GEOS-Chem

Fall 2021 Newsletter

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1. Featured News

1.1 New Release Protocol

We have adopted a new release protocol beginning with GEOS-Chem 13.2.0 that will provide a more consistent GEOS-Chem version release timeline. Major and minor GEOS-Chem versions (X.Y.0) will be released with a fixed frequency of every 3 months. Patch versions (X.Y.Z) with bug fixes and updates that do not impact benchmarking will continue to be issued as bugs are identified and fixed.

The new protocol incorporates a more flexible development pipeline. Features will be rolled in continuously as they are ready rather than bundled in advance per version as they have been in the past. To facilitate this change we have restructured the Model Development Priorities wiki page to group GEOS-Chem features in the pipeline by stage of development rather than future version number.

While the GEOS-Chem release frequency will be every 3 months users should not feel pressured to update to every new release. We encourage groups to choose an update frequency that works best for them. We will also strive to minimize structural updates and changes to required hardware and software as much as possible in minor GEOS-Chem versions (X.Y). When these changes do go into a version they will be listed in the version release table as features to help guide users on whether to update to the new version.

1.2 Tropchem simulation issues in 13.0.0 through 13.2.0

Several users reported issues in the tropchem simulation option in GEOS-Chem versions 13.0.0 through 13.2.0. In GEOS-Chem 13.0.0 the tropchem chemistry mechanism in KPP was retired in favor of a single “fullchem” mechanism. The recommended standard full-chemistry GEOS-Chem simulation includes online chemistry throughout the troposphere and stratosphere and applies linearized prod/loss rates from GMI in the mesosphere. In versions 13.0.0 through 13.2.0 a tropchem option was still available in which the online chemical mechanism would only be applied throughout the troposphere and linearized prod/loss rates archived from a standard (i.e. UCX-based) full-chemistry simulation would be applied in the stratosphere. The tropchem option was meant to save computational resources for users who weren’t focused on the stratosphere and wanted to speed up their simulations.

As reported in Github issue #732, the tropchem simulation in versions 13.0.0 through 13.2.0 was found to be problematic and resulted in extremely low OH concentrations. This only impacted users of GEOS-Chem Classic since tropchem simulations were not provided as an option in GCHP. The issue was tracked to code in FAST-JX for the old tropchem chemistry mechanism that should have been removed with the retirement of that mechanism in 13.0.0. A fix was implemented and tagged with `13.0.0+TropchemFix`. ***For users of the tropchem simulation in GEOS-Chem Classic 13.0.0 through 13.2.0, it is important that you follow these steps to apply the fix to your code and rerun any tropchem simulations.***

The investigation into the tropchem simulation issue was discussed at the last GEOS-Chem Steering Committee meeting and a decision was made to retire the tropchem option completely to avoid similar issues in the future. Therefore, in GEOS-Chem 13.2.1 we have retired the tropchem simulation option from GEOS-Chem Classic. Timing tests comparing the standard (troposphere+stratosphere chemistry) and the tropchem (tropopshere-only chemistry) simulation at both 72 and 47 levels show that the standard simulation using 47 levels has similar performance as the tropchem simulation using 47 levels. A complete set of internal 1-month benchmark and timing results are available in this Github issue. Additional tests are in progress to quantify the impact on model performance in nested-grid simulations.

1.3 New Website on the Horizon

Harvard SEAS web designer Vittorio Bucchieri has volunteered to port the GEOS-Chem website to OpenScholar and implement design changes to give the site a new look. The new site is now accessible at geos-chem.org and is a work in progress. Please send feedback and your visions for improving it to the GEOS-Chem Support Team (geos-chem-support@g.harvard.edu).

2. GEOS-Chem Version Releases

Since our last newsletter, the following GEOS-Chem versions have been released:

2.1 GEOS-Chem 13.1.0

Release Date: 17 Jun 2021

GEOS-Chem 13.1.0 contains the following updates:

- Distribute CEDS emissions vertically in the boundary layer
- Add diurnal scale factors for power plant emissions in China
- Fix H2O boundary conditions at tropopause
- Fix parallelization issues in ISORROPIA and get_ndep_mod.F90
- Add fixes and simplifications to calc_met_mod.F90
- Add initial modifications for the HEMCO internal grid
- Add updates to speed up the chemical solver (remove useless computations, etc.)
- Update the default definition of PM2.5
- Add compatibility for reading GCAP 2.0 met fields (stored at U. Rochester)
- Updated CH4 emissions (WetCharts thru 2019, Scarpelli et al Mexico emissions)
- Updated the planeflight diagnostic to archive J-values
- Retired binary diagnostics for RRTMG simulations
- Bug fix: nested-grid boundary conditions are now read continuously
- Added the initial modifications for the GCHP adjoint - CO2 simulation
- Updated GMAO submodules used by GCHP
- Now use a YAML file (logging.yml) for certain GCHP debug output
- Add monthly diagnostic capability to GCHP History diagnostics

- GCHP History diagnostics output now uses same filenames as GEOS-Chem Classic
- GCHP no longer supports the Intel compilers version 18

Please see the following pages for details on these updates, including benchmarks:

- 13.1.0 wiki page
- 13.1.0 Github milestone for geoschem/geos-chem
- 13.1.0 Github milestone for geoschem/GCHP
- 3.0.0 Github milestone for geoschem/HEMCO

2.2 GEOS-Chem 13.1.1

Release Date: 22 Jun 2021

GEOS-Chem 13.1.1 contains fixes for minor issues that were discovered during the 13.1.0 benchmarking process, as well as minor updates that do not impact benchmarking:

- Bug fix for the PM2.5 diagnostic: Force SIA_GROWTH parameter to 1.1
- Updates to facilitate running GEOS-Chem in the NASA/GEOS ESM
- GCHP: Added support for GNU Compiler Collection version 10
- GCHP: Fixed a makefile issue that caused errors when linking to the ESMF library

Please see the following pages for details on these updates:

- 13.1.1 wiki page
- 13.1.1 Github milestone for geoschem/geos-chem
- 13.1.1 Github milestone for geoschem/GCHP

2.3 GEOS-Chem 13.1.2

Release date: 06 Jul 2021

GEOS-Chem 13.1.2 contains two additional structural updates:

- Update the dry-run script download_data.py to fetch GCAP2 data from the U. Rochester server
- Added zero-diff structural updates to facilitate running GEOS-Chem in CESM2

Please see the following pages for details on these issues:

- 13.1.2 wiki page
- 13.1.2 Github milestone for geoschem/geos-chem

2.4 GEOS-Chem 13.2.0

Release date: 07 Sep 2021

GEOS-Chem 13.2.0 contains the following updates:

- CEDS v2 emissions through 2019 as the default emissions inventory
- Yuan/BNU MODIS LAI product (2000-2019) as the default LAI
- Luo et al. 2020 wet scavenging scheme (as an option)
- Blowing snow emissions of sea salt and sea salt bromide
- Trace Metals simulation
- Bug fix: Add C-to-species conversion factors for AEIC emissions
- Fix for molecular weight of ethanol (EOH) in species_database.yml
- Bug fix: corrected typo in the CloudHet function in gckpp_HetRates.F90
- Bug fix: ObsPack diagnostic pressure units are now Pa instead of hPa
- Added lon & lat bounds to netCDF files created by GEOS-Chem Classic History diagnostics
- GCHP bug fix: set “lev:positive = up” for all diagnostic files (except Emissions)
- MAPL update: Can now use some CMake versions older than 3.14
- Updates to GCHP sample run scripts

Please see the following pages for details on these updates, including benchmarks:

- 13.2.0 wiki page
- 13.2.0 Github milestone for geoschem/geos-chem
- 13.2.0 Github milestone for geoschem/GCHP
- 3.1.0 Github milestone for geoschem/HEMCO

3.2 GEOS-Chem 13.2.1

Release date: 10 Sep 2021

GEOS-Chem 13.2.1 contains fixes for issues that were discovered during the 13.2.0 benchmarking process:

- Retire tropchem simulation as an option
- Bug fix for JValO3O1D and JvalO3O3P diagnostics
- Bug fixes for the planeflight diagnostic
- Several bug fixes for nested-grid simulations
- Several bug fixes for Hg simulations
- Update the dry-run python script download_data.py to read global settings from a YAML file (this also enables download from the WashU server)
- Bug fix: Halt simulation if Restart.frequency does not match Restart.duration in the HISTORY.rc configuration file (for GEOS-Chem Classic only)

Please see the following pages for details on these updates:

- 13.2.1 wiki page
- 13.2.1 Github milestone for geoschem/geos-chem
- 13.2.1 Github milestone for geoschem/GCHP
- 3.1.1 Github milestone for geoschem/HEMCO

3. Versions in Development

As of this writing, the following GEOS-Chem versions are in development:

3.1 GEOS-Chem 13.3.0

The following updates are slated for GEOS-Chem 13.3.0:

- Several chemistry updates, including:
    - Clean up heterogeneous chemistry rate-law functions
    - Move chemistry from sulfate_mod.F90 to KPP
    - Add HMS chemistry (Moch et al 2020, JGR)
    - Add C2H2 + C2H4 chemistry (Kwon et al, 2021, Elementa)
    - Add CH3O2 + OH reaction (Bates et al, 2021, JGR)
    - Update IONO2 hydrolysis (Wang et al 2020, ACPD)
- Monthly mean NEI2016 emissions
- Updated offline dust emissions from Meng et al. (2021)
- 2020 volcano emissions
- Fix in MEGAN HEMCO extension to remove double counting of acetone from monoterpenes

Please see the following pages for details on these updates:

- 13.3.0 wiki page
- 13.3.0 Github milestone for geoschem/geos-chem
- 13.3.0 Github milestone for geoschem/GCHP
- 3.2.0 Github milestone for geoschem/HEMCO

4. Ongoing Development

4.1 Recent KPP updates

The **KPP-for-GEOS-Chem** package converts a GEOS-Chem chemical mechanism specification in plain text to highly optimized Fortran-90 source code. KPP-for-GEOS-Chem is a clean implementation of the **Kinetic PreProcessor** originally developed by Adrian Sandu et al) that has been customized for GEOS-Chem v11 and later versions. KPP-for-GEOS-Chem is our name for the KPP code stored on the GC_updates branch at https://github.com/geoschem/KPP, and the latest version is 2.3.3_gc.

GCST members **Bob Yantosca** and **Liam Bindle** have updated the KPP-for-GEOS-Chem source code so that it can be compiled with CMake. This will also facilitate inclusion of the KPP-for-GEOS-Chem package into other earth system models such as CESM and WRF.

We are working towards including the modifications that we have made in KPP-for-GEOS-Chem into the main KPP development stream, which has not been updated in several years. Stay tuned for further developments!

4.2 Migrating Chemistry Mechanisms to KPP

This year, we have undertaken a major effort to streamline GEOS-Chem's chemical mechanisms. We have concentrated on bringing chemical reaction rate computations, many of which are hardcoded into places such as sulfate_mod.F90, directly into the GEOS-Chem chemical mechanisms built with KPP-for-GEOS-Chem.

Here is a quick recap of the work done so far:

- **Mike Long** has moved the following reactions from sulfate_mod.F90 directly into the KPP mechanism:
    - SO2 aqueous reactions that convert S(IV) to S(VI)
    - Reactions for SO2, HCL, and NO3 plus sea salt aerosol alkalinity, in both fine (SALAAL) and coarse (SALCAL) modes
- **Bob Yantosca** has cleaned up and optimized all of the heterogeneous chemistry rate-law functions that were in gckpp_HetRates.F90. These are now included in a new file called fullchem_HetChemFuncs.F90.

We plan on adding these updates to GEOS-Chem 13.3.0.

4.3 Chemistry Updates in the Pipeline

The following chemistry updates are also in progress or will be worked on soon:

- Updated aromatic chemistry (Bates et al, 2021, ACPD)
- Migrating Hg chemistry to KPP (Shah et al., submitted, ES&T)
- Implementing a unified CO2-CO-CH4 "specialty" chemistry mechanism following Bukosa et al. (2019, ACP)

4.4 Replacing FAST-JX with Cloud-J

Work is in progress to replace FAST-JX with Cloud-J in GEOS-Chem. Cloud-J is a multi-scattering eight-stream radiative transfer model for solar radiation based on FAST-J.

This work evolved from our earlier goal of abstracting and refactoring FAST-JX for integration into ESMs. NCAR was interested in having a stand-alone FAST-JX module extracted from GEOS-Chem for use in MUSICA, and GMAO was interested in using GEOS-Chem's FAST-JX implementation in GMI.

Discussion with FAST-JX developer Michael Prather led to a decision to abandon refactoring FAST-JX and instead replace it with Cloud-J which is already functional as a standalone photolysis model.

This work will also include streamlining pre-processing workflow for converting cross-section and quantum yield data into averages over 18 wavelength bins, and for assumed T and p vertical profiles.

5. New Data Servers

Two new GEOS-Chem data servers have recently been activated:

1. **Rochester** (http://atmos.earth.rochester.edu): This data server is maintained by Lee Murray's research group at U. Rochester and contains the GCAP 2.0 met field data and related files. Download from this data server if you wish to run historical or future simulations driven by GCAP 2.0 meteorology.

2. **WashU** (http://geoschemdata.wustl.edu): This data server is maintained by Randall Martin's research group at Washington University in St. Louis and contains a complete archive of all GEOS-Chem meteorology and emissions data. We recommend that you download data from WashU for most GEOS-Chem and GCHP applications. A Globus endpoint named "GEOS-Chem data (WashU)" is also attached to this server.

Starting with 13.2.1, you will be able to download data from a GEOS-Chem Classic dry-run simulation from either of these servers using the data download script included in GEOS-Chem run directories. See our new dry-run Youtube video tutorial for more information.

6. Online Live Tutorials

The GEOS-Chem Support Team plans on doing live introductory tutorials (via Zoom) about getting up and running with GEOS-Chem Classic this fall. Stay tuned for more information! Additional introduction tutorials will be provided if there is demand. The live tutorials will be provided at least twice at different times of day to accommodate users around the world. They will also be recorded and posted on our Youtube channel for later viewing.

7. Steering Committee News

The GEOS-Chem Steering Committee met on 24 August 2021. We invite you to read the meeting minutes as well as the following Working Group updates:

- GEOS-Chem Steering Committee meeting minutes
- Hg and POPs Working Group updates
- Chemistry-Ecosystems-Climate Working Group updates

8. Introducing Lucas Estrada

Please join us in welcoming **Lucas Estrada** to the GEOS-Chem Support Team. Lucas comes to us from Nevo Technologies where he was a Software Engineer. He is a Williams College graduate with a Bachelor of Arts in Geoscience and Computer Science. He will be working on general GEOS-Chem development as well as scientific project support.

Thanks for your continued support of GEOS-Chem!
Happy modeling!

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