GEOS-Chem Newsletter
End-of-Year 2018 Edition

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GEOS-Chem 12 Release Series

Released versions

The GEOS-Chem 12 versions listed below were released since our last newsletter in August.

GEOS-Chem 12.0.2

Release date: 10 Oct 2018; **DOI:** 10.5281/zenodo.1455215

GEOS-Chem 12.0.2 contains minor fixes for non-full-chemistry simulations. Highlights include:

- Fix for local time averaging in ND51 and ND51b timeseries diagnostics
- Correct missing BC and OC biomass emissions in TOMAS simulations
- Correct aerosol dry-deposition in TOMAS simulations.
- Avoid double-counting of emissions in the CO2 simulation.

GEOS-Chem 12.0.3

Release date: 16 Oct 2018; **DOI:** 10.5281/zenodo.1464210

GEOS-Chem 12.0.3 contains minor fixes for GEOS-Chem with the High-Performance option (aka GCHP). Highlights include:

- Fixed incorrect configuration for offline sea-salt emissions in GCHP
- Fixed a bug in the application of CFC mixing ratios in GCHP

GEOS-Chem 12.1.0

****** THIS IS THE CURRENT STABLE VERSION OF GEOS-CHEM ******
Release date: 26 Nov 2018; **DOI:** 10.5281/zenodo.1553349

GEOS-Chem 12.1.0 contains several science and structural updates. Highlights include:

- Budget diagnostics
- AFCID: Anthropogenic PM2.5 emissions inventory
    - Reference: Sajeev Philip et al, Environ. Res. Lett., 12, 044018, 2017.
- GEOS-Chem restart file updates
- Updates and fixes for the CEDS emissions inventory
- Several "under-the-hood" fixes in HEMCO
- Applied fix for mass conservation in non-local PBL mixing
- Fix for photolysis (now allow FAST-J to use solar zenith angles up to 98 degrees)
- FlexGrid stage 1: Read met fields via HEMCO
- Added netCDF diagnostics for several simulations
- Converted RRTMG input files from bpch to netCDF for HEMCO
- Add fixes for seasonal scale factors in CH4 simulations
- Moved FAST-JX input files from the run directory to the ExtData folder
- Updated the HEMCO configuration file for tagged CO simulations
- Continuous integration with TravisCI
- Added several fixes for GCHP
- Added structural updates to facilitate interfacing GEOS-Chem with NCAR models

We have updated the GEOS-Chem New Developments and GEOS-Chem Narrative web pages to include the new features that have been added into GEOS-Chem 12.1.0.

Featured update: GEOS-Chem budget diagnostics

GEOS-Chem 12.1.0 includes a new budget diagnostic collection that you may find useful in your research. Originally proposed by Chris Holmes and based loosely on previous work done by Christoph Keller, the budget collection is a set of 2D diagnostics containing the mass tendencies [kg/s] per species across different components (e.g. chemistry) and within different regions of the column. The diagnostics are calculated by computing the differences in vertically summed column mass before and after major GEOS-Chem components.

Three columnar regions are defined: full column, PBL-only, and troposphere-only. GEOS-Chem components include chemistry, convection, transport (GEOS-Chem Classic only), mixing, emissions/dry deposition, and wet deposition. By post-processing these diagnostics you can calculate global or regional mass tendencies by summing values across the areas of interest.

You can also retrieve the mass change across a chunk of time by multiplying the time-averaged output by the number of seconds in the averaging period.

The budget diagnostics collection is available only in netCDF format. While all pre-existing diagnostics continue to be output as binary, the netCDF option is also enabled by default in 12.1.0. You can therefore compile GEOS-Chem as usual and then turn on the budget diagnostics by configuring the HISTORY.rc file prior to running. See the list of diagnostics archived to netCDF format wiki page for detailed instructions for configuring netCDF diagnostics output.

For more information on the budget diagnostic collection in GEOS-Chem please see the budget collection description on the wiki or contact the GEOS-Chem Support Team.

Ongoing GEOS-Chem Development

New GEOS-Chem code and data submission guidelines

We have introduced new guidelines for developers to follow when submitting source code or data updates to the GEOS-Chem Support Team. We now ask that users fill out an update submission form to ensure all required information is included. For more details, please see these instructions on the GEOS-Chem wiki.

New version in development: GEOS-Chem 12.1.1

This version will include the following features:

- Skip planeflight observations outside of a nested-grid region
- Always compile with the BPCH_TPBC=y option
- Minor fixes updates for GCHP
- Minor fixes for interfacing GEOS-Chem with the NASA/GEOS ESM

For a complete description of this version, please see:

- GEOS-Chem 12.1.1 (subsection of the GEOS-Chem 12 wiki page)

Model Development Priorities

The GEOS-Chem Steering Committee has prioritized several updates that will be added into versions following 12.1.1. You can read more about them here:

- Updates to be added into GEOS-Chem 12.2.0

- Updates to be added into GEOS-Chem 12.3.0

In addition, several more features have been identified as priorities for GEOS-Chem, but have not yet been assigned to a specific version.

Structural updates for interfacing GEOS-Chem into WRF

Haipeng Lin (working with Prof. Tzung-May Fu at Peking University) has begun to make structural changes in order to facilitate interfacing GEOS-Chem into WRF. Several of Haipeng's initial updates have been added "under-the-hood" into GEOS-Chem 12.1.0.

Much of this work involves moving arrays out of modules and into the state variables (State_Met, State_Chm, and State_Diag). This is necessary because WRF needs to be able to dynamically resize arrays from the global grid dimensions to the regional grid dimensions on each node of a distributed-memory computing environment. Even though GEOS-Chem currently passes most global quantities via the state variables, there remains a significant amount of legacy and/or 3rd-party code where arrays are passed from one module to another via USE statements.

The necessary structural updates will impact several areas of GEOS-Chem, especially in the aerosol, SOA, and microphysics modules. We believe that the necessary updates can be made "under-the-hood" in a way that will minimize disruption to GEOS-Chem users.

Removal of binary punch file format

We are continuing to work towards the removal of the binary punch (aka "bpch") file format from GEOS-Chem. The binary punch format is not only cumbersome to use, but it presents a bottleneck to interfacing GEOS-Chem with external models that run in high-performance computing environments, such as the NASA GEOS ESM.

In GEOS-Chem 12.1.0, we have added netCDF diagnostics for the CH4, CO2, and POPs simulations. We are continuing to add netCDF diagnostic capability into the Hg, RRTMG, and TOMAS simulations, as well as certain custom diagnostics (e.g. ND51 satellite timeseries output).

Restart files in GEOS-Chem 12.1.0 are archived as a special type of netCDF diagnostic output, known as the Restart collection. This development will also allow us to convert the nested-grid boundary condition files to netCDF in a future version. (The netCDF boundary condition files are similar to restart files in that they both contain instantaneous species concentrations.)

For the time being, we are currently keeping both netCDF and binary punch diagnostic options in GEOS-Chem. This will allow us to work on implementing the remaining netCDF diagnostic

quantities while preserving the existing diagnostics capabilities. For more information, please see our *List of diagnostics archived to netCDF format* wiki page.

GCHP Updates

Changes to GCHP run directory retrieval

GEOS-Chem 12.1.0 includes an important update to GCHP run directory retrieval. Starting in this version, GCHP no longer requires the GEOS-Chem unit tester. Run directories are instead created directly from the GCHP source code repository using an interactive shell script, createRunDir.sh, in new subdirectory Run/. These updates are intended to improve user experience and increase transparency of run setting updates by storing them in the same history as source code changes.

New run directory features include:

1. Create run directories directly from the GCHP source code repository
2. Interactively choose simulation type, meteorology source, run directory name, and target path when creating a run directory
3. Put run directories under version control with default values as the initial commit (optional)
4. Automatically point to the source code the run directory was created from
5. Lookup the GEOS-Chem version the run directory is compatible with in file rundir.version
6. Use shell script setEnvironment to set symbolic link gchp.env to your environment file stored anywhere on your system

Benefits of the updates include elimination of the following steps in GCHP setup:

1. Syncing versions of the GCHP and GEOS-Chem-UnitTest repositories
2. Editing a config file before run directory creation
3. Manually editing MetDir and ExtData.rc to switch meteorology source
4. Setting CodeDir to point to source code
5. Manually sourcing the environment file prior to compiling
6. Editing the run script to include environment filename

The GCHP Online Manual is up-to-date with both the new and old methods for creating GCHP run directories. Please contact the GEOS-Chem Support Team with questions and feedback.

From the GEOS-Chem Support Team

Requesting assistance with GEOS-Chem

Please take a moment to view our new *Submitting GEOS-Chem support requests* wiki page. This page contains a checklist of items that you should always include when reporting GEOS-Chem bugs or technical issues. Including these items in your support requests will help to ensure that we have all of the information that we need in order to diagnose your issue and to suggest a solution.

Use the Spack package manager to install libraries locally

As described in the GEOS-Chem manual, GEOS-Chem requires a netCDF library installation. While many GEOS-Chem users have access to shared computer systems with pre-built netCDF libraries, many other GEOS-Chem users must install netCDF on their own.

For the past several years, we have maintained the GEOS-Chem-Libraries installer, which is a set of Makefiles and scripts that built specific versions of the HDF5 and netCDF4 libraries. But we have recently become aware that HDF5 and netCDF4 versions contained in the GEOS-Chem-Library installer are no longer compatible with the most recent Intel and GNU compilers. Therefore, we no longer support the GEOS-Chem-Libraries installer.

If you need to install netCDF on your own, we recommend that you use Spack, which is a modern package manager. Spack can install libraries that are compatible with many different types of compilers and operating systems (including Unix and MacOS). For more information about using Spack, please see our *Installing libraries for GEOS-Chem* wiki page.

Updated wiki pages

We have updated several wiki pages in order to reflect the changes that have taken place in the GEOS-Chem 12 release series. These include:

- Submitting GEOS-Chem support requests
- GEOS-Chem restart files
- GEOS-Chem Output Files
- GEOS-Chem coding and debugging
- Working with netCDF data files
- Preparing data files for use with HEMCO

We are also in the process of identifying and removing obsolete information from the wiki.

GEOS-Chem python tools

The GEOS-Chem Support Team is currently developing **GCPy**, a free, open-source, Python-based data visualization and analysis package. GCPy is lightweight, leveraging the existing functionality of several "off-the-shelf" Python packages (such as xbpch, xarray, cartopy, numpy, and matplotlib). It also contains customized functions and example Jupyter notebooks specifically designed for creating plots from GEOS-Chem 1-month and 1-year benchmark simulations. It will eventually include regridding and handling of the cubed sphere grid.

Migrating our benchmarking tools to GCPy will allow us to finally retire the older IDL-based benchmark plotting code, which was cumbersome and difficult to maintain. Using GCPy will also improve the portability of the benchmark plotting code, and it can be used as a general-purpose data analysis and visualization package by GEOS-Chem users.

From the GEOS-Chem Steering Committee

Redesigning the benchmark

The GEOS-Chem Steering Committee is discussing how the plots from the 1-month and 1-year benchmark simulations can be more easily presented online, as well as what species to include. Mat Evans is heading this effort.

As of this writing, the following features in GCPy supporting the new benchmarking capabilities have been implemented by GCST:

1. Creation of 3x2 panel plots showing values, differences, and fractional differences on the same page per species, for either one level or zonal mean, and using either netcdf or bpch diagnostic output.
2. Inclusion of species bookmarks automatically displayed upon opening PDF files.
3. Calculation of lumped species to be included in benchmarking plots.
4. Generation of separate benchmarking files for different species categories.

IGC9 will take place in May 2019!

IGC9 will be held at Harvard on May 6-9, 2019, with the Young Scientists' social on May 5. Registration will open up in December. More information will be posted to the IGC9 website at a later date. For now, mark your calendars, and see you in May!

The GCSC is working on a new logo for GEOS-Chem!

The GEOS-Chem Steering Committee is currently working with several graphic designers on the creation of a new GEOS-Chem logo. Several prototype designs have been submitted and are under review. The new logo will replace the unofficial (and ad-hoc) logos that are presently on the GEOS-Chem web and wiki sites. Stay tuned for more news!

Other GEOS-Chem News

Running GEOS-Chem in the Amazon cloud

Jiawei Zhuang has created a tutorial that shows how you can run GEOS-Chem "Classic" (GCC) on the Amazon Web Services EC2 cloud computing platform. A copy of the GEOS-Chem "gcgrid" data directories has been synchronized to the Amazon S3 storage system and is available for use with your GEOS-Chem simulations.

Using machine learning to speed up the chemistry solver

Several current GEOS-Chem research projects are focusing on machine learning as a way to produce a faster chemical solver. You will hear more about this at the upcoming IGC9 meeting!

And on the lighter side …

With the GEOS-Chem 12.1.0 release, the GEOS-Chem Support Team has noted that GEOS-Chem now has the same version number as the Apple iPhone operating system (iOS 12.1). But with GEOS-Chem 12.1.1 on the horizon, this distinction may be short-lived.

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

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