Development and Applications of CMAQ Adjoint

Rob Pinder and Amir Hakami

10th Annual CMAS Workshop
October 25, 2011

Who is involved?

- Carleton University: Shunliu Zhao and Amir Hakami
- Georgia Tech: Shannon Capps, Thanos Nenes, and Ted Russell
- University of Colorado: Matthew Turner and Daven Henze
- University of Iowa: Jaemeen Baek, Charles Stanier, and Greg Carmichael
- University of Houston: Peter Percell
- Virginia Tech: Adrian Sandu
- ICS Prague: Jaroslav Resler
- USEPA: Rob Pinder and Sergey Napelenok, Havala Pye, Gill-Ran Jeong, Jesse Bash
- NOAA: Tianfeng Chai and …

Daewon Byun

Outline

- Adjoint models
- Examples
- CMAQ-ADJ status and timeline
- Community feedback and involvement

CMAQ-ADJ history

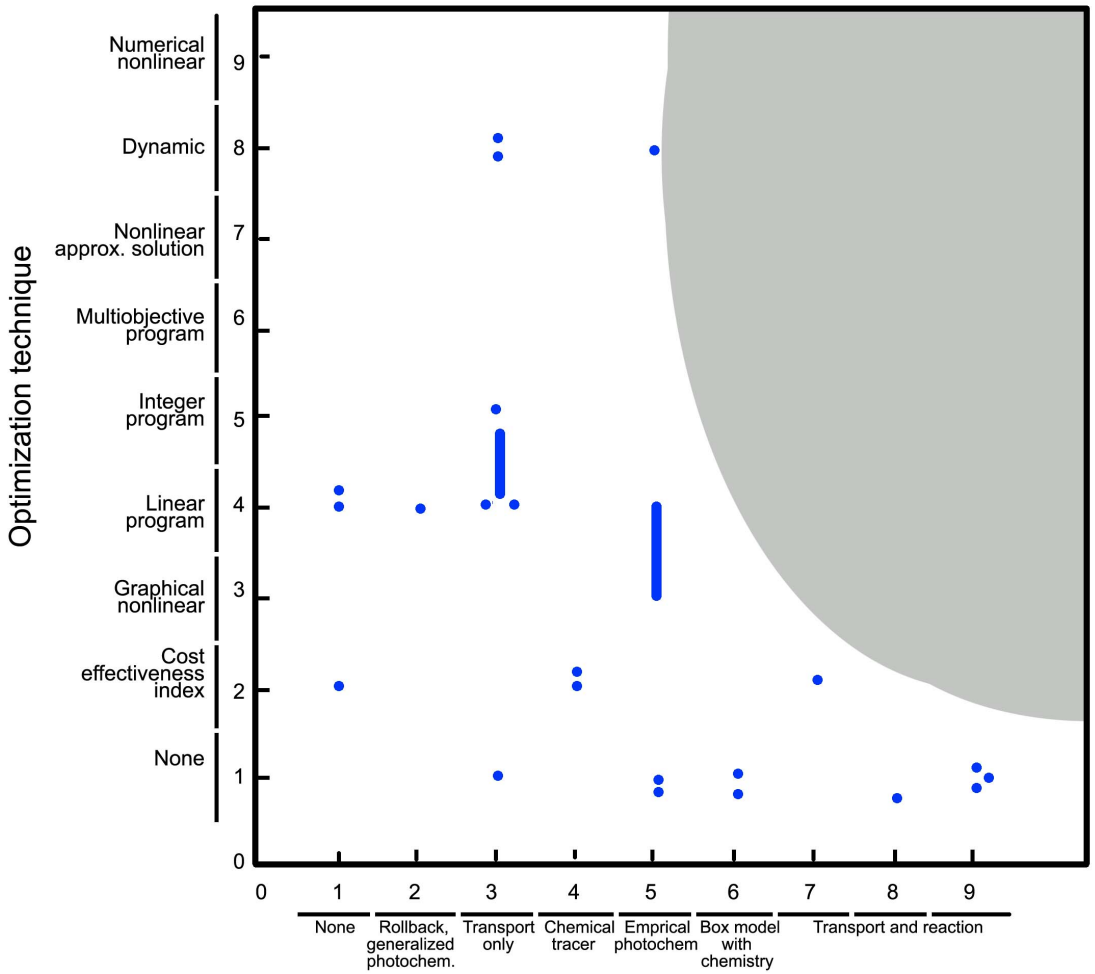
- Gas-phase adjoint in 2006
  - Caltech, Virginia Tech, U. Iowa, U. Houston
- Multi-phase adjoint
  - Core project funded by API
    - Carleton, GaTech, U. Colorado
  - Expanded team and scope to include multiple organizations

Air quality modeling and decision-making

- Integrating air quality models and decision models has always been the goal

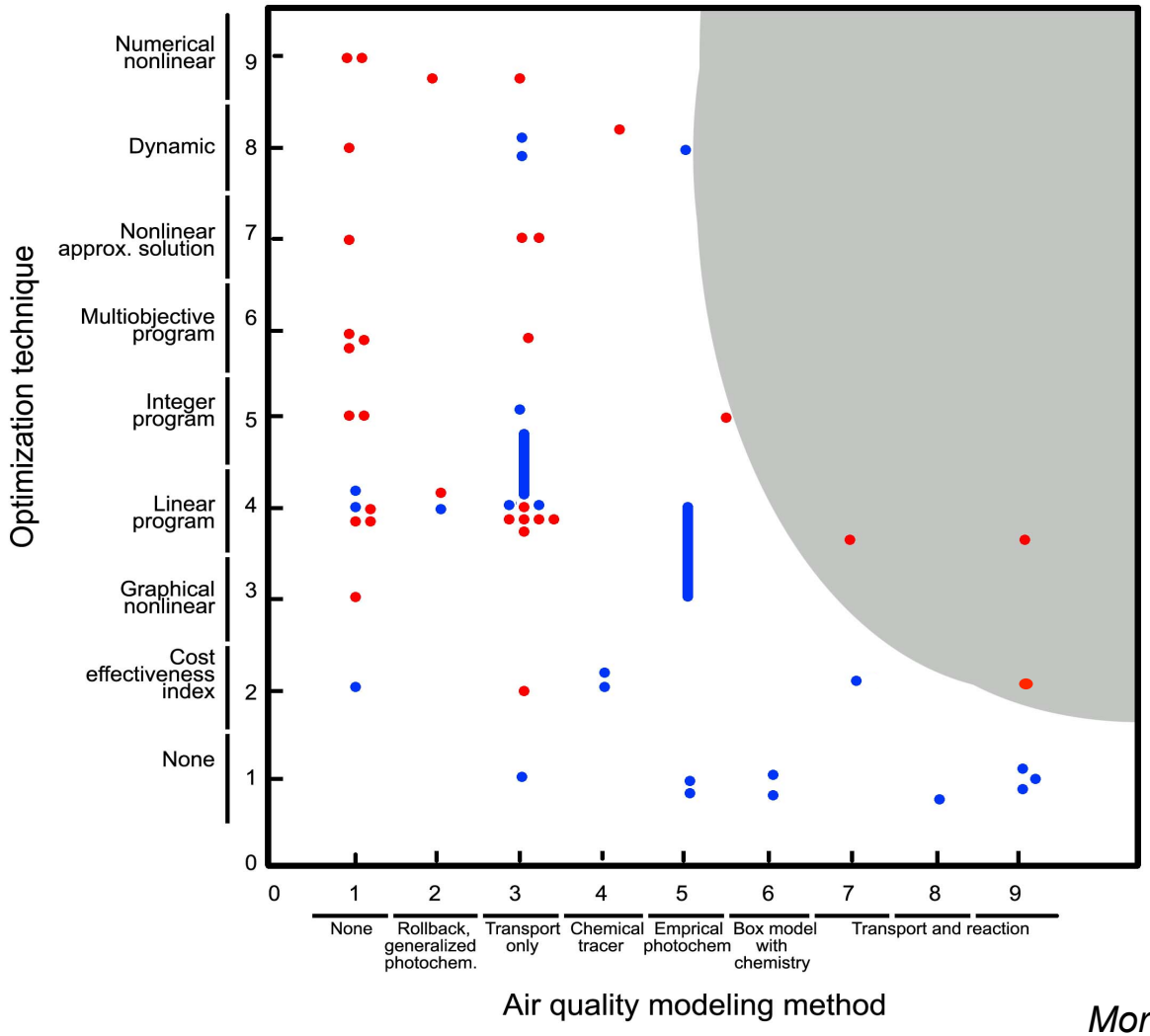
- This integration often requires sensitivity information, explicitly or implicitly

Air pollution decision making



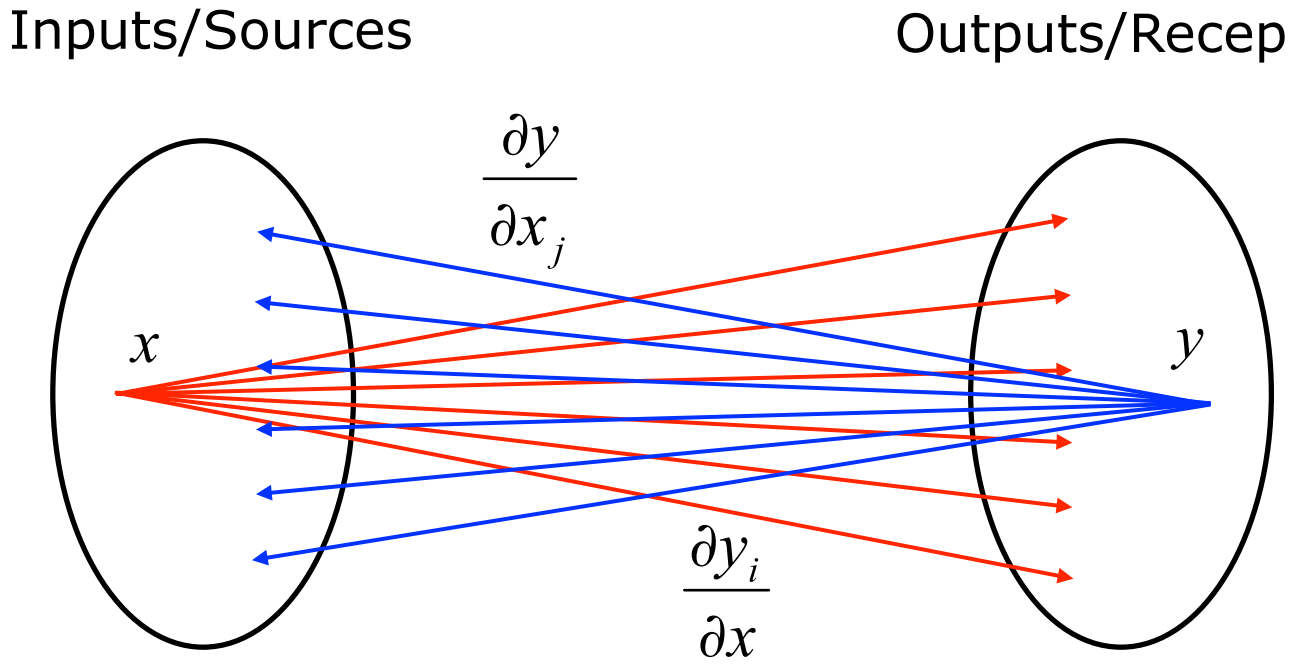
McRae and Cass (1981)

30 years later!



Morteza Mesbah, Carleton

What is an adjoint model?

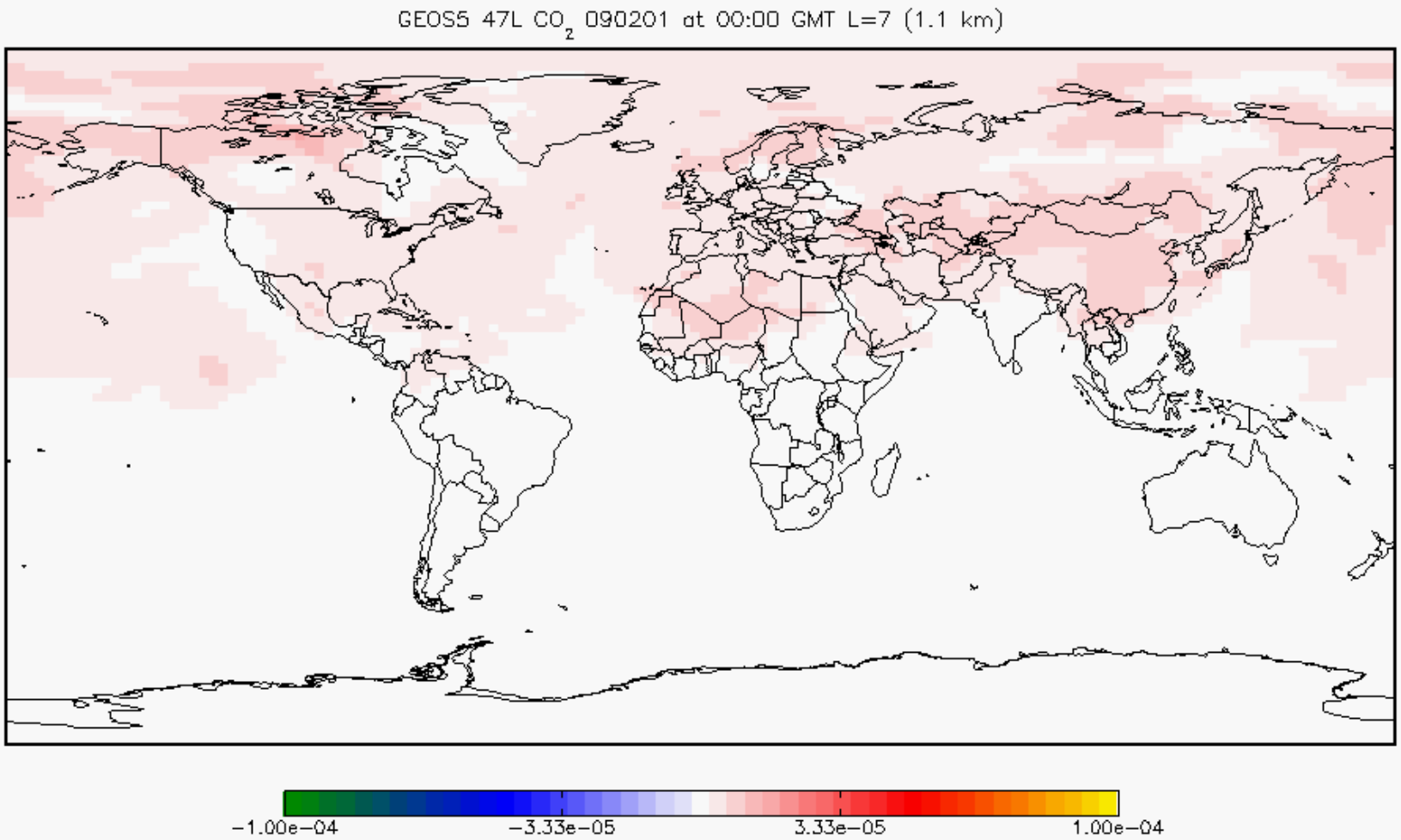


What is an adjoint model (cont'd)?

- Forward sensitivity:
  - Source-oriented
  - Receptor specificity
  - Where "influences" go from source(s)

- Backward/adjoint sensitivity:
  - Receptor-oriented
  - Source specificity
  - Where "influences" at receptor(s) come from

Where pollution comes from …



Adjoint applications

An adjoint application

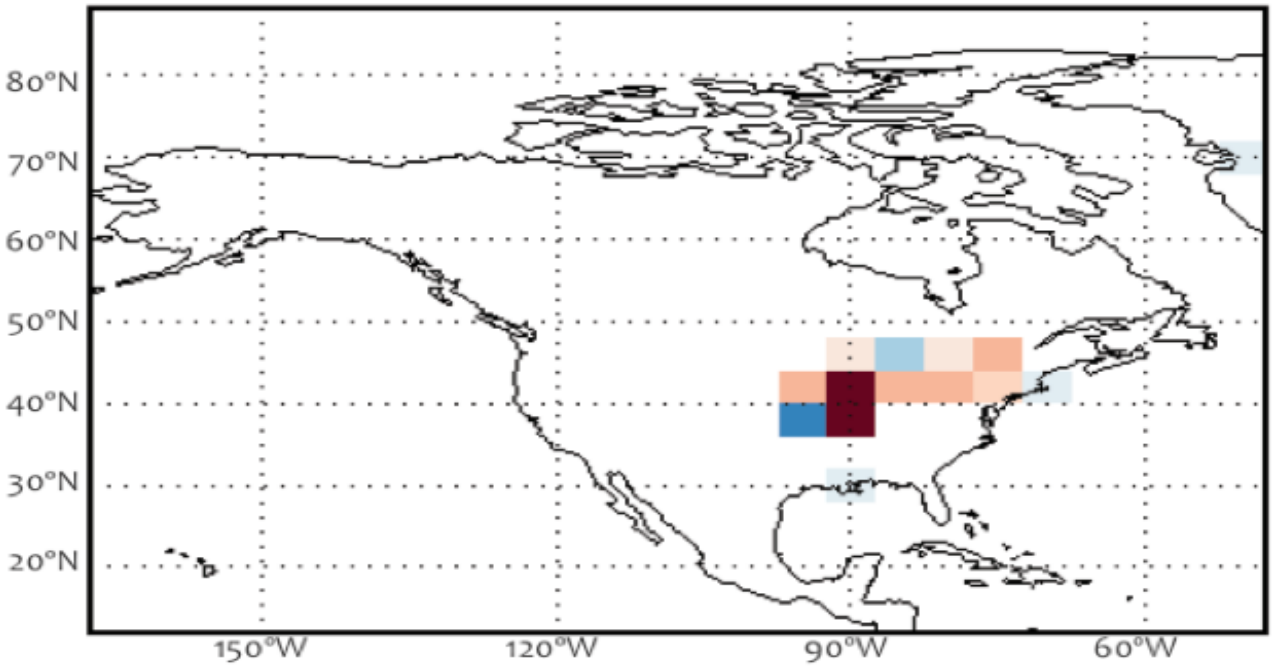
1. Sensitivity of what?
2. Sensitivity to what?
3. How to use sensitivities?

Lots of room to get creative about “1” and “3”

1- Concentrations

$PM_{2.5}$ over the US by GEOS-Chem wrt to emission the prior day

$$\frac{\partial [PM_{2.5}]_{U.S.}}{\partial (NO_{x,an}\ Emissions)} (NO_{x,an}\ Emissions)$$



Shannon Capps, Ga Tech

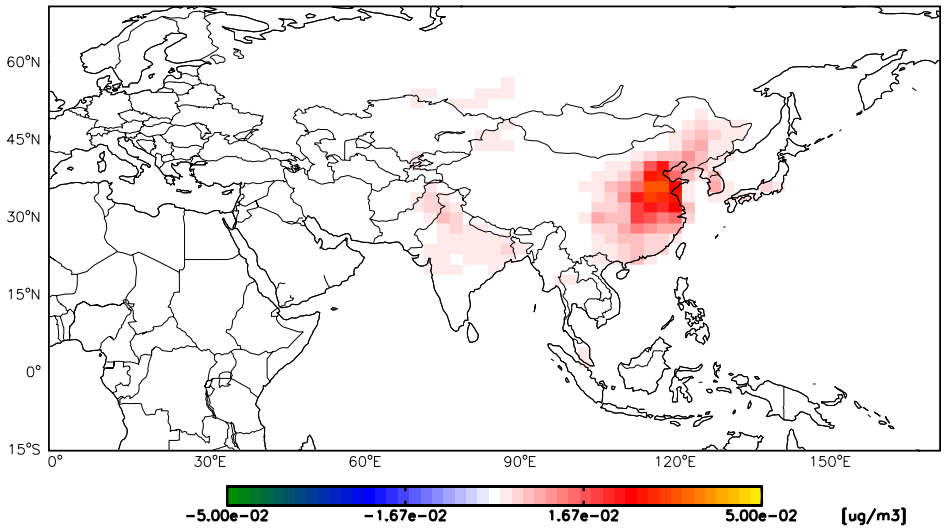
2- Concentration-based metrics

- A number of policy issues can be addressed as a concentration-based metric
  - Average concentration
  - Vegetation stress
  - Nonattainment
  - Exposure, mortality, health costs, etc
  - etc

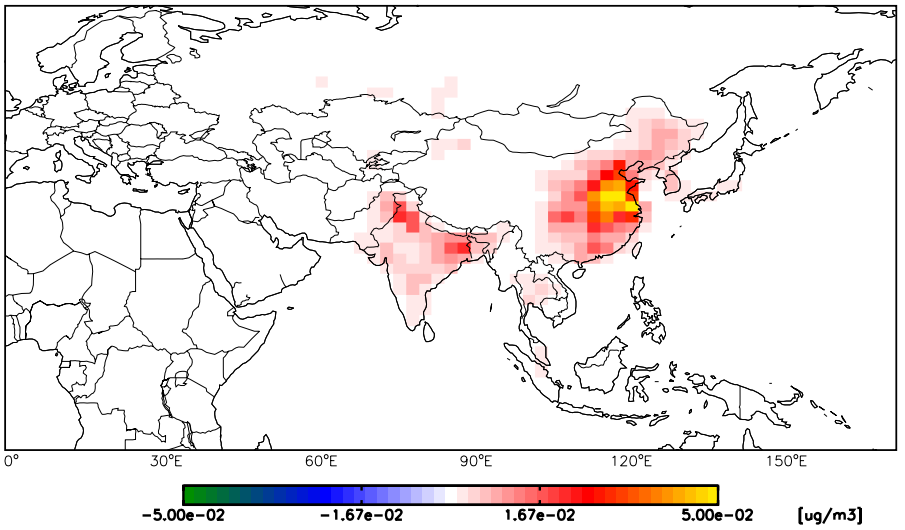
2.1. Average concentration

Sensitivity of Asian inorganic fine PM (sulfate + ammonium + nitrate) average concentrations [ug/m3] during the second week of October, 2008, with respect to emissions from the prior two weeks

Sensitivity with respect to NH_3 emissions



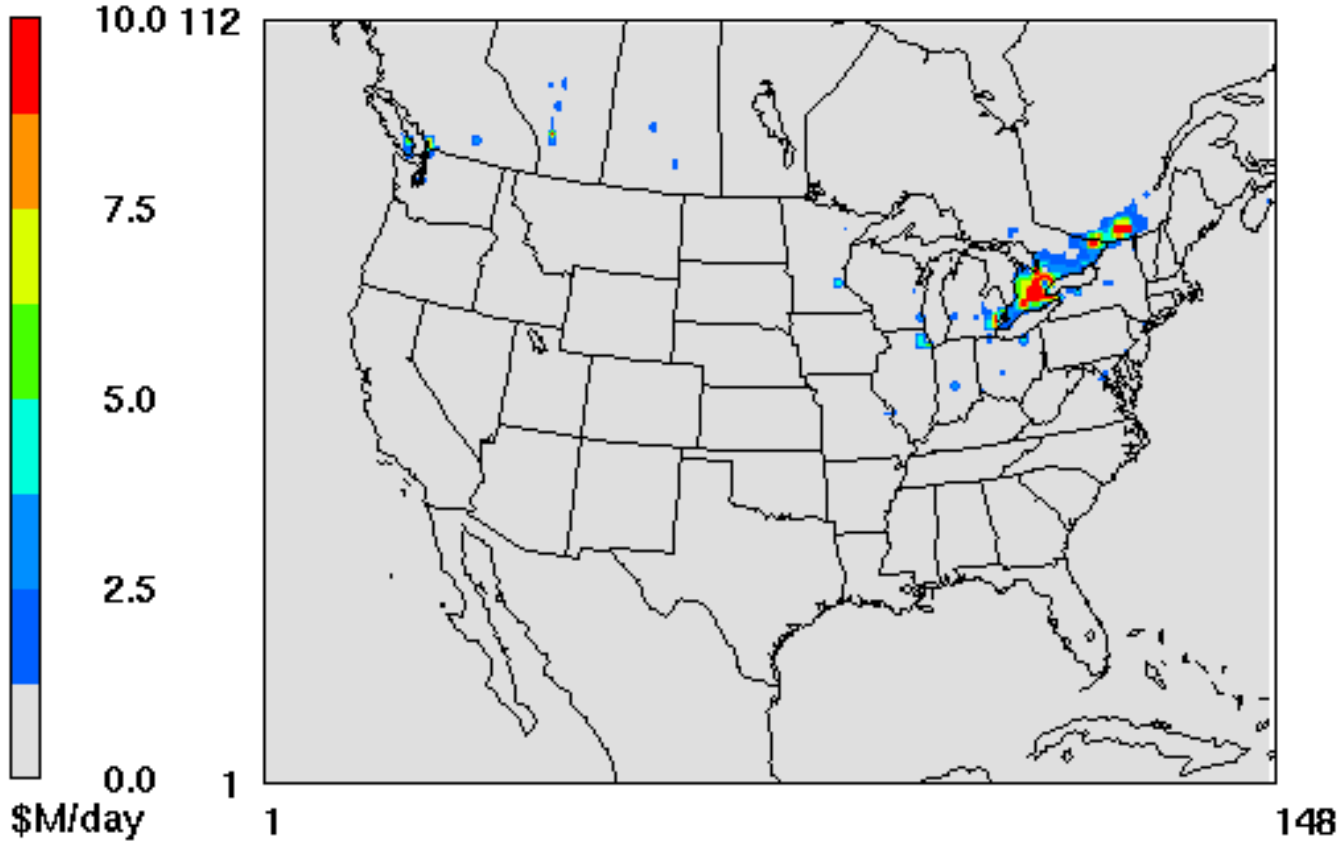
Sensitivity with respect to NO_x emissions



Daven Henze, CU Boulder

2.2. Health metrics (short term O_3 mortality)

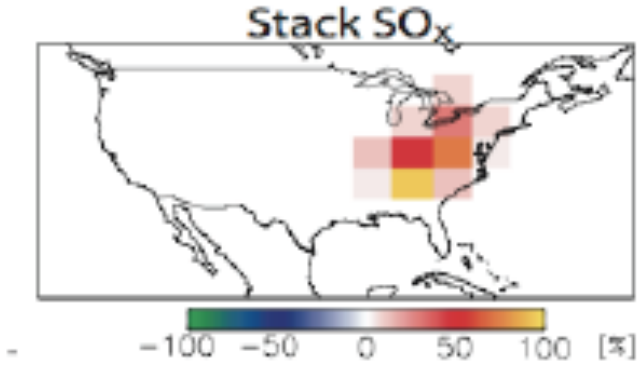
Canadian health benefit sensitivities (semi-normalized) wrt NOx emissions at each locations

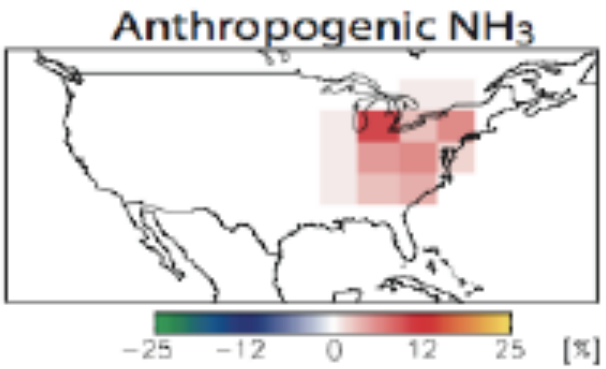


Amanda Pappin, Carleton

2.3. Attainment metrics

$$J = \frac{1}{2} \sum \mathrm{MAX}[(\text{inorganic } \mathrm{PM}_{2.5})_{24\mathrm{h}} - 10\mu\mathrm{g/m}^3, 0]^2$$

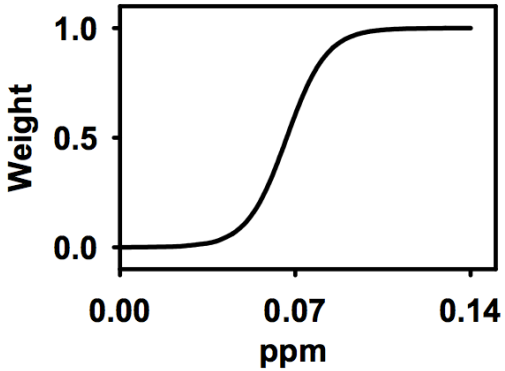




Henze et al., 2009

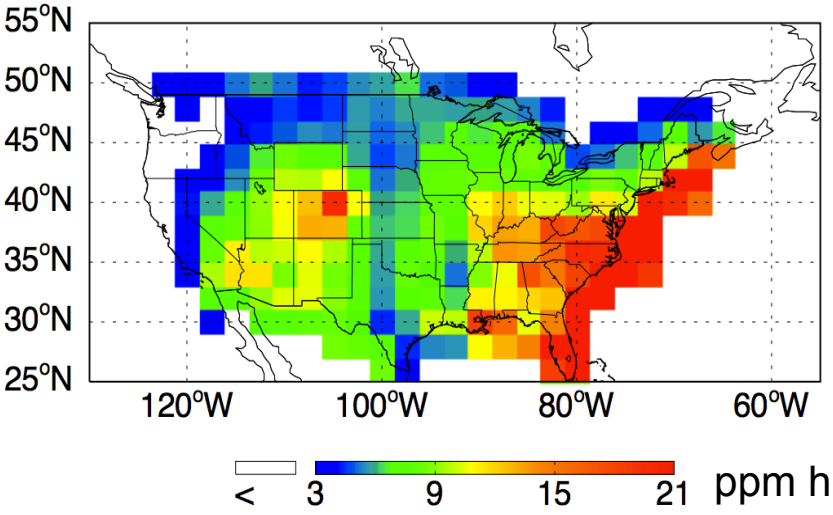
2.4. W126 in continental US

W126 cost function evaluated in GEOS-Chem for April, 2006

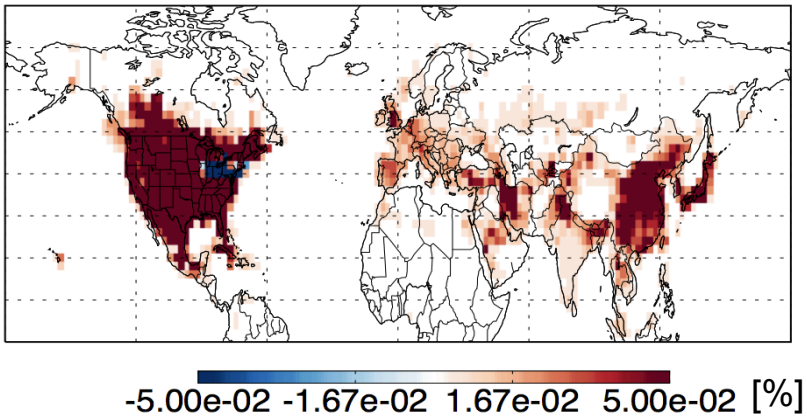


$$\mathrm{W126\ (ppm)} = \sum_{i=1}^{n} w_i\,[C_{O_3}]_i.$$

$$w_i = 1/\{1 + 4403\,\exp[-0.126\,(C_{O_3})_i]\}.$$



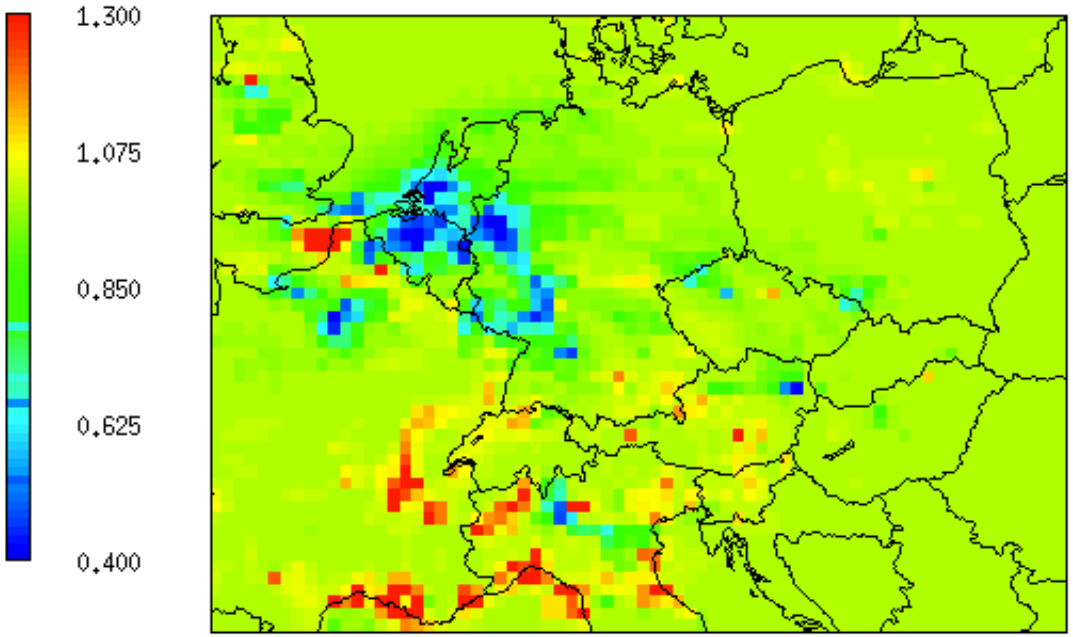
Impact on W126 from NOx emissions



Kateryna Lapina, CU Boulder

3. Inverse modeling and 4D-Var DA

Cost function as a measure of distance between model and observations

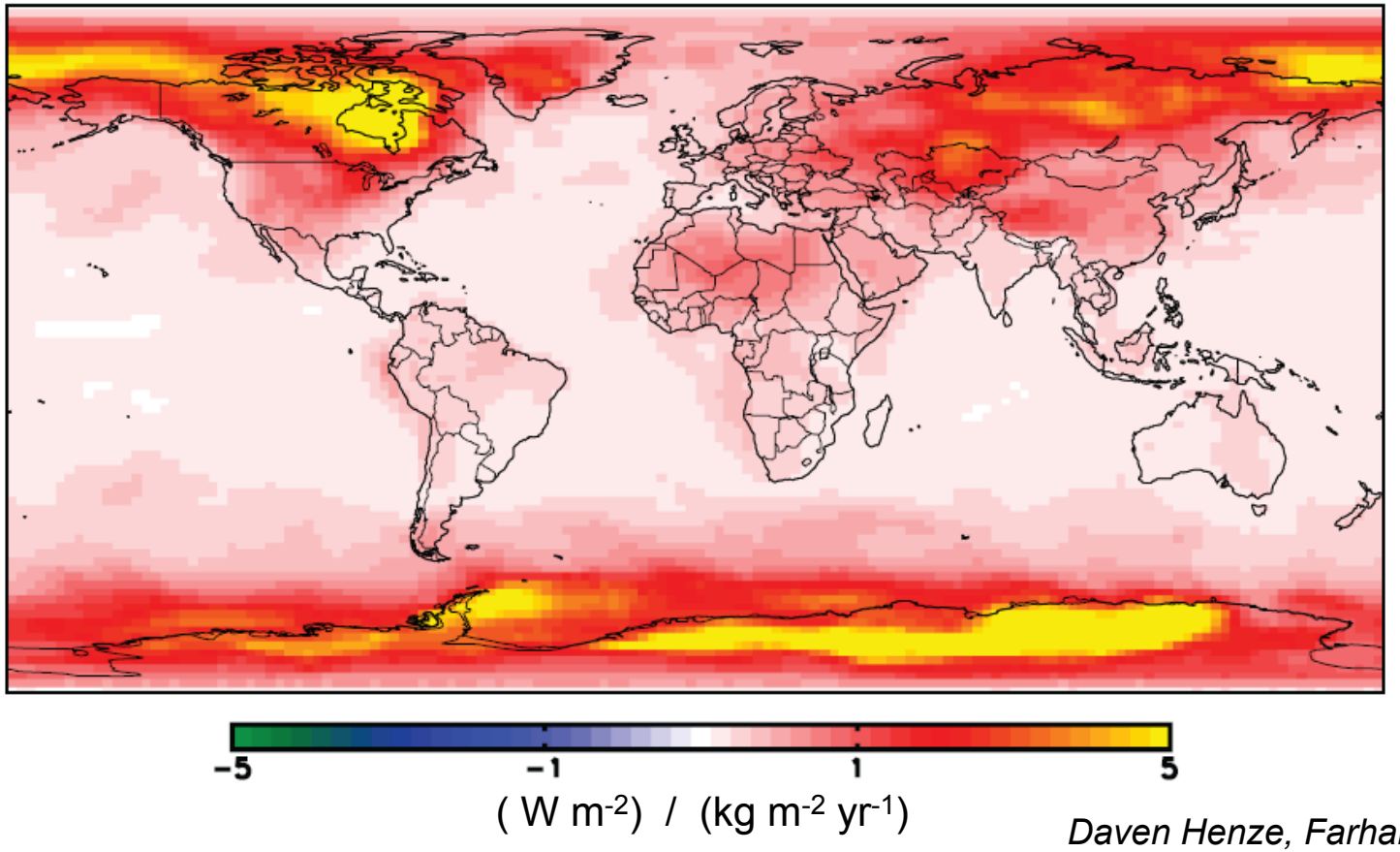


Emission scaling factors based on ozone surface observations

Jaroslav Resler, ICS Prague

4. Radiative forcing

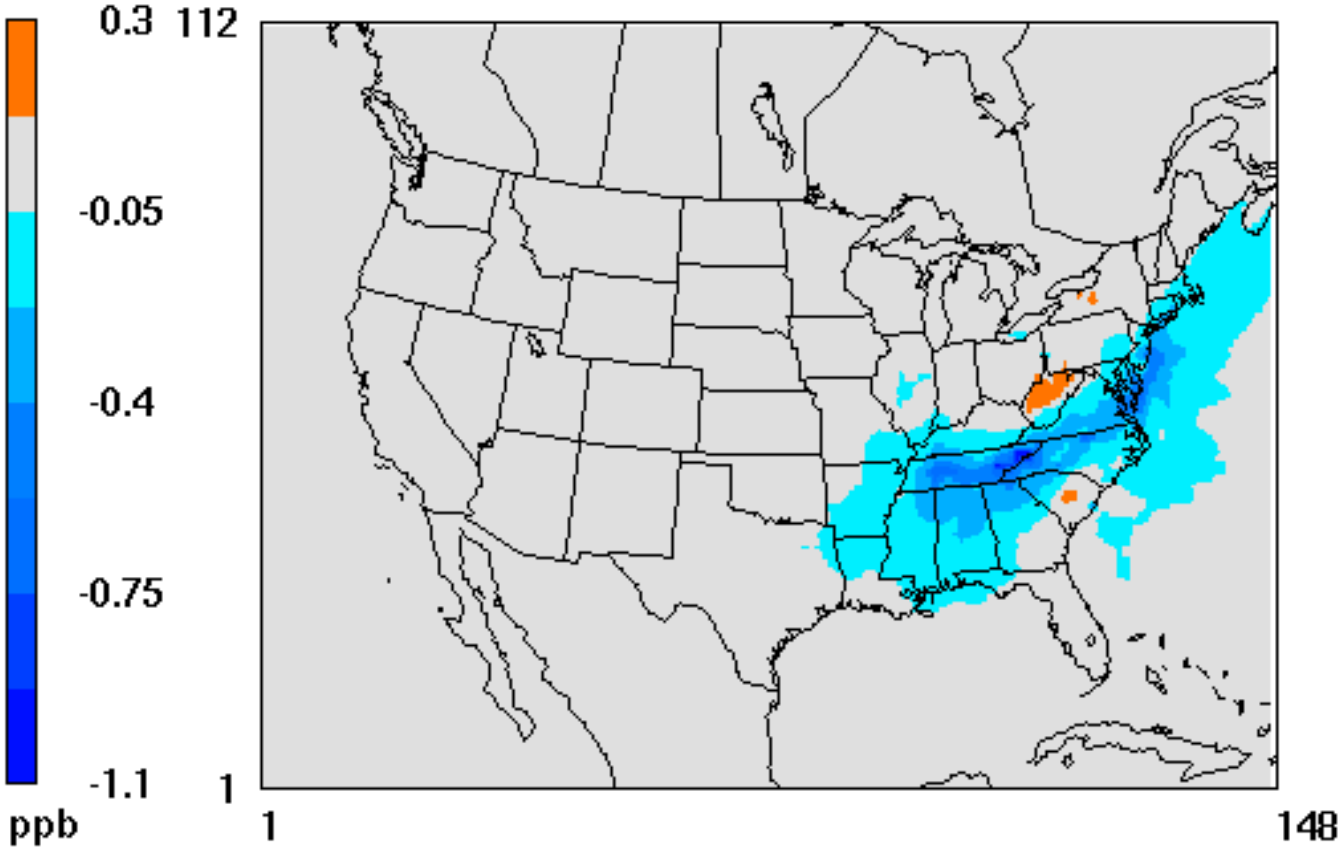
Sensitivity of global direct radiative forcing to black carbon emissions



Daven Henze, Farhan Akhtar

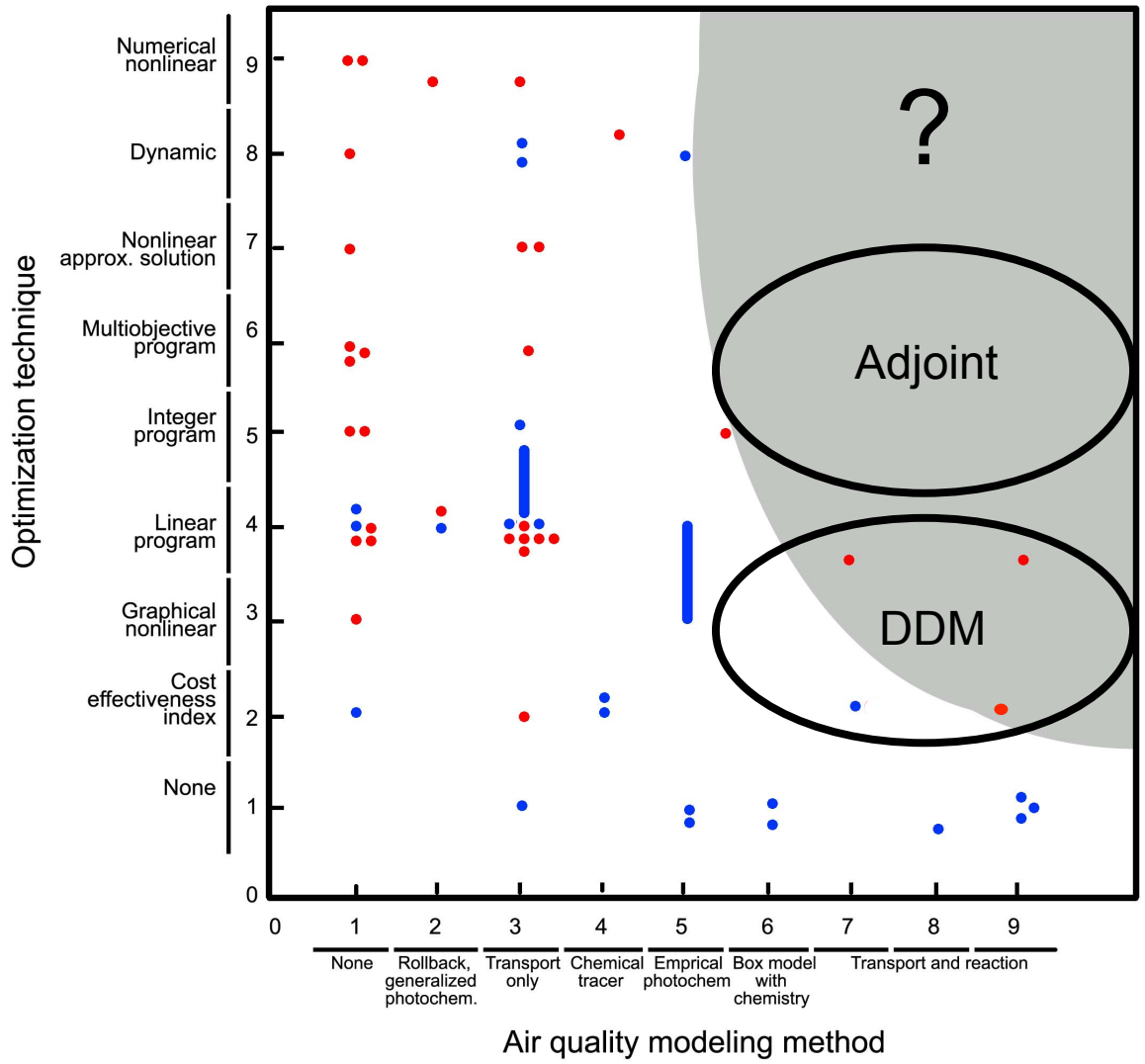
5. NOx cap-and-trade

Cap-and-trade system enhanced by emission exchange rates



Morteza Mesbah, Carleton

Decision-making: the adjoint paradigm



CMAQ Adjoint

- Currently based on CMAQv4.7.1
- EPA collaborators have kept the team updated about upcoming changes
  - Aerosol is based on CMAQv5.0
- The adjoint for CMAQv5.0 is planned as the final product

Science routines

- Transport (Peter Percell, old CMAQ-ADJ team)
  - ACM2 inline vertical diffusion
- Aerosol thermodynamics (Shannon Capps)
- Aerosol dynamics (Shunliu Zhao and Matt Turner)
- Aqueous chemistry (Jaemeen Baek)
- Clouds (Shunliu Zhao)
- Gas-phase chemistry (Amir Hakami)
- Checkpointing (Jaroslav Resler)
- Parallelization (Peter Percell and Jaroslav Resler)
- …

Status

- All default science routines have a working (?) adjoint.
  - There is lots of debugging, testing, and evaluation left
  - Computational efficiency should be improved

Planned release: CMAS 2012

CMAQ-ADJ as a community model

- How best to prepare CMAQ-ADJ for use by the community
  - How to propagate the “adjoint way” of thinking in the community?
  - Ease of use and user interfaces with the adjoint model
  - Computational limitations

There is a lot that can be learned from the DDM experience

How the user will interact with the model

- There are two levels of interaction that require user input:
  - How to define the cost function
    - What function, what species, where, and when?
  - How to process calculated sensitivities
    - Integrated over time, space, species (e.g. VOCs or NOx), emission sectors, etc?

What type of applications?

- Source attribution (marginal source apportionment)
- Attainment analysis
- Control strategy design
- Health impact analysis
- Ecosystem impact analysis

- Forecasting
- Emission inversion
- Other types of parameter estimation

- …

Feedback

- This is the best time to influence the direction CMAQ-ADJ is taking in terms of user interaction
- Let us know: amir_hakami@carleton.ca
- Check the status and give feedback: pontus.cee.carleton.ca/cmaq-adj

Comments, questions?

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