Aerosol Processes in the CMAQ Adjoint

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Introduction

The Community Multiscale Air Quality (CMAQ) modeling system is utilized by the US EPA to develop emission control regulations for air quality improvements and by research groups around the world to investigate air pollution. Still, air quality models contain uncertainty which drive a continual process of model refinement. Developing a constraint on emissions using 4D-Variational data assimilation is a valuable method for reducing such uncertainty. Towards this goal, a large consortium of researchers are working together to build a complete 4D-Var system for CMAQ. The original CMAQ adjoint model was developed for CMAQ 4.5.1 and was limited to gas-phase processes. The current effort includes the addition of aerosol dynamics and thermodynamics, cloud processes, and heterogenous chemistry. The model will also include parallelization, 4D-Variational capabilities, and improved modularity. Once the adjoint has been completely implemented and validated, the model will be publicly released.

Objectives

Air quality models are important for EPA efforts to improve health, but models contain large uncertainty. This project focuses on reducing uncertainty in sources of aerosols by developing a constraint on emissions using observations with the 4D-Var data assimilation technique. Through this approach, this project will address the following research objectives:

1. More accurately distinguish between natural and anthropogenic sources of aerosol.
2. More accurately distinguish between local and long-range sources of aerosol.
3. Better predict the effects that policy change will have on the future evolution of atmospheric composition.

Motivation

Particulate Matter (PM) is an air pollutant consisting of a mixture of solid and liquid particles suspended in the air. Knowledge of PM concentrations is important for many reasons, two of which are that PM has an adverse effect on human health, and PM also has an effect on climate change.

- Many atmospheric chemical transport models (CTM) have been modified recently to include aerosols, however the models still contain considerable uncertainty.
- There are many methods to decrease model uncertainty such as:
  - Developing a better understanding of physical processes
  - Data Assimilation
  - Using an ensemble of models
- This project focuses on the 4D-Variational data assimilation technique
  - Requires development of an adjoint model for use in inverse modeling of a currently existing CTM.
- Currently no other regional chemical transport model has an adjoint that includes aerosols.

Effects of PM on Climate Change

Aerosols have both a direct and indirect effect on radiative forcing (Figure 1).

- Direct effect caused by scattering and absorption of solar and infrared radiation in the atmosphere
- Indirect effect caused by changes in cloud properties due to aerosols

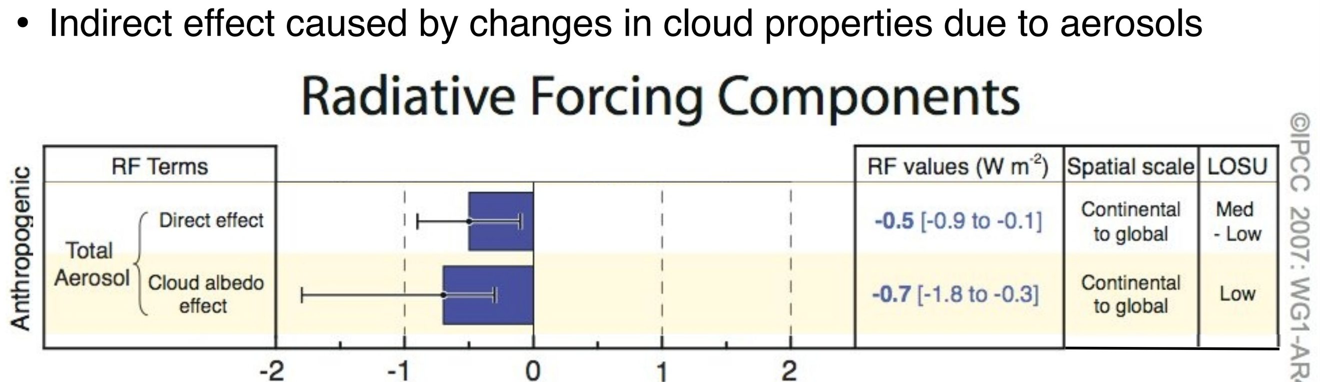
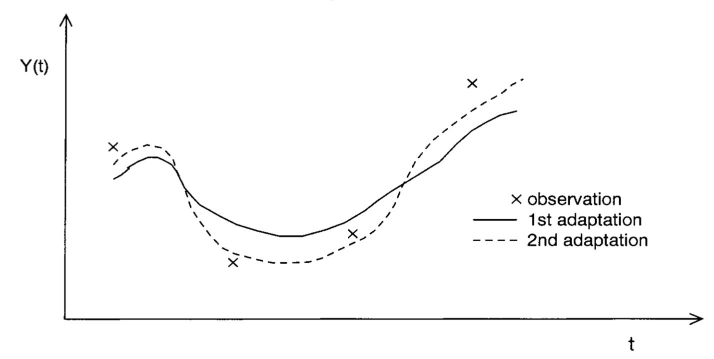


Figure 1: Aerosol Radiative Forcing Components (IPCC, 2007)

What Are Adjoints?

- Adjoint models are used for studies that require an estimate of sensitivity of a model output with respect to an input.
- In air quality studies, adjoints are often used for data assimilation
  - Atmospheric chemical transport models have large amount of uncertainty
  - An adjoint model used in conjunction with the 4D-Var data assimilation technique allows model trajectory to be brought as close as possible to observed data (see Figure 2) by varying control variables (emission scaling factors, initial condition scaling factors, etc.)
- To quantify misfit of model prediction, a cost function is introduced
  - Cost function is reduced through an iterative process
- Adjoint method has 2 main advantages over finite difference:
  - Especially for large number of parameters, adjoint model saves run time
  - Computed gradient is exact

Figure 2: Schematic representation of variational methods (Giering and Kaminski, 1998)



Checkpointing and Parallel Efficiency

Checkpointing and parallel efficiency results courtesy of Jaroslav Resler (ICS Prague).

- 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. Also different frequency of the recording of output files can be configured.
- Current implementations include:
  - Serial I/O through IOAPI3/PARIO (equivalent to the present state)
  - MPI I/O using the Parallel NetCDF library and NetCDF4/HDF5 libraries
  - Multiple local files strategy implemented by direct calls of NetCDF

Tests have been performed to analyze the time to run the CMAQ Adjoint model (Figure 3a), and the parallel efficiency of the CMAQ Adjoint (Figure 3b) for various checkpointing methods.

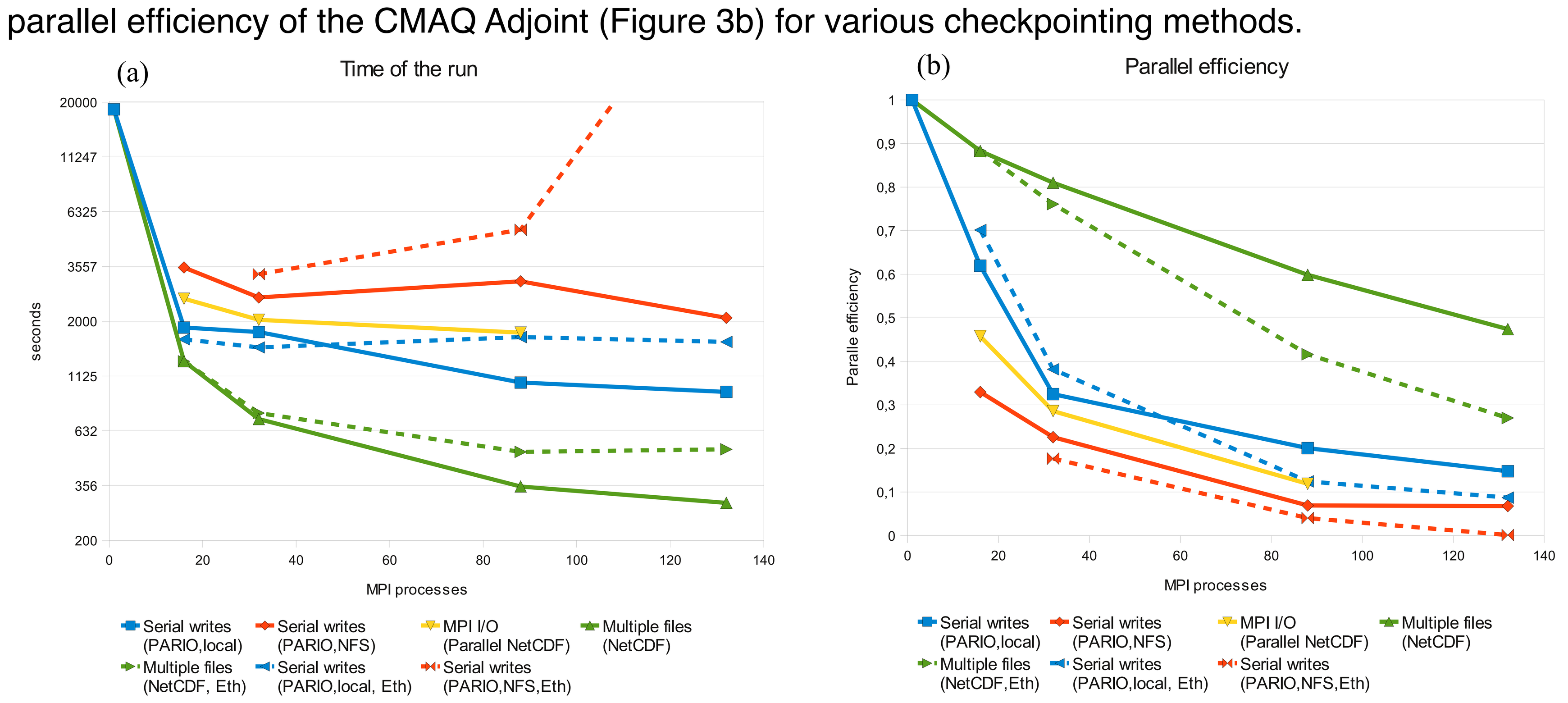


Figure 4: (a) Total time of forward and backward run of the model, and (b) Parallel efficiency of the CMAQ Adjoint model in different testing configurations. Testing configuration: Linux cluster, NFS cluster storage, Infiniband interconnection, MVAPICH2

Adjoint of Aerosol Processes

ISOROPIA Adjoint results courtesy of Shannon Capps (Georgia Tech.)

Aerosol Thermodynamics

- Adjoint of aerosol thermodynamics model ISOROPIA-II has been developed and validated.
  - Validation by comparison of adjoint sensitivities to complex variable method (CVM) results (See Figure 4).
  - Results show significant agreement between adjoint and CVM sensitivities

Adjoint of Aerosol Processes (cont.)

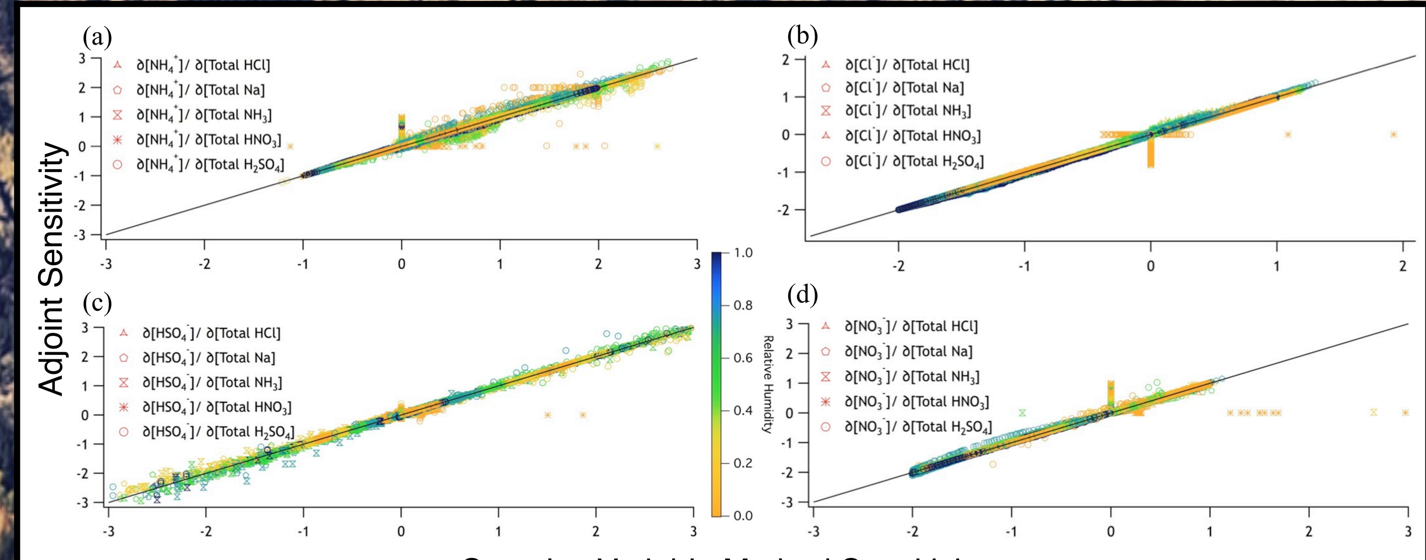


Figure 4: Comparison of Adjoint sensitivity to CVM sensitivity for Adjoint of ISOROPIA-II for (a) NH_4^+, (b) CL^-, (c) HSO_4^-, (d) NO_3^-

Aerosol Dynamics

- Adjoint has been developed for the aero5 aerosol module utilized by CMAQ.
  - Individual subroutines have been validated by comparing finite difference sensitivities to adjoint sensitivities (See Figure 5a for validation of HCOND3).
  - Adjoint of aerosol dynamics has been verified as a whole by the same method (See Figure 5b).

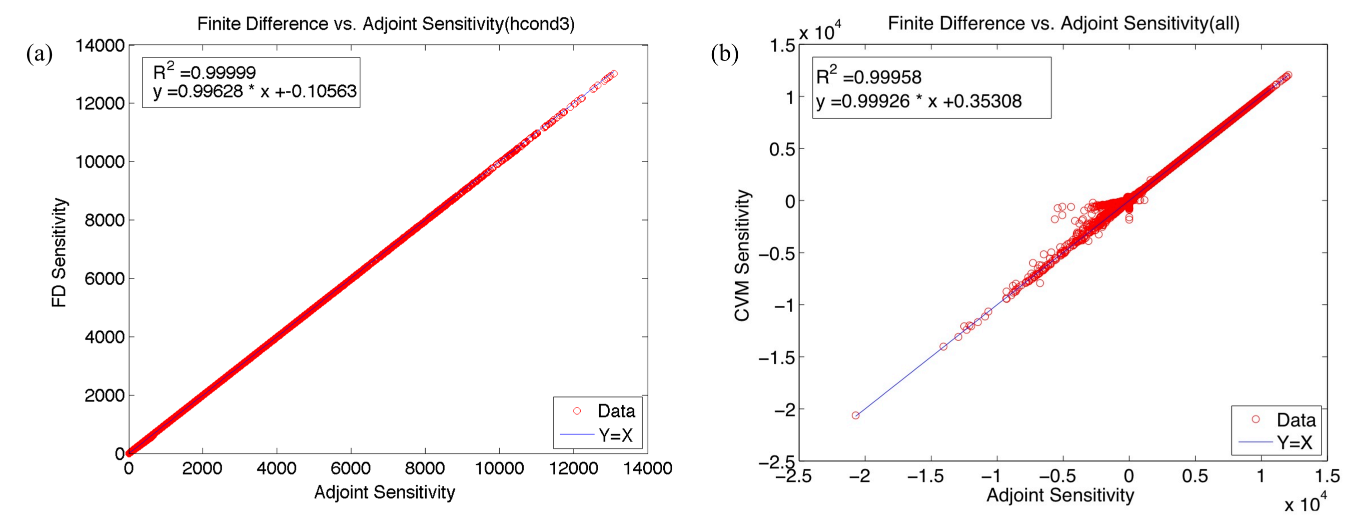


Figure 5: Aerosol dynamics adjoint validation for (a) subroutine HCOND3, and (b) entire aerosol module, excluding aerosol thermodynamics.

Sensitivity Analysis

- Initial sensitivity calculations have been performed to test the current adjoint model.
- Tests were performed to determine the sensitivity of NO_2 inert tracer concentrations with respect to entire species concentration array.
  - Results are shown for the sensitivity of NO_2 with respect to NO_2 initial conditions in grid cell (50, 50, 1).

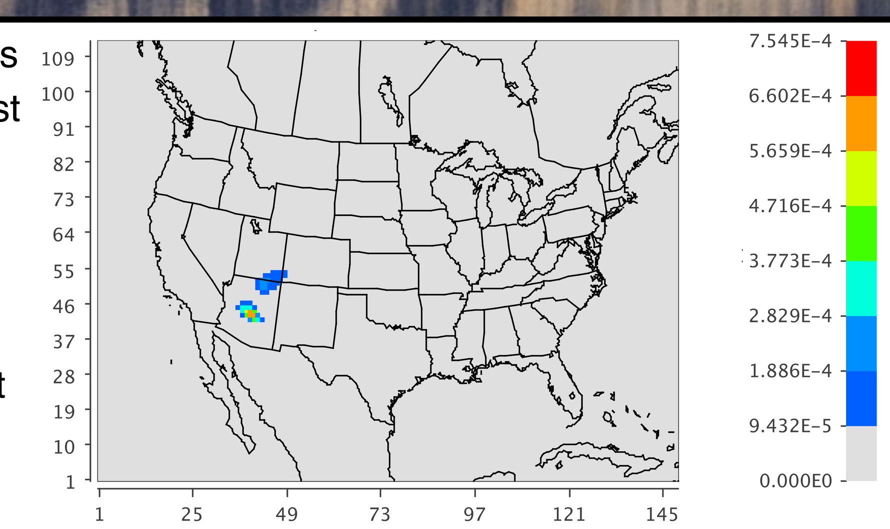


Figure 6: Sensitivity of NO_2 with respect to initial conditions of NO_2 in grid cell (50, 50, 1)

Data obtained from week long adjoint run (transport only) using CMAQ input data from April 2008.

References

- Bousquet et al., 2005; Intergovernmental Panel on Climate Change (IPCC), 2007
- Giering, R. and Kaminski, T.: Recipes for Adjoint code Construction, ACM Trans. Math. Softw., 24, 437–474, 1998.

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