

GEOS-Chem

Spring 2021 Newsletter

GEOS-Chem Support Team (GCST)

Bob Yantosca, Melissa Sulprizio, Lizzie Lundgren,

Will Downs, Liam Bindle, and Yanshun Li

18 March 2021

Table of Contents

| | | |
|--------|--|---|
| 1. | GEOS-Chem 13.0.0 is officially released! | |
| 1.1. | Updates included in GEOS-Chem 13.0.0 | 2 |
| 1.1.1. | GEOS-Chem updates | 2 |
| 1.1.2. | GCHP updates | 3 |
| 1.1.3. | GCPy updates | 3 |
| 1.1.4. | Outstanding issues | 3 |
| 1.2. | GEOS-Chem 13.0.0 validation | 3 |
| 2. | GEOS-Chem 13.0.1 will contain minor fixes | 4 |
| 3. | Recent developments | 4 |
| 3.1. | GCHP can now be built with Spack! | 4 |
| 3.2. | Updates to the Kinetic PreProcessor (KPP) | 5 |
| 3.3. | GCPy version 1.0.2 | 5 |
| 4. | Cloud computing updates | 5 |
| 4.1. | GEOS-Chem Classic | 5 |
| 4.2. | GCHP | 5 |
| 5. | Ongoing GEOS-Chem development | 6 |
| 5.1. | Speeding up reaction rate computations | 6 |
| 6. | News from the GEOS-Chem Steering Committee | 6 |
| 7. | Introducing Yanshun Li | 7 |

GEOS-Chem 13.0.0 is officially released!

We are pleased to announce the official release of GEOS-Chem 13.0.0! This major release includes:

GEOS-Chem Classic 13.0.0

- Github: <https://github.com/geoschem/geos-chem>
- DOI: [10.5281/zenodo.4618180](https://doi.org/10.5281/zenodo.4618180)
- Manual: [Getting Started with GEOS-Chem](#) (wiki doc)
 - NOTE: This manual will be migrated to ReadTheDocs in the near future.

GCHP 13.0.0

- Github repository: <https://github.com/geoschem/GCHP>
- DOI: [10.5281/zenodo.4618205](https://doi.org/10.5281/zenodo.4618205)
- Manual: gchp.readthedocs.io

HEMCO “release candidate” 3.0.0-rc.1

- Github: <https://github.com/geoschem/HEMCO>
- DOI: [10.5281/zenodo.4618254](https://doi.org/10.5281/zenodo.4618254)
- Manual: hemco.readthedocs.io

GCPy 1.0.2

- Github repository: <https://github.com/geoschem/HEMCO>
- DOI: [10.5281/zenodo.4618391](https://doi.org/10.5281/zenodo.4618391)
- Manual: gcpy.readthedocs.io

Tutorial videos may be viewed at our Youtube channel: youtube.com/c/geos-chem

Updates included in GEOS-Chem 13.0.0

We have been busy fixing several user-reported issues since the GEOS-Chem 13.0.0 release candidate evaluation period began on 8 January 2021. Here is a quick summary of issues that were fixed. These fixes have now been included in the GEOS-Chem 13.0.0 final release.

GEOS-Chem updates

1. [Species concentrations, oxidant fields, and similar quantities](#) from the GEOS-Chem Classic 10-year benchmark simulation are now archived. These quantities can be used as [inputs to the various specialty simulations](#). This archive also [restores the aerosol-only simulation](#).
2. [The EMISSIONS MENU is removed from input.geos](#). All emissions settings should now be handled in the HEMCO configuration file.

3. Several [issues that had prevented the TOMAS15 and TOMAS40 simulations](#) from executing properly in GEOS-Chem 13.0.0 are fixed.
4. [An issue in the tagged O3 simulation](#) when using the extended set of O3 species is fixed.
5. Several issues in various areas of the diagnostics, including the [planeflight diagnostic](#), [ND51 satellite timeseries diagnostic](#), and [potential temperature diagnostic](#) are fixed. [BrO](#) is now added to the ConcAboveSfc diagnostic collection.
6. [An issue in toms_mod.F90](#) that only occurs on older compilers (e.g. ifort 12) is now fixed.

GCHP Updates

1. The run/GCHP/runScriptSamples folder now includes an [expanded set of example GCHP run scripts](#) using the SLURM, PBS and LSF schedulers. The scripts will now be helpful to an expanded set of users.
2. The isCoords script can now properly parse GCHP History files to check for configuration errors.
3. GCHP integration tests are now fully functional.
4. The GCHP user guide is now available on [ReadTheDocs](#) at gchp.readthedocs.io.

GCPy updates

1. Cubed-sphere regriding [no longer takes an excessive amount of time](#) to complete.
2. File regriding now works properly [when the dataset only has one vertical level](#).
3. Minor issues in core plotting routines were resolved.

Outstanding issues

1. [The global mass of MSA is much lower in GCHP](#) than in GEOS-Chem Classic. This is only a problem when compiling GCHP with the Intel compilers.
2. Impact of using offline vs. online emissions (especially for dust) in the benchmark simulations. New recommendations for scale factors will be provided in 13.2.0.

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

We have also performed 1-month benchmarks with **GEOS-Chem Classic 13.0.0-rc** and **GCHP 13.0.0-rc** (rc = “release candidate”) to investigate the impact of using offline vs. online emissions:

- [GEOS-Chem Classic offline vs. online emissions](#)
- [GCHP offline vs. online emissions](#)
- [GCHP offline emissions vs. GEOS-Chem Classic offline emissions](#)

GEOS-Chem 13.0.1 will contain minor fixes

We are currently working on **patch version GEOS-Chem 13.0.1**, which will be available soon. This version will include minor fixes that were not able to be included in the official 13.0.0 release, including:

- [A minor bug fix for the planeflight diagnostic](#)
- Fixes for issues in the GEOS-Chem dry-run (see [here](#) and [here](#))

Recent developments

GCHP can now be built with Spack!

We're happy to announce that GCHP is now available through [Spack](#). Spack is an open source package manager that automatically builds packages and their dependencies. You can use Spack to build GCHP and install all of its external software dependencies (such as NetCDF-Fortran and ESMF) in a single **spack install gchp** command. You can also use **spack install --only dependencies gchp** to only install GCHP's dependencies if you wish to build GCHP's source code on your own.

The main advantage of using Spack to install GCHP is its ability to automatically install all dependencies. This is particularly useful on fresh computing environments such as new GCHP setups on the AWS Cloud. You can also command Spack to use existing installations of specific dependencies external to Spack without building new versions.

The main disadvantage of building GCHP through Spack is that you cannot modify the GCHP source code and recompile it with Spack. Spack provides you with a copy of the GCHP source code, but this is intended only for run directory creation and general perusal.

For more information on using Spack to install GCHP and its dependencies, including build customization options and interfacing Spack-built GCHP with Slurm, please visit [our Spack usage guide on the GCHP Read The Docs site](#).

Updates to the Kinetic PreProcessor (KPP)

KPP ([The Kinetic PreProcessor](#), by A. Sandu et al), translates a chemical mechanism specification from plain-text format to source code. You may select the numerical integrator to be used (Runge-Kutta, LSODES, Rosenbrock, etc.) and the language for the generated source code (Fortran-90, Fortran-77, C, Matlab). The resulting source code files may then be integrated into an atmospheric chemistry model, chemical box model, or other application.

KPP-for-GEOS-Chem is KPP that has been customized specifically for GEOS-Chem. You can use KPP-for-GEOS-Chem to modify existing GEOS-Chem chemistry mechanisms or create new mechanisms from scratch.

The latest KPP-for-GEOS-Chem version is now 2.3.1_gc. This version contains some important fixes and under-the-hood improvements since the prior version (2.2.4_gc). If you are editing GEOS-Chem mechanisms, you should update to KPP-for-GEOS-Chem 2.3.1_gc. You will find detailed installation instructions at the KPP-for GEOS-Chem manual (kpp.readthedocs.io).

GCPy version 1.0.2

GCPy 1.0.0 was released concurrently with the **GEOS-Chem 13.0.0-rc** and **GCHP 13.0.0-rc** release candidate versions in early January 2021. Since then, minor fixes were added to GCPy; namely to improve the speed of cubed-sphere regridding and also to fix minor plotting issues. We have released these updates as **GCPy 1.0.2**, which is available for installation using Conda through the **conda-forge** channel. You can find installation and usage instructions on the [GCPy Read the Docs site](#).

Cloud computing updates

GEOS-Chem Classic

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 can be found with the AMI ID **ami-0ef2c8a2d3464485c**.

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

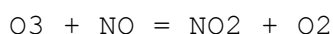
Setting up GCHP on the cloud is easier than ever thanks to the release of GCHP on Spack. We are currently benchmarking the performance of GCHP 13.0.0 on the AWS Cloud. We plan to release official documentation on the use of GCHP on the AWS Cloud in the next few months.

Ongoing GEOS-Chem development

Speeding up reaction rate computations

Bob Yantosca has been working on speeding up computation of chemical reaction rates. These updates should be ready for inclusion into an early GEOS-Chem 13 version.

For example, consider the reaction



The JPL chemical data evaluation (Feb 2017) specifies that the rate of this reaction may be computed according to the Arrhenius law

$$k = a_0 + (300 / \text{TEMP})^{b_0} + \text{EXP}(c_0 / \text{TEMP})$$

and that its Arrhenius coefficients are $a_0 = 3.0e-12$; $b_0 = 0$; $c_0 = 1500$. Because $b_0 = 0$, the middle term $(300 / \text{TEMP})^{b_0}$ evaluates to 1. Therefore, when we compute k , we can skip computing the b_0 term, and thus rewrite the reaction rate computation as:

$$k = a_0 + \text{EXP}(c_0 / \text{TEMP})$$

By adding modifications such as these into the rate law functions included in GEOS-Chem chemistry mechanism, we can gain significant speedup. **Preliminary tests on Harvard's Cannon cluster suggest that modifications of this type can halve the time spent in computing reaction rates.** This translates into approximately 20 minutes of time saved when using the "out-of-the-box" GEOS-Chem 4° x 5° benchmark simulation. For further information, see [Github discussion thread #598](#).

News from the GEOS-Chem Steering Committee

The **GEOS-Chem Steering Committee** met on February 24, 2021. We invite you to read the [meeting minutes](#) as well as the following **Working Group updates**:

- [GCHP Working Group update](#)
- [Transport Working Group update](#)
- [Stratospheric Working Group update](#)

Hongyu Liu (Transport Working Group co-chair) and **Susan Strahan** (Stratospheric Working Group co-chair) are stepping down from the GCSC. We would like to extend our warmest thanks to Hongyu and Susan for their service to the GEOS-Chem community.

Please join us in welcoming the following people to their new roles on the GCSC:

- **Andrew Schuh** (NOAA) has joined the GCSC and will co-chair the [Transport Working Group](#) with Andrea Molod.
- **Pam Wales** (NASA/GSFC) has joined the GCSC and will co-chair the [Stratospheric Working Group](#) with Seb Eastham and Dylan Jones.
- **Melissa Sulprizio** and **Lizzie Lundgren** now serve as Model Engineers alongside Bob Yantosca. All three will co-chair the [Software Engineering Working Group](#).

Introducing Yanshun Li

It is a pleasure to welcome **Yanshun Li** to the GEOS-Chem Support Team. Yanshun is a doctoral student working with Randall Martin at Washington University in St. Louis. He brings adept computational skills along with experience developing and using GEOS-Chem. His research experience includes developing and testing the effects of dry deposition schemes on the diel variation of PM_{2.5}. He will begin in the area of processing and archiving the GEOS meteorological data used by GEOS-Chem.

Please join us in welcoming Yanshun to the GCST!

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

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