A Multiphase Adjoint Model for CMAQ

Shunliu Zhao, Amir Hakami (Carleton University); Matt D. Turner, Shannon L. Capps, and Daven K. Henze (University of Colorado); Peter B. Percell (University of Houston); Jaroslav Resler (ICS Prague); Jesse O. Bash, Sergey L. Napelenok (USEPA); Rob W. Pinder; Armistead G. Russell and Athanasios Nenes (Georgia Tech); Jaemeen Baek, Greg R. Carmichael, and Charlie O. Stanier (University of Iowa); Adrian Sandu (Virginia Tech); Tianfeng Chai (University of Maryland); Daewon Byun (NOAA)

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

Benefits-per-ton of NO$_x$ Control
At 2007 Emission Levels
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

<table>
<thead>
<tr>
<th>Process</th>
<th>Sub-processes</th>
<th>Validation Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td></td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Aerosol</td>
<td>Secondary organic aerosol, Heterogeneous chemistry, Coagulation, Nucleation, Condensation, Thermodynamics (Isorropia; Capps et al., 2012)</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Transport</td>
<td>Horizontal/vertical advection, Horizontal/vertical diffusion</td>
<td>Finite difference</td>
</tr>
<tr>
<td>Cloud</td>
<td>Convective cloud, Resolved cloud, Aqueous chemistry</td>
<td>Finite difference Complex variable Tangent linear model</td>
</tr>
</tbody>
</table>
## Process-by-process validation

<table>
<thead>
<tr>
<th>Process</th>
<th>Sub-processes</th>
<th>Validation Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td></td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Aerosol</td>
<td>Secondary organic aerosol, Heterogeneous chemistry, Coagulation, Nucleation,</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td></td>
<td>Condensation, Thermodynamics (Isorropia; Capps et al., 2012)</td>
<td></td>
</tr>
<tr>
<td>Transport</td>
<td>Horizontal/vertical advection, Horizontal/vertical diffusion</td>
<td>Finite difference</td>
</tr>
<tr>
<td>Cloud</td>
<td>Convective cloud, Resolved cloud, Aqueous chemistry</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Tangent linear model</td>
</tr>
</tbody>
</table>
Th adjoint of chemistry: Limitations of the FDM

Adjoint

Finite difference

\[ \frac{\partial O_3}{\partial HCL} \]
The adjoint of chemistry

Adjoint

Complex variable
The adjoint of chemistry: Full Jacobian

Adjoint

Complex variable
## Process-by-process validation

<table>
<thead>
<tr>
<th>Process</th>
<th>Sub-processes</th>
<th>Validation Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td></td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Aerosol</td>
<td>Secondary organic aerosol, Heterogeneous chemistry, Coagulation, Nucleation, Condensation, Thermodynamics (Isorropia; Capps et al., 2012)</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Transport</td>
<td>Horizontal/vertical advection, Horizontal/vertical diffusion</td>
<td>Finite difference</td>
</tr>
<tr>
<td>Cloud</td>
<td>Convective cloud, Resolved cloud, Aqueous chemistry</td>
<td>Finite difference Complex variable Tangent linear model</td>
</tr>
</tbody>
</table>
The adjoint of aerosol: secondary organic aerosol

\[
\frac{\partial PM_{2.5}}{\partial AALK}\quad\quad \frac{\partial PM_{2.5}}{\partial SV_{BNZ}}
\]

Complex variable

Adjoint
The adjoint of aerosol: heterogeneous chemistry
The adjoint of aerosol: coagulation
The adjoint of aerosol dynamics

\[ \frac{\partial PM_{2.5}}{\partial ANH4J} \]
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
The adjoint of aerosol: aerosol dynamics and thermodynamics
<table>
<thead>
<tr>
<th>Process</th>
<th>Sub-processes</th>
<th>Validation Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td></td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Aerosol</td>
<td>Secondary organic aerosol, Heterogeneous chemistry, Coagulation, Nucleation,</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td></td>
<td>Condensation, Thermodynamics (Isorropia; Capps et al., 2012)</td>
<td></td>
</tr>
<tr>
<td>Transport</td>
<td><strong>Horizontal/vertical advection, Horizontal/vertical diffusion</strong></td>
<td><strong>Finite difference</strong></td>
</tr>
<tr>
<td>Cloud</td>
<td>Convective cloud, Resolved cloud, Aqueous chemistry</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Tangent linear model</td>
</tr>
</tbody>
</table>
The adjoint of transport: horizontal advection

- Horizontal advection at the $X$ direction / discrete adjoint
The adjoint of transport: vertical diffusion

Adjoint  Finite Difference
The adjoint of vertical diffusion and chemistry

\[
\frac{\partial O_3}{\partial NO}
\]

Adjoint

0.1 ppbV

1 ppbV

10 ppbV

Finite Difference
## Process-by-process validation

<table>
<thead>
<tr>
<th>Process</th>
<th>Sub-processes</th>
<th>Validation Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td></td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Aerosol</td>
<td>Secondary organic aerosol, Heterogeneous chemistry, Coagulation, Nucleation, Condensation, Thermodynamics (Isorropia; Capps et al., 2012)</td>
<td>Finite difference Complex variable</td>
</tr>
<tr>
<td>Transport</td>
<td>Horizontal/vertical advection, Horizontal/vertical diffusion</td>
<td>Finite difference</td>
</tr>
<tr>
<td>Cloud</td>
<td><strong>Convective cloud, Resolved cloud, Aqueous chemistry</strong></td>
<td>Finite difference Complex variable Tangent linear model</td>
</tr>
</tbody>
</table>
The adjoint of clouds

- Aqueous chemistry (KPP; Kathleen Fahey, EPA)
Test run of the full adjoint model

\[ \frac{\partial PM_{2.5}}{\partial ASO4f} \]

Day 1

Day 4
Test run of the full adjoint model

\[ \frac{\partial PM_{2.5}}{\partial ASO_4J} \]

Day 1

Day 4
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