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Evaluation of CMAQ adjoint and Future Steps

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ABSTRACT

A cross-institutional team of researchers has worked for the past few years on the development of a full adjoint for CMAQ (including aerosol, clouds and aqueous chemistry, gas-phase chemistry, and transport). CMAQ-ADJ development is now complete. This poster presents final evaluations of the adjoint model, a retrospective view of challenges faced, limitations, and future steps in adjoint model development.

BACKGROUND

An adjoint air quality model provides location- and time-specific gradients of an air quality metric to model inputs and lends itself to various scientific and policy applications such as:

- backward sensitivity analysis,
- source attribution,
- optimal pollution control,
- data assimilation and inverse modeling.

An adjoint model is complimentary to other tools for forward sensitivity analyses, e.g. CMAQ-DDM (Napelenok et al., 2006), which provide spatially distributed gradients with respect to a single model input.

A gas-phase adjoint model for CMAQ was previously developed (Hakami et. al, 2007) and has been used in a variety of ozone-related applications.

The current work is to develop a multiphase adjoint which can be employed for both gas-and aerosol-related applications, on topics such as human health and climate.

MODEL DEVELOPMENT

There are two approaches to develop an adjoint. In the discrete approach, differentiation is applied directly on a numerical model. The gradient values produced by a discrete adjoint model are exact due to the nature of algorithmic differentiation (AD). The process could be automated with AD tools (autodiff.org).

The other continuous approach starts with the adjoint equations which are discretized and then numerically solved.

The science processes of the CMAQ model include gas-phase chemistry (CHEM), aerosols (AERO), cloud chemistry (AQCHEM) and dynamics (RESCLD/CONVCLD), horizontal and vertical diffusion (HDIFF/VDIFF), and horizontal and vertical advection (HADV/VADV).

Discrete adjoints are implemented for all the science processes, with an additional continuous adjoint for horizontal advection.

Distinctive AD tools have been employed in the development of discrete adjoints which include

- KPP (Kinetic Pre-Processor; Damian et al., 2002) for CHEM/AQCHEM
- Tapenade (Hascoët and Pascual, 2013) for AERO/RESCLD/CONVCLD
- TAMC (Giering and Kaminski, 1998) for HDIFF/VDIFF/HADV/VADV.

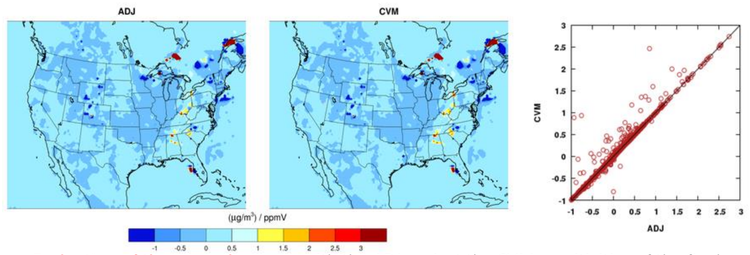
The continuous adjoint of advection is developed manually by using the same PPM scheme as implemented for CMAQ.

MODEL EVALUATION

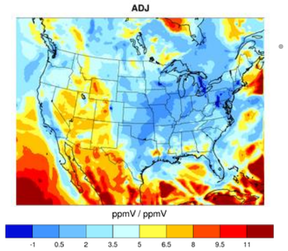
- Evaluations of the adjoints are performed on a process-by-process basis and finally as a full model.
- The Complex Variable Method (CVM) is employed when a mismatch between the Finite Difference Method (FDM) and the adjoint sensitivities appears.
- Although the CVM is only 2nd-order accurate, it is not subject to subtraction errors and could produce accurate derivatives using as small a step size as allowed

$$J'(p) = \Im(J(p + ih))/h + O(h^2)$$

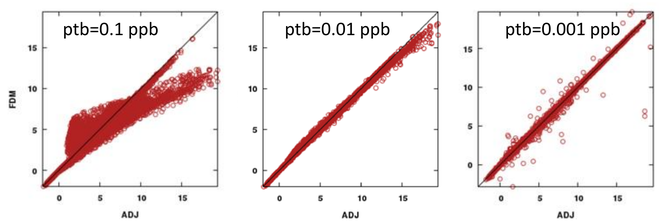
- Experimental setups: An episode in April 2008 for the North American domain with a 36km-by-36km resolution and 24 vertical layers.

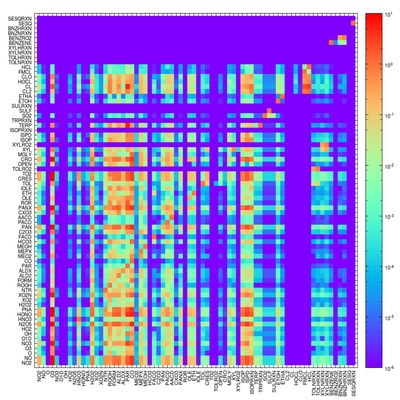


- **Evaluation of the aerosol process** with the ADJ against the CVM sensitivities of the final concentrations of an accumulation-mode aerosol species ASO4J (μg/m³) with respect to the initial concentrations of NH3 (ppmV) from a one-day test run.

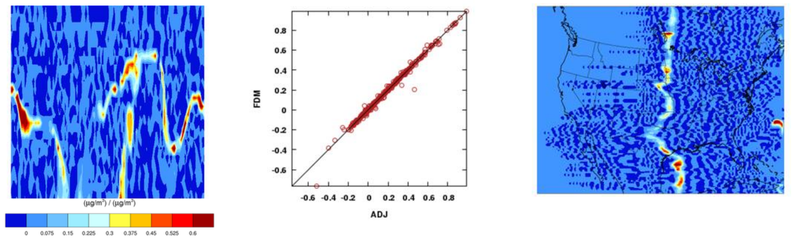


- **Evaluation of gas-phase chemistry** with the ADJ (Adjoint) against the FDM (Finite Difference Method) sensitivities of the final O_3 concentrations (ppmV) with respect to the initial NO_2 concentrations (ppmV) from a one-day test run. The perturbation sizes (ptb) are 0.1, 0.01 and 0.001 ppb for the FDM.

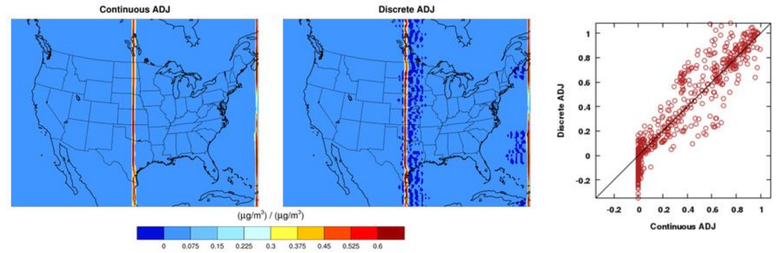




- **Jacobian of sensitivities** is used when necessary for a thorough comparison. On the left is an example from the evaluation of the gas-phase chemistry (CHEM) of the Jacobians of ADJ sensitivities at a grid cell. The X and Y axes represent all species involved in gas-phase chemistry.



- **Evaluation of horizontal advection** in the x-direction with sensitivities of final ASO4J to initial ASO4J from a one-day test run. The left figure shows the discrete ADJ (DADJ) sensitivities across the plane of the column where the cost function (CF) is defined; the middle figure compares DADJ with FDM; the right figure shows the nonphysical oscillatory DADJ sensitivities across the surface.
- Shown below are ADJ sensitivities from a one-hour test run. Continuous ADJ with a smooth solution is desirable for sensitivity analysis. (CF defined in the middle and right border.)



Gradient exploding could occur for adjoint simulations over a week. What happens is that the gradient values grow gradually and eventually lead to NaN's. The gradient clipping technique is often used to deal with the exploding problem in machine learning, in which arbitrary threshold values are used to curb the growth (Baydin et al., 2016). However, implemented for the adjoint at the science-process level the technique only caused the gradients to grow to the threshold values over time.

Presented below is a solution that gets rid of the spurious growth. Similar techniques have been implemented for clouds and aerosols.

Suppose we have a function of concentrations

$$f_i = w_i \cdot C$$
$$w_i = C_i / \sum_j C_j.$$

Here, $C = C(C_1, C_2, \ldots)$. The first-order derivative is then

$$f_i' = w_i \cdot C' + \frac{\sum_j C_j - C_i}{(\sum_j C_j)^2} \cdot C$$

The second term on the RHS could cause significant growth. Omitting the second term does the trick; essentially, the sensitivities are redistributed just as the concentrations.

CONCLUSIONS

- Process-by-process validation of the adjoint against the FDM or the CVM has been successful.
- The discrete adjoint of advection produces gradients that are accurate but with spurious noises; the continuous adjoint is preferable for sensitivity analysis.
- Special treatment is required to treat gradient exploding which could occur over long-term simulations.
- **The adjoint of CMAQ will be publicly released in near future.**

References

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