Fall-Winter 2019 Newsletter

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Featured News

Upcoming major release: GEOS-Chem 13 (TBD 2020)

We wanted to let everyone know that we anticipate having a major GEOS-Chem release sometime in early 2020. This release---**GEOS-Chem 13.0.0**---will contain the following new updates:

1. Retire the GNU Make build system in both GEOS-Chem Classic and GCHP and replace with CMake.

2. Retire the GEOS-Chem Unit Tester repository and move GEOS-Chem run directory creation to the GEOS-Chem source code repository.

3. Retire the existing GCHP repository and replace with a new wrapper repository that uses ESMF as an external library and integrates GEOS-Chem and NASA/GMAO GEOS-ESM git repositories as git submodules.

These changes are necessary in order for GEOS-Chem to keep pace with rapid developments that are taking place at NASA/GMAO and elsewhere in the GEOS-Chem modeling community.

GEOS-Chem 13.0.0 will most likely follow the GEOS-Chem 12.7.0 and 12.8.0 releases, which will bring several important chemistry updates into the standard code base.

Most binary punch diagnostics removed in GC 12.7.0

All binary punch diagnostics not ported to NetCDF format will be removed in GEOS-Chem 12.7.0, currently in development. We ask that you now use the netCDF (aka "History") diagnostics to archive fields from GEOS-Chem.

We will preserve a few specialty binary diagnostics for backwards compatibility with existing simulations. These are:

1. TOMAS (ND59, ND60, ND61, ND65 and ND44 drydep fluxes)
2. RRTMG (ND72)
3. Hg (ND03)
4. POPs (ND53)
5. Planeflight diagnostic (ND40)
6. Satellite timeseries (ND51, ND51b)

GEOS-Chem now uses Continuous Integration & Deployment

We are thrilled to announce a new and exciting GEOS-Chem feature! Liam Bindle (GCST) has implemented **Continuous Integration** and **Continous Deployment** pipelines for GEOS-Chem 12.6.1 (Classic) and later versions. Work for the same functionality in GCHP is in progress and expected to be ready for GEOS-Chem 13.0.0.

- With **Continuous Integration (CI)**, any updates to GEOS-Chem's Github repository (e.g. commits or pull requests) will trigger automatic tests. The rigor of these tests depends on the type of update—quick tests for single commits and more substantial tests for pre-releases. At present, these automated tests can only check if GEOS-Chem Classic compiles properly. But in the near future, we would like to extend these tests so that they not only compile GEOS-Chem but also run a short simulation. This will help us to better ensure the integrity of the GEOS-Chem source code.

- With **Continuous Deployment (CD)**, each official GEOS-Chem release that is made at the Github repository will trigger an automatic pipeline that (1) builds GEOS-Chem executables for various configurations, (2) creates corresponding container images, and (3) pushes the container images to DockerHub. The container images hold all of the necessary libraries (e.g. netCDF) that you need to run GEOS-Chem Classic. You can then download the container images from our DockerHub site to your cluster or AWS cloud instance, so that you can quickly initialize your GEOS-Chem runtime environment.

We will post more documentation about these CI/CD pipelines for GEOS-Chem very soon. In the meantime, you can see the results of GEOS-Chem builds and releases at our Microsoft Azure DevOps site: https://dev.azure.com/geoschem/geos-chem.

A GEOS-Chem "dry-run" option will be available soon

Haipeng Lin (Harvard), Jiawei Zhuang (Harvard), and the GEOS-Chem Support Team are working on implementing a GEOS-Chem dry-run option. This would allow GEOS-Chem to timestep through any simulation without actually reading any data from disk or performing any computation. This dry-run option would have the following advantages:

1. You can easily check if your Unix environment is properly configured with a GEOS-Chem dry-run. Any missing libraries or incorrectly specified data paths would immediately cause the GEOS-Chem dry-run to exit with an error.

2. You can produce a list of all of the input files (e.g. met fields and emissions) that are needed for any GEOS-Chem simulation. Then you can check if all of those files are present on disk before doing the actual simulation.

3. Lastly, from the output of any dry-run simulation, you would be able to create a script that downloads only as much data as is required for that simulation. This would be an easy way to generate the download commands to transfer data from the s3://gcgrid bucket on Amazon Web Services (AWS) to your AWS cloud computing instance. This could also be used to create a more generalized data download tool for GEOS-Chem.

We hope to have a working dry-run available soon, perhaps in GEOS-Chem 12.7.0.

We are migrating support requests to Github issues

We encourage all GEOS-Chem users to report bugs and technical issues via the GEOS-Chem Github issue tracker rather than by direct email. Each Github issue is given its own page with a unique URL. Issues can be searched by label (e.g."bug", "feature", "waiting-for-release", etc.) or by version number, aka milestone (e.g. "12.6.1", "12.7.0"), or from the search box at the GEOS-Chem issue tracker page.

We also highly recommend watching the GEOS-Chem GitHub repository to receive email notifications when new releases are issued. You can further configure your GitHub notifications to stay aware of bug fixes and new issues and follow GEOS-Chem discussions on GitHub.

We will post new tutorials about using Github to create support requests, search existing issues, and set automatic notifications in order to stay up-to-date with the latest GEOS-Chem fixes for bugs and technical issues. These tutorials will be posted at our GEOS-Chem YouTube channel (**youtube.geos-chem.org**) very soon. We will email the GEOS-Chem user community once these tutorials go live. In the meantime, please see *How can I make a support request?* and our checklist of items to include in a support request on the GEOS-Chem wiki.

GEOS-Chem Version Updates

Recently released GEOS-Chem versions

The GEOS-Chem 12 versions listed below were released since our last newsletter (Sep 2019):

12.6.0

Release date: 18 Oct 2019; **DOI:** 10.5281/zenodo.3507501

This version includes the following features:

- N2O5, NO3, NO2 reactive uptake updates
- Subgrid cloud NOy chemistry
- HNO3 cold temperature deposition
- Quick fix for aerosol pH calculation when dry
- Remove isoprene in VBS (leaving aqueous)
- Updates for aerosol hygroscopicity and optics
- Add simple parameterization for CO2 dependence of stomatal resistance
- Add option for nitrate aerosol photolysis (off by default)
- Enable CMake to build the GEOS-Chem executable (GC "Classic" only)
- Add "Subset" capability (regional grid output) to the History diagnostics
- Add surface timeseries diagnostic for O3 and HNO3 with user selected height
- Re-integrate APM microphysics (from F. Yu group @ Albany) with GEOS-Chem
- Optional historical biomass burning inventory (BB4CMIP6 + LPJ-LMfire) for 1750-2014

For more information about the updates in GEOS-Chem 12.6.0, please click here. Also see our *GEOS-Chem Narrative Description* and *New GEOS-Chem Developments* pages, which have been updated for version 12.6.0.

12.6.1

Release date: 28 Oct 2019; **DOI:** 10.5281/zenodo.3520966

This version fixes a few issues that were identified during or since the 12.6.0 benchmarking process:

- Fix CMake error message for when NetCDF is not found
- Fix units for PRECANV, PRECCON, PRECLSC, PRECTOT in state_met_mod.F90
- Various minor structural updates:
    - ObsPack uses to hourly sampling if a sampling interval is not found in data files
    - GEOS-Chem now prints the full path of each file that is read

- - GNU Fortran 9.2.1 can now compile GEOS-Chem
    - Use Microsoft Azure DevOps instead of TravisCI for continuous integration
  - Fix GCHP regridding bug at poles, introduced in 12.5.0, that caused MERRA2 runs to crash at high resolution

For more information about the updates in GEOS-Chem 12.6.1, please click here.

Versions in development

GEOS-Chem 12.7.0 is currently in development. This version contains a new small alkyl chemistry mechanism, and also adds methanol as a chemical species (instead of a background species), plus several other updates. Starting in this version, GCHP run directory creation and high-level files that interface between GEOS-Chem and ESMF/MAPL are included in the GEOS-Chem repository.

GEOS-Chem 12.8.0 is slated to include updated isoprene chemistry and wet deposition. This version will likely be followed by the new major release 13.0.0, as described above.

Upcoming Events

Interactive GEOS-Chem clinics: January 17, 2020 at Harvard

We plan on holding a day of interactive GEOS-Chem model clinics on January 17, 2020 at Harvard University. This date was chosen to dovetail with the American Meteorological Society (AMS) January meeting in Boston. We anticipate offering clinics on (1) basic GEOS-Chem usage, (2) advanced GEOS-Chem usage, (3) GCHP, and (4) running GEOS-Chem on the AWS cloud computing platform.

We will post more information about this event on the GEOS-Chem website very soon. In the meantime, please mark your calendars!

GCA2 Meeting: May 18-20, 2020 in Hangzhou, China

The 2nd GEOS-Chem Asia meeting (GCA2) will be held on May 18-20 in Hangzhou, China. GCA meetings are organized every two years by the Joint NUIST-Harvard Laboratory for Air Quality and Climate (JLAQC) to benefit the Asian community using GEOS-Chem and to supplement the International GEOS-Chem meetings (IGC) held at Harvard in alternate years.

Registration for GCA2 will commence in December 2019. In the meantime, please see the GCA2 meeting website.

GCE1 Meeting: June 22-24, 2020 in Leeds, UK

The first GEOS-Chem Europe meeting (GCE1) will be held on June 22-24 in Leeds, UK at the National Centre for Atmospheric Science (NCAS) organised by [Mathew Evans](#) (York), [Eloise Marais](#) (Leicester), and [Paul Palmer](#) (Edinburgh).

Registration will commence in December 2019. In the meantime, please see the [GCE1 meeting website](#).

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

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