Development of a Multiphase Adjoint for CMAQ

The team

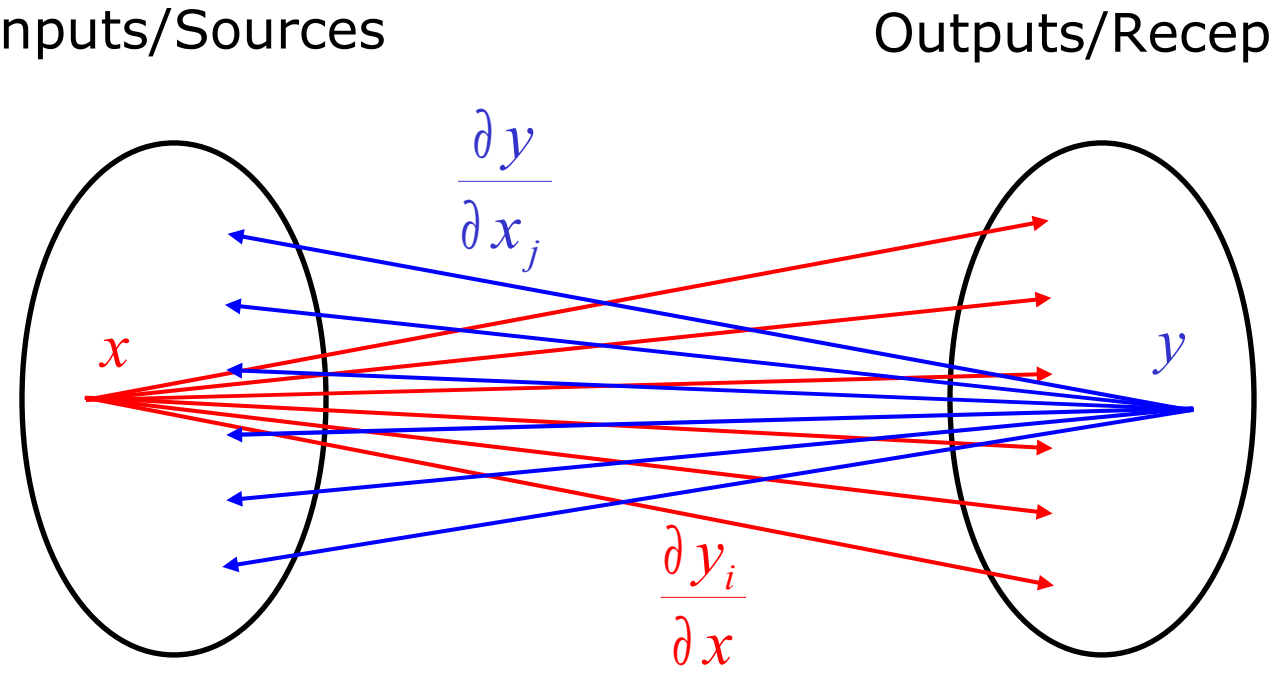
- Carleton University (CU): ShunLiu Zhao and Amir Hakami
- Georgia Tech (GT): Shannon Capps, Athanasios Nenes, and Ted Russell
- University of Colorado (UC): Matthew Turner and Daven Henze
- University of Houston (UH): Peter Percell
- University of Iowa (UI): Jaemeen Baek, Greg Carmichael, and Charles Stanier
- Virginia Tech (VT): Adrian Sandu
- ICS Prague: Jaroslav Resler
- NOAA: Tianfeng Chai and Daewon Byun
- EPA: Rob Pinder, Sergey Napelenok, and Havala Pye

- Past Contributions from Kumaresh Singh and Tianyi Gou (VT) and John Seinfeld (Caltech)

Outline

- History and background
- Collaboration structure
- Status
  - Gas-phase model
  - Thermodynamics
  - Dynamics
- Outlook

Forward vs. backward sensitivity analysis



- Complementary methods (Source-based vs. Receptor-based), each suitable for specific types of problems.
  - Adjoint useful for calculations of sensitivities of few metrics with respect to many parameters
- Numerous applications for adjoint such as data assimilation and sensitivity analysis.

History of CMAQ-ADJ

- Gas-phase version based on CMAQ 4.5.1 was developed in 2006 (Hakami et al., 2007)
  - available for download at: http://people.cs.vt.edu/~asandu/Software/CMAQ_ADJ/CMAQ_ADJ.html
- Gas-phase CMAQ-ADJ rapidly diverged into multiple versions
  - VT version
    - VT/UH version (chemistry update, parallelization, data assimilation tools)
    - ICS Prague version (chemistry update, parallelization, data assimilation)
  - CU/Caltech version (chemistry update, parallelization)

History of CMAQ-ADJ (Cont'd)

- There was a strong need to
  - Consolidate versions
  - Update to a more recent version of CMAQ
  - **Include all processes, particularly aerosols**
- Funding from the American Petroleum Institute (API) initiated multi-phase CMAQ-ADJ development (CU, GT, UC)
- High level of interest and activity among various developer and user groups resulted in the wider collaborative effort.

Objective: Develop multi-phase CMAQ-ADJ that is based on latest CMAQ, computationally efficient, easy to use, easy to update, modular, and capable of data assimilation and various types of sensitivity analysis

Structure

- Aerosol thermodynamics: GT
- Aerosol dynamics: CU and UC
- Aqueous chemistry: UI and EPA
- Data assimilation and gradients: VT, NOAA, UH, ICS, and CU
- Gas-phase: UH and CU
- Parallelization: UH and ICS
- Nesting: CU

CMAQ-ADJ

- Based on a hybrid version of CMAQ
  - General structure, transport and gas-phase chemistry based on v4.7.1
  - Aerosols based on “alpha” version of aerosol processes in v5.0

- Wanted to have CMAQ-ADJ based on latest release but could not wait for v5.0 (2011). This hybrid version adjoint allows us to quickly update to v5.0 once it is released.

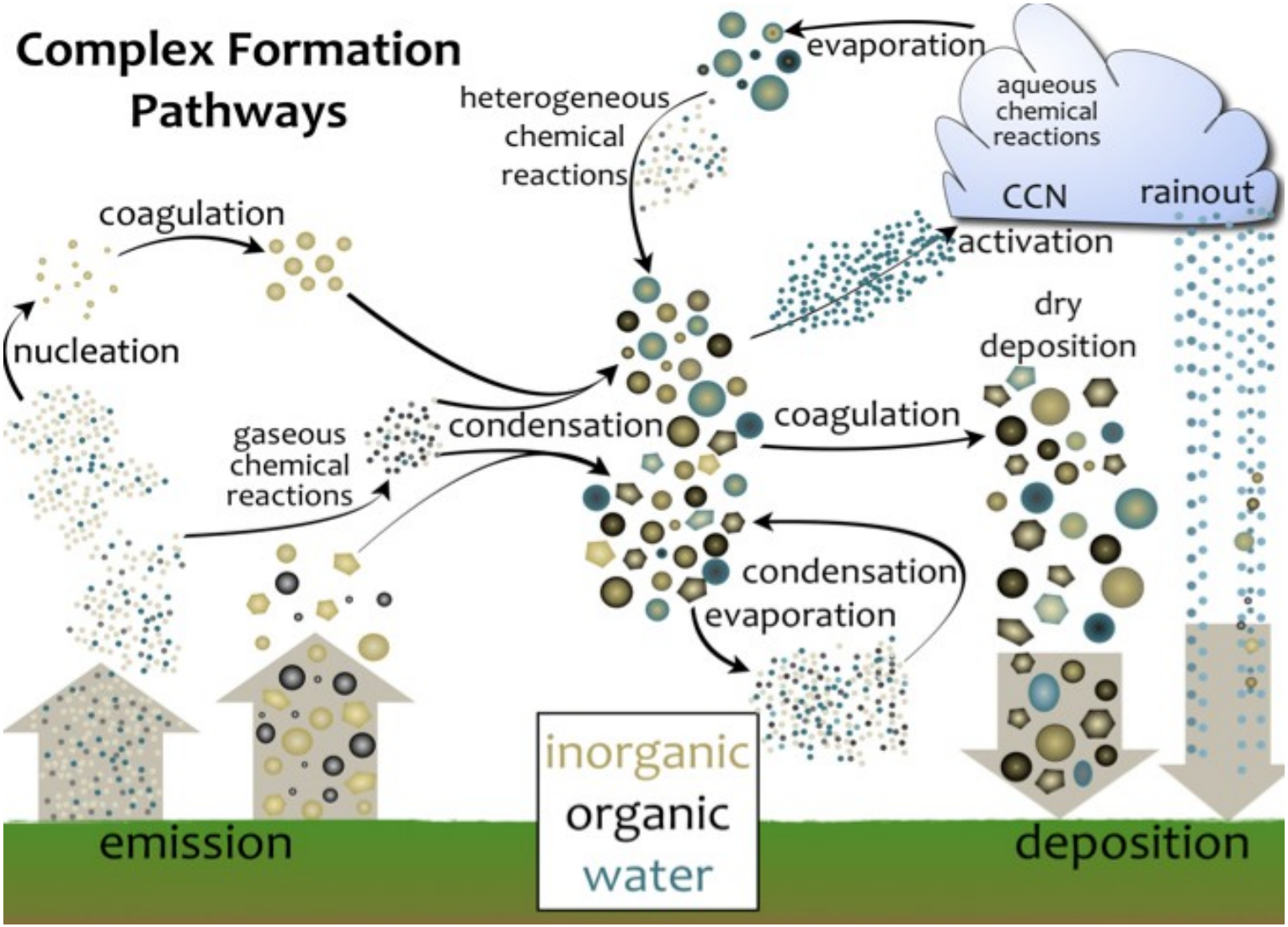
Adjoint code development

- Isolate the process of concern
- If the process is too complicated, break down into small pieces
- Develop the adjoint code
  - By automatic differentiation
    - Requires further code preparation
  - Manually
- Evaluate on a process-by-process basis
  - Finite difference (FD) comparisons
  - Complex variable method (CVM)
    - Avoid cancellation errors and allow small perturbations

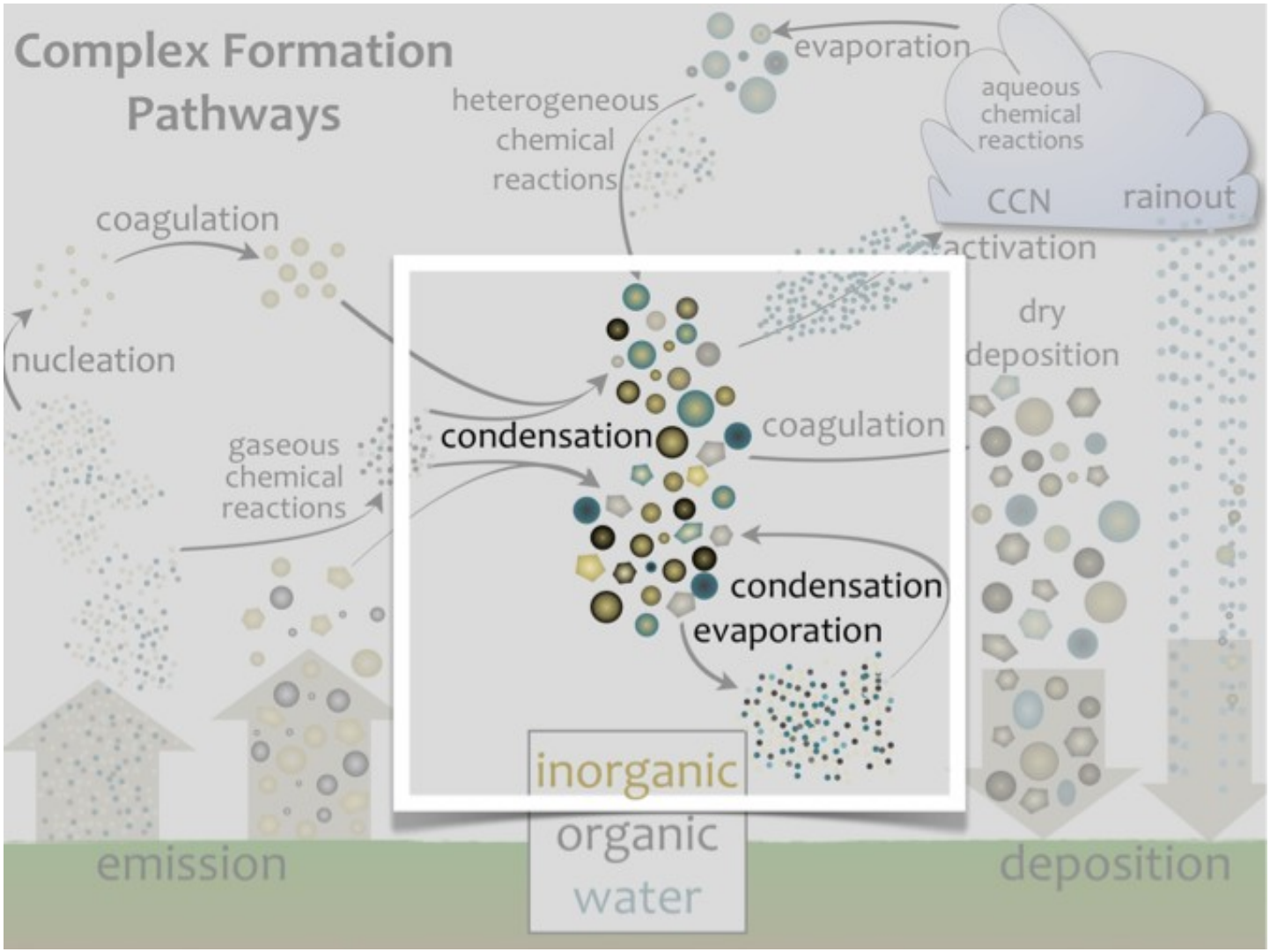
Gas-phase processes

- Updated to v4.7.1
  - Adding backward (adjoint) solvers for transport module options not previously supported:
    - YAMO advection, but without the “hidden” modification of horizontal wind (using the same forward and backward solvers for horizontal advection in both PPM and YAMO)
    - ACM2 and ACM2_INLINE options for vertical diffusion
  - To include CB05
  - Focusing on adjoint backbone (not gradient calculation) at the moment

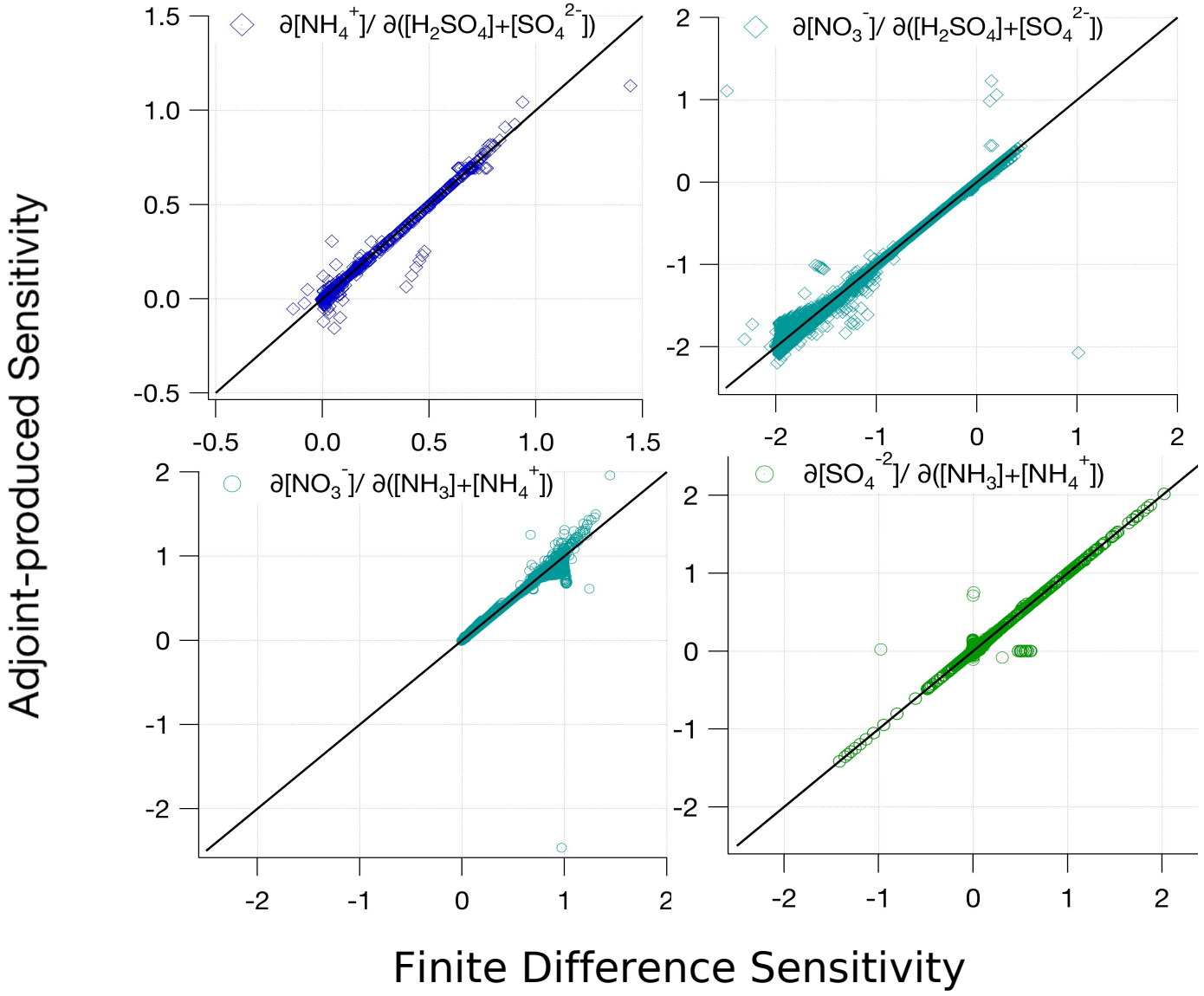
Aerosol Processes



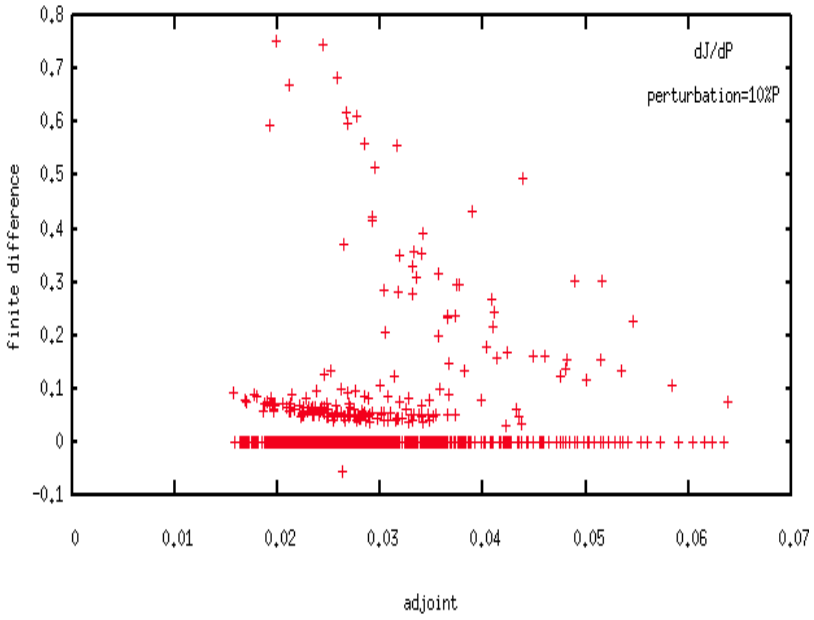
Aerosol Thermodynamics: ISORROPIA

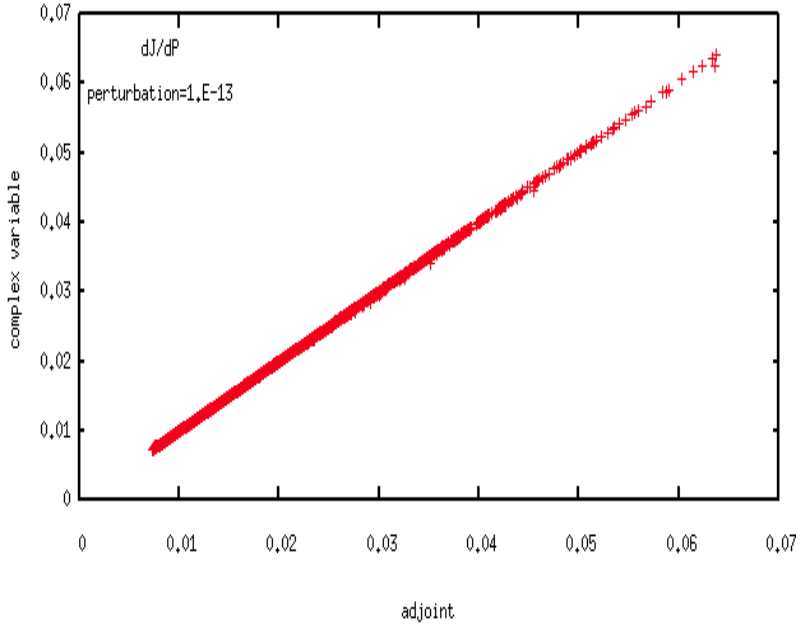


Sample ISORROPIA results



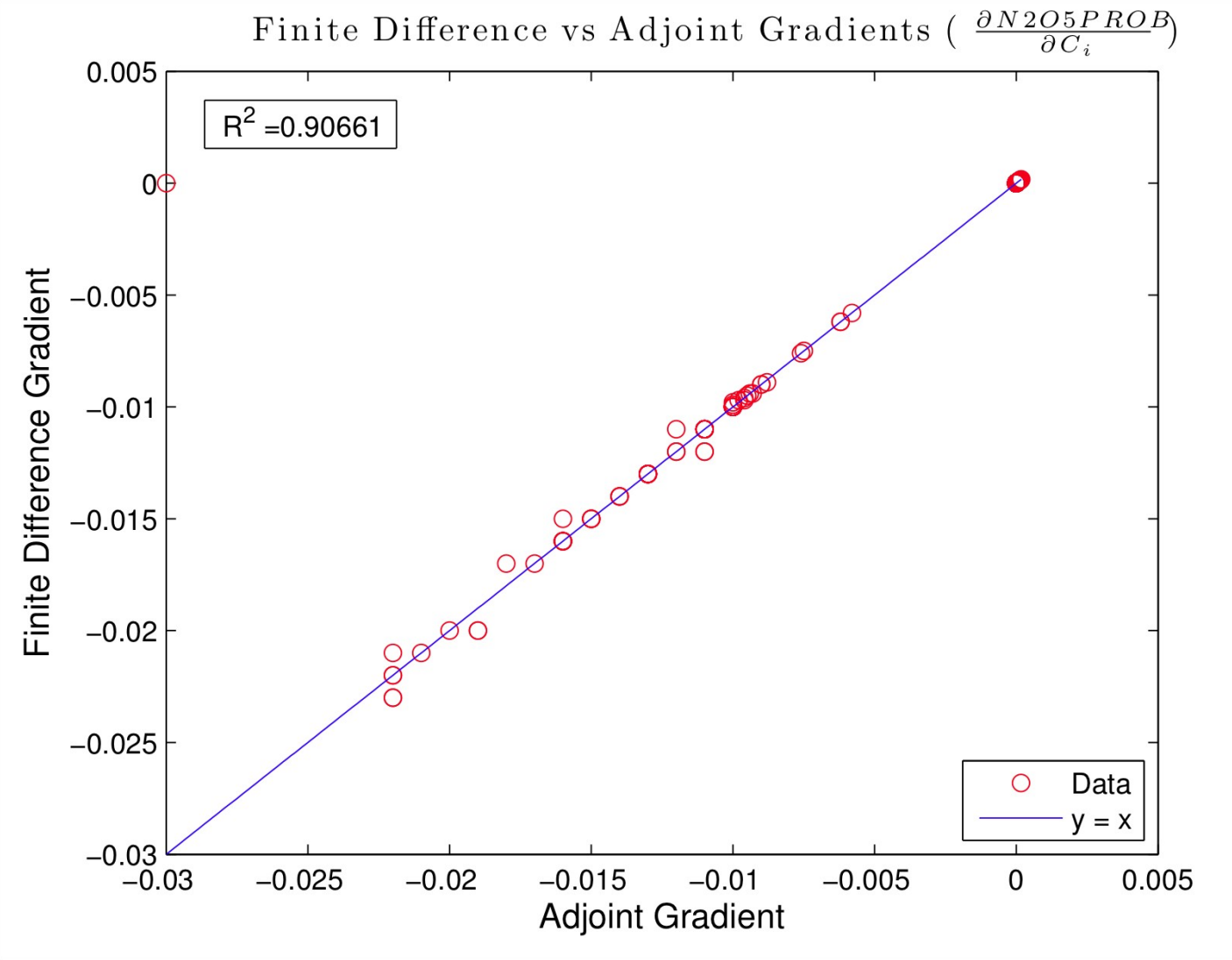
Aerosol Dynamics – example: SOA



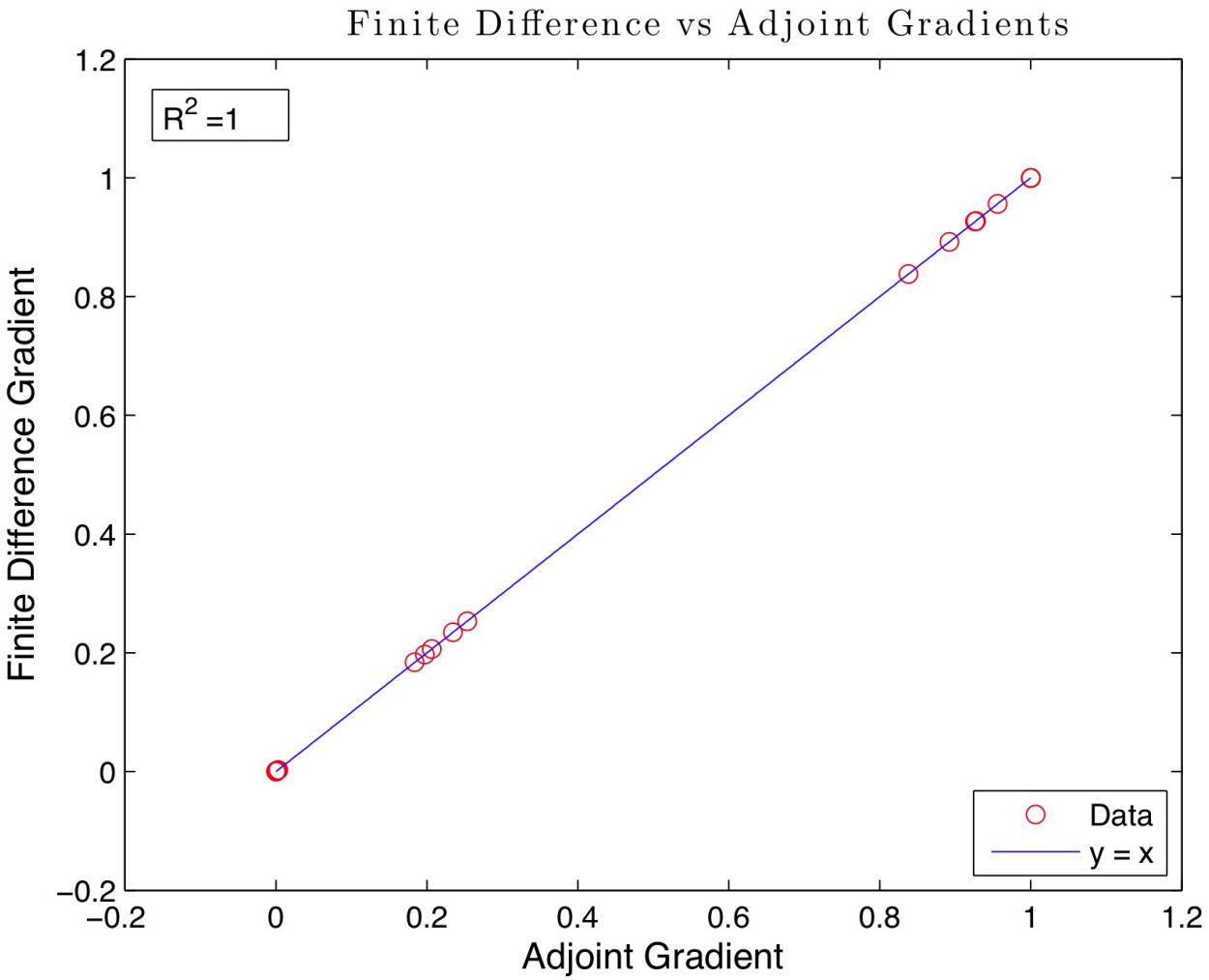


Sensitivities of SOA mass
w.r.t. J-mode ABNZ2

Heterogeneous chemistry

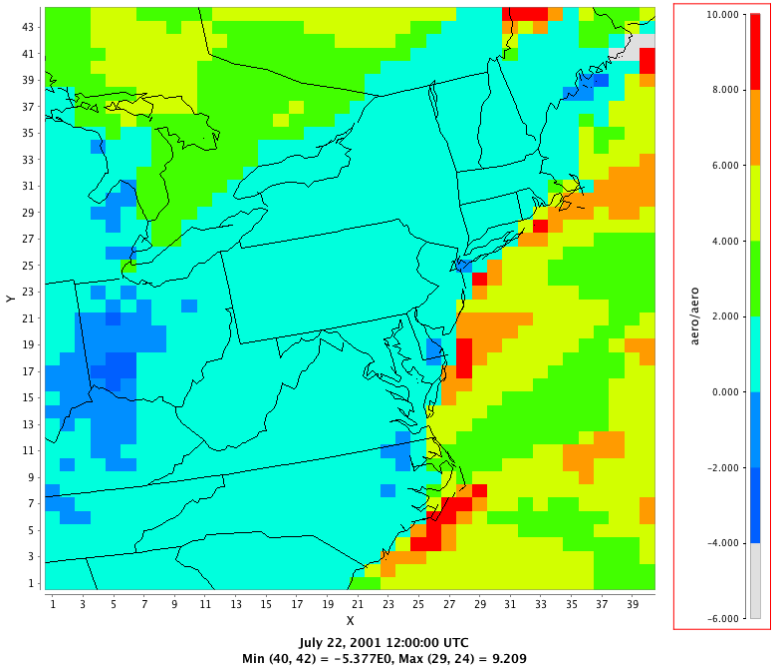


Coagulation

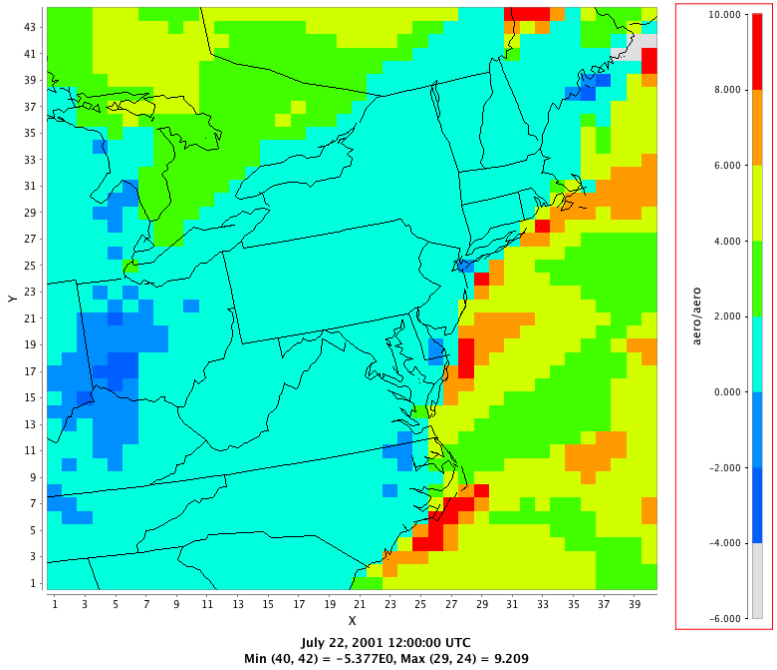


Aerosol dynamics – all processes

CVM



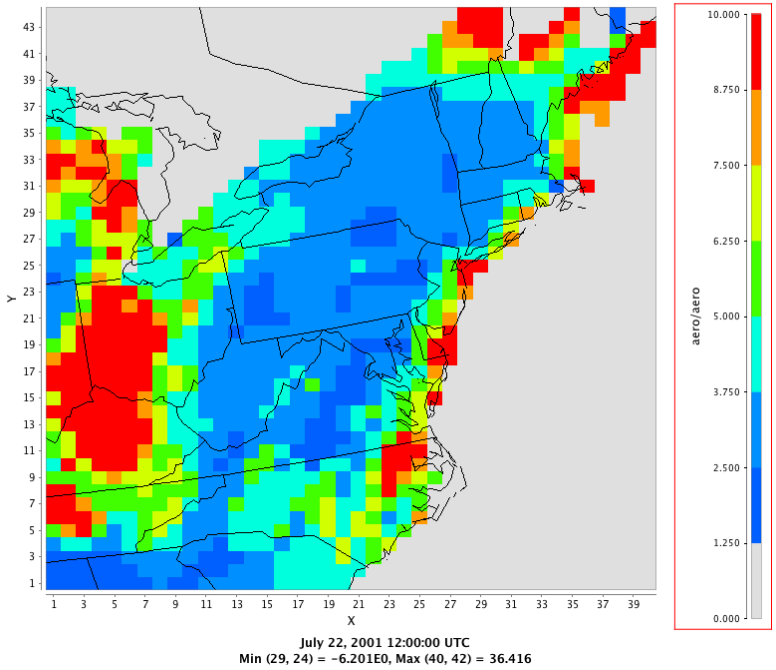
ADJ



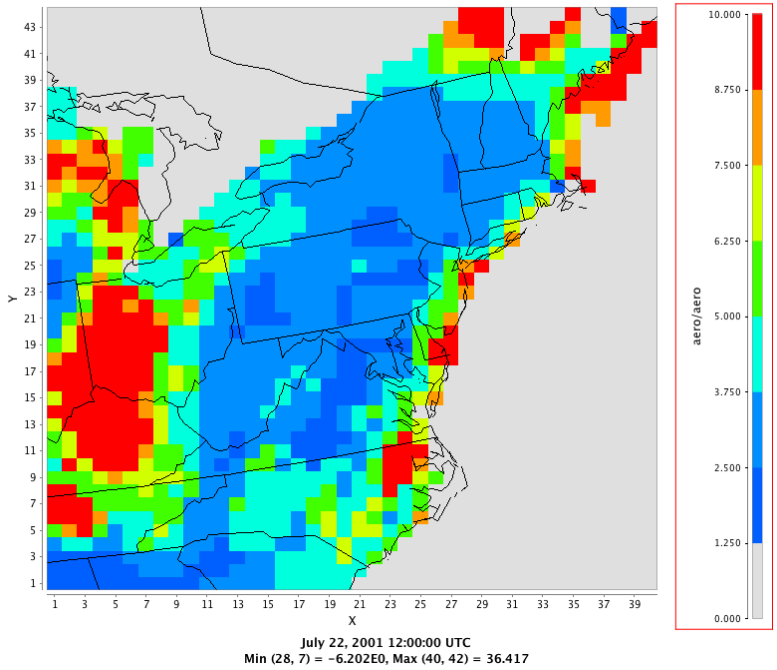
Sensitivities of all j-mode aerosol mass
w.r.t. j-mode SO4

Aerosol dynamics – all processes

CVM



ADJ



Sensitivities of all j-mode aerosol mass
w.r.t. j-mode NH4

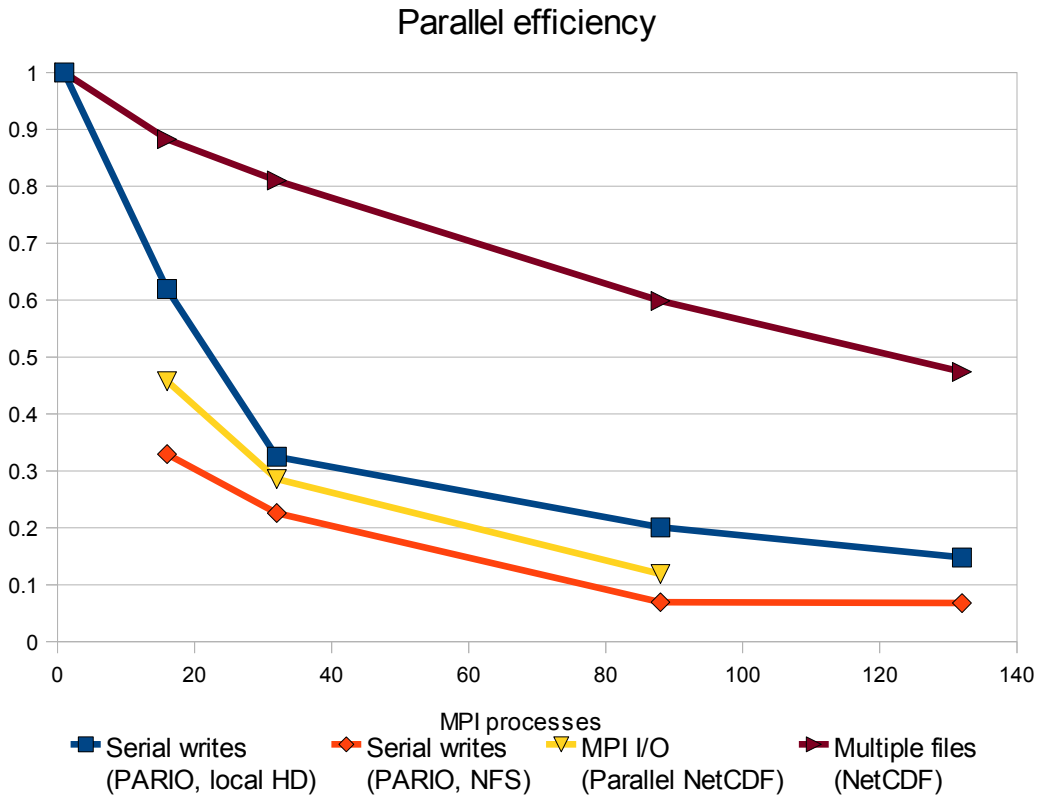
Aqueous Chemistry

- Use KPP-generated Rosenbrock solver for aqueous chemistry
  - Stay compatible with Carlton et al. (2009)
- Recast the equilibrium reactions as simultaneous forward and back reactions following Li [2006] and Kamens et al. [1999].
- Forward (k_f) and backward (k_b) reaction rates should be
  - consistent with Henry's Law and dissociation constants
  - fast enough that equilibrium will be reached within a given time step in the aqueous chemistry module

Parallelization

- Write I/O operations in CMAQ are preformed serially
  - Data from all processes are collected to process 0 by calls of MPI routines
  - Parallelization of CMAQ is suboptimal and it does not scale well on large clusters
- At the moment, we follow CMAQ parallelization
  - Parallelization of CMAQ adjoint scales worse than original CMAQ (due to frequent checkpointing), especially for large domains with fine resolution.
  - Other issues: observation operators and minimization in data assimilation applications

Efficiency of parallelization



Testing domain: 266x194, 3km resolution
Cluster: AMD Opteron, 152 cores, SAS-2, Infiniband Mellanox
System: OpenSuse11.2, OFED 1.4, MVAPICH2 1.2p1 with Gen2-IB RDMA + SHMEM
Parallelization: From 16 to 132 MPI processes.

Details on the poster Resler et al.: Fine resolution modeling with CMAQ-adjoint

Current status

- An adjoint model development working session is scheduled for November 12-15. We hope to put many pieces together at or before the meeting.
  - This will give us a draft version
  - Other topics remain:
    - Gradients calculation
    - 4D-Var tools
    - Nesting
    - Additional modules in CMAQ
- Working version to be ready in spring 2011

Summary and conclusions

- Majority of aerosol subroutines are already differentiated
- Code optimization and efficiency are next
- Next year we will have an operational multi-phase adjoint for CMAQ

- The development is geared towards the user community. If there are capabilities you like to see in CMAQ-ADJ, this is the time to ask for them (amir_hakami@carleton.ca).

Acknowledgements

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