# Spring 2021 Newsletter

**GEOS-Chem Support Team (GCST)**
**Bob Yantosca, Melissa Sulprizio, Lizzie Lundgren, Will Downs, Liam Bindle, and Yanshun Li**
**20 May 2021**

## Table of Contents

1. GEOS-Chem version updates
   - 1.1. GEOS-Chem 13.0.1 2
   - 1.2. GEOS-Chem 13.0.2 2
   - 1.3. GEOS-Chem 13.1.0 2

2. Ongoing GEOS-Chem developments 3
   - 2.1. Consolidating chemistry mechanisms with KPP 3
   - 2.2. Compatibility with GCAP 2.0 4
   - 2.3. HEMCO 3.0.0 development 4

3. Ongoing GCHP developments 5
   - 3.1. GCHP updates in 13.1.0 5
   - 3.2. GCHP timing results 5

4. News from the GEOS-Chem Steering Committee 6

5. Congratulations to Will Downs! 7

# GEOS-Chem Version updates

In the Spring 2021 edition of this Newsletter, we announced the official release of GEOS-Chem 13.0.0! Since then, we have released a couple of patch updates in order to fix minor issues, after the 13.0.0 release.

## GEOS-Chem 13.0.1

**Release Date:** 23 Mar 2021 **DOI:** 10.5281/zenodo.4632275

GEOS-Chem 13.0.1 contains the following updates:

- Force GEOS-Chem Classic restart file to match the simulation start date
- Bug fixes for GEOS-Chem dry-run simulations
- Updated the MAX_RO2 parameter for the Planeflight diagnostic
- Set offline dust emissions to FALSE until further notice
- Add fix for adding P and L species to the species database

For a complete description of these issues, see the GEOS-Chem 13.0.1 Milestone on Github.

## GEOS-Chem 13.0.2

**Release Date:** 12 Apr 2021 **DOI:** 10.5281/zenodo.4681204

GEOS-Chem 13.0.2 contains the following updates:

- Bug fix: Introduce HEMCO time cycle flag EFYO for restart files (which are only read once), and use time cycle flag EFY for met fields (which are read in at the start of each day)

For a complete description of these issues, see the GEOS-Chem 13.0.2 Milestone on Github.

And as of this writing, we are currently benchmarking the next version in the GEOS-Chem 13 series:

## GEOS-Chem 13.1.0

**Release Date TBD**

GEOS-Chem 13.1.0 will contain the following updates:

- HEMCO 3.0.0 official release, with initial modifications for HEMCO internal grid
- Fix H2O boundary conditions at the tropopause
- Compatibility with GCAP 2.0 horizontal and vertical grids
- Capability to distribute emissions vertically in the boundary layer
- Diurnal scale factors for Chinese power plant emissions
- Updates to speed up the chemical solver

- Removal of RRTMG binary diagnostics
- J-value output via the Planeflight diagnostic
- Initial modifications for GCHP adjoint
- Updated GMAO submodules for GCHP
- Use new GCHP config file logging.yml
- GCHP monthly mean diagnostic output
- Update GCHP diagnostic filenames to match GEOS-Chem Classic
- Retire ifort18 support in GCHP

For a complete description of these issues, see the GEOS-Chem 13.1.0 Milestone on Github.

# Ongoing GEOS-Chem development

## Consolidating chemistry mechanisms with KPP

This year, we have undertaken a major effort to bring all GEOS-Chem chemistry mechanisms into the Kinetic Pre-Processor (KPP) framework. This involves several different phases.

### Speeding up chemical rate computations in KPP

As reported in our Spring 2021 Newsletter, GCST member **Bob Yantosca** was able to speed up the computation of the reaction rates in KPP by avoiding useless computations. New rate-law functions were introduced in order to avoid computing terms that would evaluate to either 0 or 1. Also, Bob identified terms that only needed to be computed once instead of at each grid box, which greatly reduces computational overhead. These modifications, which will be included in GEOS-Chem 13.1.0, resulted in a 44% speedup in the chemistry computation time.

### Porting sulfur chemistry into KPP

Many chemical reactions for sulfur gas and aerosol species have historically been performed outside of KPP (i.e. in sulfate_mod.F90). This was likely done for expediency, as well as to avoid modifying the indecipherable SMVGEAR solver code that we used up until GEOS-Chem v11-01. But this separation of code has proved to be brittle and difficult to maintain.

**Mike Long** has been working on migrating the remaining sulfur chemistry reactions into the KPP solver framework. This work has involved:

- Defining chemistry reactions for sulfur gas-phase and aerosol species within KPP;
- Migrating rate law functions (e.g. CALC_*) from sulfate_mod to KPP;
- Adding HMS chemistry reactions (Moch et al, 2020) into KPP;
- Applying Holmes et al, 2019 cloud fraction method to reactions migrated into KPP.

When complete, this will result in the complete removal of sulfate_mod.F90 from GEOS-Chem.

### Cleaning up heterogeneous chemistry rate law functions

**Bob Yantosca** is currently cleaning up the heterogeneous chemistry code. Currently, functions that compute rates for heterogeneous reactions (aka the “rate-law functions”) are included in a module (gckpp_HetRates.F90) that is separate from the chemical mechanism definition. But this module has proven difficult to maintain and extend, and is a common source of errors. Bob has been porting the rate law functions from gckpp_HetRates.F90 into the KPP configuration file, so that they will be integrated into the chemical mechanism specification.

### Migrating specialty simulation mechanisms to KPP

At present, many of the “specialty” simulations (e.g. Hg, CH4, CO2, tagged CO, etc.) use chemistry reactions that are defined in separate modules rather than in KPP mechanisms. We plan on bringing all of these “specialty” simulation chemistry mechanisms into KPP.

- **Viral Shah** (Harvard) is working on a KPP mechanism for the Hg simulation, continuing with work originally done by **Colin Thackray** (Harvard). It is currently in testing.
- **Beata Bukosa** (Wollongong/NIWA) has provided a unified CO2-CO-CH4 specialty simulation. We plan on converting this into a KPP mechanism very soon.
- The aerosol-only and tagged O3 mechanisms can be created as subsets of the full-chemistry mechanism.

### Making KPP a submodule of GEOS-Chem

Recent modifications to KPP (such as described in our Spring 2021 Newsletter) mean that newer KPP versions can only be used with certain versions of GEOS-Chem. To reduce version confusion, we propose to make the KPP-for-GEOS-Chem package a submodule of GEOS-Chem (much like HEMCO already is). This will allow updates to KPP to be seamlessly integrated with new GEOS-Chem versions. We hope to start on this work in the near future.

## Compatibility with GCAP 2.0

**Lee Murray** (U. Rochester) has submitted updates that will allow GEOS-Chem to be driven by the GCAP 2.0 meteorological data. This has mostly involved importing the GCAP vertical and horizontal grid definitions into both GEOS-Chem and HEMCO, as well as adding in hooks for external function calls. See the submitted GCAP 2.0 paper for details. This feature will debut in GEOS-Chem 13.1.0.

## HEMCO 3.0.0 development

GEOS-Chem 13.1.0 will contain the official release of HEMCO 3.0.0 (as described in this GMDD preprint by **Haipeng Lin**). One of the new features of HEMCO 3.0.0 will be an intermediate grid, which can allow masking and scaling to be done at higher resolution than the grid on which emissions will

eventually be computed. This feature will be off by default pending inspection of impact on performance.

# Ongoing GCHP development

## GCHP Updates in 13.1.0

Starting in version 13.1.0 all GCHP diagnostic output files will have the same default filename format as GEOS-Chem Classic. This includes prefixing the filenames with GEOS-Chem rather than GCHP and timestamping with start time rather than mid-point time for time-averaged diagnostics. Users should update GCPy to version 1.1.0 which allows backwards compatibility with the old file format. As a reminder, users may also customize the GEOS-Chem output filename format in the HISTORY.rc configuration file.

GCHP monthly mean diagnostics are now fully supported by MAPL History. Users will no longer need to post-process daily files or split up runs into 1-month chunks in order to generate monthly means. All HSTORY.rc files now contain the monthly mean option for all time-averaged collections and it is enabled by default in benchmark and transport tracer simulation run directories. Users may toggle it on and off within the configuration file runConfig.sh.

GCHP contains a new logging capability that users may configure from new configuration file logging.yml. The logging feature is made possible by the pFlogger library developed by Tom Clune at GMAO and is based on python logging which uses a hierarchy of loggers, such as info, warnings, error, and debug. It replaces the previous method of generating MAPL ExtData debug prints. We look forward to expanding its use in GCHP in the future.

Please note that due to updates in GMAO libraries you will no longer be able to build GCHP with Intel 18 fortran compiler. Please switch to a more recent Intel compiler or use GNU fortran compiler versions 8 or 9.

## GCHP timing results

Timing tests of GCHP version 13.0 have shown that the I/O bottleneck in previous versions of GCHP is now resolved, and that the model is scaling well and consistently on different systems. Figure 1 shows results for 7-day timing tests done at WashU, Harvard, and AWS. Resolving the I/O bottleneck has made high-core-count simulations (e.g., >500 cores) more efficient at all resolutions; at C48 and C90 resolution, throughputs of up to 150–200 days/day are possible. Generally, we are seeing comparable performance with GNU and Intel compilers, and that ordinary interconnects like Gigabit Ethernet are sufficient for simulations with less than 500 cores.

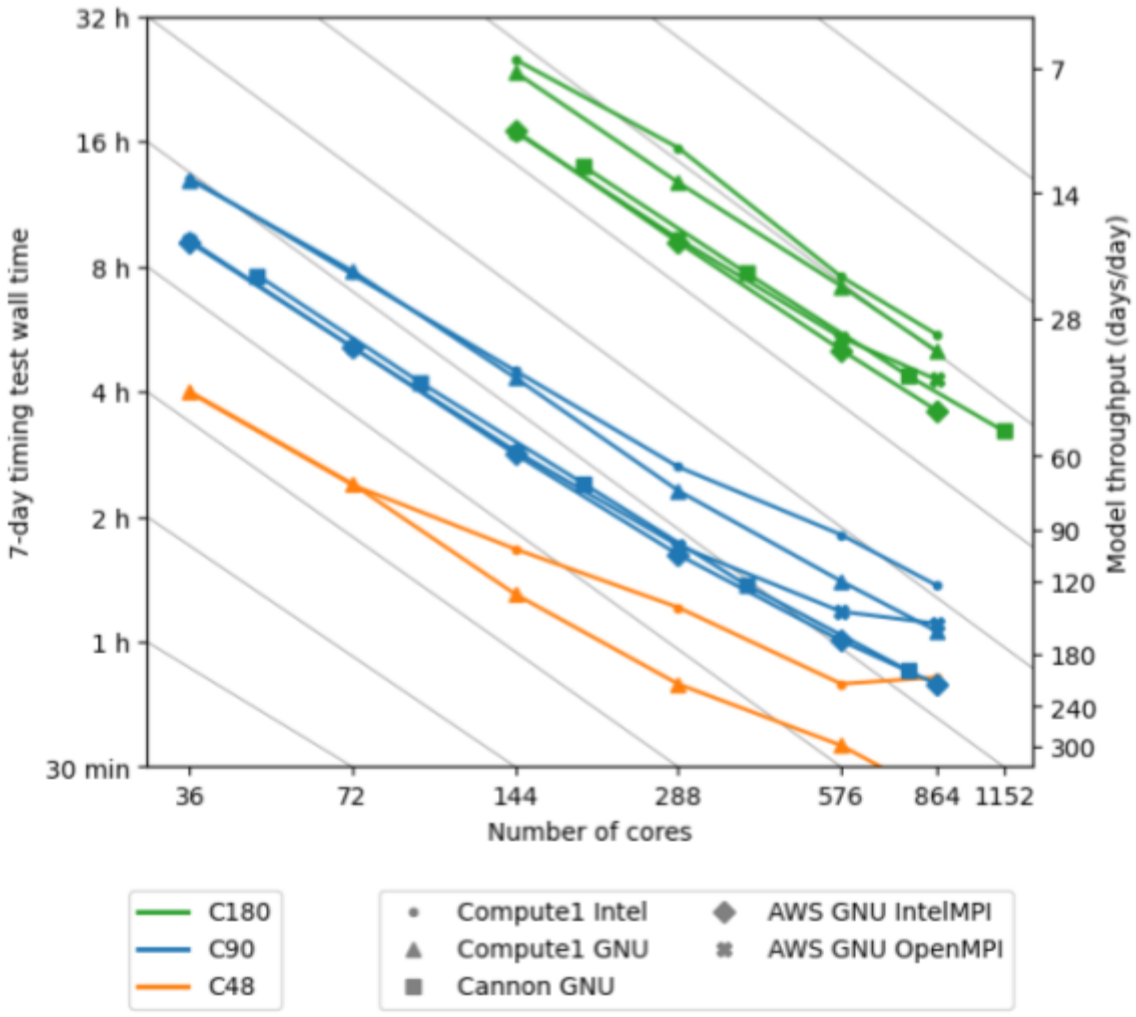


Figure 1: 7-day timing test results for GCHP 13.0.

# News from the GEOS-Chem Steering Committee

The **GEOS-Chem Steering Committee** met on May 19th, 2021. We invite you to read the **meeting minutes** as well as the following **Working Group updates**:

- Aerosols Working Group update
- Software Engineering Working Group update
- Carbon Cycle Working Group update

# Congratulations to Will Downs!

Please join us in congratulating **Will Downs** as he steps down from his role on the GCST to attend graduate school in the fall. Will has enrolled in the Atmospheric Sciences PhD program at the University of Miami (FL), where he will study the evolution and development of hurricanes.

Will has been an instrumental part of the GCST for the past 2 years. He contributed greatly to both GCPy and GCHP development. Thanks to Will's efforts, GCPy is now much more user friendly and efficient than it was, and can easily be installed by the Conda package manager. Will also implemented a one-line installation of GCHP and its required libraries with Spack, and successfully ported GCHP to the Amazon Web Services cloud.

Thanks again Will, and congratulations from all of us!!

---

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