



13.0.0 Release Candidate Edition

GEOS-Chem Support Team (GCST):

Bob Yantosca, Melissa Sulprizio, Lizzie Lundgren, Will Downs, & Liam Bindle

08 Jan 2021

1.	Overview	2
1.1.	The release candidate period for GEOS-Chem 13.0.0 has begun!	2
1.2.	GEOS-Chem 13.0.0 validation	2
1.3.	GEOS-Chem 13.0.0 final release (and beyond)	2
2.	Important new features in GEOS-Chem 13.0.0	3
2.1.	GCHP is now easier to build than ever!	3
2.2.	GCHP has some impressive new capabilities	3
2.3.	Run directory creation has been simplified	4
2.4.	MERRA-2 is recommended over GEOS-FP	4
2.5.	Several emissions updates have been added	5
2.6.	Important updates in other areas	5
3.	Structural Modifications in GEOS-Chem 13.0.0	6
4.	Release of GCPy, GEOS-Chem's Python Toolkit	7
5.	Instructions for downloading and use	7
5.1.	GEOS-Chem Classic 13.0.0-rc.0	7
5.2.	GCHP 13.0.0.rc.0	8
5.3.	HEMCO 3.0.0-rc.0	8
5.4.	GCPy 1.0.0	9

Overview

The release candidate period for GEOS-Chem 13.0.0 has begun!

After many months of development, we are excited to announce the release of the **GEOS-Chem 13.0.0 release candidates** as:

- **GEOS-Chem Classic 13.0.0-rc.0:** GEOS-Chem in “Classic” mode
- **GCHP 13.0.0-rc.0:** GEOS-Chem in “High performance” mode

As well as the **HEMCO 3.0.0** release candidate::

- **HEMCO 3.0.0-rc.0** The Harmonized Emissions Component

And the official release of:

- **GCPy 1.0.0:** The GEOS-Chem Python toolkit

During the release candidate period, we encourage you to **download and run GEOS-Chem 13.0.0** (as GEOS-Chem Classic and/or GCHP) and to [report any bugs or technical issues](#) via Github.

GEOS-Chem 13.0.0 validation

As of this newsletter, the following benchmarks have been approved:

- [1-month full-chemistry benchmarks](#) with GEOS-Chem Classic and GCHP
- [1-year full-chemistry benchmarks](#) with GEOS-Chem Classic and GCHP
- [1-year TransportTracers benchmarks](#) with GEOS-Chem Classic and GCHP

While the following benchmarks are still running:

- [10-year stratospheric benchmarks](#) with GEOS-Chem Classic and GCHP

GEOS-Chem 13.0.0 final release (and beyond)

We will issue the GEOS-Chem 13.0.0 final release once the 10-year stratospheric benchmarks have been approved and when we are sure that all user-reported issues with the 13.0.0 release candidates have been resolved.

For a list of updates that will be considered for the GEOS-Chem 13 series, please see our [GEOS-Chem model development priorities](#) wiki page.

Important new features in GEOS-Chem 13.0.0

GEOS-Chem 13.0.0 includes many new features, the most important of which are listed below. A complete list of updates may be found at our [GEOS-Chem 13.0.0 wiki page](#).

GCHP is now easier to build than ever!

Our collaboration with NASA/GMAO has resulted in many “under-the-hood” developments that make GCHP much more easier to compile than in previous versions. These include:

ESMF is now an external dependency

Prior versions of GCHP included the ESMF software library, but this was brittle to maintain. GCHP now uses ESMF as an external software dependency. We hope to soon have the proper ESMF version for GCHP distributable via the Spack package manager.

NASA-maintained libraries are now submodules

When you clone a new copy of GCHP via Git, the GCHP source code will now point to the latest version of external libraries (such as MAPL) that are developed by NASA/GMAO. This greatly simplifies the build process, as we no longer have to keep these libraries bundled in the GCHP repository.

GCHP (and GEOS-Chem Classic) now compile with CMake

In order to keep pace with developments at NASA/GMAO, we have migrated the GEOS-Chem build system from GNU Make to CMake. This greatly simplifies the build system as well, especially for GCHP. As a result, **we have now retired GNU Make in GEOS-Chem 13.0.0**.

GCHP has some impressive new capabilities

Stretched-grid option

You can choose to increase the horizontal resolution of one of the cubed-sphere faces over an area of interest. (This will decrease the resolution of the other faces accordingly.) For more information about the GCHP stretched-grid option and its validation, please see Bindle et al, 2020 ([doi:10.5194/gmd-2020-398](https://doi.org/10.5194/gmd-2020-398)).

Prepackaged software containers

We hope to have prepackaged software containers (Docker images) with all of the required libraries for GCHP to ship soon. We will post these on our GEOS-Chem DockerHub site.

Multi-node simulations on Amazon EC2

We are working on the capability to run GCHP across multiple nodes on the Amazon EC2 cloud computing platform. A few technical hurdles (mostly pertaining to how MPI works on the EC2 fabric) first had to be solved. Stay tuned for more news soon.

Run directory creation has been simplified

You will find that it is now much easier to create GEOS-Chem Classic and GCHP run directories in version 13.0.0 than in prior versions.

You can now create run directories from the source code

Instead of having to generate GEOS-Chem run directories with the GEOS-Chem Unit Tester, you can use a run-directory generation script contained within the GEOS-Chem source code itself. When you run the script, you will be prompted to supply the run directory parameters: simulation type, horizontal and vertical resolution, met field type, etc. A properly-configured run directory will be generated for you for the type of GEOS-Chem simulation that you requested.

We have made GCHP and GEOS-Chem Classic configuration files more consistent with each other

As part of the run directory migration work, we took the opportunity to make the GEOS-Chem Classic and GCHP configuration files as similar to each other as possible. Removing all possible configuration-file differences in GCHP and GEOS-Chem Classic will facilitate comparisons between GCHP and GEOS-Chem Classic benchmark simulations. This in turn helps us to identify any unforeseen issues.

We have retired the GEOS-Chem Unit Tester

Because the run directory generation has now been migrated to the GEOS-Chem source code, we have retired the GEOS-Chem Unit Tester in 13.0.0.

MERRA-2 is recommended over GEOS-FP

For the reasons listed below, we recommend that you choose the MERRA-2 assimilated data product to drive your GEOS-Chem Classic and GCHP simulations:

MERRA-2 is a stable long-term reanalysis meteorology product

The MERRA-2 assimilated meteorology product, which contains data from 1980-present, is kept free of assimilation system updates. In other words, the same data streams and the same GEOS-GCM model version are used to create all years of MERRA-2 data. On the other hand, GEOS-FP is an operational product, and is frequently updated as new data or GCM features

become available. MERRA-2 is thus more suitable for running multi-year GEOS-Chem simulations.

Benchmark simulations now use MERRA-2 data

Because we are recommending MERRA-2 over GEOS-FP, we have updated our GEOS-Chem Classic and GCHP benchmark simulations to use 2019 MERRA-2 data instead of 2016 GEOS-FP data.

Several important emissions updates have been added

Carbon-based units for VOC species have been removed

Prior to 13.0.0, some species (e.g. ALK4) were treated as an equivalent number of carbon atoms. We have now discontinued this practice, which was a source of confusion and a holdover from the earliest versions of GEOS-Chem.

CEDS GBD-MAPS is now the default anthropogenic inventory

Starting in 13.0.0, the CEDS GBD-MAPS total anthropogenic emissions (i.e. summed over all fuel sectors) will be the default global inventory.

You may still use the CEDS GBD-MAPS sectoral emissions as a research option. However, using this option will incur additional I/O overhead due to the amount of data that must be read from disk.

Regional emissions inventories are now turned off by default.

You can reactivate any of these inventories by editing the HEMCO configuration file.

Important updates in other areas

We have retired the “tropchem” full-chemistry mechanism

We now use the same GEOS-Chem mechanism (UCX) whether chemistry is performed up to the tropopause or up to the mesopause. Additional chemistry options (e.g. complex SOA, aciduptake, etc.) can be requested during run directory generation.

We have resolved several issues with RRTMG diagnostics

We have resolved several issues with inconsistent diagnostic output from RRTMG. You can now use the RRTMG radiative transfer model to compute diagnostic forcings in both GCHP and GEOS-Chem Classic simulations.

Structural modifications in GEOS-Chem 13.0.0

In [GEOS-Chem 13.0.0](#) and later versions, the GEOS-Chem source code has been split up into these Github repositories:

Repository https://github.com/...	Description
geoschem/geos-chem	This is the GEOS-Chem "science codebase" repository. It contains all of the GEOS-Chem science code, plus: <ul style="list-style-type: none">• Scripts to create GEOS-Chem run directories• Scripts to create GEOS-Chem integration tests• Interfaces (i.e. the driver programs) for GEOS-Chem "Classic", GCHP, etc.
geoschem/HEMCO	This is the HEMCO (Harmonized Emission Component) repository. It contains code to read and regrid data such as emissions, met fields, chemistry data, etc.
geoschem/GCClassic	A lightweight wrapper (aka the "superproject") for GEOS-Chem Classic, which uses GEOS-Chem and HEMCO as submodules . This is the directory that contains files for configuring and building GEOS-Chem classic.
geoschem/GCHP	A lightweight wrapper (aka the "superproject") for GCHP, which uses GEOS-Chem and HEMCO (as well as other relevant software libraries such as MAPL) as submodules . This is the directory that contains files for configuring and building GCHP.

You may be wondering why this was done. Recent structural updates to GCHP and HEMCO have also necessitated corresponding structural changes to GEOS-Chem Classic. In particular, HEMCO is no longer being developed exclusively for GEOS-Chem. It is now also being developed for the NCAR models (CESM2 and next-generation models) as well as for models at NOAA. Because of this, it made sense to split off HEMCO from GEOS-Chem and to store HEMCO in its own Github repository. We hope that this will spur feedback and innovation from users outside of the GEOS-Chem community.

This new setup also has the advantage that the GEOS-Chem code itself no longer can be described as a self-contained model, but of a science codebase that can be integrated into several modeling contexts: as GEOS-Chem Classic, as GCHP, as WRF-GC, as GEOS-Chem within the NASA/GEOS ESM, as GEOS-Chem within CESM, etc. This better aligns with our [GEOS-Chem Vision](#) and [Mission](#) statements.

Release of GCPy, GEOS-Chem's Python Toolkit

Coinciding with the release of the GEOS-Chem 13.0.0 release candidates, we are pleased to announce the release of **GCPy 1.0.0**. GCPy is a Python-based toolkit containing useful functions for working with GEOS-Chem model input and output. GCPy aims to build on the well-established scientific Python technical stack, leveraging tools like cartopy and xarray to simplify the task of working with model output and performing atmospheric chemistry analyses.

GCPy's intended functionality includes:

- Producing plots and tables from GEOS-Chem output using simple function calls
- Generating the standard evaluation plots and tables from GEOS-Chem benchmark output
- Obtaining GEOS-Chem's horizontal/vertical grid information
- Implementing GCHP-specific regridding functionalities (e.g. cubed-sphere to lat-lon regridding)
- Providing examples for creating specific types of plots or analysis from GEOS-Chem output

Version 1.0.0 is the first official release of GCPy. Main additions over previous versions (which have been available on Github but unpublicized until now) include:

- Complete documentation on a new ReadTheDocs site
- conda-forge installation support
- File regridded for NetCDF restarts and output between GEOS-Chem's horizontal grid types
- Plotting supports automatic regridding between lat/lon, cubed-sphere, and stretched-grid formats

Full details on installing and using GCPy are available at <https://gcpy.readthedocs.io>. Source code, version history, and a user issues page are available at <https://github.com/geoschem/gcpy>.

Instructions for downloading and use

GEOS-Chem Classic 13.0.0-rc.0

Getting started

You can find detailed instructions on how to download and run GEOS-Chem Classic at manual.geos-chem.org. This currently points to our [Getting Started with GEOS-Chem](#) wiki manual;

however, we will migrate this documentation to **readthedocs.io** in the near future. This will allow us to keep the GEOS-Chem manual under version control (i.e. you can easily find the instructions for previous GEOS-Chem versions).

Please also take a few moments to watch our tutorial video [Getting started with GEOS-Chem "Classic" 13.0.0](#), which you can find at the [GEOS-Chem Youtube channel](#). This video will walk you through the process of setting up GEOS-Chem 13.0.0 on your system.

Using GEOS-Chem Classic on the Amazon EC2 cloud computing platform

We generate images on the AWS Cloud for each GEOS-Chem release that contain pre-compiled GEOS-Chem Classic code and minimal sample data. You can generate an instance on AWS EC2 using one of these images as a baseline for running GEOS-Chem Classic on the AWS Cloud. An AMI for 13.0.0-rc.0 can be found with the AMI ID **ami-097f1b62def179f42**.

Please see [our Quick Start Guide at cloud.geos-chem.org](#) for detailed instructions on getting started with GEOS-Chem on the AWS cloud. Using [GEOS-Chem's dry-run capability](#), you can quickly download required input files for any GEOS-Chem simulation from AWS S3 to your cloud instance.

GCHP 13.0.0-rc.0

You can find detailed instructions on how to download and run GCHP at <https://gchp.readthedocs.io>. This is the new location of our GCHP User's Guide.

Please also take a few moments to view these new GCHP tutorial videos GEOS-Chem Youtube Channel:

- [Getting started with GCHP 13.0.0 -- Building GCHP](#)
- [Getting started with GCHP 13.0.0 -- Running GCHP](#)

These videos will guide you through the process of installing GCHP on your system. If you have used older GCHP versions in the past, you should find a much better user experience with GCHP 13.0.0-rc.0!

HEMCO 3.0.0-rc.0

As mentioned above, the HEMCO code has now been split off into its own repository. This allows GEOS-Chem Classic or GCHP to treat HEMCO as a submodule instead of as internally-embedded code. If you are only interested in running GEOS-Chem or GCHP simulations, you will NOT need to install HEMCO as a separate package.

However, if you wish to develop new emissions inventories or validate an existing HEMCO configuration, **you can run HEMCO in standalone mode independently of GEOS-Chem**. With the HEMCO standalone mode, you can generate hourly, daily, monthly, or annual emissions output. This

can be useful if you wish to combine the results from one or more emissions inventories into an inventory of total emissions.

To download the HEMCO 3.0.0-rc.0 release candidate, please follow the instructions specified at hemco.readthedocs.io. This is the new location of the HEMCO User's Guide.

Please also take a few moments to view our [Getting Started with the HEMCO 3.0.0 standalone](#) tutorial video, which you can find on our GEOS-Chem Youtube channel.

GCPy 1.0.0

GCPy is now available for installation using Conda through the **conda-forge** channel. You can find detailed instructions on installing and using GCPy on the new [GCPy Read the Docs site](#).

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

The GEOS-Chem Support Team:
Bob, Melissa, Lizzie, Will, and Liam
geos-chem-support@g.harvard.edu