GEOS-Chem Adjoint Model and the Data Assimilation Working Group

IGC6
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Daven K. Henze, CU Boulder, Adjoint Model Scientist
Kevin W. Bowman, JPL, Data Assimilation WG Co-Chair
Dylan B. A. Jones, U Toronto, Data Assimilation WG Co-Chair

with contributions from the entire group*

* ~50 registered adjoint users at more than 20 institutions
An adjoint model...

...efficiently calculates gradients of a scalar model response with respect to all model parameters (emissions, rate constants, ...) at the native model resolution.
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Sensitivity analysis

Modes response = US cumulative O3 (W126).

Adjoint calculates how sources of CO emissions anywhere in the world impact this response.

Katerya Lapina, CU Boulder
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Sensitivity analysis

Inverse modeling / 4D-Var

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Adjoint calculates how sources of CO emissions anywhere in the world impact this response.

Katerya Lapina, CU Boulder

top-down CH3OH emissions using TES
Kelly Wells, UM
Adjoint model: current features

Standardized code: v34i, maintained / distributed via GIT
Code base: v8-02-01 with relevant fixes / updates up to v9-01-03

Meteorology: GEOS-3, GEOS-4, GEOS-5
Simulations: full chem; offline CO, O\textsubscript{x}, CO\textsubscript{2}, CH\textsubscript{4}, BC, Dust
Resolution: 4x5, 2x2.5, 0.5 x 0.667
Sensitivities: emissions, initial conditions, rate constants, stratospheric prod/loss rates

Processes: all main forward model process excluding:
- non-local pbl mixing scheme
- aerosol microphysics, online heterogeneous chemistry

Species: forward full chemistry model species excluding:
- SOA, SO4s, NITs, Br

see GC adjoint wiki page and Trello board for details
Adjoint model: current features

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Overview

BETA RELEASE

Previous version: GEOS-Chem_Adjoint_v33

What's new in this version

GEOS-Chem Adjoint v34 contains the following major updates and improvements.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Type</th>
<th>Submitted by</th>
<th>Committed by</th>
<th>Version</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Building Process Updated</td>
<td>Adjoint Update</td>
<td>Daven Henze (CU Boulder), Yanko Davila (CU Boulder)</td>
<td>Yanko Davila (CU Boulder)</td>
<td>v34</td>
<td>Approved 14 Nov 2012</td>
</tr>
<tr>
<td>Add support for GFED3 Emissions</td>
<td>Forward Model Update</td>
<td>Melissa Payer (Harvard)</td>
<td>Yanko Davila (CU Boulder)</td>
<td>v34</td>
<td>Approved 14 Nov 2012</td>
</tr>
<tr>
<td>Checkpoint files creation updated</td>
<td>Adjoint Update</td>
<td>Daven Henze (CU Boulder), Yanko Davila (CU Boulder)</td>
<td>Yanko Davila (CU Boulder)</td>
<td>v34</td>
<td>Approved 14 Nov 2012</td>
</tr>
</tbody>
</table>

New: benchmarking procedures

see GC adjoint wiki page and Trello board for details
Developments: rank by priority (high, med, low) and assign point people or groups

<table>
<thead>
<tr>
<th>Model development</th>
<th>Development group</th>
<th>Priority level</th>
<th>Readiness</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Off-diagonal error covariance matrix</td>
<td>JPL</td>
<td>high</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>Inverse Hessian</td>
<td>Tang (Purdue), JPL</td>
<td>high</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>Methane</td>
<td>Wecht (Harvard), Tang (Purdue)</td>
<td>high</td>
<td>high</td>
<td>low</td>
</tr>
<tr>
<td>CH4 obs operators: SCIA, AIRS, TES</td>
<td>Harvard / Purdue</td>
<td>med</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>generalized DOAS obs operator</td>
<td>Bousserez (Dal)</td>
<td>high</td>
<td>high</td>
<td>low</td>
</tr>
<tr>
<td>generalized TES obs operator</td>
<td>Lee (JPL)</td>
<td>med</td>
<td>med</td>
<td>med</td>
</tr>
<tr>
<td>full chemistry nested</td>
<td>Zhe Jiang (UT)</td>
<td>highest</td>
<td>low</td>
<td>med</td>
</tr>
<tr>
<td>CO/CO2</td>
<td>Jones (UT), Bowman (JPL)</td>
<td>high</td>
<td>low</td>
<td>med</td>
</tr>
<tr>
<td>BC offline adjoint</td>
<td>Yuhao Mao, Qinbin Li (UCLA)</td>
<td>high</td>
<td>low</td>
<td>low</td>
</tr>
<tr>
<td>heterogeneous chemistry (RDAER)</td>
<td>Henze (CU Boulder)</td>
<td>med</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>GISS tracer advection adjoint</td>
<td>Henze (CU Boulder)</td>
<td>low</td>
<td>low</td>
<td>low</td>
</tr>
<tr>
<td>GCAP convection</td>
<td>Henze (CU Boulder)</td>
<td>low</td>
<td>low</td>
<td>med</td>
</tr>
</tbody>
</table>

Focusing on the development of high priority items implemented in the last two years:

<table>
<thead>
<tr>
<th>Sensitivity</th>
<th>Development group</th>
<th>Priority level</th>
<th>Readiness</th>
<th>Difficulty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dust</td>
<td>Xu (UNL), Park (SNU), Li (UCLA)</td>
<td>high</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>Satellite obs operator sensitivity</td>
<td>Bowman, Lee (JPL)</td>
<td>med</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>Generic surface obs operator</td>
<td>Jones (UT)</td>
<td>med</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>Output rxn rate sensitivities</td>
<td>Paulot (Caltech/Harvard)</td>
<td>med</td>
<td>med</td>
<td>low</td>
</tr>
<tr>
<td>Joint initial condition &amp; emissions opt</td>
<td>?</td>
<td>high</td>
<td>low</td>
<td>low</td>
</tr>
<tr>
<td>ISORROPIA adjoint</td>
<td>Shannon Capps (Georgia Tech)</td>
<td>med</td>
<td>med</td>
<td>med</td>
</tr>
<tr>
<td>Scaling factor &quot;hooks&quot; in forward model work w/Bob and emissions group</td>
<td></td>
<td>high</td>
<td>low</td>
<td>low</td>
</tr>
</tbody>
</table>

Many high priority items implemented in the last two years.
Recent and current applications:
Inverse modeling

Aerosol and aerosol precursor emissions:
- Carbonaceous PM using IMPROVE (Mao, UCLA; Egan-Pimblett, Dalhousie)
- Asia BC with OMI AAOD (Zhang, CU Boulder)
- Aerosols with MODIS (Xu, Wang, UNL)
- Aerosols with POLDER (Meland, CU Boulder/CUD)
- NH$_3$ using TES (Zhu, CU Boulder; Capps, US EPA)
- NH$_3$ using wet deposition (Paulot, Harvard)

Greenhouse gases:
- CH$_4$ (Wecht, Turner, Harvard; Tan, Purdue)
- CO$_2$ from GOSAT (Liu, Lee, JPL; Deng, UT; Zhu, Purdue; Shim, KEI)

Reactive gas-phase species
- CO from MOPITT (Jiang, UT) and BORTAS (Parrington, Edinburgh)
- CH$_3$OH from TES (Wells, UMN)
Recent and current applications: Sensitivity analysis

Climate / chemistry:
- Radiative forcing (Henze, Lacey, CU Boulder; Bowman, JPL)
- Arctic $O_3$ and $NO_y$ (Walker, UT) and Antarctic nitrate (Lee, CU Boulder)
- CCN (Karydis, GIT)
- Adjoint of ISORROPIA aerosol thermodynamics (Capps, GIT/US EPA)

Satellite design and analysis
- GEOCAPE (Lee, JPL; Henze, CU Boulder; Wecht, Harvard)
- XCO2 sensitivity analysis (Liu, JPL)
- Column constraints (Turner, Harvard; Padmanabhan, Dalhousie)

Emissions mitigation strategies
- PM2.5 in Asia (Kharol, Dalhousie)
- O3 W126 vegetative exposure (Lapina, CU Boulder)
- PM2.5 and O3 health impacts (Lee, Dalhousie; Henze, CUB; Koo, MIT)
- N deposition (Henze, CU Boulder; Paulot, Harvard)
Research Highlights:
Source attribution of PM$_{2.5}$ related mortality

What is the health-related benefit for reducing a ton of emissions, and how does this vary by location?
Recent and current applications

Theory
- Weak constraint 4D-Var (Keller, UT)
- Inverse Hessian (Bousserez, CU Boulder)

Other Data Assimilation activities
- 3D-Var assimilation of ozone from TES and MLS (Lee, Neu JPL)
- 3D-Var assimilation of CO2 from TES and GOSAT (Lee)
- EnKF CO2 flux estimates (Denning, CSU; Palmer, Univ Edinburgh)

Software Engineering
- pyEnsemble Manager (Perkins, UW)
- Multi-mission observation operator M2O2 (Lee, JPL)
- full-time adjoint model code support (Yanko Davila, CU Boulder)
New: code tracking with GitLab

http://adjoint.colorado.edu:8080

Daven Henze 21 days ago
Shouldn't it also be possible to use LKGNHAYR for NHx deposition?

Fabien Paulot 16 days ago
but NH3 and NH4 are not in CSPEC so I think it's fine
Future directions

- Additional adjoint model capabilities
  - Additional offline simulations ($N_2O$, ...)
  - more sensitivity output: convection, ...
  - more sophisticated optimization and DA analysis tools
  - further consolidation of observation operators (e.g., M2O2)
  - additional meteorology: MERRA, GCAP...
  - chemistry update when SMVGEAR is retired

- Keep an eye on grid-independent forward model development

- More connection/shared code with other assimilation methods (3D-Var and other sequential methods)

- Switch from quarterly to ~monthly WG telecons

- Adjoint Model Co-Scientist: assist with development, benchmarking, code maintenance and support
the end