CMAQ Adjoint Development and Initial Applications

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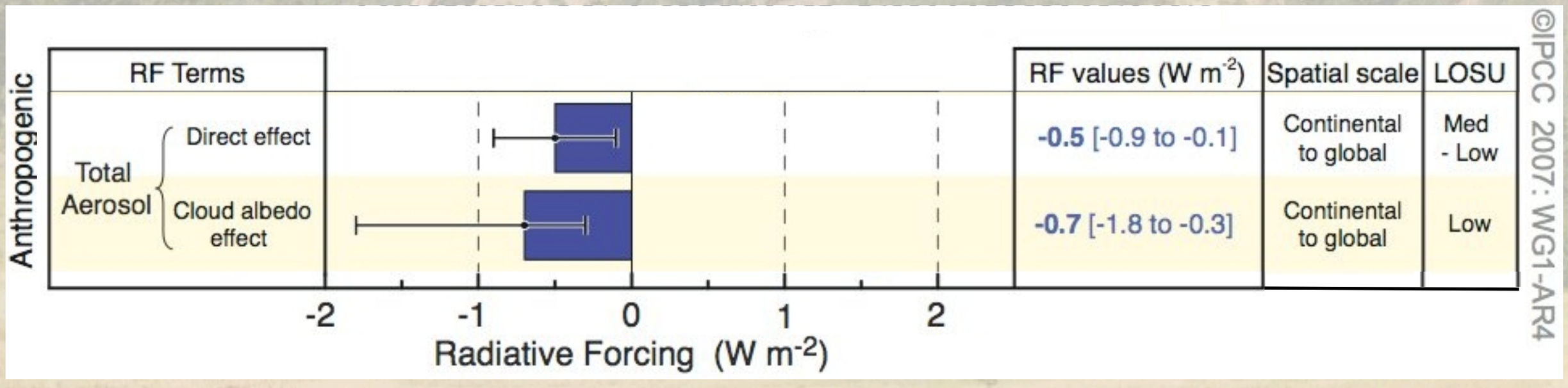
Motivation

- Many atmospheric CTMs now include aerosols
  - Models still contain large amounts of uncertainty.
- Many methods to decrease uncertainty
  - Develop better understanding of physical processes.
  - Data assimilation.
  - Using ensemble of models.
- This project focuses on 4D-Variational data assimilation
  - Requires an adjoint model.
- Currently no other regional CTM has an adjoint that includes aerosols.

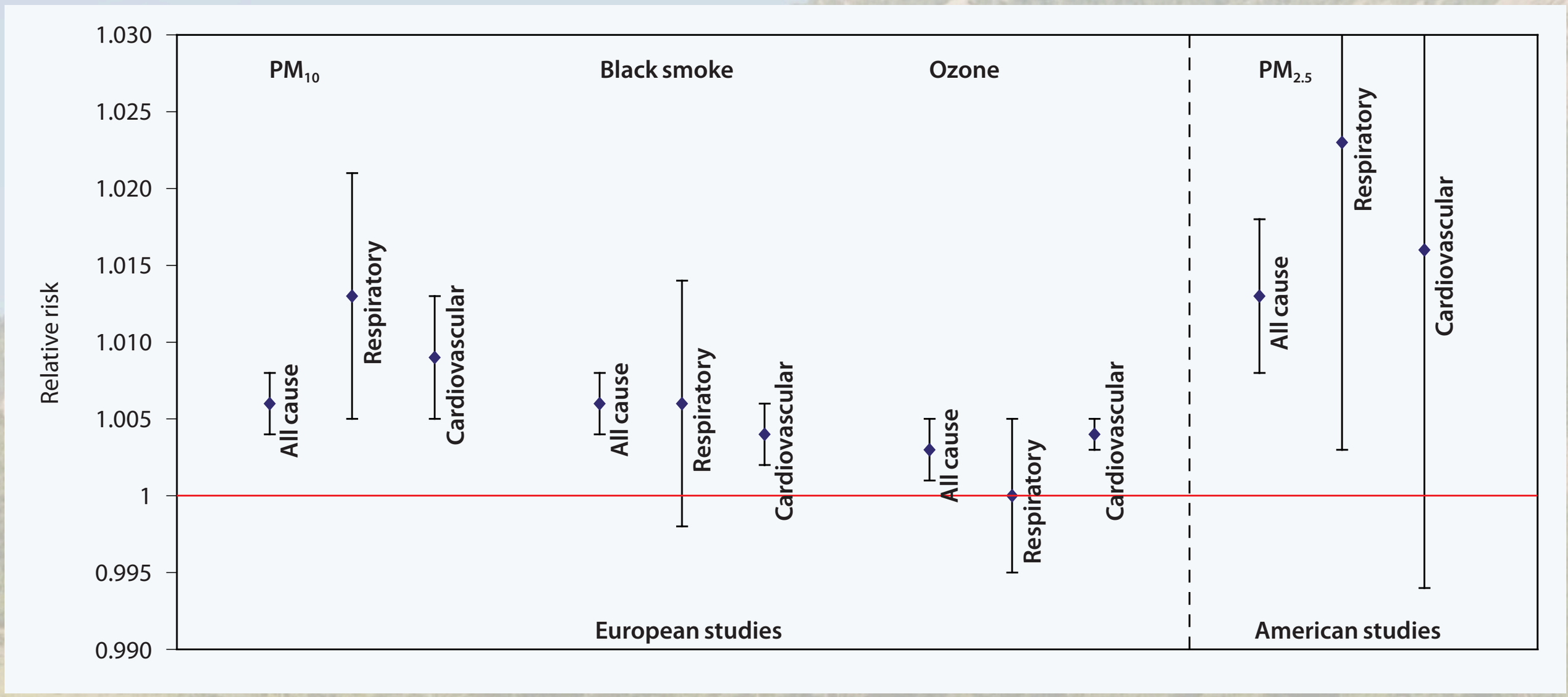
Aerosol Effects on Climate Change

- Both direct and indirect effect on radiative forcing.
- Direct effect:
  - Scattering
  - Absorption
- Indirect effect:
  - Changes in cloud properties due to aerosols



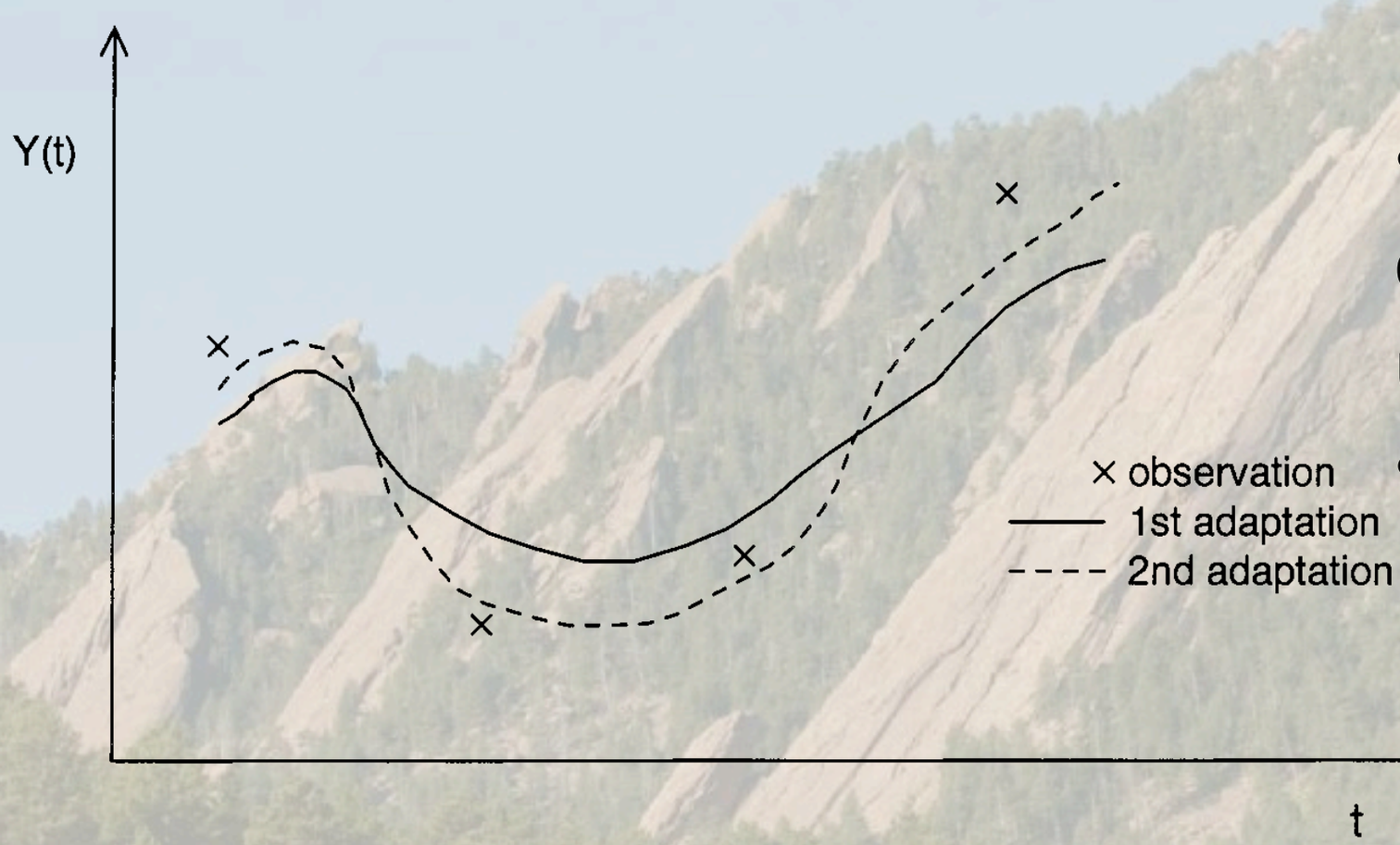
Aerosol Radiative Forcing Components (IPCC, 2007)

Health Effects of PM



Estimates for Relative Risks for Mortality and different air pollutants (WHO, 2006)

Adjoint Models



Schematic representation of the benefit of adjoint models (Giering and Kaminski, 1998)

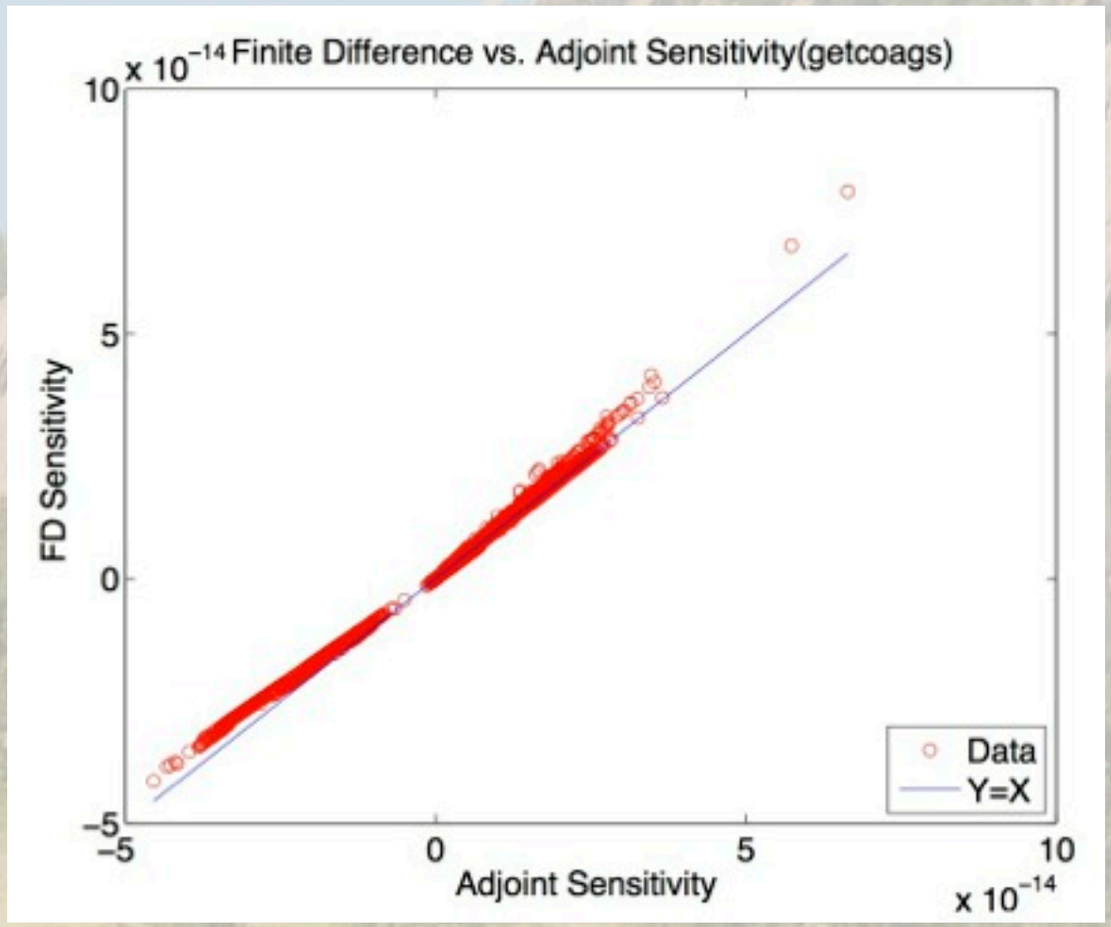
- Atmospheric CTMs contain large amounts of uncertainty.
- 2 types of adjoints:
  - Discrete
  - Continuous

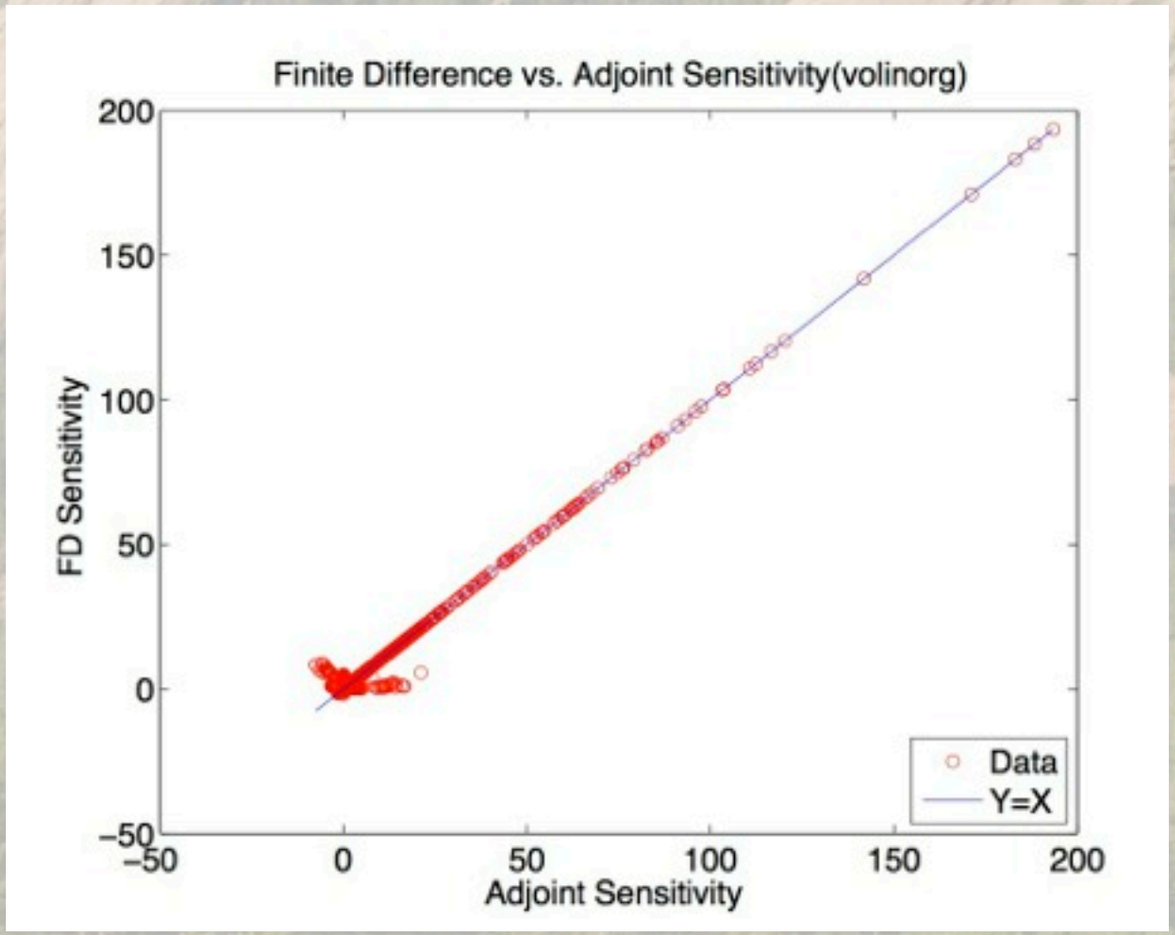
- In order to quantify misfit, cost function introduced.
  - Cost function then reduced through iterative process.
- Adjoint method has 2 main advantages over FD:
  - Especially for large *n*, adjoint model saves run time
  - Computed gradient is exact.

Adjoint Validation

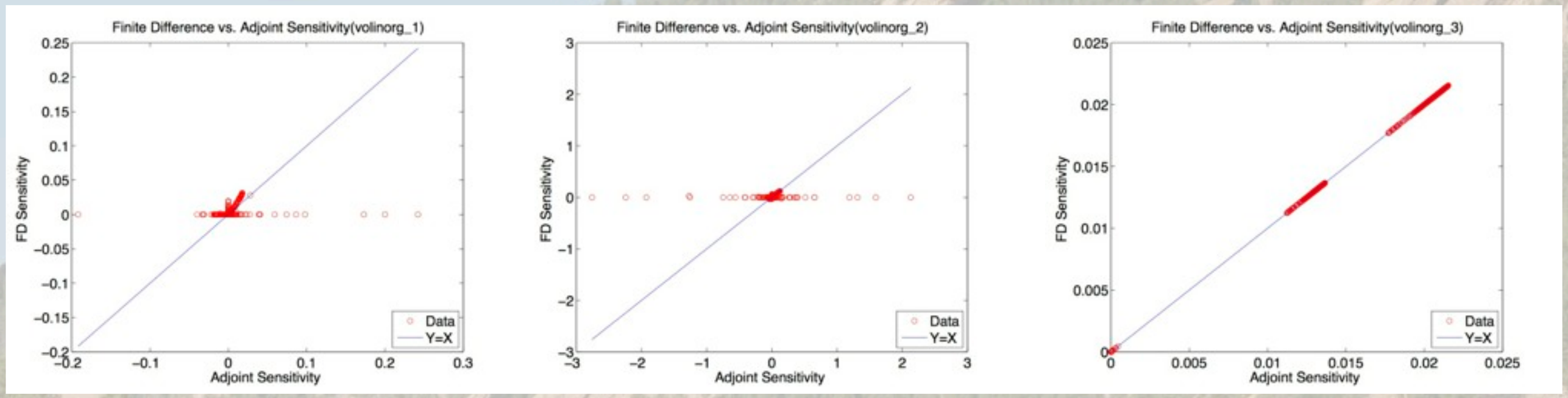
- Validate adjoint by comparing Finite Difference sensitivities to Adjoint sensitivities.
- Finite Difference:
  - Run simulation --> store output values
  - Run simulation after perturbing parameter --> store output values
  - FD = (Perturbed output - base output) / perturbation
- Adjoint:
  - Specify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

Aerosol Dynamics Validation





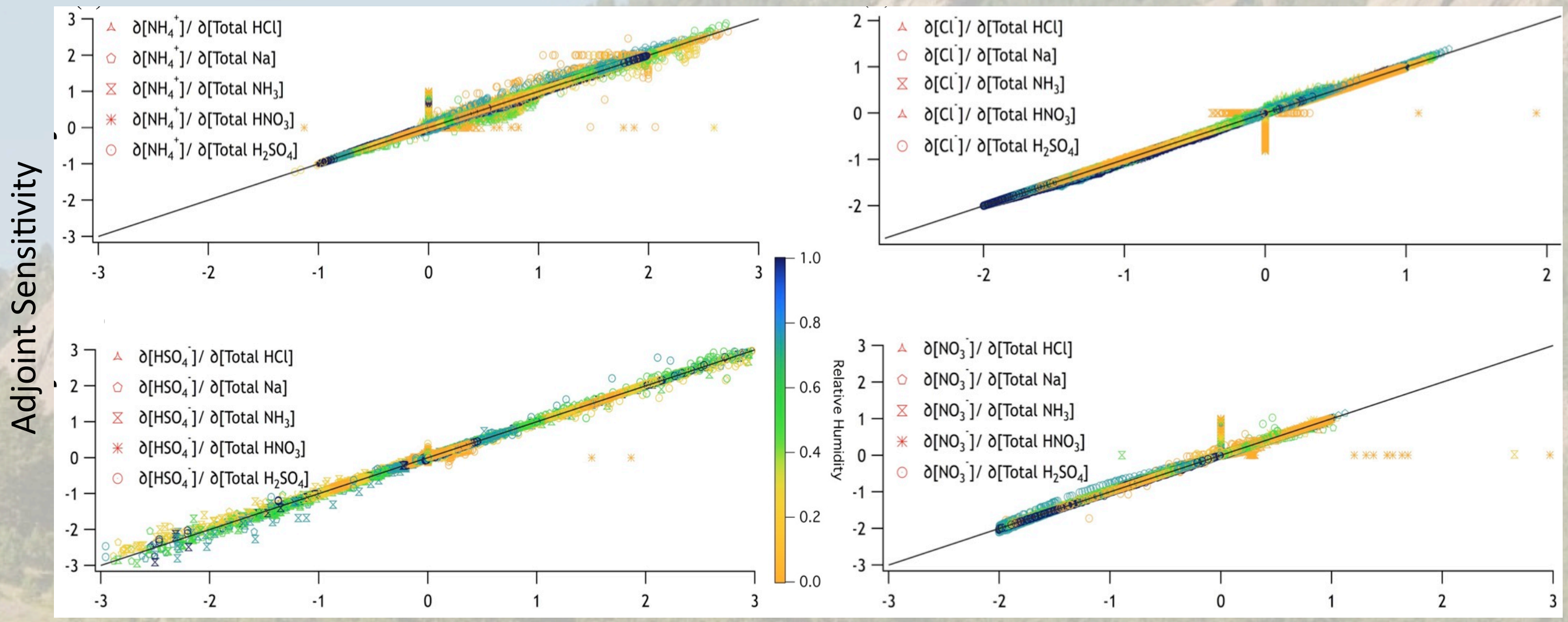
VOLINORG Validation



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

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

Aerosol Thermodynamics



Complex Variable Sensitivity

Courtesy of Shannon Capps, Georgia Tech.

Checkpointing

- The I/O in CMAQ Adjoint code has been altered so that particular strategies for I/O operations on checkpoint and output files can be chosen at configuration time.
- Current implementations include:
  - Serial I/O through IOAPI3/PARIO
  - MPI I/O using the Parallel NetCDF library and NetCDF4/HDF5 libraries
  - Multiple local files

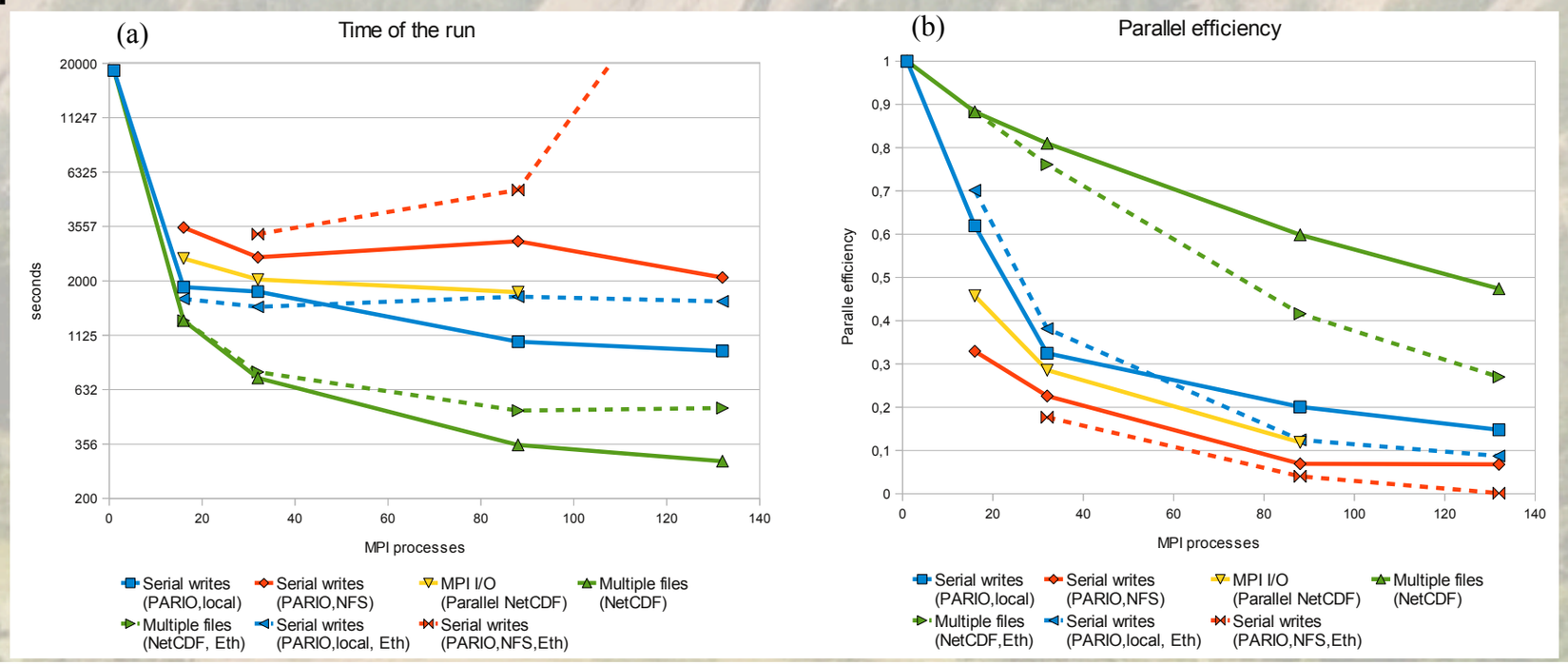
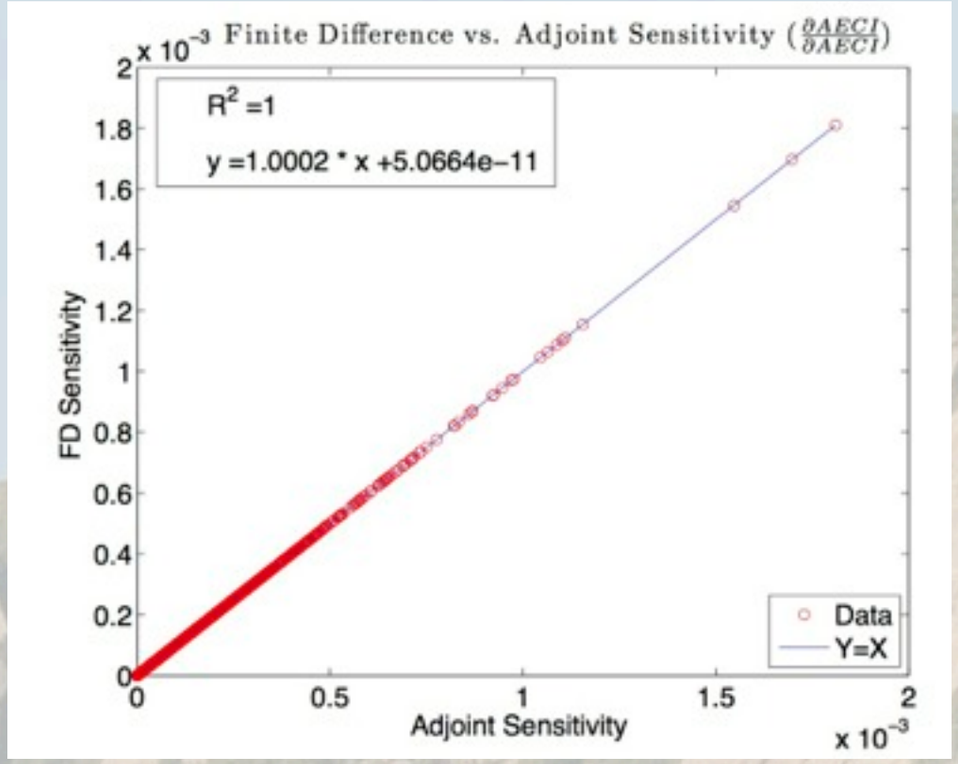
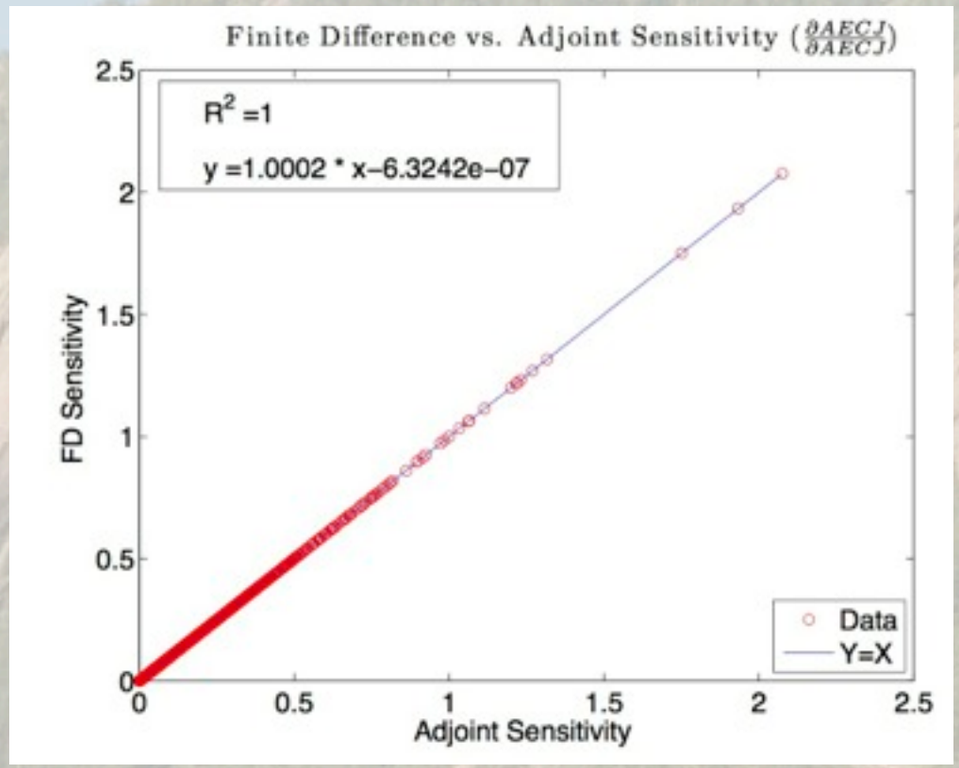


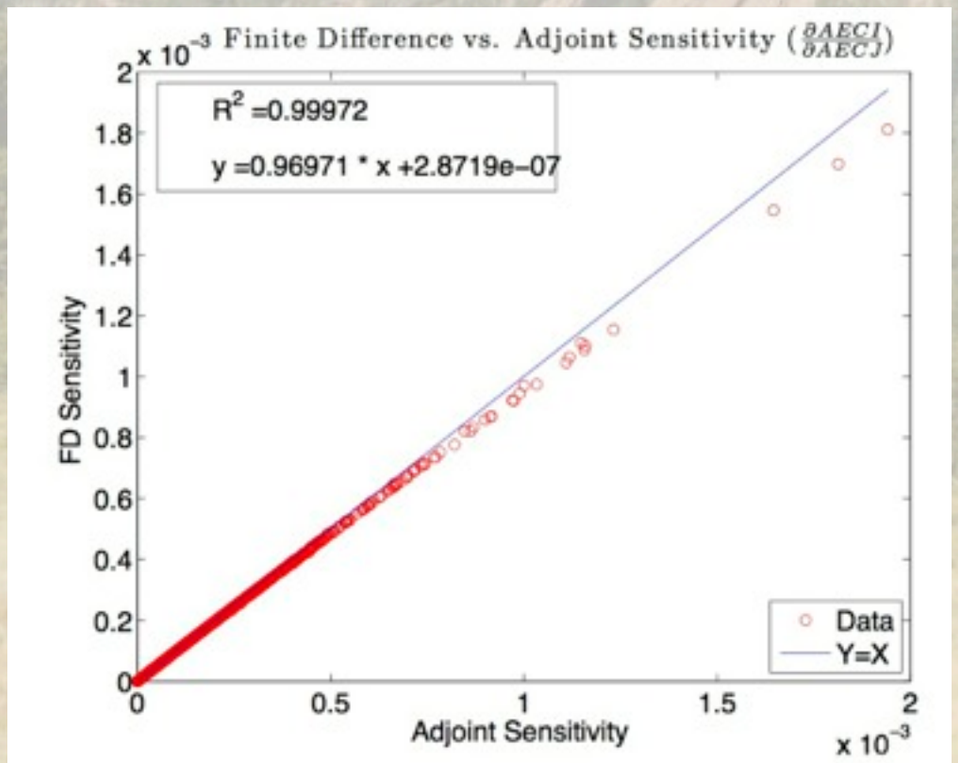
Figure 4: (a) Total time of forward and backward run of the model, and (b) Parallel efficiency of the CMAQ Adjoint model in different testing configurations. Testing configuration: Linux cluster, NFS cluster storage, Infiniband interconnection, MVAPICH2

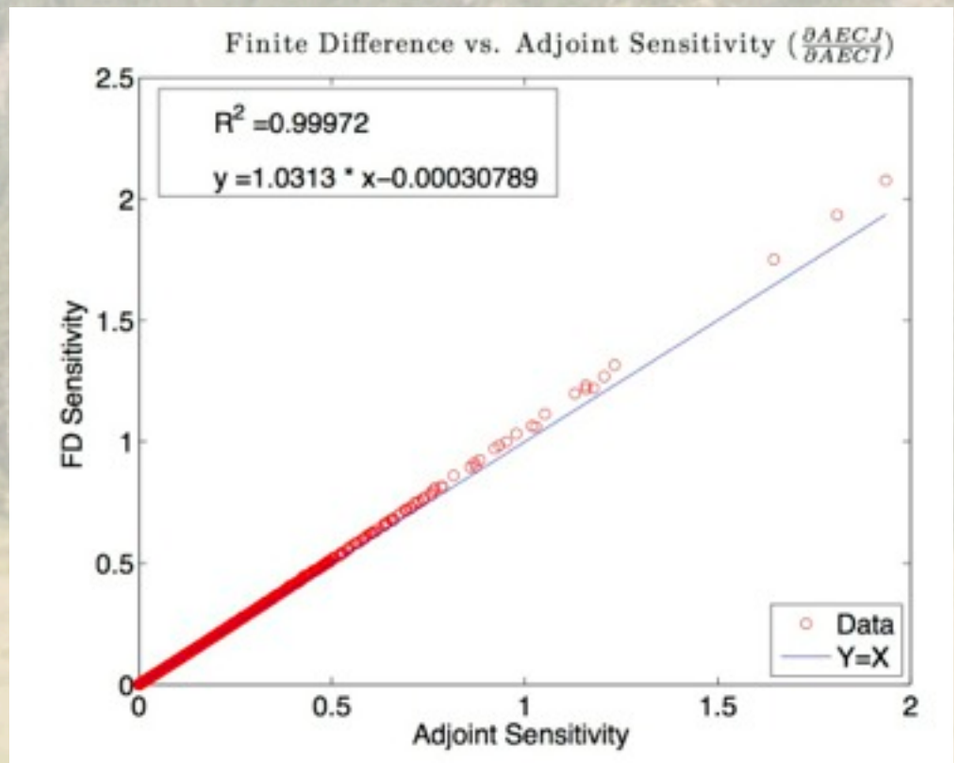
Courtesy of Jaroslav Resler, ICS Prague

Aerosol Dynamics - Full Model

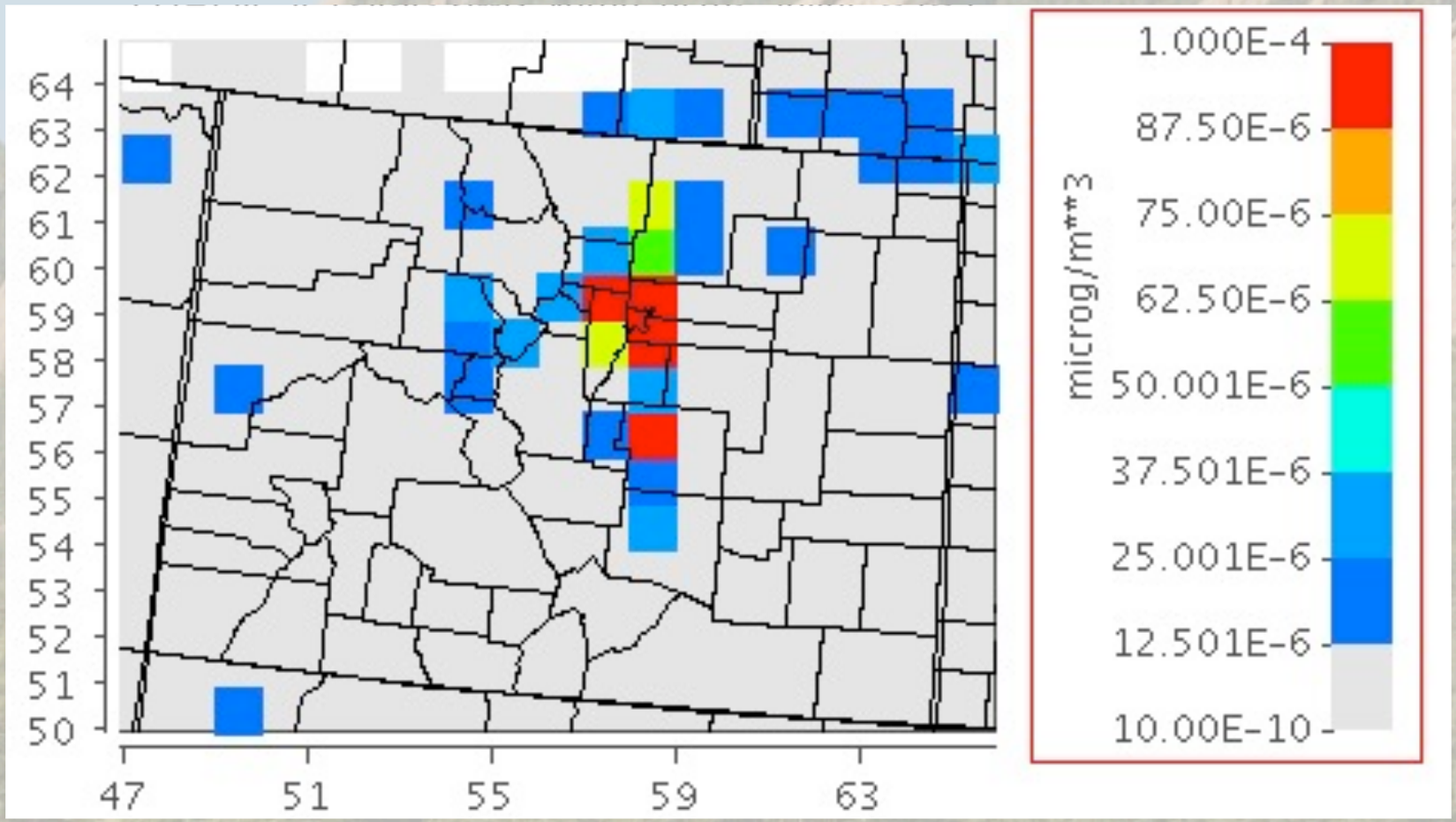








Black Carbon Analysis



Sensitivity of Black Carbon concentrations in Colorado with respect to Black Carbon emissions. Simulation time period: April 4, 2008.

Future Work

- Finish development of aerosol adjoint module
  - VOLINORG incorrect for modes 1 and 2
- Expand simulation period to 1 week.
- Modify cost function to calculate sum of excess mortalities in Colorado due to concentrations of Black Carbon
  - Use adjoint to determine sensitivity of excess mortality due to Black Carbon emissions throughout entire domain.

Supplemental Slides

Discrete Adjoint Example

- **Forward code:**

GAMMA = GAMMA2 + (ASO4 / (ASO4 + ANO3))* (GAMMA1 - GAMMA2)

- **Active variables**: ASO4, ANO3

$$\partial\gamma = \overbrace{(\gamma 1 - \gamma 2)\left(\frac{1}{ASO4 + ANO3} - \frac{ASO4}{(ASO4 + ANO3)^2}\right)}^{a_1}\partial ASO4$$

$$\underbrace{-(\gamma 1 - \gamma 2)\left(\frac{ASO4}{(ASO4 + ANO3)^2}\right)}_{a_2}\partial ANO3$$

Discrete Adjoint Example

$$\begin{bmatrix} \partial ASO4 \\ \partial ANO3 \\ \partial \gamma \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ a_1 & -a_2 & 0 \end{bmatrix} \begin{bmatrix} \partial ASO4 \\ \partial ANO3 \\ \partial \gamma \end{bmatrix}$$

$$\begin{bmatrix} ASO4* \\ ANO3* \\ \gamma* \end{bmatrix} = \begin{bmatrix} 1 & 0 & a_1 \\ 0 & 1 & -a_2 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} ASO4* \\ ANO3* \\ \gamma* \end{bmatrix}$$

- **Adjoint Equations:**

  ASO4_ADJ = ASO4_ADJ + a_1 * GAMMA_ADJ

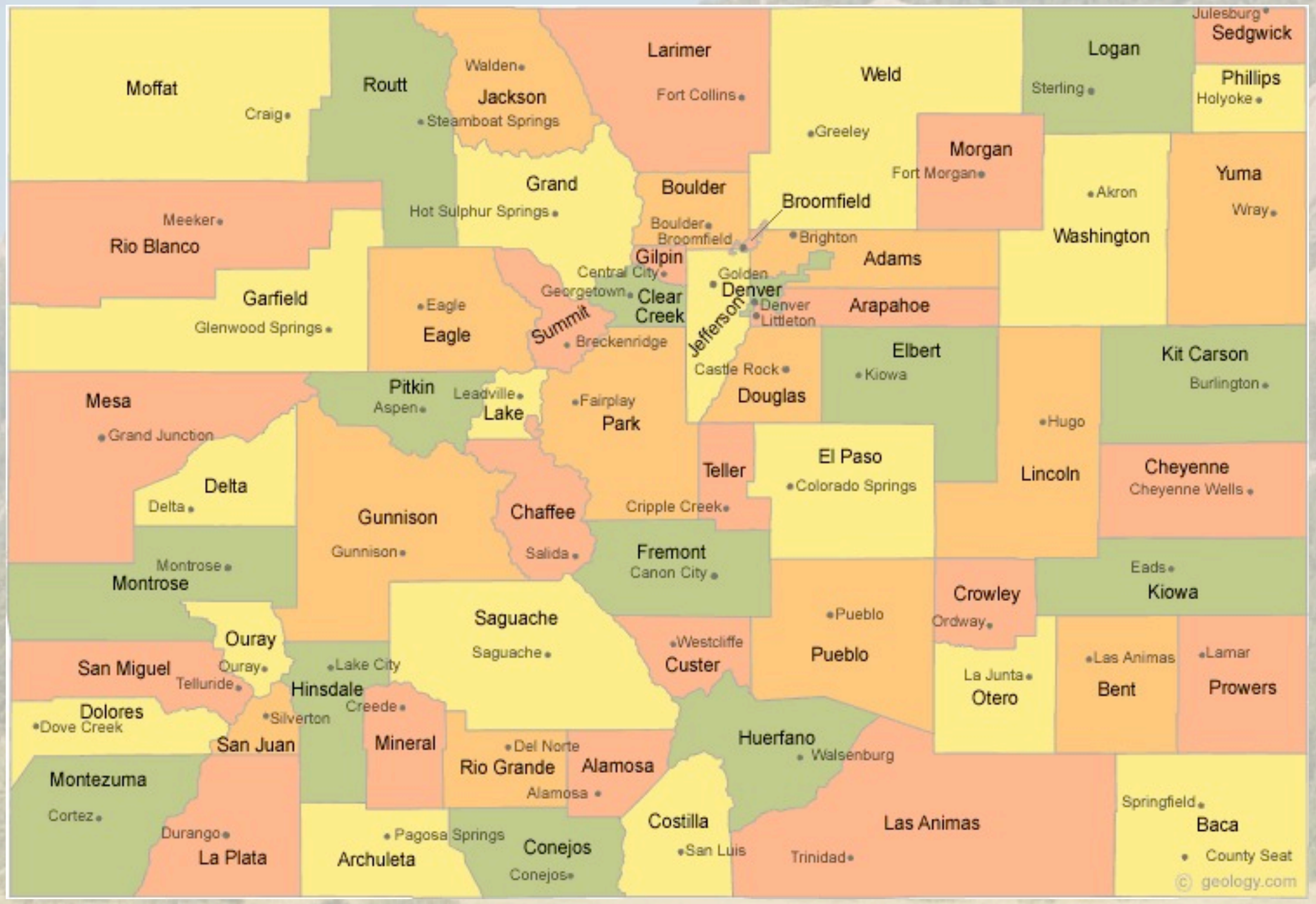
  ANO3_ADJ = ANO3_ADJ – a_2 * GAMMA_ADJ

  GAMMA_ADJ = 0.0

Objectives

- Reduce uncertainty in sources of aerosols.
- More accurately distinguish between local and long-range sources of aerosol.
- Better predict the effects that policy change will have on the future evolution of atmospheric composition.

Colorado Counties

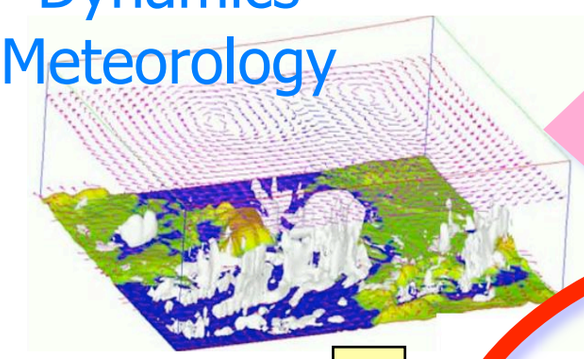


Why Air Quality Models?

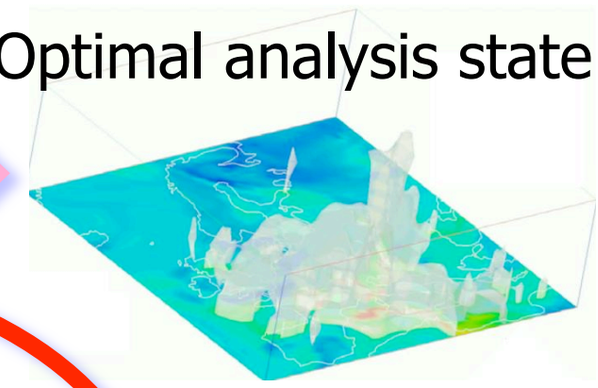
- Air Quality concerns:
  - Contribution of source to concentration of pollutants in area?
  - Most cost-effective way to reduce pollutant concentrations?
  - Where to place future source to minimize environmental impacts?

Information feedback loops between CTMs and observations: data assimilation and targeted meas.

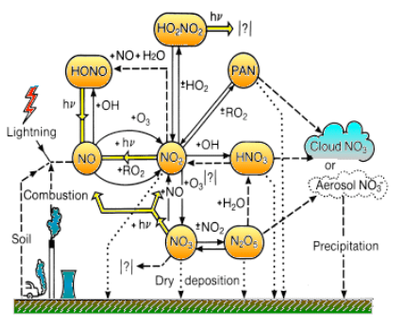
Dynamics
Meteorology

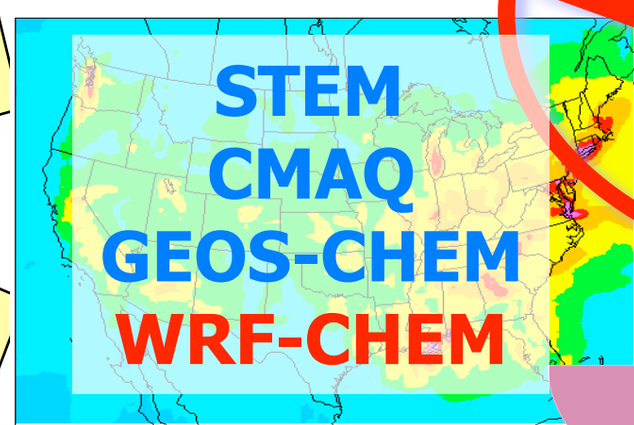


Optimal analysis state



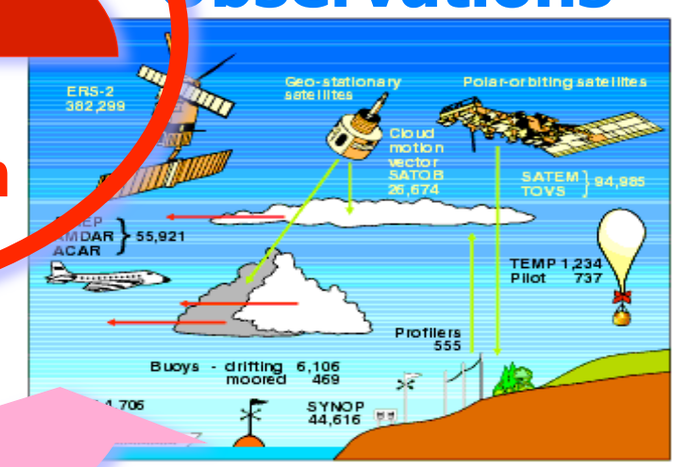
Chemical kinetics



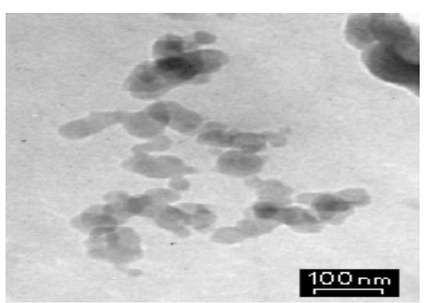


4D-Var
Data
Assimilation

Observations



Aerosols



Emissions

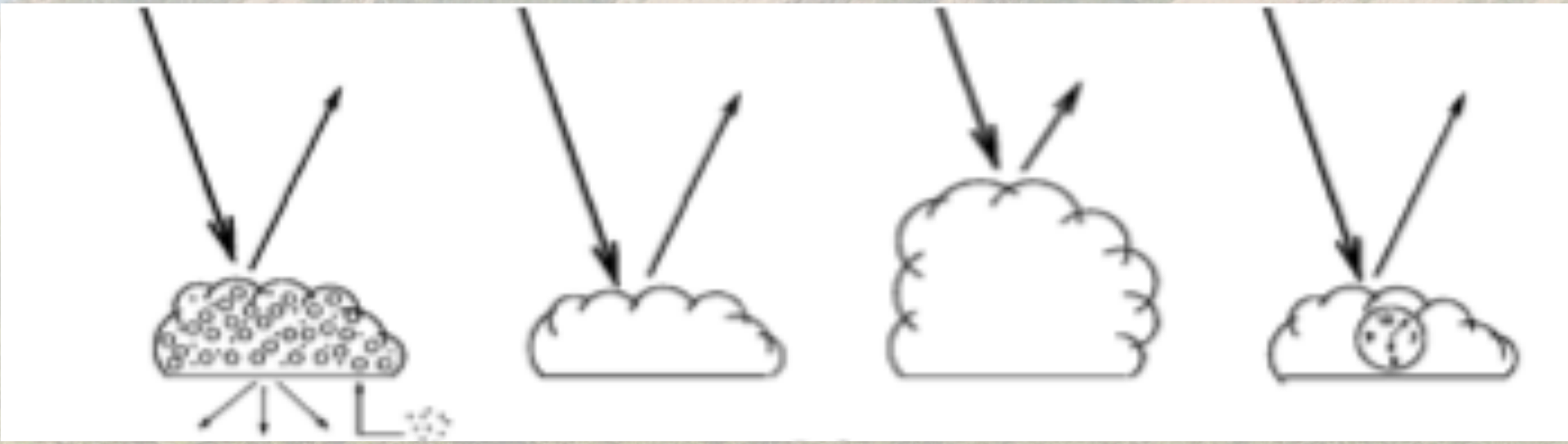
Targeted
Observ.

Improved:
- forecasts
- science
- field experiment design
- models
- emission estimates

Slide courtesy of Adrian Sandu, Virginia Tech.

Aerosol Effects on Climate Change

- Indirect effect:
  - Alteration of cloud properties



Schematic of aerosol indirect effects. Haywood and Boucher (2000)

Air Quality Models

Solve 3D chemical continuity equations
on regional Eulerian grid

Modules
- Emissions
- Aerosols
- Chemistry
- Transport
- Deposition

Comparison to Observations

Model Adjoint

Sensitivity Analysis

Input Data
- Emissions
- Meteorological Data
- Chemical Transformations
- Removal Processes