GEOS-Chem

Spring 2019 Newsletter

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GEOS-Chem 12 Release Series

Released versions

The GEOS-Chem 12 versions listed below were released since our last newsletter (Dec 2018):

GEOS-Chem 12.1.1

Release date: 13 Dec 2018; **DOI:** **10.5281/zenodo.2249246**

GEOS-Chem 12.1.1 contains minor fixes that do not affect the full-chemistry simulations:

- Bug fix for tagged CO: don't multiply the emissions timestep by 60.
- Bug fixes for nested-grid simulations:
    - Skip Planeflight diagnostic observations that lie outside of a nested domain.
    - Always compile with BPCH_TPBC=y so that transport BC files will be archived.
- Fixes for minor compilation issues.
- Bug fix: Prevent instant propagation from troposphere to stratosphere in GCHP.
- GCHP updates:
    - Fix transport to prevent instant propagation from troposphere to stratosphere.

GEOS-Chem 12.2.0

Release date: 19 Feb 2019; **DOI:** **10.5281/zenodo.2572887**

GEOS-Chem 12.2.0 contains several science and structural updates. Highlights include:

- Retire BRAVO emissions and use CEDS emissions for Mexico instead.
- Bug fix: Update mask file used for NEI2011 emissions.
- Renamed the Rn-Pb-Be simulation to the TransportTracers simulation.

- ○ Added several passive species for benchmarking purposes. These species will be used to compare transport in GEOS-Chem and the NASA GEOS ESM.
- Added the ObsPack diagnostic, which outputs model quantities at point locations.
- Added GFAS biomass burning emissions as an optional inventory.
- Fixed bug in stratospheric aerosol surface area diagnostic.
- Updated HEMCO from 2.1.010 to 2.1.011 to make the HEMCO standalone compatible with the FlexGrid updates from GEOS-Chem 12.1.0.
- GCHP updates:
  - ○ Upgrade from ESMF v5.2.0rp2 to v7.1.0r.
  - ○ Add extra fields to GCHP output restart file to facilitate multi-segmented runs.

GEOS-Chem 12.2.1

***THIS IS THE CURRENT STABLE VERSION OF GEOS-CHEM ***
Release date: 28 Feb 2018; **DOI:** **10.5281/zenodo.2580198**

GEOS-Chem 12.2.1 contains fixes and updates that do not affect the benchmark simulation:

- Bug fix: netCDF diagnostics with frequency "End" now properly span leap year days
- TOMAS updates for compatibility with GEOS-Chem 12
- Structural updates to facilitate WRF-GC development
- The polar bromine explosion is now the default option for the Hg simulation.
- Bug fix for Henry's law coefficient for C2H6 in the species database.
- Add RRTMG fluxes to netCDF diagnostics: *NOTE: still needs validation!*
- Fix for the CO2 simulation chemical source.
- GCHP updates:
  - ○ Update MODIS LAI source to match GEOS-Chem Classic.
  - ○ Correct pressure units for MERRA-2 simulations.
  - ○ Use online sea flux emissions by default (offline used since 12.0.0).

Featured topic: Running GEOS-Chem in the cloud

It is now easier than ever to run GEOS-Chem on the Amazon Web Services (AWS) cloud computing platform! Running GEOS-Chem in the cloud lets you take advantage of computational resources that otherwise might not be available to you. The cloud is also a way for you to request additional computational resources that you might only need for a short period of time (e.g. to accommodate a special research project).

We have synced the GEOS-Chem "gcgrid" data directories to the Amazon S3 storage system. These directories contain all of the necessary meteorology and emissions data that you will need for your GEOS-Chem simulations on the cloud.

Jiawei Zhuang (Harvard) is spearheading GEOS-Chem development on the AWS cloud. He writes:

> *Dear GEOS-Chem Users,*
>
> *The description of the GEOS-Chem on AWS cloud capability has just been submitted to the Bulletin of the American Meteorological Society (BAMS). You can access it by clicking on the link:*
>
> > *Zhuang, J., D.J. Jacob, J. Flo-Gaya, R.M. Yantosca, E.W. Lundgren, M.P. Sulprizio, and S.D. Eastham, Enabling immediate access to Earth science models through cloud computing: application to the GEOS-Chem model, submitted to Bull. Amer. Met. Soc., 2019. [click here for PDF]*
>
> *You can start using GEOS-Chem on the cloud immediately by following our hands-on online tutorial* **http://cloud.geos-chem.org**. *Please also feel free to browse the project source code (https://github.com/geoschem/geos-chem-cloud) and post any questions on the GitHub issue tracker (https://github.com/geoschem/geos-chem-cloud/issues).*
>
> *Best,*
>
> *Jiawei*

Jiawei is currently exploring how to make GCHP (GEOS-Chem with the High-Performance option) compatible for cloud-computing simulations using a single AWS computational node. But scaling to multiple nodes on the AWS cloud with MPI parallelization presents some technical challenges, and this is where Jiawei will focus his efforts.

Featured diagnostic: ObsPack

GEOS-Chem 12.2.0 and later versions include the ObsPack diagnostic output module. This diagnostic can be used to archive species concentration along with several meteorological data variables at point locations, corresponding to individual observation locations -- either at the surface or aloft.

The GEOS-Chem ObsPack diagnostic is currently configured to read coordinate data from netCDF files that adhere to NOAA's ObsPack format, and will archive output with the same format. A brief overview of the Obspack framework is given at the ObsPack web site:

> *Observation Package (ObsPack) data products are intended to stimulate and support carbon cycle modeling studies. A variety of ObsPack products are available and vary from one another depending on their intended use. Products may include providers' original data and metadata reformatted into the ObsPack framework (Masarie et al.,*

2014) or may contain averages or subsets of original data. ObsPack data products are prepared by NOAA in consultation with data providers.

The ObsPack framework (Masarie et al., 2014) is designed to bring together direct atmospheric greenhouse gas measurements derived from one or more national or university laboratories, prepare them with specific applications in mind, and package and distribute them in a set of self-documenting files. ObsPack products include a set of prepared data sets and metadata, a summary of included data sets, an e-mail address list of all data providers, and the complete set of configuration files used by NOAA to prepare the product.

-- ObsPack web site (https://www.esrl.noaa.gov/gmd/ccgg/obspack/)

Andy Jacobson (NOAA) mentions that many important observational data sets are now being produced using the ObsPack netCDF format:

NOAA is committed to providing data in ObsPack format specifically for modelers, and both ICOS and the World Data Center for GHG are considering/planning to publish their measurements in ObsPack format. In addition to our GLOBALVIEW+ and NRT ObsPacks for CO2, we've rolled out an AirCore ObsPack, an SF6 ObsPack, and are working on a major new GLOBALVIEW+ methane ObsPack.

For those of you who are using GEOS-Chem for carbon-cycle research, the new ObsPack diagnostic might prove to be a useful tool for comparing GEOS-Chem output to observations.

The ObsPack diagnostic in GEOS-Chem can potentially be used as an alternative to the existing Planeflight diagnostic, provided that you first convert existing flight track coordinate data to the ObsPack format (e.g. by writing a Python script).

Featured simulation: TransportTracers

The Transport Working Group proposed implementing a common set of transport tracers in GEOS-Chem for benchmarking purposes and for diagnosing transport in GEOS-Chem compared to the NASA GEOS ESM.

- The GMI tracer suite is implemented via the tracer gridded component "TR_GridComp" in the NASA GEOS ESM.

- In GEOS-Chem, the tracer suite now has been added as an extension of the Rn-Pb-Be simulation (simulation type "1") by default, but may be added to any GEOS-Chem simulations by following these instructions.

The common set of transport tracers was introduced in GEOS-Chem 12.2.0. In this version, the Rn-Pb-Be simulation has now been renamed to the **TransportTracers** simulation, as the new transport tracers are included by default. Additional transport tracers will be added to this simulation in the future.

Ongoing GEOS-Chem Development

New version in development: GEOS-Chem 12.3.0

This version will include the following features:

- Update ISORROPIA v2.0 to v2.2 to remove persistent noise in output.
- Update MODIS LAI to the BNU product (Yuan et al, 2011), covering the years 2005-2016.
- Update the plant functional type (PFT) file used in MEGAN biogenic emissions.
- Use OMI-based volcanic emissions as the default emissions inventory
- Update HEMCO to version 2.1.012 to fix a bug in the HEMCO interpolation algorithm

For a complete description of this version, please see:

- GEOS-Chem 12.3.0 (subsection of the GEOS-Chem 12 wiki page)

Alpha release of WRF-GC

We are excited to announce that an alpha version of WRF-GC (GEOS-Chem interfaced with the WRF ESM) is now ready! This work is being carried out by Prof. Tzung-May Fu and her students at Peking University. She writes:

Dear GEOS-Chem users,

We are excited to announce that the alpha version of WRF-GC (v0.1) is now available for test users to play with. The development of WRF-GC was led by my students Haipeng (Jimmie) Lin and Xu Feng. You can check out our brief description and user's guide at: http://wrf.geos-chem.org

To download, please send me your github account. We will give you access to our private github repository, where you can download the WRF-GC code along with a tested version of GEOS-Chem (v12.1.1). As the code is still under development, please do not directly redistribute the code to other users. Instead, please direct interested users to our download page. That way we can make sure that bug fixes and updates are

delivered to all test users. Future stable versions will be made available from public repositories.

A few notes about the WRF-GC alpha version:

1. *So far, the coupling between WRF and GEOS-Chem is one-way only, i.e., there is no feedback from GEOS-Chem to WRF. We are working on a two-way coupled version.*

2. *The nested domain capability of WRF is not yet supported. This is a high-priority item that we hope to resolve in the beta version.*

3. *We aim to have a more stable beta release by the time of IGC9 in May 2019.*

*If you encounter any problems running WRF-GC or have suggestions for model improvements, please email me at **tmfu@pku.edu.cn**.*

Thanks!

Regards,
Tzung-May Fu

ESMF and MAPL library updates for GCHP

GCHP 12.2.0 features ESMF v7.1.0r released in 2018. Prior versions of GCHP used ESMF version 5.2.0rp2 released in 2012. The update to a more recent version removes deprecated library issues some users ran into when compiling with certain compilers. It also paves the way for future updates to install and build ESMF as an external library outside of GCHP. Separating ESMF from GCHP will reduce GCHP compilation time and memory requirements by making ESMF setup a separate one-time only task. For more information about the new ESMF version please see documentation at www.earthsystemcog.org/projects/esmf.

Lizzie Lundgren is actively working with GMAO to develop a cutting edge version of their Modeling, Analysis and Prediction Layer software (MAPL) that will replace the current MAPL used in GCHP. MAPL is an interface between GCHP and ESMF that includes specialized implementations not available in standard ESMF. The updated version will include new functionalities such as ESMF online regridding and parallel I/O to address the I/O bottleneck currently impeding GCHP performance. The update will also solve an open issue in GCHP 12.2.0 that prevents running GCHP built with the GNU compiler gfortran, an important fix for running GCHP in software containers (such as Singularity) and on AWS Cloud.

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.

Users are also encouraged to open issues on our GEOS-Chem Github repository site, which is located here: https://github.com/geoschem/geos-chem. Opening issues on GitHub brings greater visibility of issues and their resolutions to the GEOS-Chem community.

Python tools for analyzing GEOS-Chem output

GEOS-Chem Python tutorial

Jiawei Zhuang has created an excellent tutorial on how you can use Python to read, manipulate, and plot GEOS-Chem data. Most basic plotting and analysis operations can be achieved with only a handful of Python packages. For more information, please see:

- https://github.com/geoschem/GEOSChem-python-tutorial

GCPy development

We are 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).

Included in GCPy is a benchmark library with customized functions for comparing GEOS-Chem run output. This includes the capability to produce plots and emissions totals for the GEOS-Chem benchmark simulations. 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.

A prototype of the 1-month benchmark materials generated using GCPy is now available for review. Lizzie Lundgren writes:

As you know, the GCST, in consultation with Mat Evans, has been developing new benchmarking tools using Python to replace IDL GAMAP. Part of this work includes designing a new set of visualizations and a new, easy-to-use display for browsing.

We now have a [prototype demonstration for the 1-month benchmark](#) available for you to view. Please take a moment to look through the page if you have time.

Thanks in advance for what I know will be very valuable feedback!

Primarily developed for 1-month and 1-year benchmarks, the GCPy benchmark functions may also be used more generally by users for comparing GEOS-Chem output for any two runs, including comparison of binary and netcdf output, lat-lon and cubed sphere grids, and different grid resolutions. This is made possible because GCPy now leverages the regridding capability provided by the [xESMF](#) Python package. xESMF, which is written by Jiawei Zhuang (Harvard), lets you easily regrid data on rectangular and/or cubed-sphere grids..

While GCPy will contain some general-purpose functions, we do not envision that it will become as comprehensive a plotting package as GAMAP was. This is because most basic plotting and analysis operations can already be done with existing Python packages (as illustrated in our [Python tutorial](#)). Nevertheless, we plan on adding several examples in the form of Jupyter notebooks to illustrate how to create different types of plots from GEOS-Chem output using GCPy. We will also encourage users to share their own GEOS-Chem python tools with the rest of the community.

Although GCPy is still in development, we encourage interested users to take GCPy for a spin. GCPy can be downloaded via Git clone from our Github site: https://github.com/geoschem/gcpy.

Plan to remove binary punch format from GEOS-Chem

We would like to update you on our plans to remove [binary punch (aka "bpch") file format](#) from GEOS-Chem. Removing the binary punch file format will not only result in cleaner GEOS-Chem source code, but will also facilitate interfacing GEOS-Chem with external models such as NASA GEOS ESM, WRF, and CESM.

Several developments must occur before binary punch format is removed from GEOS-Chem. These are:

1. **A mature GCPy release.** As explained above, the GCPy package will contain several new Python-based benchmarking utilities. We are currently validating and finalizing these benchmarking utilities and are in the process of preparing an official GCPy release.

2. **The release of GEOS-Chem 12.3.0.** GEOS-Chem 12.3.0 will ship with a new HEMCO diagnostics configuration file (aka HEMCO_Diagn.rc) for each type of simulation. This will make it possible to schedule diagnostics for all emitted species and to archive them to the HEMCO_diagnostics*.nc netCDF files. Once this happens, essentially all of the existing bpch diagnostics for emissions will be rendered obsolete.

3. **A benchmark comparing netCDF diagnostic output to bpch diagnostic output.** Before removing the binary punch file format from GEOS-Chem, we will perform benchmark simulations for the same GEOS-Chem version so that we can compare the diagnostic output in binary punch format against the diagnostic output in netCDF format.This will help to flag any issues with the implementation of the netCDF diagnostics.

While most of the bpch diagnostics can be removed after these criteria are met, a few binary punch diagnostics might need to be preserved for a longer period of time. This includes satellite observation diagnostics as well as several diagnostics in the [Hg](#), [POPs](#), [RRTMG](#), and [TOMAS](#) simulations. The latter still need to be converted from binary punch to netCDF format, and to do so will probably require assistance from members of the relevant Working Groups. In order to not break any backwards compatibility for these simulations, we plan on keeping these binary punch diagnostics active for the time being. In addition, the planeflight diagnostic output, which is currently output as text, will remain text file output.

For more information about the existing diagnostics in GEOS-Chem, please visit these pages of the GEOS-Chem wiki:

- [List of diagnostics archived to bpch format](#)

- [List of diagnostics archived to netCDF format](#)

Use the Spack package manager to install local libraries

As described in the GEOS-Chem manual, GEOS-Chem requires a netCDF library installation. GEOS-Chem with the High-Performance option (GCHP) also requires a version of the Message Passing Interface (MPI) library. While many GEOS-Chem users have access to shared computer systems with pre-built libraries, many other GEOS-Chem users must install libraries on their own.

If you need to install libraries such as netCDF and MPI on your own, we recommend that you use [Spack](#). Spack is a modern package manager that can install libraries that are compatible with many different types of compilers and operating systems, including Unix/Linux and MacOS.

Please see our [*Installing libraries for GEOS-Chem* wiki page](#) with improved instructions for using Spack..

From the GEOS-Chem Steering Committee

New GEOS-Chem logo

The GEOS-Chem Steering Committee selected a new logo for GEOS-Chem ([this design](#), plus a few variants). We have already started using the logo on the GEOS-Chem web, wiki, and tutorial pages. An official "Rollout" of the new logo will happen at the IGC9 meeting in May.

IGC9 Meeting: May 6-9 at Harvard

The 9th International GEOS-Chem Meeting (IGC9) will take place at Harvard University from May 6-9, 2019. Registration for the meeting is now closed.

Please visit our IGC9 website (**igc9.geos-chem.org**) for all of the latest updates! We plan on posting a draft agenda shortly.

We will have live-streaming of the plenary sessions for those of you who are unable to attend IGC9. A link will be available via the IGC9 website during the meeting.

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

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