Winter 2020 Newsletter

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Featured News

GEOS-Chem 12.7.0 is now released!

GEOS-Chem 12.7.0 is now released and ready for use! This version contains several science updates and bug fixes. For installation instructions, please see the GEOS-Chem 12.7.0 section of the wiki.

If you are using GEOS-Chem on the Amazon Web Services cloud, we have prepared a new AMI containing a pre-compiled GEOS-Chem Classic 12.7.0 executable, plus the required software libraries. Please see our *Quick Start Guide* at cloud.geos-chem.org for detailed instructions.

GEOS-Chem 12.7.0 now contains a "dry-run" capability! This exciting new feature can generate a list of files that are required for any GEOS-Chem Classic simulation. The files can then easily be downloaded to your local computer cluster or AWS cloud instance by executing a simple Python script that ships with each GEOS-Chem run directory. For more information about the new "dry-run" capability, please see the following resources:

1. *Downloading data with the GEOS-Chem dry-run option* (on the GEOS-Chem wiki)

2. *Video Tutorial: Downloading data with a "dry-run" simulation* (@ Youtube)

We would also like to invite you to do the following:

1. Sign up for notifications from (aka "watch") our GEOS-Chem Github repository (**`https://github.com/geoschem/geos-chem`**). This will ensure that you'll

receive notifications for all GEOS-Chem version releases. GCST member Lizzie Lundgren has prepared a video tutorial that will walk you through the process.

2. Subscribe to our GEOS-Chem Youtube Channel and click on the bell to be notified of new videos. Help us reach 100 subscribers so that we can receive URL youtube.com/geoschem!

Updated GEOS-Chem narrative and new developments

The GEOS-Chem narrative description and GEOS-Chem new developments web pages are updated to highlight the contributions of individual developers to GEOS-Chem 12.7.0.

For more information, please follow these links:

1. **http://www.geos-chem.org/geos_new_developments.html**
2. **http://www.geos-chem.org/geos_chem_narrative.html**

Major update to GEOS-FP meteorology

NASA's Global Modeling and Assimilation Office (GMAO) has announced a major update to the GEOS-FP ("Forward-processing") data stream. The switchover to GEOS-FP version 5.25.1 occurred on January 30, 2020. This new version contains the following updates to the GCM:

1. New convection scheme:
    a. The RAS convection scheme used to date has now been replaced with Grell & Freitas deep convection plus Park & Bretherton shallow convection.

2. New radiation scheme:
    a. The Chou-Suarez shortwave model has been replaced by RRTMG.

For more details, please read the full announcement about the update to GEOS-FP 5.25.1.

Because the GEOS-FP meteorological product is an operational dataset, system changes and updates such as these are made at regular intervals. This ensures that the GEOS-FP data product reflects the state of the science. If you use GEOS-FP met fields to drive GEOS-Chem simulations for model dates after January 30, 2020, note that the convection and radiation variables might show substantial differences with respect to prior dates.

We plan on performing benchmark simulations in order to assess the impacts of this GEOS-FP system update. Stay tuned for more information.

If you would prefer using a meteorology product that does not contain any system changes, then consider using the GMAO MERRA-2 reanalysis product. MERRA-2 has a native resolution of 0.5 degree x 0.625 degree native resolution, and is generated with a “frozen” assimilation system based on the GEOS GCM version 5.12.4. There are more than 30 years of assimilated MERRA-2 data available (~1980-present) for you to use with GEOS-Chem.

GEOS-Chem Version Updates

Recently released GEOS-Chem versions

The GEOS-Chem 12 versions listed below were released since our last newsletter (Nov 2019):

12.6.2

Release date: 15 Nov 2019; **DOI:** 10.5281/zenodo.3543702

This version includes the following features and bug fixes:

- Now make sure the HEMCO standalone gets the proper met field name and grid resolution (Jun Meng and Bob Yantosca, GCST)
- Prevent overwriting restart variables H2O2AfterChem and SO2AfterChem if present (Lizzie Lundgren, GCST)
- Fix incorrect vertical flipping of MAPL 3D imports impacting mesospheric chemistry (Lizzie Lundgren, GCST; Seb Eastham, MIT)
- Fix incorrect mapping between internal state H2O2AfterChem and the equivalent State_Chm field (Lizzie Lundgren, GCST)
- Fix two timestep delay in update time for LAI upon day change (Lizzie Lundgren, GCST)

For more information about the updates in GEOS-Chem 12.6.2, please click here.

12.6.3

Release date: 25 Nov 2019; **DOI:** 10.5281/zenodo.3552959

This version contains a bug fix for GCHP:

- Fix bug preventing successful transport tracer simulation runs (Lizzie Lundgren, GCST)

For more information about the updates in GEOS-Chem 12.6.3, please click here.

12.7.0

Release date: 03 Feb 2020; **DOI:** 10.5281/zenodo.3634864

****** THIS IS THE CURRENT STABLE VERSION OF GEOS-Chem ******

This version contains the following features and fixes:

- Small alkyl nitrate chemistry (Jenny Fisher, Wollongong)
- Methanol added to standard chemical mechanism (Xin Chen and Dylan Millet, UMN; Katie Travis, NASA)
- Now use Yuan-process MODIS LAI fields for 2005-2016 by default (GCST)
- Latitudinally and monthly resolved fixed surface concentrations for long-lived organohalogen species (1750-2014) and prior to 1979 (Tomas Sherwen, U. York; Lee Murray, U. Rochester)
- Bug fix: Prevent differences in chemistry caused by toggling the ND65 bpch diagnostics off or on (Bob Yantosca, GCST)
- Fix incorrect uptake coefficient for N2O5 in heterogeneous chemistry (Hyeonmin Kim, Seoul National U.; Chris Holmes, FSU)
- Fix offline dust scale factors (Jun Meng, GCST)
- Add GEOS-Chem "dry-run" capability (Haipeng Lin and Jiawei Zhuang, Harvard; Bob Yantosca, GCST)
- Update to HEMCO 2.2.0 (Melissa Sulprizio, GCST)
- Implement Luo et al (GMD-12-3439-2019) wetdep as an option (Gan Luo and Fangqun Yu, SUNY Albany; Bob Yantosca, GCST)
- Add CH4 soil absorption from MeMo model (Melissa Sulprizio, GCST)
- Removal of most binary punch diagnostics (GCST)
- Add netCDF diagnostics for UV fluxes from FAST-JX (Jonathan Moch, Harvard; Bob Yantosca, GCST)
- Bug fix for HEMCO standalone using high-resolution input grids (Chris Holmes, FSU)
- Fix Incorrect units returned from GET_OH in sulfate_mod.F (Rong Tian, NUIST)
- Several fixes for GCHP (Lizzie Lundgren, GCST)

For more information about the updates in GEOS-Chem 12.7.0, please click here.

Versions in development

GEOS-Chem 12.7.1 is currently in development. This version contains fixes for minor issues that were reported during the 12.7.0 benchmarking process.

GEOS-Chem 12.8.0 is slated to include updated isoprene chemistry (Bates and Jacob, 2019), updated wet deposition parameterization (Safieddine and Heald, 2017), and ozone deposition to the ocean (Pound et al., 2019).

GEOS-Chem 12.9.0 will contain an updated halogen chemistry mechanism (Wang et al., 2019).

This version will likely be followed by the next major release, GEOS-Chem 13.0.0, which will feature structural updates to GEOS-Chem Classic and GCHP.

GEOS-Chem development news

Resolving differences when restarting GEOS-Chem runs

GCST members **Will Downs** and **Lizzie Lundgren** have been investigating differences that occur between GEOS-Chem simulations that run in a single phase as opposed to running as multiple phases (i.e. when a 1-year simulation is broken up into 12 individual 1-month simulations). They have identified and corrected several issues that were causing these differences. These updates have been added into GEOS-Chem 12.7.0.

A further issue that still needs to be addressed is the precision of the GEOS-Chem and HEMCO restart files. This issue impacts GEOS-Chem Classic only. The restart files are currently archived data with 32-bit (aka REAL*4) precision values. But GEOS-Chem uses 64-bit (aka REAL*8) precision internally for species concentrations. When reading in 32-bit data from disk to a 64-bit variable, roundoff errors are incurred. These roundoff errors can cause differences when comparing restarted runs to a single run that spans the entire period. Therefore, this results in non-negligible numerical drift whenever a GEOS-Chem Classic simulation is broken up into multiple run phases. A full resolution of this issue will involve updating the GEOS-Chem Classic History component, as well as HEMCO.

Another outstanding issue is in the Rn-Pb-Be HEMCO extension and occurs only when running GCHP. It causes differences in restarted versus single runs in the transport tracer simulation. That simulation has zero differences if this extension is turned off. This issue will be investigated at a future date. In addition, any remaining differences in the GCHP full chemistry simulation will be reevaluated once the GEOS-Chem Classic restart precision issue discussed above is fixed.

HEMCO restructuring

GCST members **Melissa Sulprizio** and **Lizzie Lundgren** along with **Haipeng Lin** (Harvard) are leading the effort to restructure the HEMCO emissions component so that it can be more easily implemented into external ESMs. This work will involve the following:

1. Move model-specific code (i.e. I/O, regridding, and model-to-HEMCO interfaces) into separate layers that can be turned on or off depending on which external model is being connected to HEMCO.

2. Move HEMCO out of the GEOS-Chem source code repository and into its own Github repository. This will allow updates that are pushed to the HEMCO repository to be

seamlessly linked into other modeling applications. HEMCO will then become a Git submodule in GEOS-Chem.

3. Implement an optional internal HEMCO grid on which masks and scale factors may be applied to emissions before emissions are regridded to the coarser model resolution.

4. Implement HEMCO as a gridded component in GCHP.

This work is ongoing and many of the updates listed above will be included in GEOS-Chem 13.0.0

GCHP stretched-grid capability

GCST member **Liam Bindle** is currently working on adding a stretched-grid capability into GCHP. This will allow you to define a high-resolution cubed-sphere face over an area of interest (such as North America, Europe, or Asia), while reducing the resolution of the remaining grid faces.

One of the great benefits of using a stretched-grid simulation over a nested-grid simulation is that you will no longer need to generate transport boundary conditions from a separate global simulation. The stretched-grid simulation implicitly handles the two-way nesting (transport of species into and out of the high-resolution grid face).

This work is still in the development stage but rapid progress is being made. A preliminary stretched grid capability will be available in GCHP as part of release 13.0.0.

GCHP Restructuring

GCST members **Lizzie Lundgren** and **Liam Bindle** are currently working on restructuring GCHP to provide a new framework for running high performance GEOS-Chem. The new framework will feature GEOS-Chem, HEMCO, and updated NASA/GMAO libraries as git submodules, will use ESMF as an external library, and will incorporate a CMake build system to streamline the compilation process. The upgrade will be part of the next major GEOS-Chem release (13.0.0).

Upcoming Events

GCA2 Meeting: May 18-20, 2020 in Hangzhou, China

The 2nd GEOS-Chem Asia meeting (GCA2) will be held on May 18-20 in Hangzhou, China. GCA meetings are organized every two years by the Joint NUIST-Harvard Laboratory for Air Quality and Climate (JLAQC) to benefit the Asian community using GEOS-Chem and to supplement the International GEOS-Chem meetings (IGC) held at Harvard in alternate years.

See the GCA2 meeting website to register for the meeting. The registration deadline is March 1, 2020.

GCE1 Meeting: June 22-24, 2020 in Leeds, UK

The first GEOS-Chem Europe meeting (GCE1) will be held on June 22-24 in Leeds, UK at the National Centre for Atmospheric Science (NCAS) organised by Mathew Evans (York), Eloise Marais (Leicester), and Paul Palmer (Edinburgh).

See the GCE1 meeting website to register for the meeting. The registration deadline is March 30, 2020.

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

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