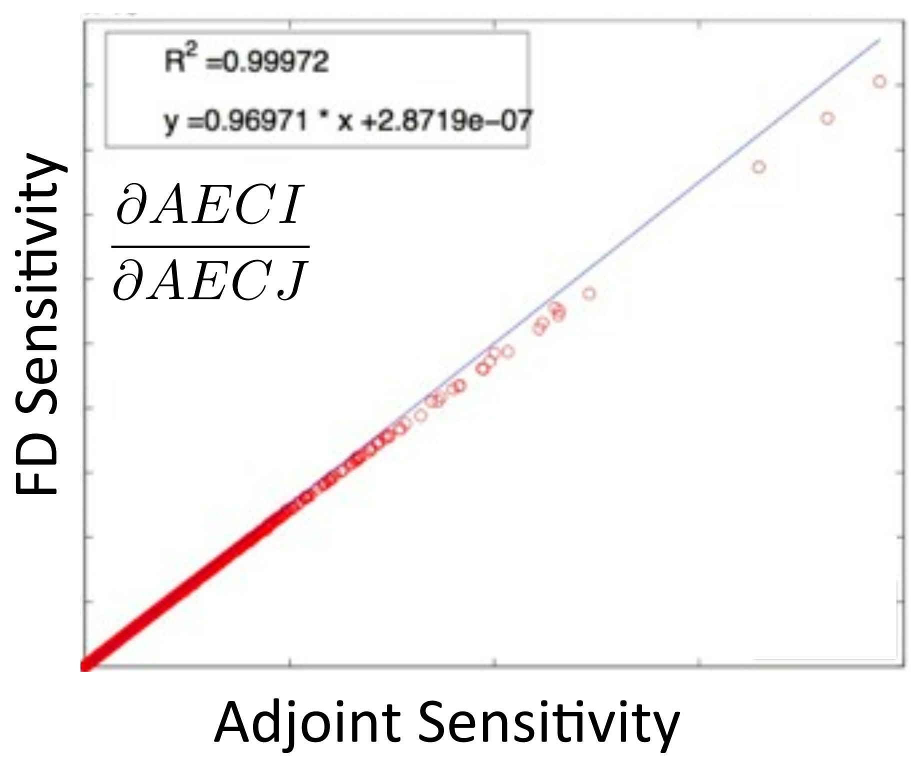
Validation of Calc_H2O Subroutine.
Finite Difference perturbation of 0.0001

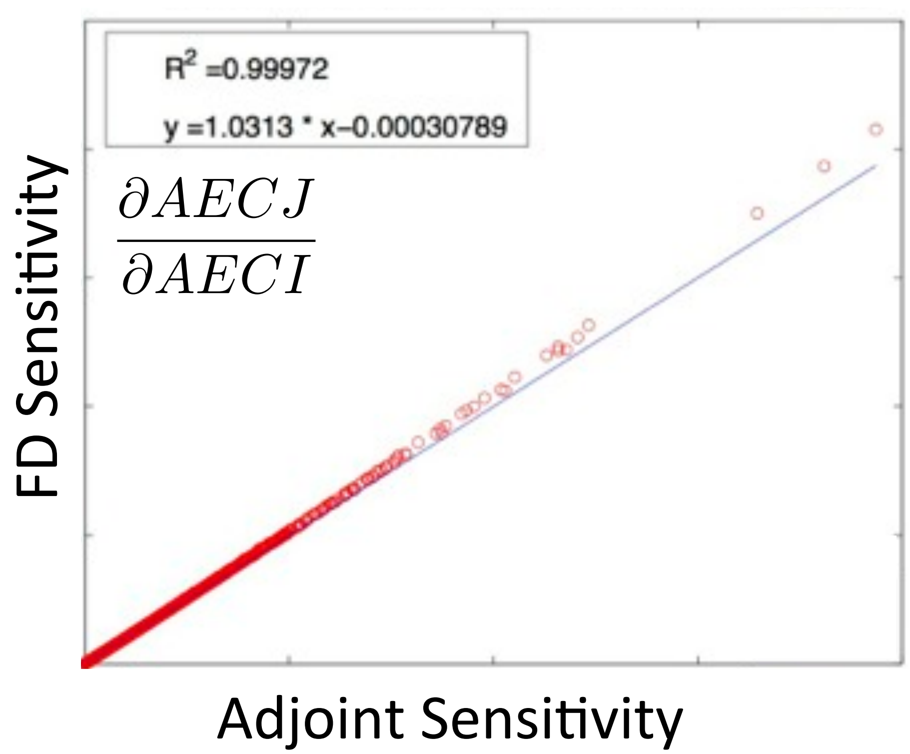
Adjoint may be correct even if it does not match finite difference results

Black Carbon Validation

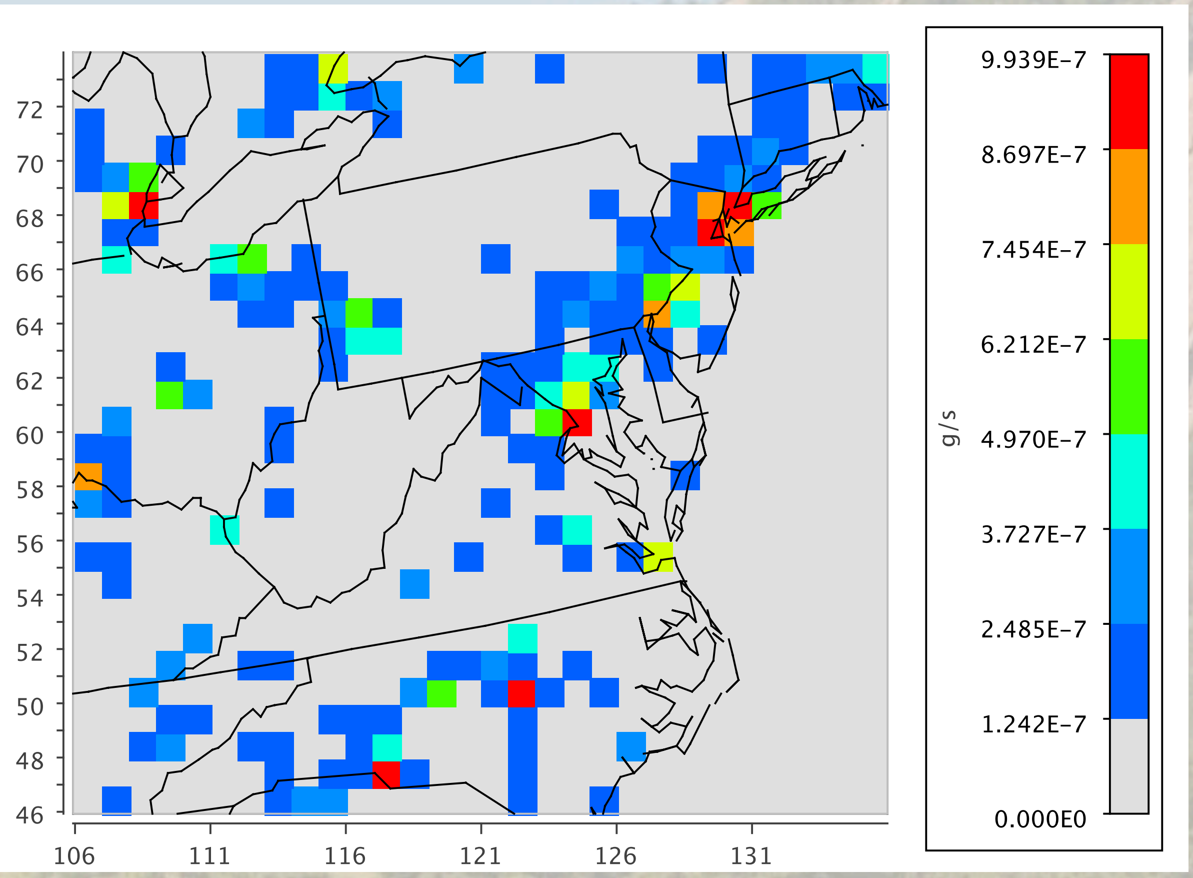




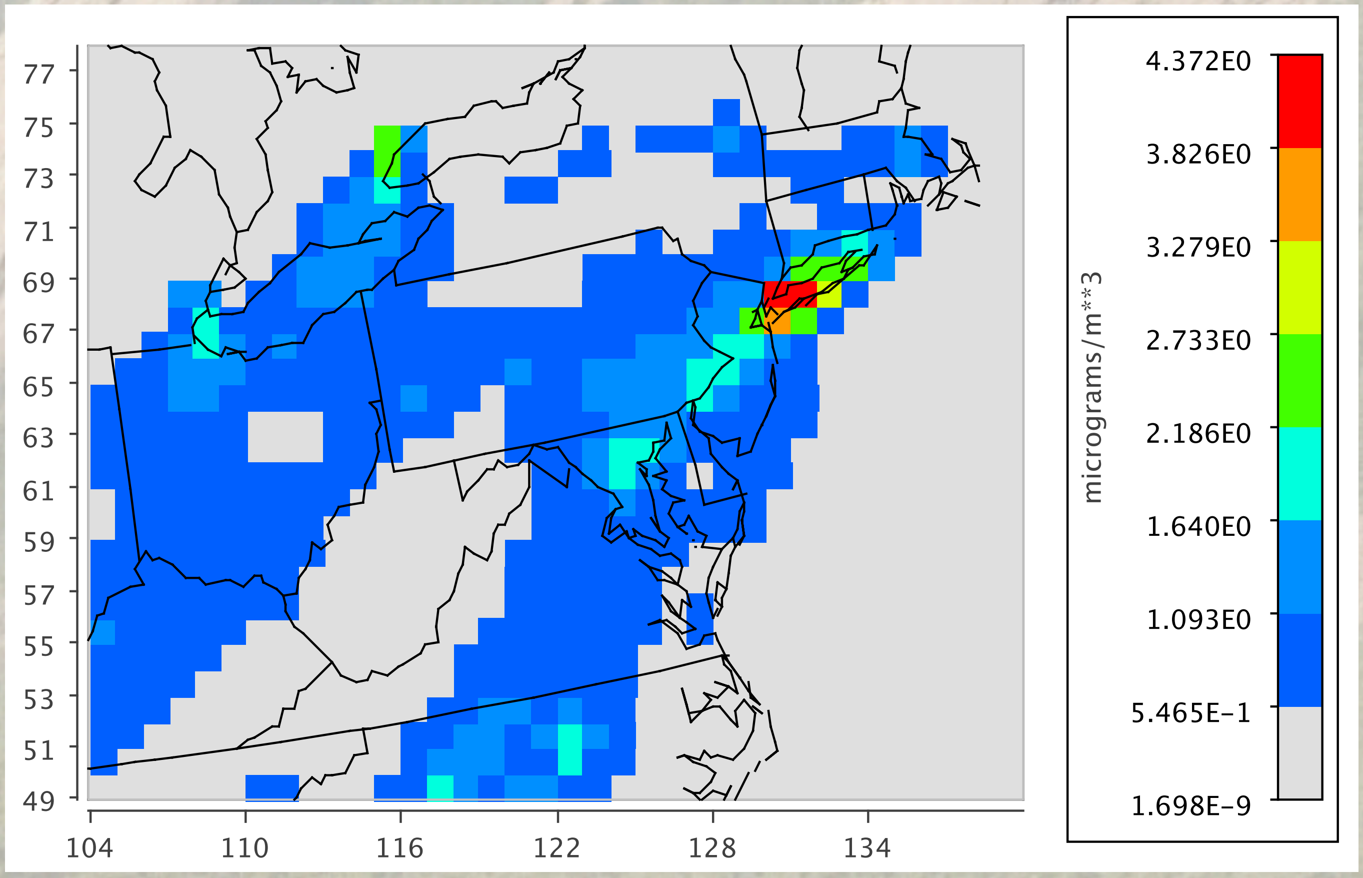




Black Carbon Analysis



AECJ Emissions



AECJ Concentrations

Black Carbon Analysis

Health Impact Function: $\Delta Mort = y_0(1 - exp^{-\beta \Delta X})Pop$

- y_0 = baseline mortality rate
- ß = Concentration Response Factor
- X = concentration
- Pop = population

J = Health Impact Function

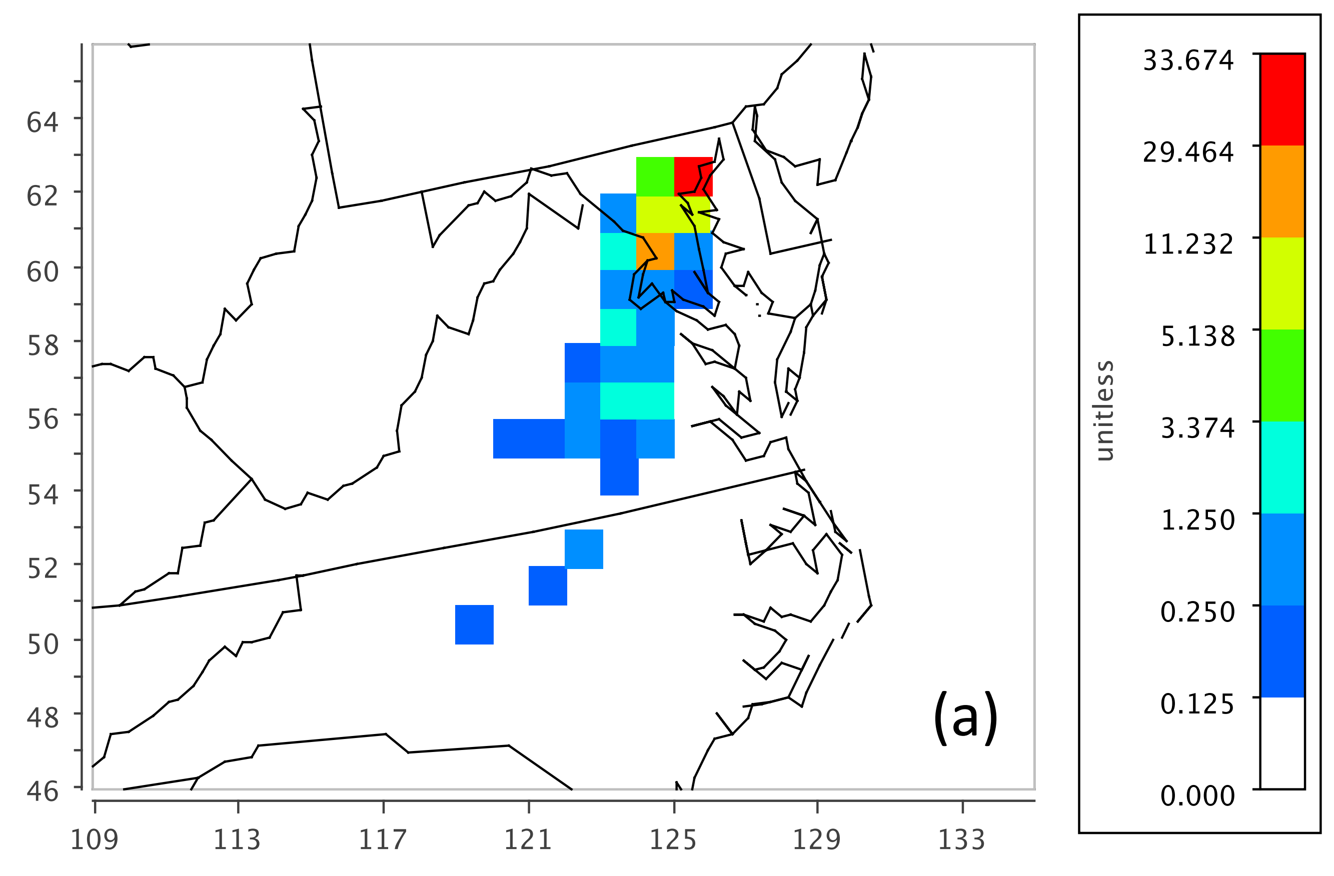
Adjoint model driven by:

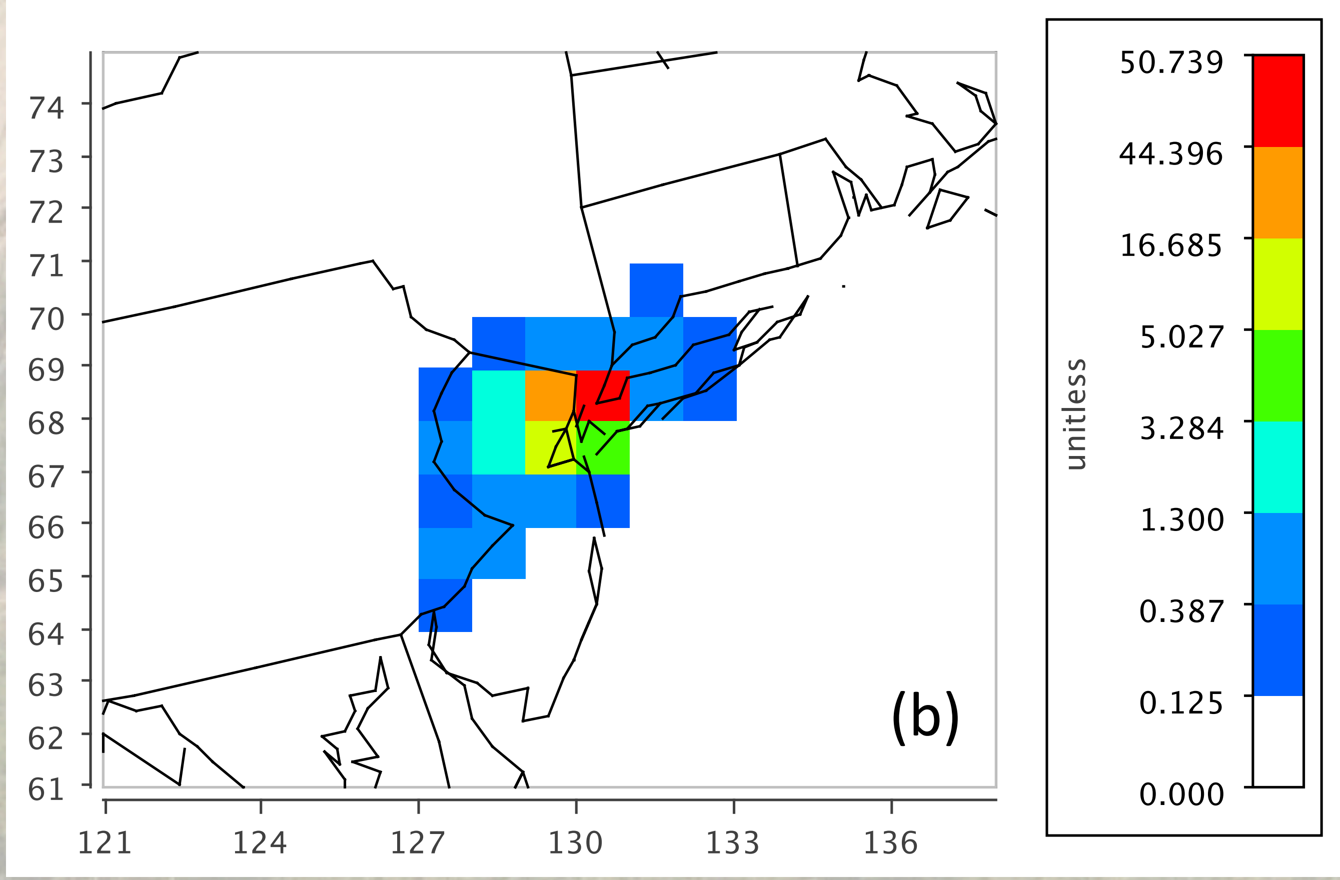
$$\frac{\partial Mort}{\partial X} = \beta * y_0 * Pop * exp^{-\beta X}$$

	Baltimore	NY
y_0	1.02	0.634
β	0.005827	0.005827
Pop	636919	8363710

Black Carbon Analysis

$$\frac{\partial J}{\partial E_{i,j,k}} \frac{E_{i,j,k}}{J} \times 100\%$$





J = 748.25 J = 13490.4

Sensitivity of mortalities caused by black carbon in (a) Baltimore, MD and (b) NY, NY with respect to black carbon emissions.

April 3, 2008, 7:00 PM Local to April 4, 2008, 7:00 PM Local

Summary and Future Work

- Adjoint of CMAQ aerosol module has been developed and validated for black carbon.
  - Needs further validation/debugging of other processes
  - Compare to CVM
- Sensitivities with respect to emissions have been obtained for single day simulations for Baltimore, MD and New York city.
  - Need to extend to multiple month simulations
  - Use monthly average concentrations in Health Impact Function
- Extend work to inverse modeling (4D-Var) of emissions.