A Multiphase Adjoint Model for CMAQ

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CMAS 2015

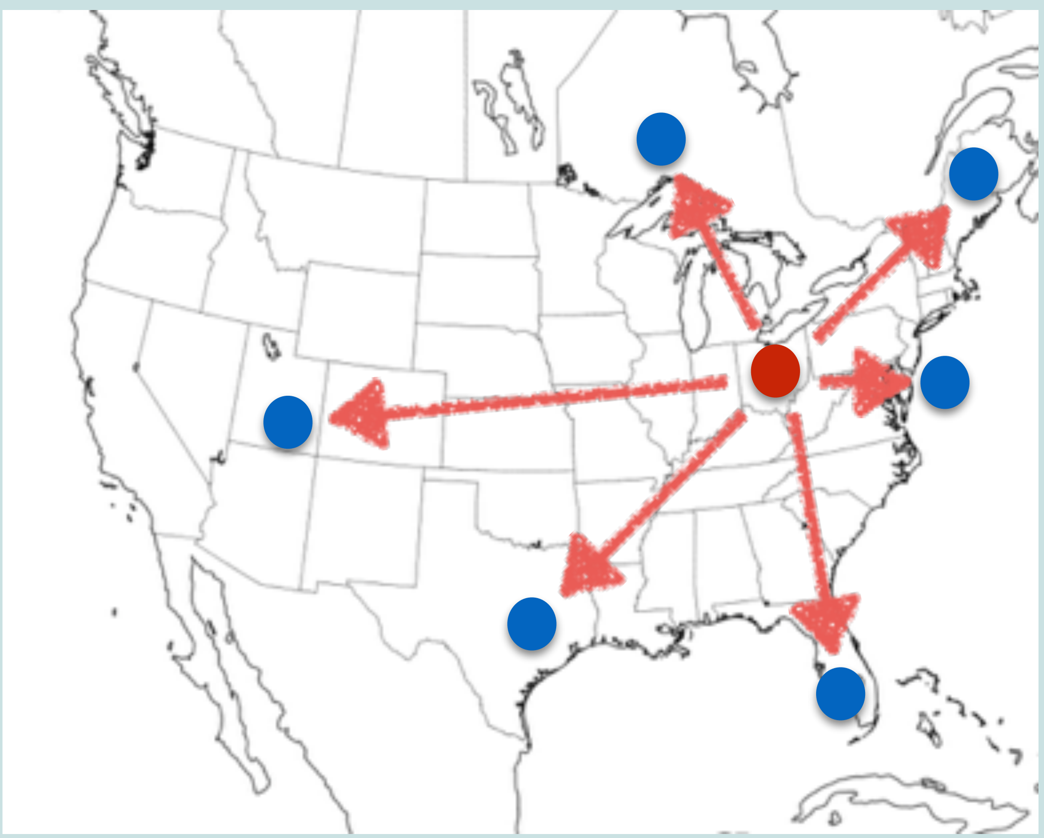
Outline

- Motivation for developing a multiphase adjoint model
- The current status of the development
    - Adjoint code
    - Process-by-process validation
    - Test run of the full adjoint model
- Concluding remarks

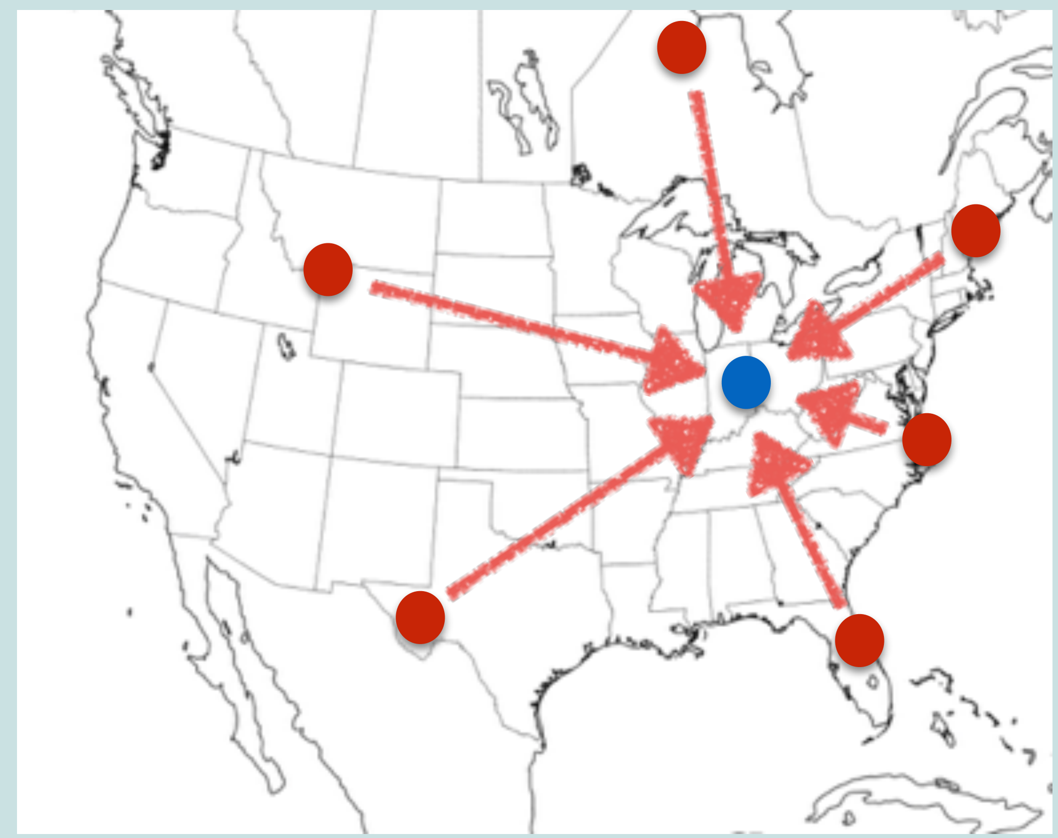
Motivation

- CMAQ: Evolution of atmospheric gas and aerosol species
- Forward sensitivity analysis (Decoupled Direct Method, DDM)

● source ● receptor



Forward

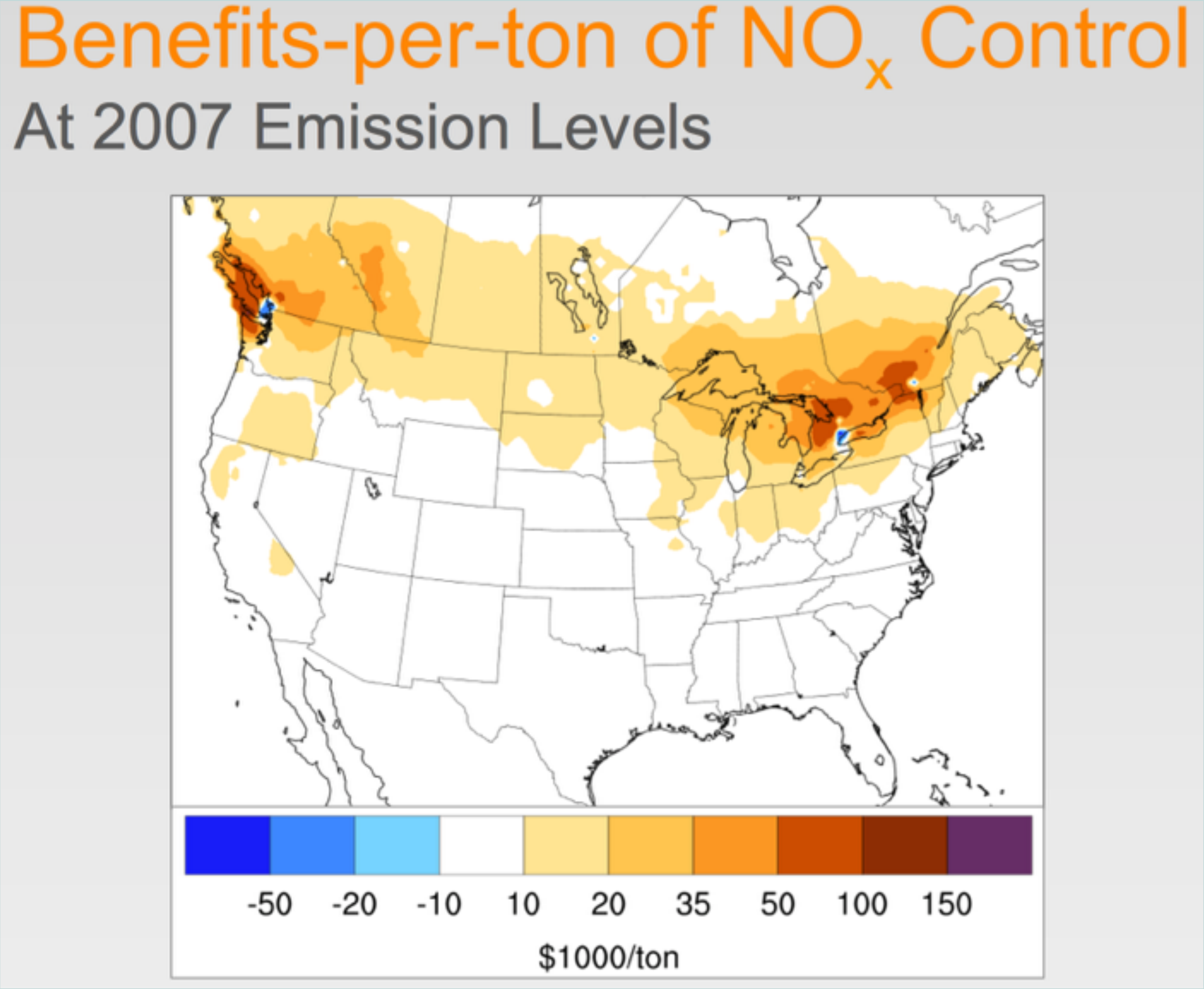


Backward

- Backward/Adjoint sensitivity analysis

Adjoint sensitivity analysis: An example

Pappin et al., “Compounding Benefits of Air Pollution Control: A Revised View of Air Pollution Economics”, Wednesday Presentation



The current status of the adjoint development

- CMAQ scientific processes: chemistry, aerosol, transport, cloud
- Adjoint code generated by tools (KPP, Tapenade, TAMC) or by hand
- Code validating using
  - Finite Difference Method (FDM)

$$f'(x) = \frac{f_{x+h} - f_{x-h}}{2h} + O(h^2)$$

  - Complex Variable Method (CVM)

$$f'(x) = \frac{\Im(f(x+ih))}{h} + O(h^2)$$

  - and sometimes DDM/TLM

Process-by-process validation

Process	Sub-processes	Validation Methods
Chemistry		Finite difference Complex variable
Aerosol	Secondary organic aerosol, Heterogeneous chemistry, Coagulation, Nucleation, Condensation, Thermodynamics (Isorropia; Capps et al., 2012)	Finite difference Complex variable
Transport	Horizontal/vertical advection, Horizontal/vertical diffusion	Finite difference
Cloud	Convective cloud, Resolved cloud, Aqueous chemistry	Finite difference Complex variable Tangent linear model

Process-by-process validation

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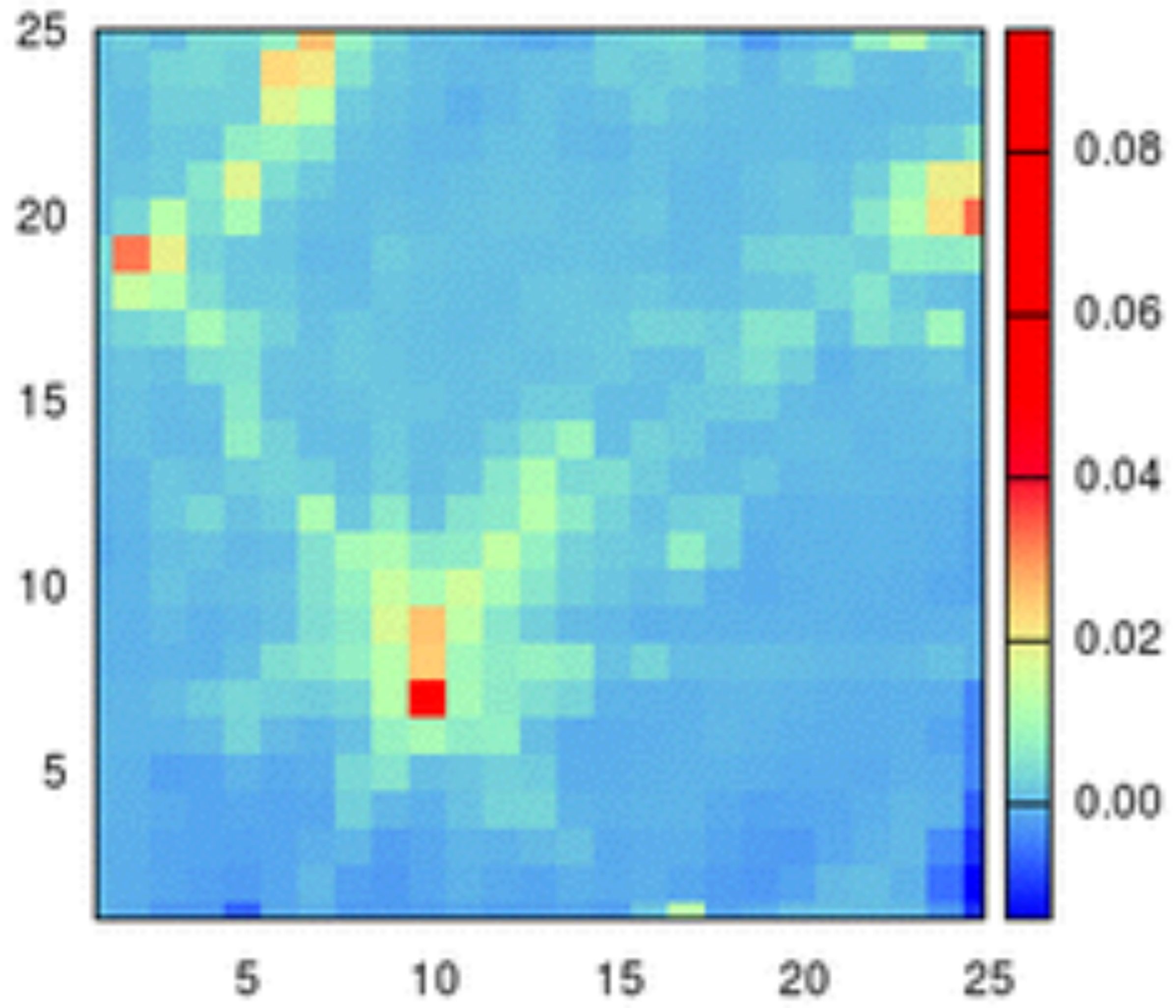
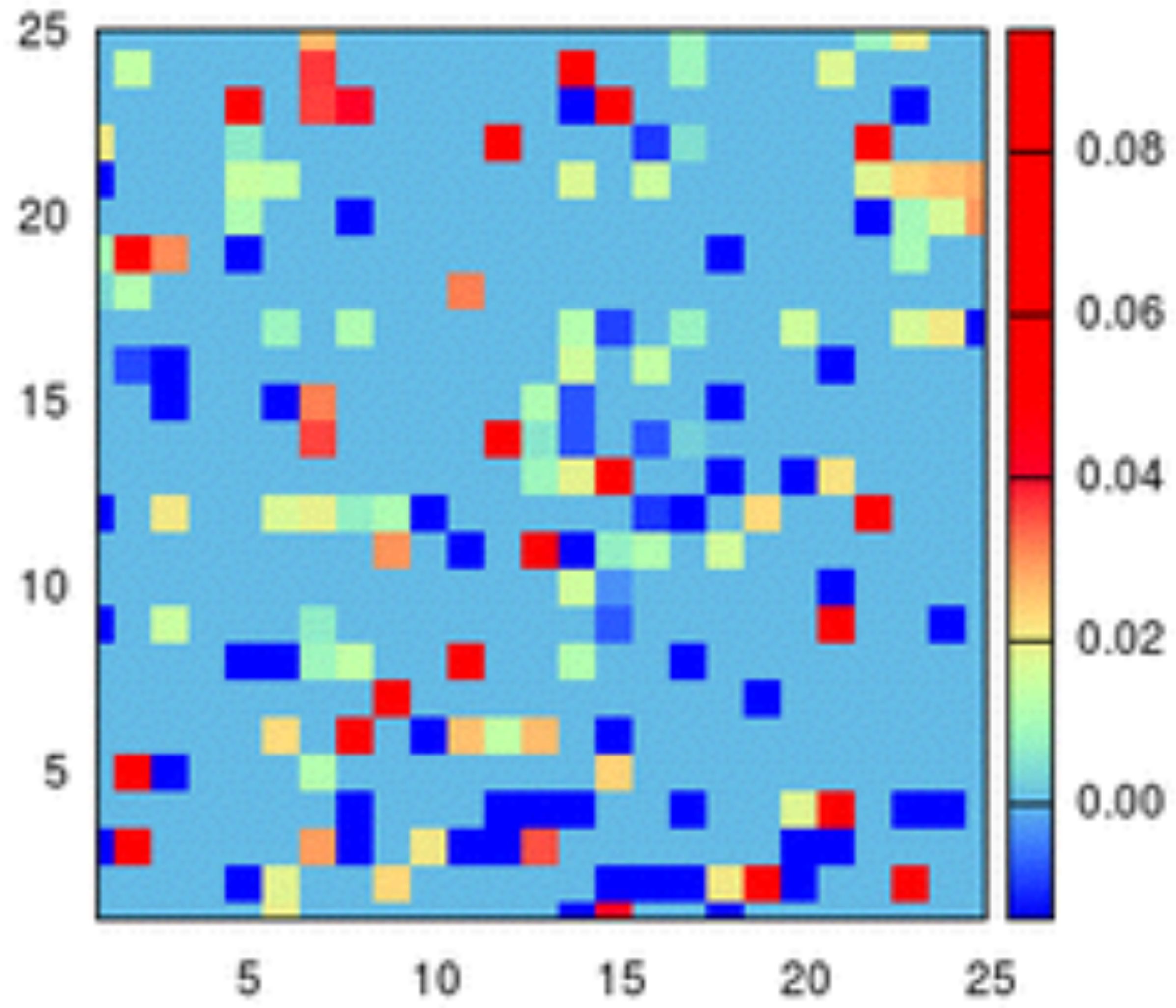
Th adjoint of chemistry: Limitations of the FDM

Adjoint



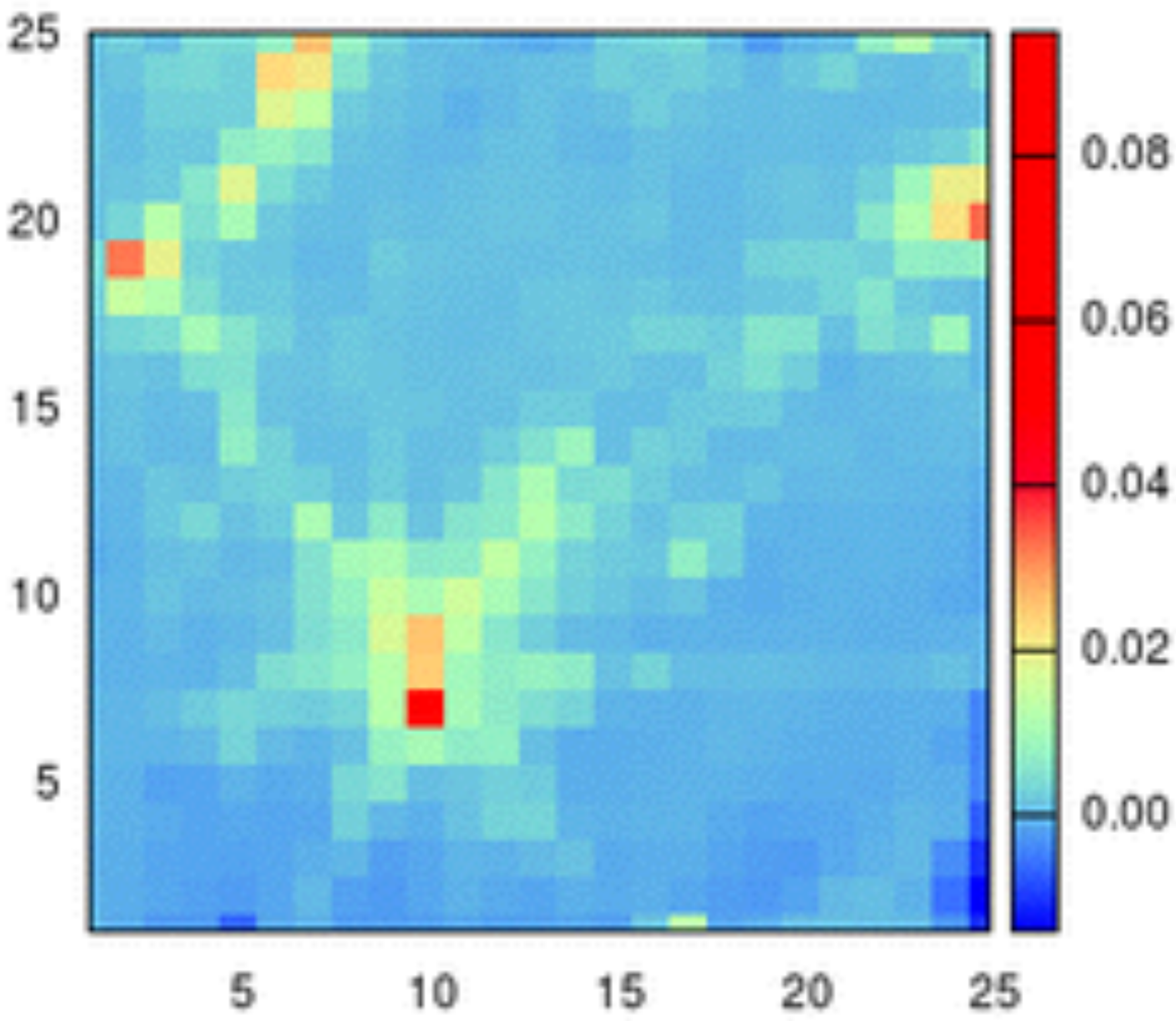
Finite difference

$$\frac{\partial O3}{\partial HCL}$$



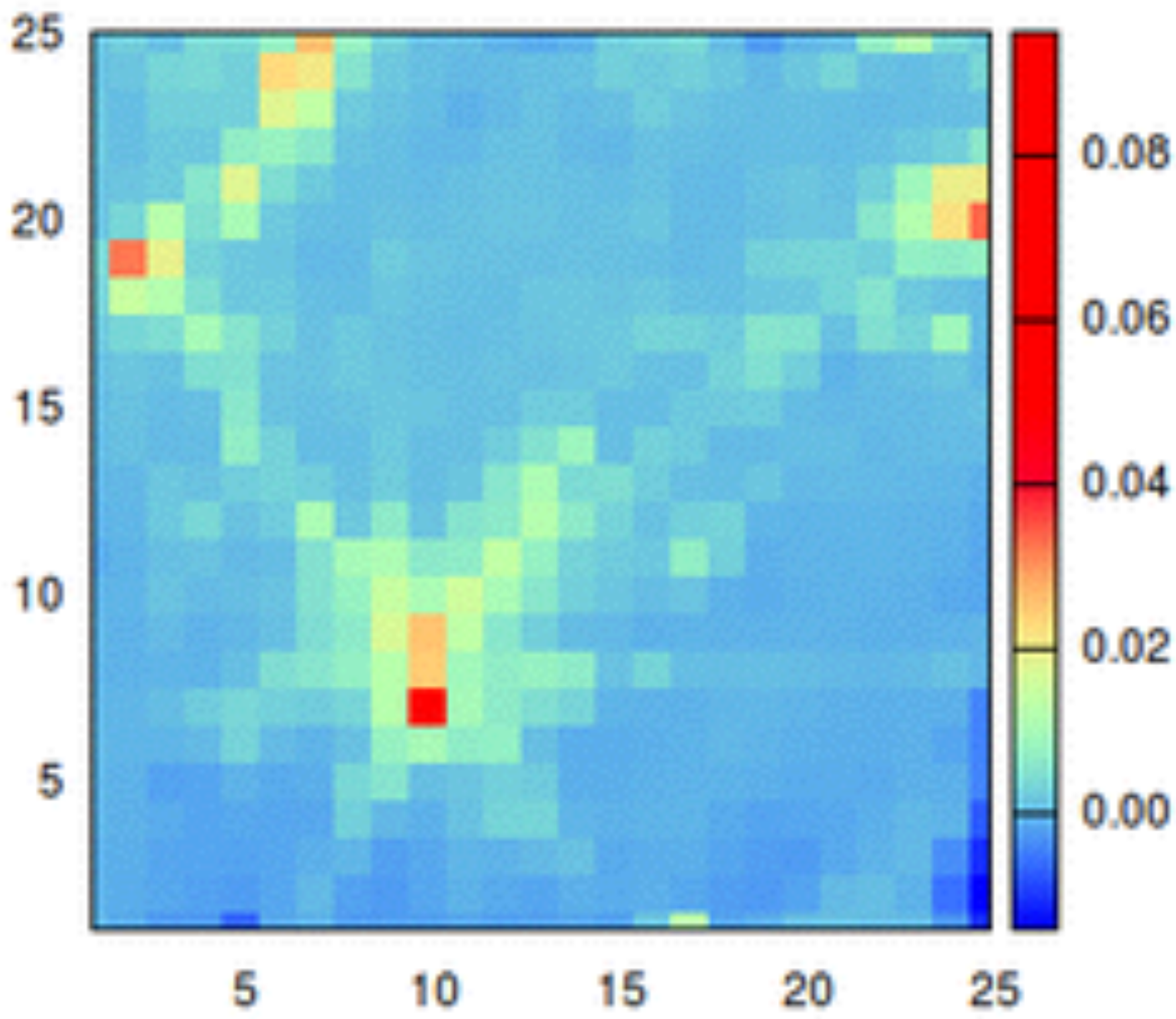
The adjoint of chemistry

Adjoint



Complex variable

$$\frac{\partial O3}{\partial HCL}$$

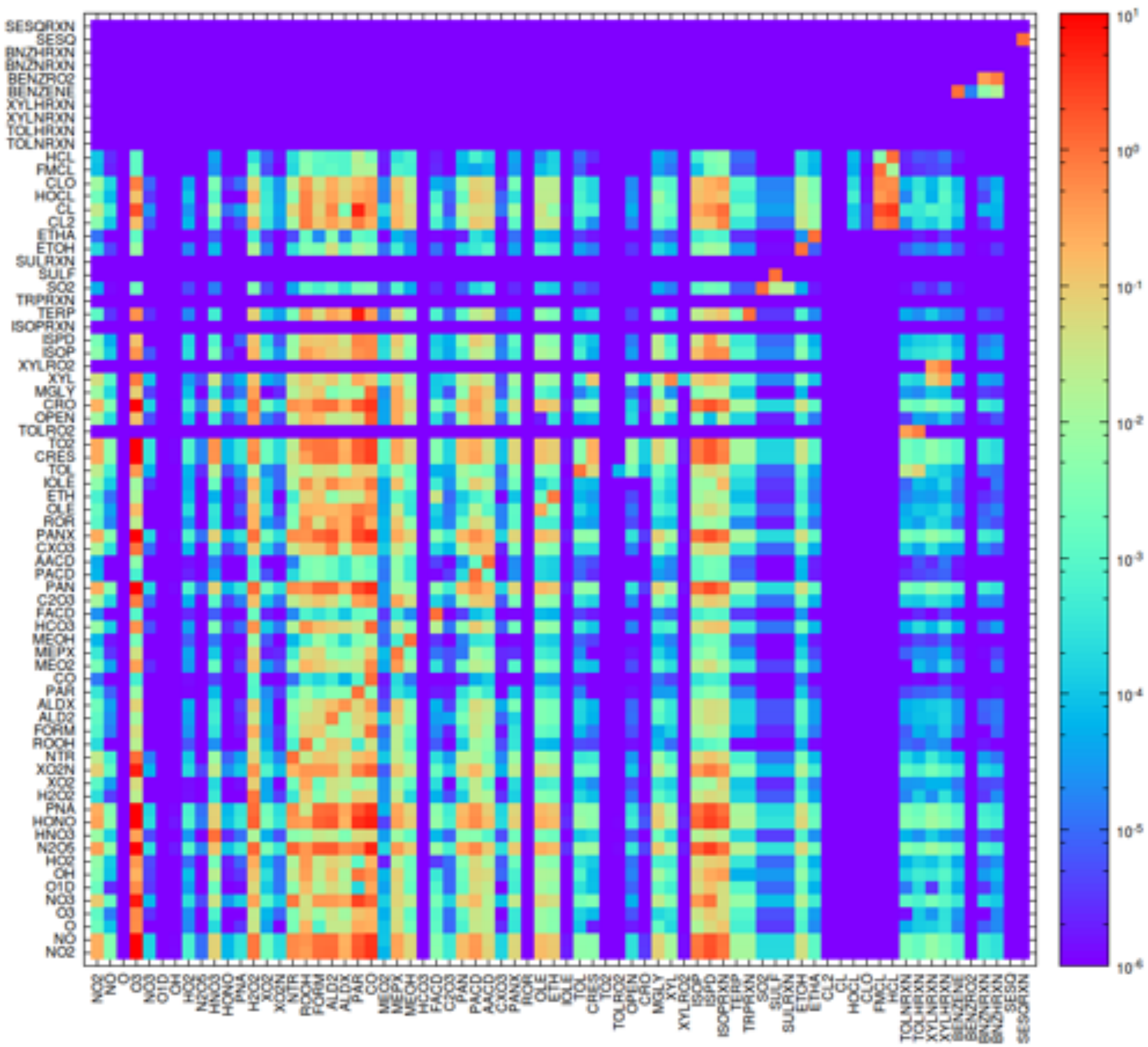


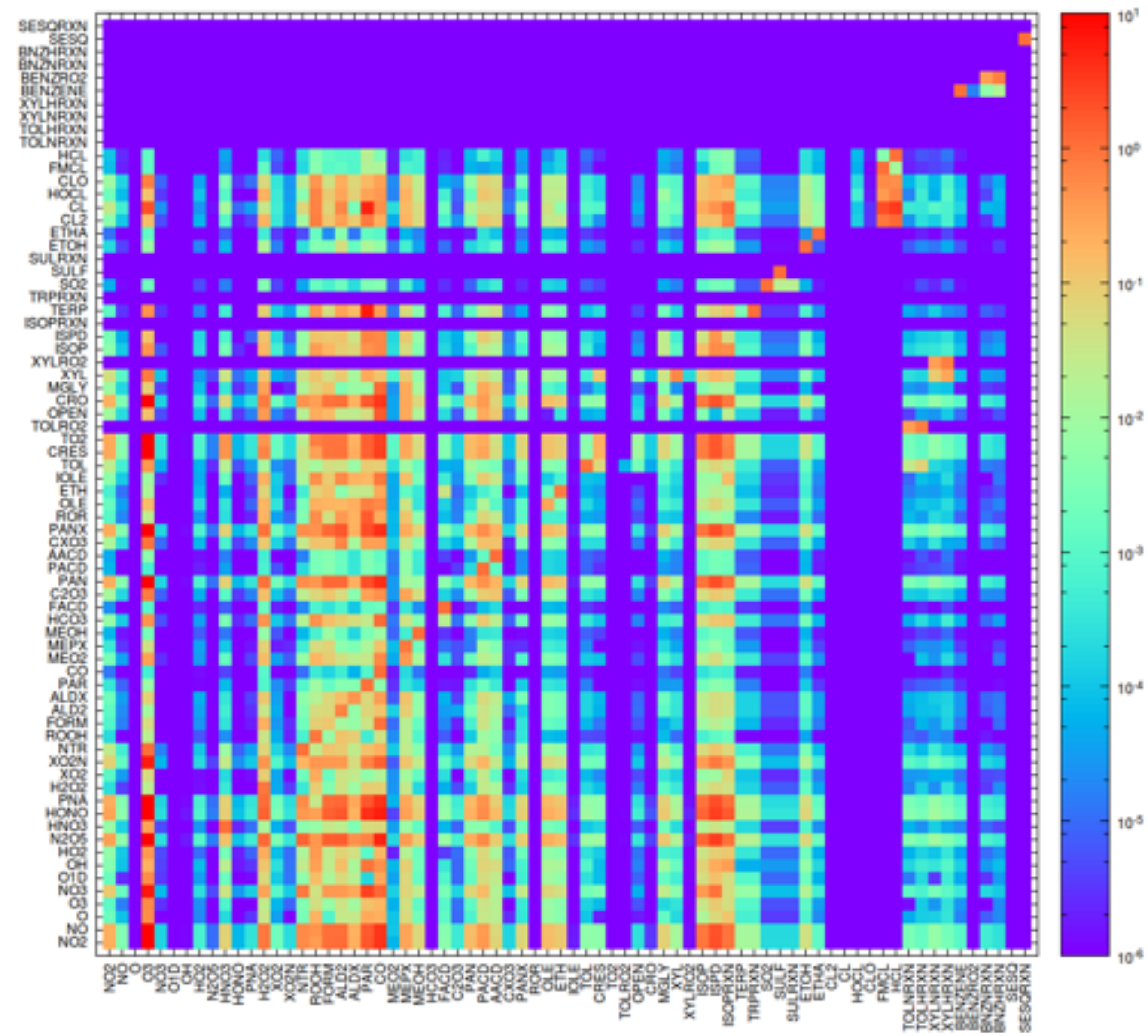
The adjoint of chemistry: Full Jacobian

Adjoint

Complex variable

$$\frac{\partial Gas_i}{\partial Gas_j}$$





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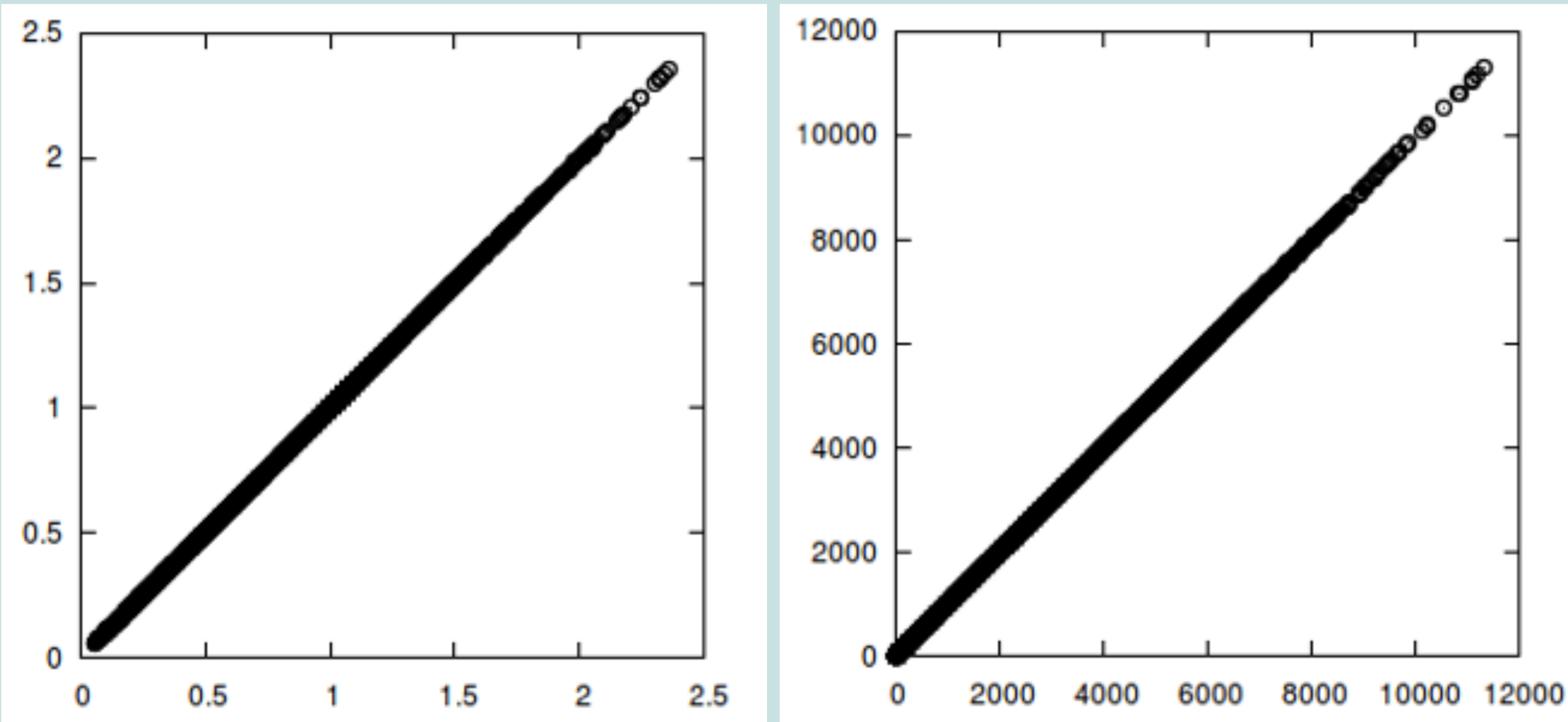
The adjoint of aerosol: secondary organic aerosol

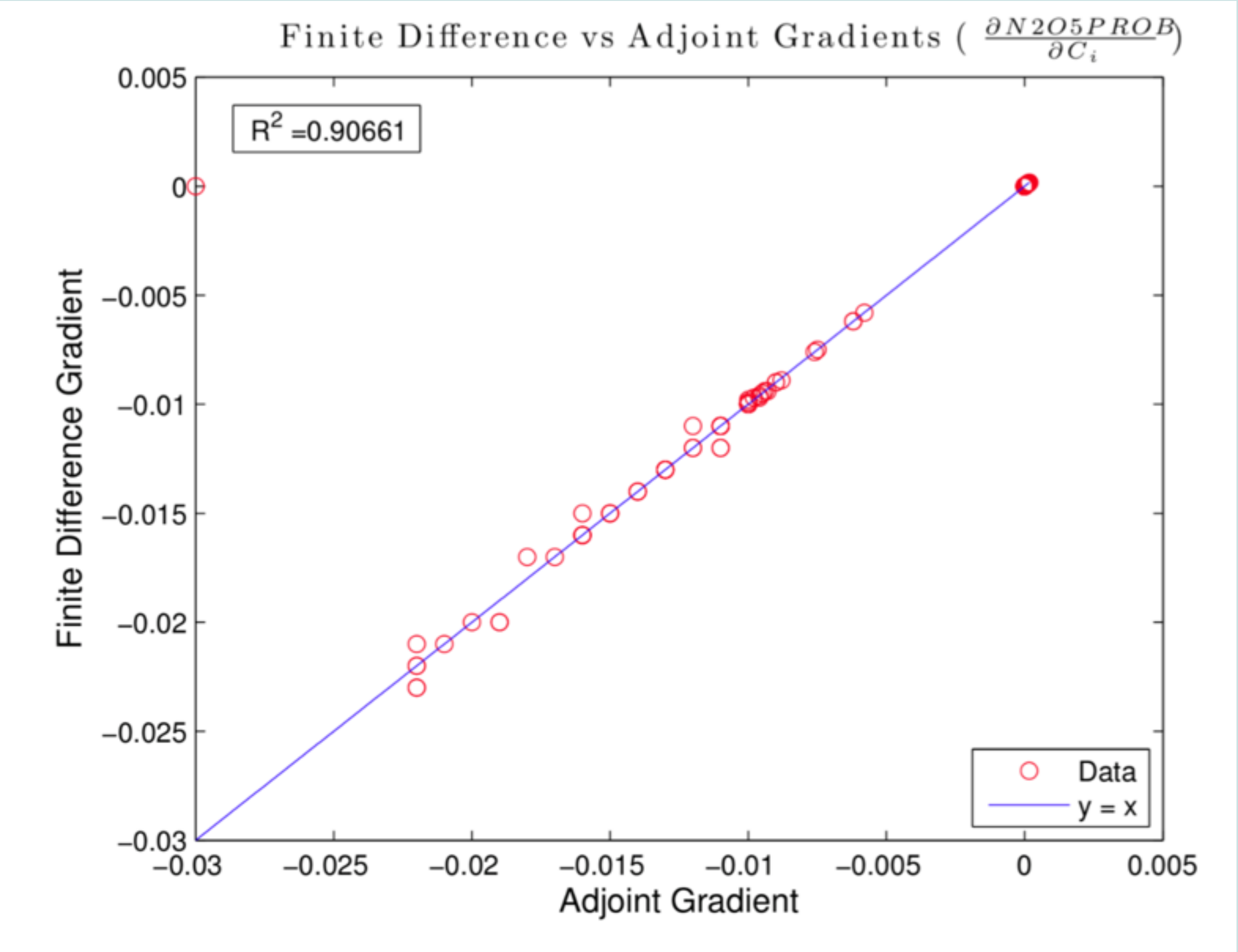
$$\frac{\partial PM_{2.5}}{\partial AALKJ} \qquad \frac{\partial PM_{2.5}}{\partial SV\_BNZ1}$$

Complex variable

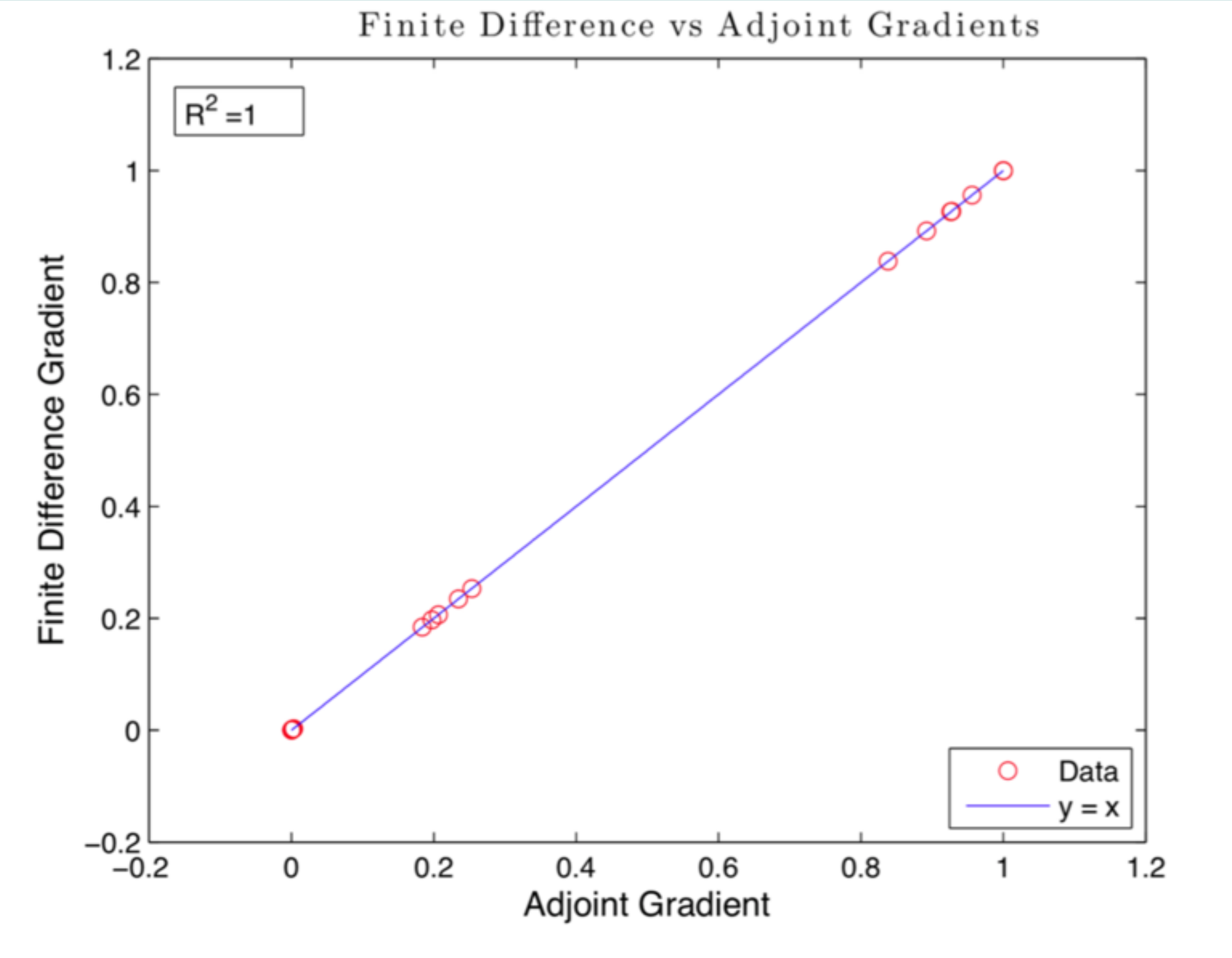


Adjoint

The adjoint of aerosol: heterogeneous chemistry

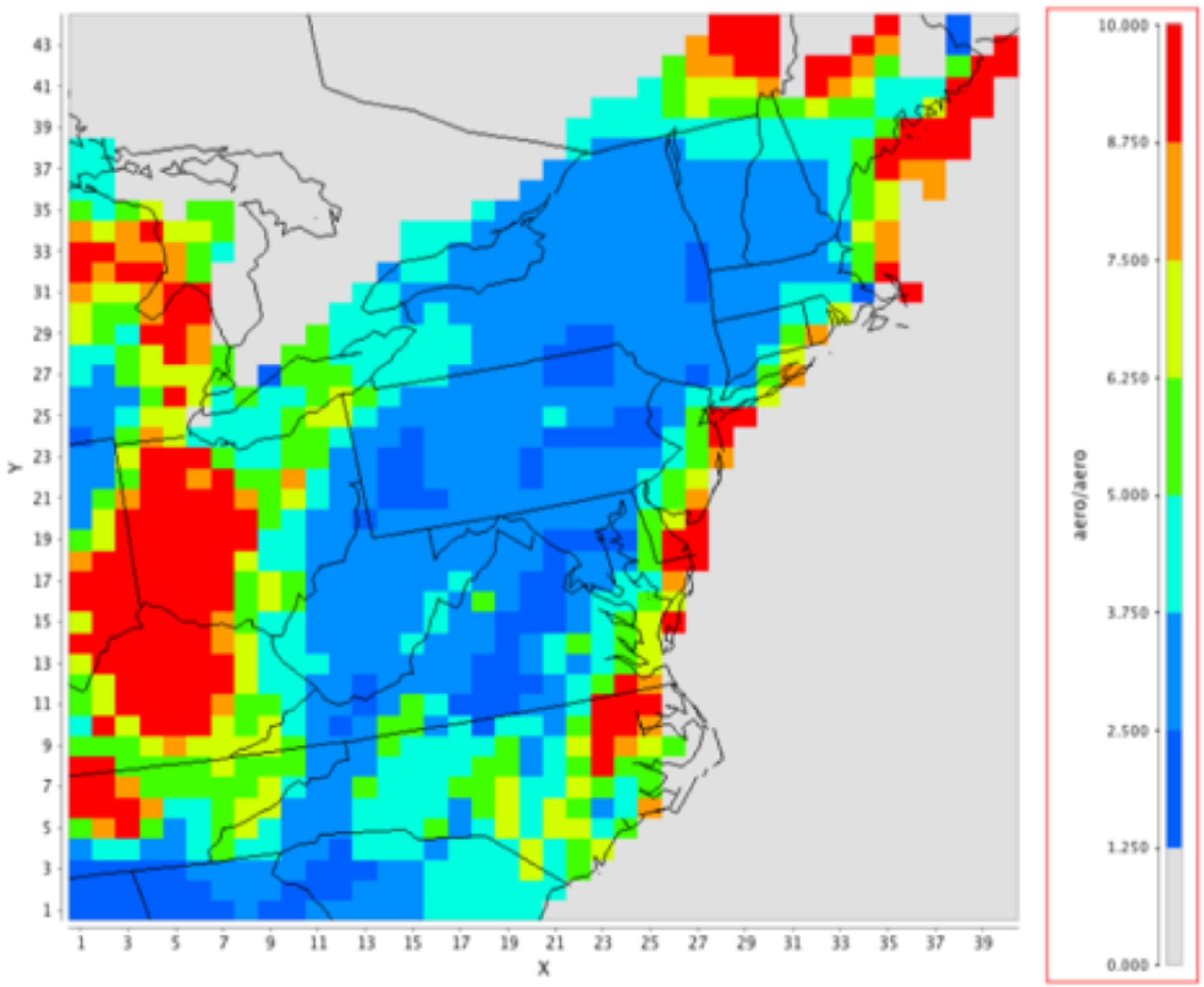


The adjoint of aerosol: coagulation

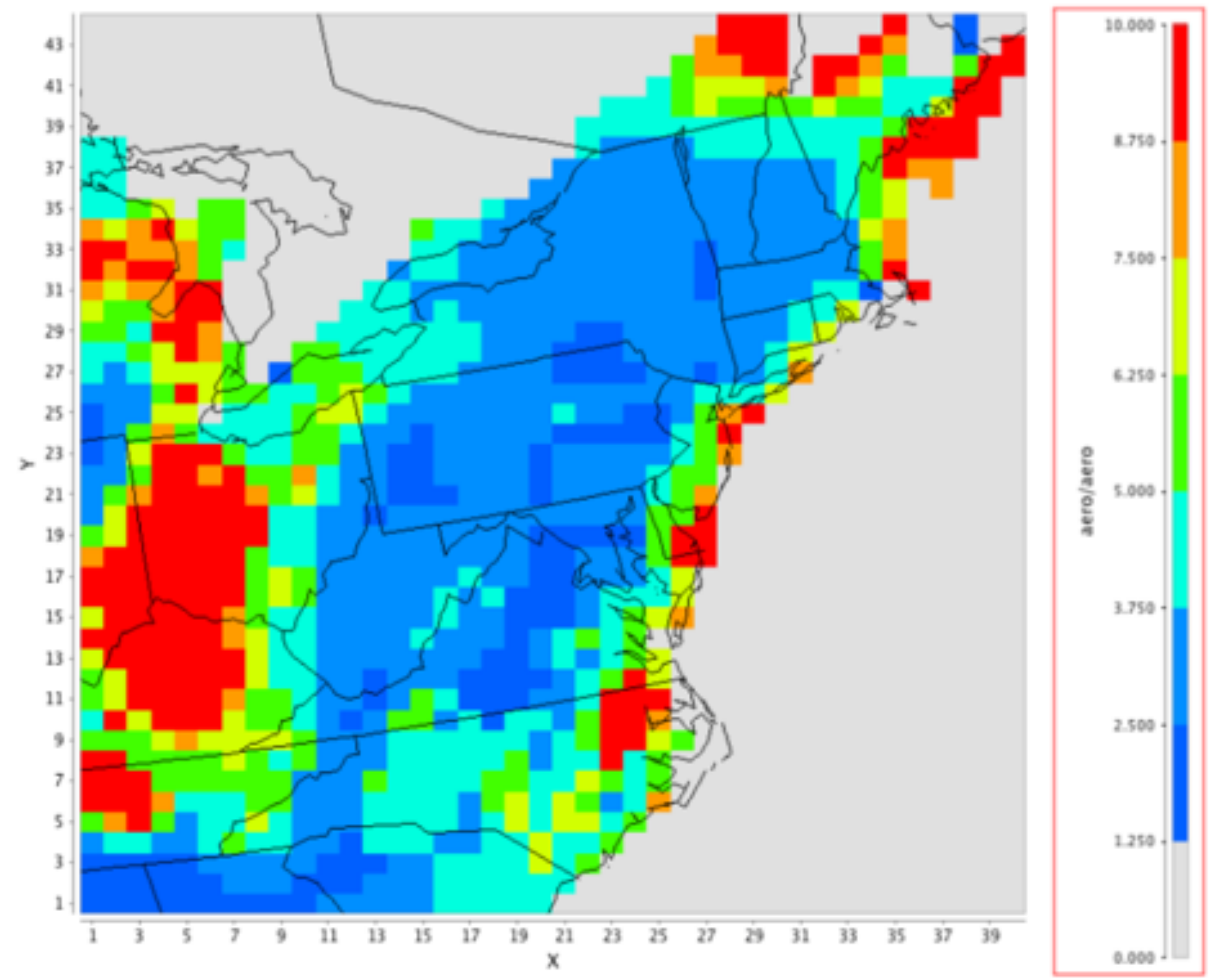


The adjoint of aerosol dynamics

$$\frac{\partial PM_{2.5}}{\partial ANH4J}$$



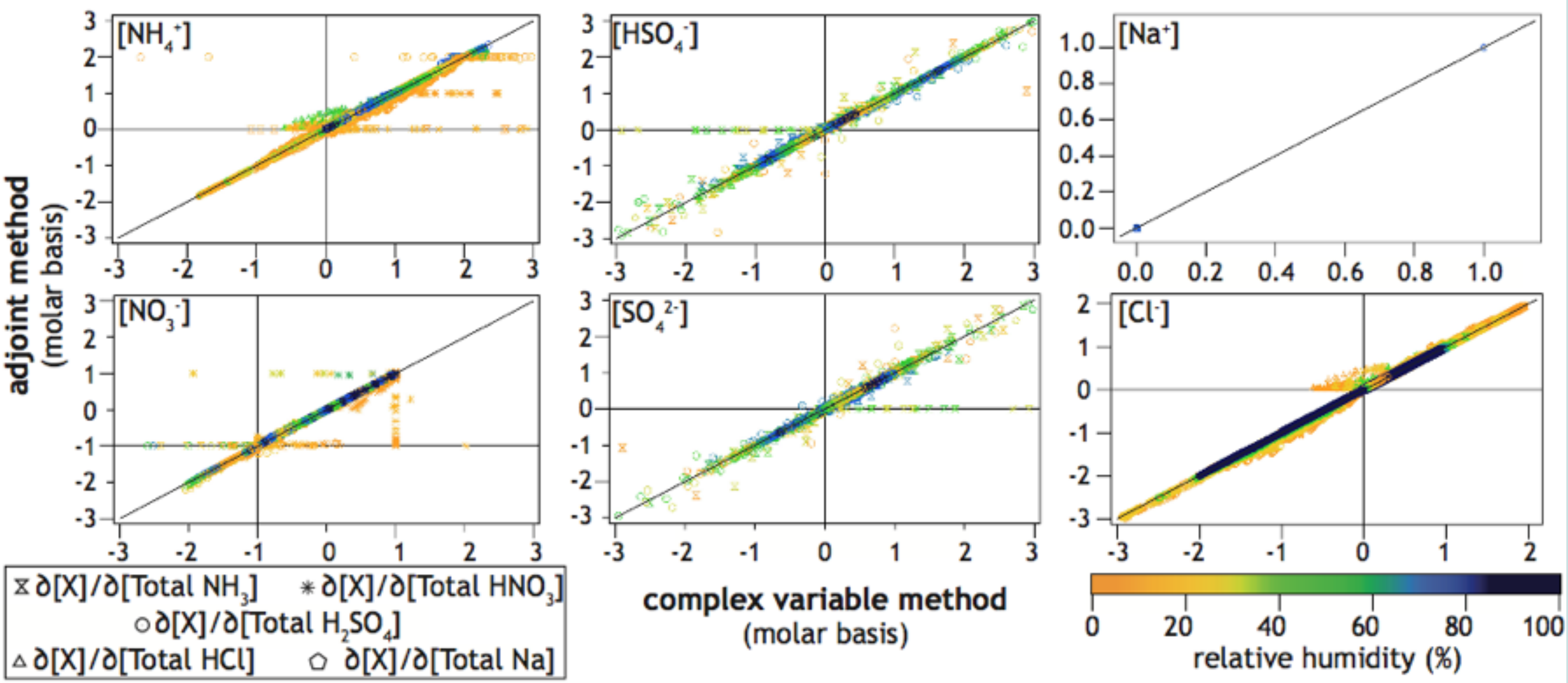
Adjoint



Complex variable

The adjoint of aerosol: Isorropia

ANISORROPIA Evaluation

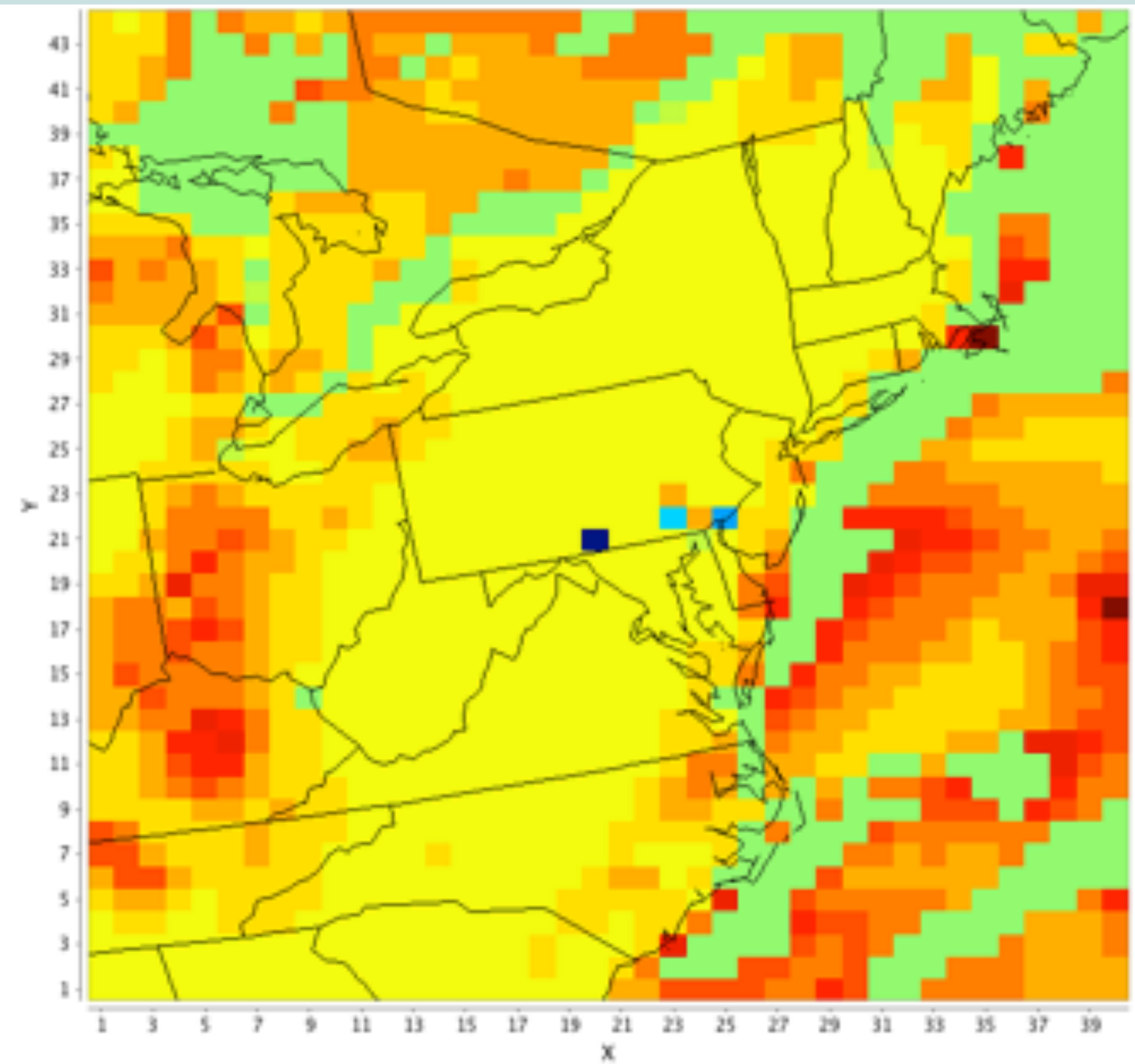


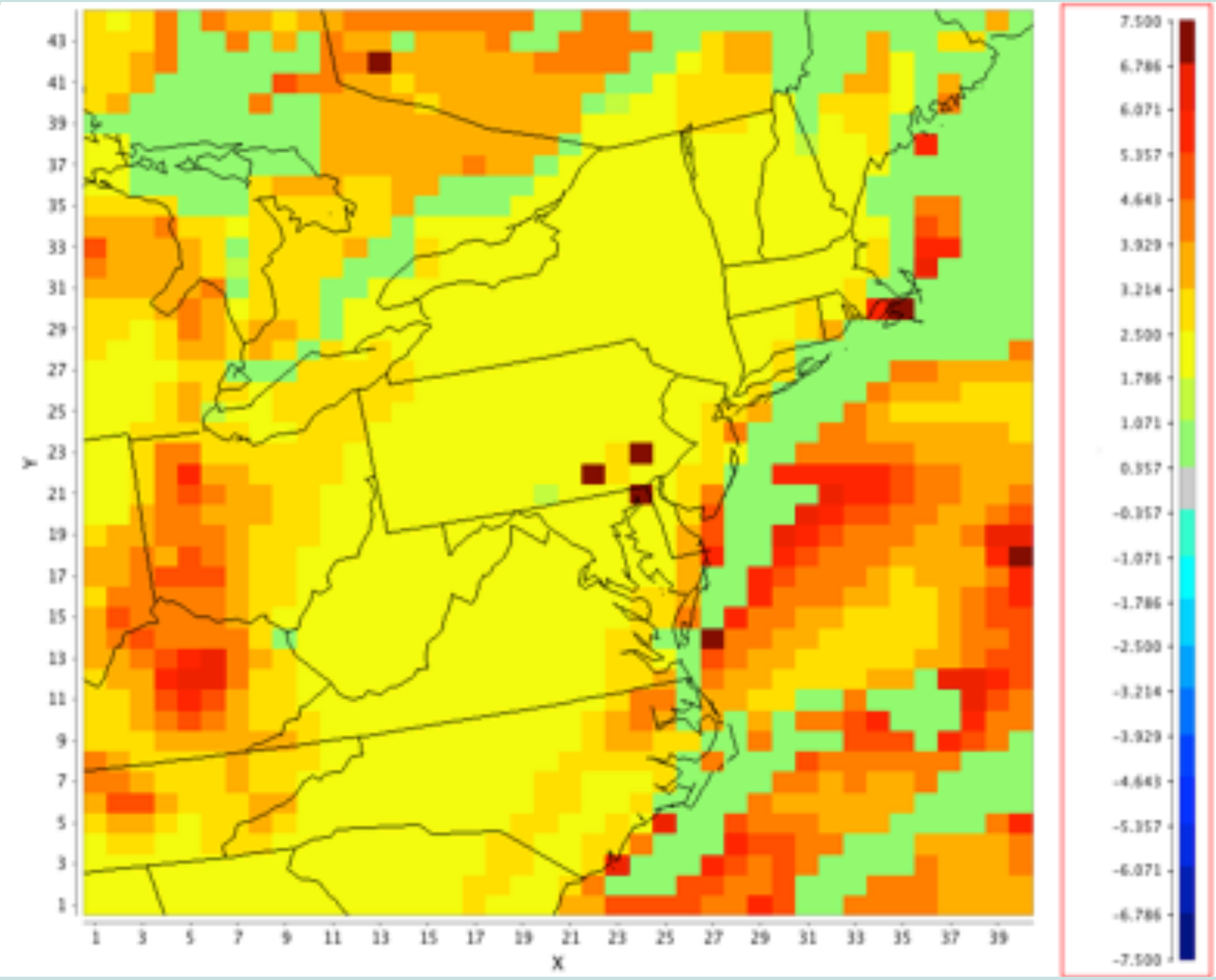
across an atmospherically relevant range of concentrations
268-308 K

Capps, Henze, Hakami, Russell, and Nenes, *ACP*. 2012

The adjoint of aerosol: aerosol dynamics and thermodynamics

$$\frac{\partial PM_{2.5}}{\partial ASO4J}$$



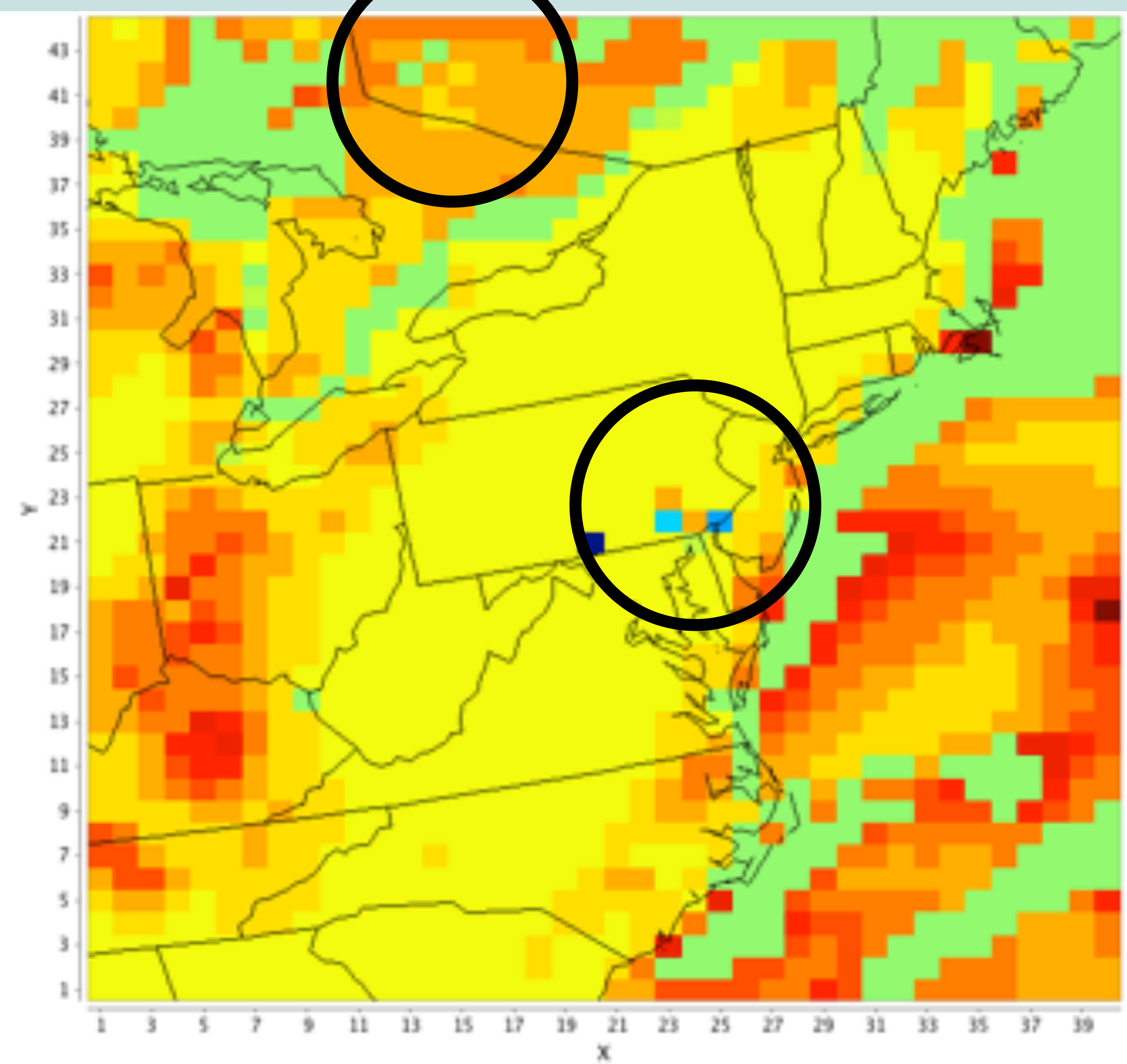


Adjoint

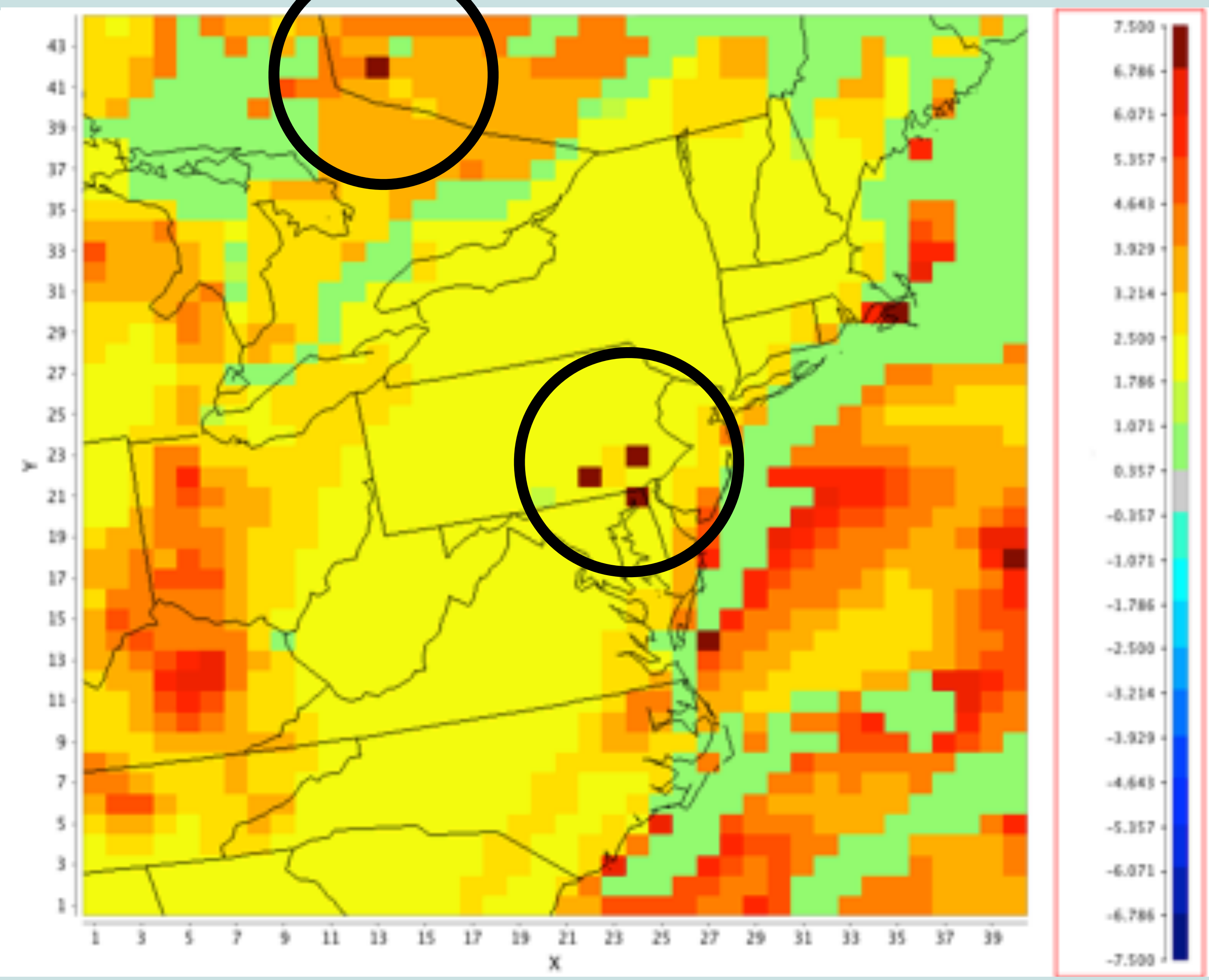
Finite difference

The adjoint of aerosol: aerosol dynamics and thermodynamics

$$\frac{\partial PM_{2.5}}{\partial ASO4J}$$



Adjoint



Finite difference

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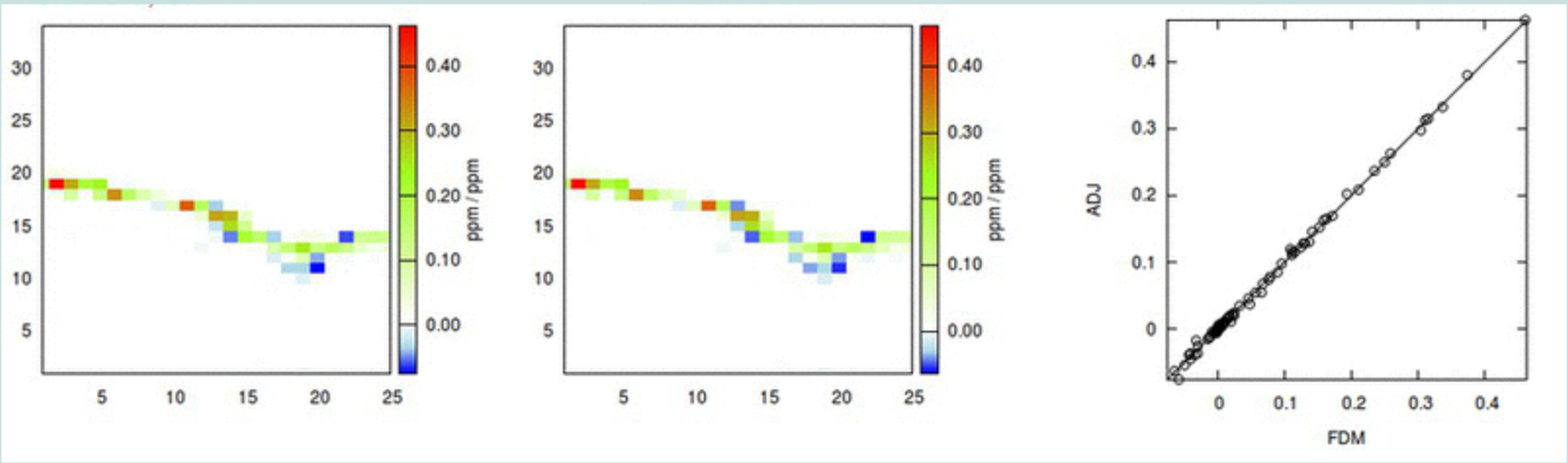
The adjoint of transport: horizontal advection

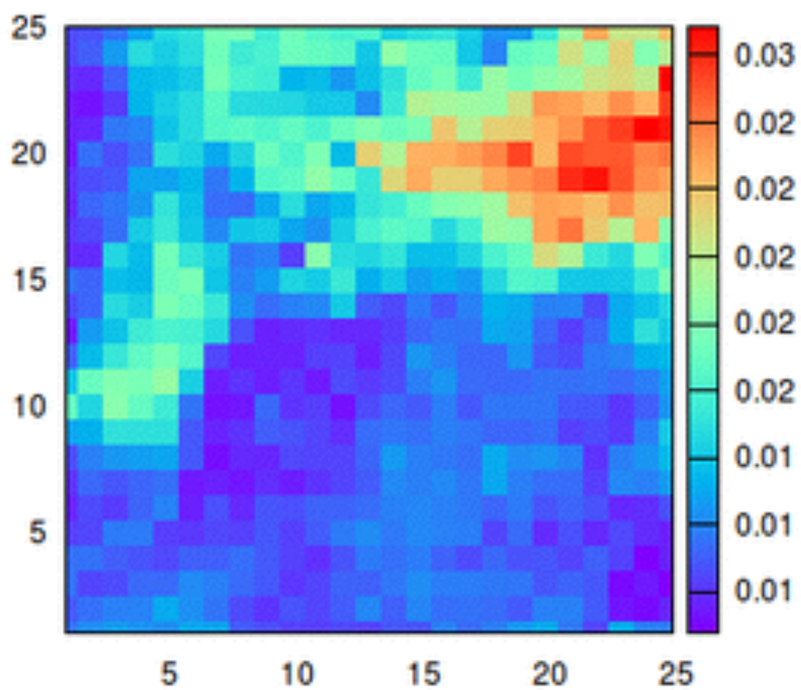
- Horizontal advection at the *X* direction / discrete adjoint

Adjoint Finite Difference $\frac{\partial O3}{\partial O3}$

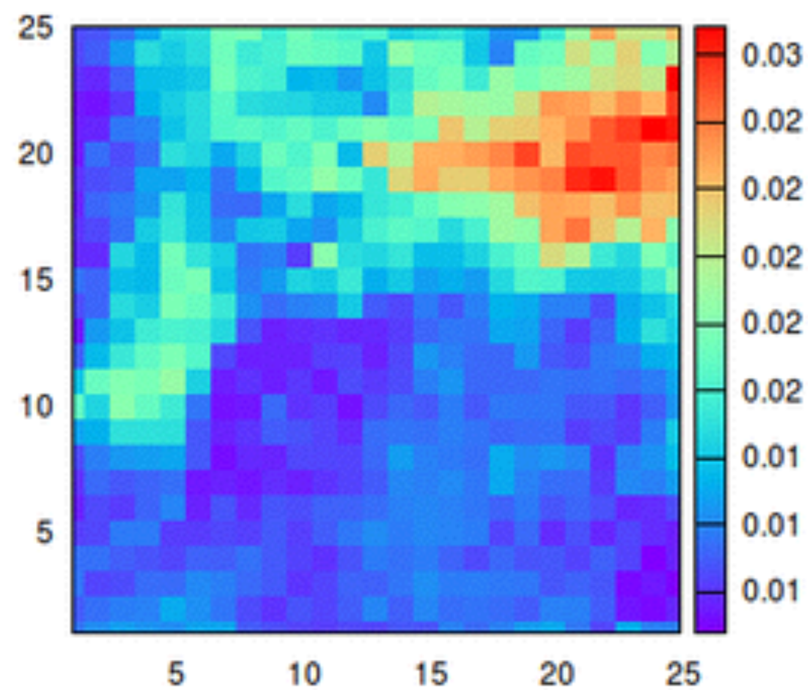


The adjoint of transport: vertical diffusion

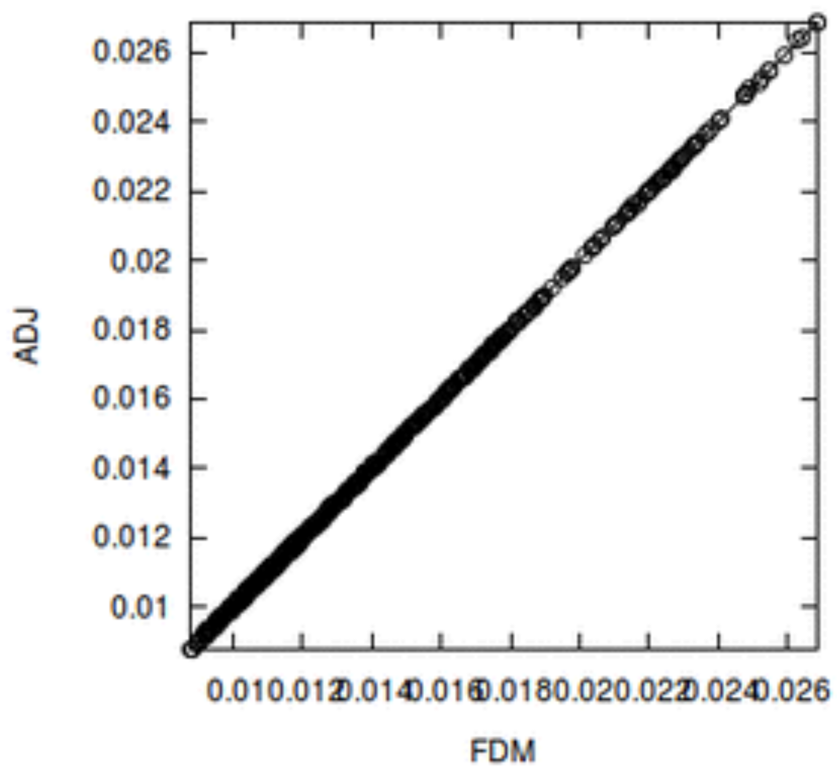
$$\frac{\partial O3}{\partial O3}$$



Adjoint



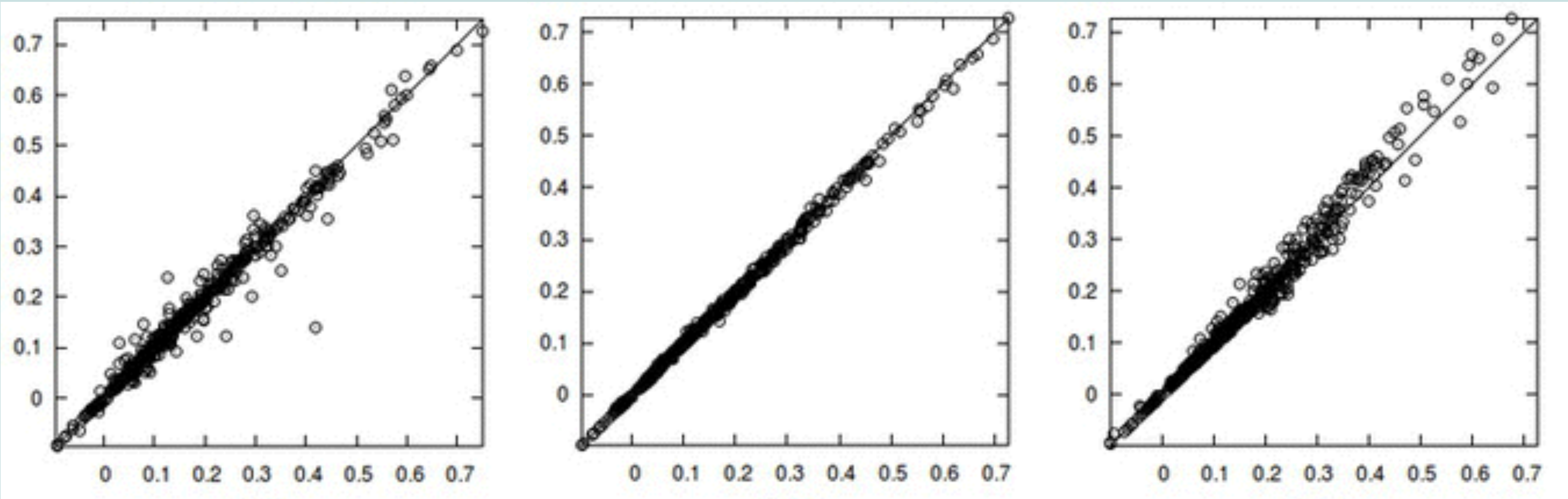
Finite Difference



The adjoint of vertical diffusion and chemistry

$$\frac{\partial O3}{\partial NO}$$

Adjoint



0.1 ppbV | 1 ppbV | 10 ppbV

Finite Difference

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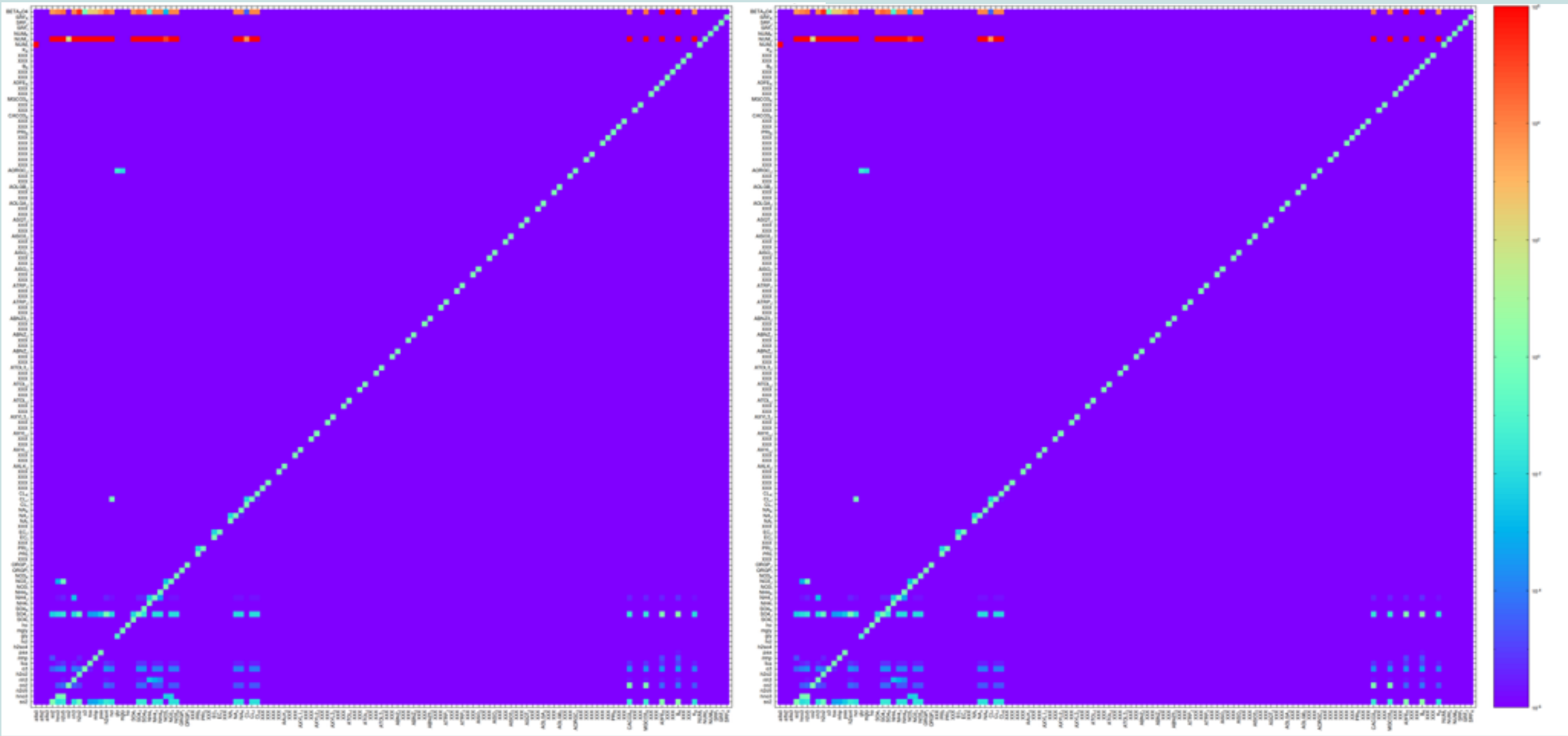
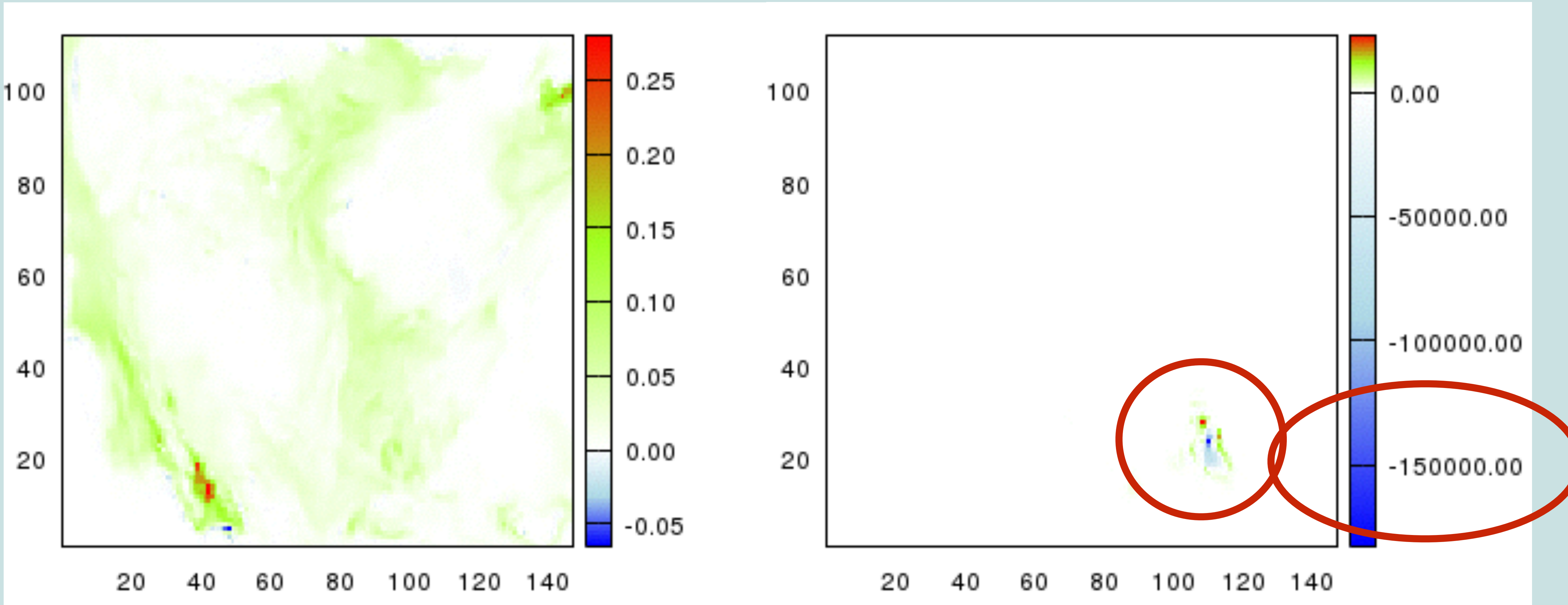
The adjoint of clouds

- Aqueous chemistry (KPP; Kathleen Fahey, EPA)

Adjoint DDM



Test run of the full adjoint model

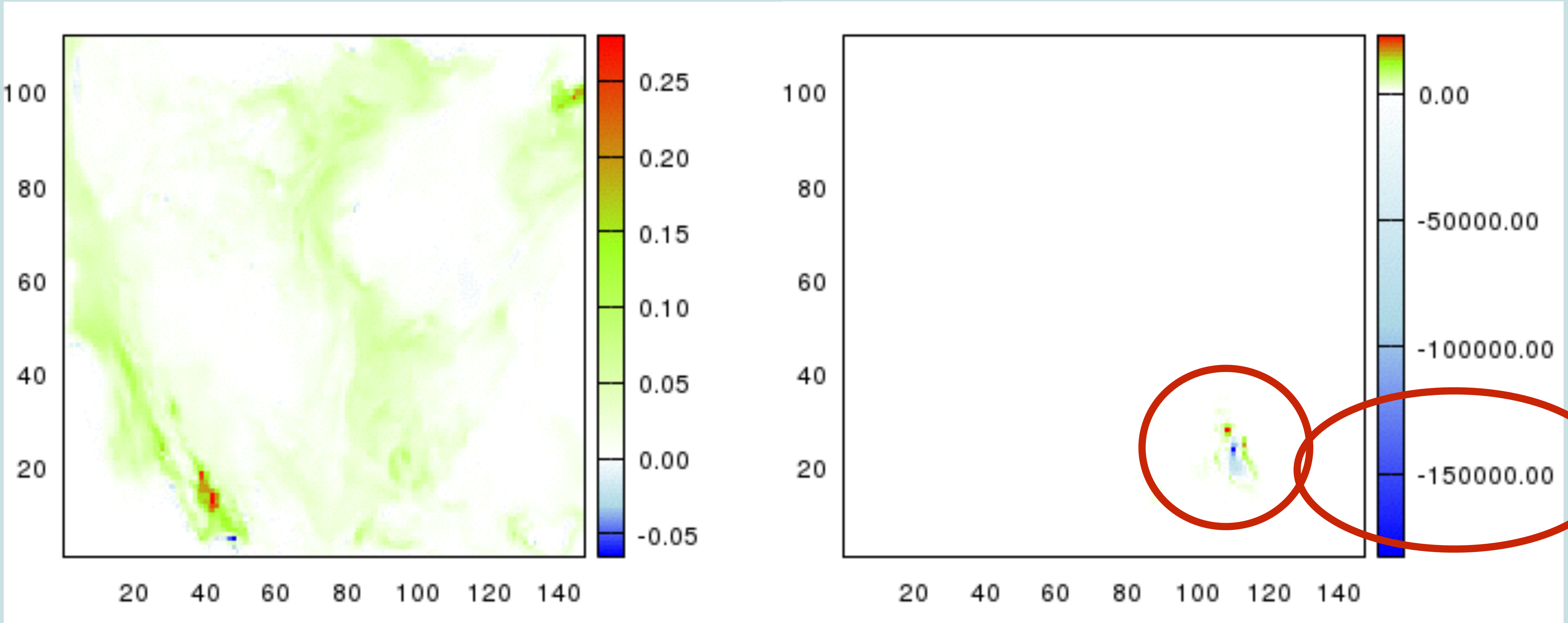


Day 1

Day 4

$$\frac{\partial PM_{2.5}}{\partial ASO4J}$$

Test run of the full adjoint model

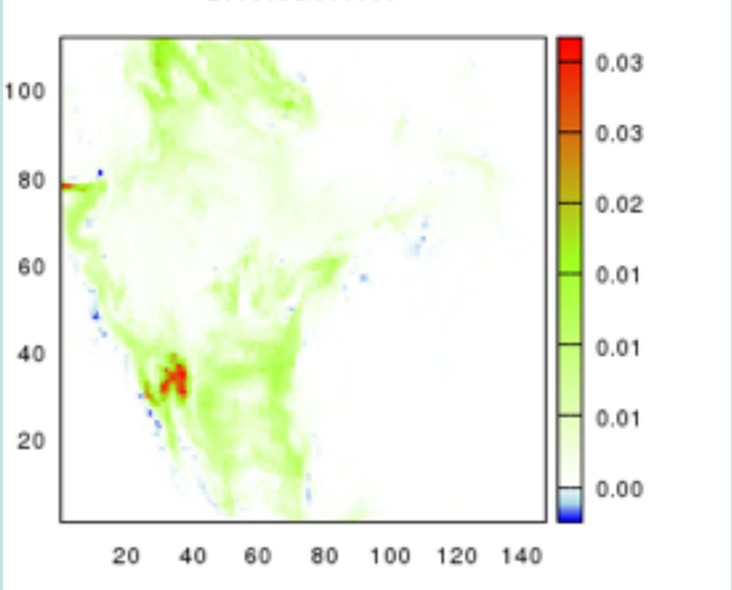


Day 1

Day 4

$$\frac{\partial PM_{2.5}}{\partial ASO4J}$$

without *AQCHEM*



Lessons learned

- Automatic differentiation entails a number of problems
  - Significant clean-up debugging is necessary
  - Single/double precision
  - Active variables passed by modules not visible to some top routines
  - Uninitialized variables in the adjoint code
- Problems that can be ignored in process-by-process tests may become more serious in interaction with other processes
- A number of issue can be avoided if forward model development is mindful of differentiation
  - Fractured response surface for a number of processes

Concluding remarks

- When testing with the full adjoint model, blow-ups in the adjoint sensitivities caused by various reasons have been observed. Despite numerous bug fixes, large numbers still exist.
- Process-by-process validations are positive in general. But there seems to be interactions between processes which cause the abnormal growth in sensitivities.

Acknowledgements

- Funding:
  - API, NSERC
- Model support:
  - USEPA