End-of-Summer 2019 Newsletter

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Featured News

Updated GEOS-Chem narrative

The GEOS-Chem Steering Committee (GCSC) has updated the narrative description of the current standard version of GEOS-Chem. You may find this new narrative on the GEOS-Chem website:

- geos-chem.org/geos_chem_narrative.html

This narrative serves two purposes.

- To provide you with a quick overview of GEOS-Chem components and capabilities;
- To assist you in correctly citing relevant model components in your publications.

New GEOS-Chem developments list

As described in the GEOS-Chem narrative, the GCSC strongly encourages you to be generous in citations—this not only recognizes the developer's work but also increases the traceability of your paper. Offering co-authorship to developers is encouraged for new developments as flagged in this narrative if they are important for your work.

To facilitate this, the GCSC has updated the list of new GEOS-Chem developments, which is posted here:

- geos-chem.org/geos_new_developments.html

Please check the list of new developments to find out more specific information about the developer(s) who should be credited.

New GEOS-Chem logo

As officially announced at the IGC9 meeting last May, the GEOS-Chem Steering Committee selected a new logo for GEOS-Chem. We encourage you to start using these logos in your GEOS-Chem presentations and posters. You may download these logos at geos-chem.org/geos_chem_logo.html.

Our GEOS-Chem Youtube channel is live!

We are excited to announce the launch of **youtube.geos-chem.org**, our new GEOS-Chem Youtube channel! We plan on uploading a few tutorial videos per quarter to this channel, covering various aspects of GEOS-Chem, GCHP, and GCPy. If you are interested in creating a video tutorial on certain aspects of GEOS-Chem, then please contact us at geos-chem.support@g.harvard.edu.

Software Engineering Working Group now formed

The new GEOS-Chem Software Engineering Working Group (SEWG) consists of GEOS-Chem users and engineers interested in model software development. Its purpose is to coordinate:

- optimizing model performance
- improving usability
- facilitating extensibility to ESMs
- developing tools for visualization and data analysis
- expanding model quality assurance

All SEWG activities are documented in a publicly viewable Google document accessible, along with quarterly telecon minutes, at the GEOS-Chem Software Engineering Working Group wiki page. For more information about how to get involved, contact group co-chairs Lizzie Lundgren (elundgren@seas.harvard.edu) and Melissa Sulprizio (mpayer@seas.harvard.edu).

Beta version WRF-GC v0.9 is now ready to use!

Tzung-May Fu wrote:

> *We are excited to announce a major update to WRF-GC (v0.9), which is an online, coupled model of WRF and GEOS-Chem. WRF-GC is developed by Haipeng Lin, Xu Feng, and Tzung-May Fu. This update includes significant bug fixes and improvements for better simulation results and compatibility with the WRF model.*

Major changes which may impact your simulations with WRF-GC include:

- *Updated compatibility with the latest release of GEOS-Chem v12.3.2*
- *Fixes to the chemical boundary conditions, as they were previously incorrectly passed to GEOS-Chem in WRF-GC.*
- *Fixes to the conversion of wet air pressure, optical depth of water/ice clouds, visible optical depth and downward PAR direct/diffusive flux from WRF to GEOS-Chem. This fix will impact photolysis, biogenic emissions, and chemistry in GEOS-Chem in WRF-GC.*

Furthermore, WRF-GC now supports the GNU C and Fortran compilers and the OpenMPI library, in addition to the existing supported Intel compilers & MVAPICH2 MPI library, allowing users to use fully free and open-source software to run WRF-GC. We have also fixed multiple compile issues, streamlining the installation process for WRF-GC users.

As WRF-GC is still in testing stages, distribution is currently through a private GitHub repository. Please do not directly redistribute the code to other users. Instead, please contact Tzung-May Fu ***(fuzm@sustech.edu.cn****) to be added to our GitHub repository, where the latest code can be downloaded. That way we can make sure bug fixes and updates are delivered to all test users. Future stable versions will be made available from a public repository*

We would like to thank the test users for feedback and support of the WRF-GC model. Please do not hesitate to contact us if you have any questions regarding WRF-GC. We also have an official documentation page at ***http://wrf.geos-chem.org.***

GEOS-Chem Version Updates

Recently released GEOS-Chem versions

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

12.3.0

Release date: 01 Apr 2019; **DOI:** 10.5281/zenodo.2620535

GEOS-Chem 12.3.0 contains several science updates as well as bug fixes:

- Update ISORROPIA from v2.0 to v2.2
- Use updated plant functional type (PFT) file for MEGAN biogenic emissions
- Add a bug fix for eruptive volcanic emissions
- Update HEMCO from v2.1.011 to v2.1.012

- Bug fix for netCDF diagnostics for intervals spanning leap years
- Bug fixes for tagged CO simulation
- Enable time to run backwards in GCHP (to facilitate GCHP adjoint)

For more information about the updates in GEOS-Chem 12.3.0, please click here.

12.3.1

Release date: 19 Feb 2019; **DOI:** 10.5281/zenodo.2633278

GEOS-Chem 12.3.1 contains fixes for issues that were identified in 12.3.0:

- Fix for noontime J-value netCDF diagnostic
- Planeflight diagnostic now writes out data for last timestep of the day
- Reduce memory footprint in stratospheric chemistry

For more information about the updates in GEOS-Chem 12.3.1, please click here.

12.3.2

Release date: 02 May 2019; **DOI:** 10.5281/zenodo.2658178

GEOS-Chem 12.3.2 contains fixes for issues that were still outstanding as of 12.3.1:

- Fix inconsistency in species H2402 between GC “Classic” and GCHP
- Bug fixes for the FAST-JX photolysis mechanism
    - Species DHDC was listed as not photolyzing; now fixed
    - Removed duplicate entry for ClNO2 in a FAST-JX input file
- Updates for HEMCO diagnostics
- Extended the CEDS anthropogenic emissions inventory back to 1750
- Several updates for GCHP

For more information about the updates in GEOS-Chem 12.3.2, please click here.

12.4.0

Release date: 05 Aug 019; **DOI:** 10.5281/zenodo.3360635

This version includes the following features:

- FlexGrid Stage 2: Defining custom grids
- Grid-independent dust emissions
- Grid-independent lightning NOx emissions
- Grid-independent biogenic VOC emissions
- Grid-independent sea-salt emissions

- Grid-independent soil NOx emissions
- Updated volcano emissions (1978-2019)
- Bug fix: rebuild chemical mechanisms w/ FAST-JX updates from version 12.3.2
- Read FAST-JX input files from a central directory instead of the run directory

For more information about the updates in GEOS-Chem 12.4.0, please click here.

12.5.0

Release date: 09 September 2019; **DOI:** 10.5281/zenodo.3403111

This version will include the following features:

- Update GCHP to use MAPL tagged version "gchp/v1.0.0"
- Make sure stratospheric Bry emissions are read properly each month
- Retire obsolete emissions inventories
- Fixes for GFED4 emissions
- Scale DICE-Africa emissions to address errors in inventory
- Add corrections for CFCs in the chemistry mechanism
- Enable accurate cloud pH diagnostic (involves post-processing)
- Bug fix for proposed Henry's law constants

For more information about the updates in GEOS-Chem 12.5.0, please click here.

Version in development: 12.6.0

This version will include 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.

From the GEOS-Chem Support Team

Introducing Will Downs

Will Downs has joined the GEOS-Chem Support Team as a Scientific Programmer this fall. Will hails from New Orleans and recently graduated from Williams College with a degree in Geosciences and Computer Science.

Binary punch diagnostic removal begins

The GEOS-Chem 12.5.0 1-month benchmark includes a comparison of the binary punch (bpch) format diagnostic output against the netCDF format diagnostic output. This was done in order to document any differences between bpch and netCDF diagnostics and flag any issues. We have accounted for all observed differences between the binary punch and netCDF diagnostics. **Therefore, we will begin to remove most of the binary punch diagnostics starting in GEOS-Chem 12.7.0**.

A few binary punch diagnostics, such as those for specialty simulations, will be preserved for a longer period of time in order to preserve backwards compatibility. The planeflight diagnostic, which currently outputs to text files, will remain unchanged. However, the ObsPack netCDF diagnostic may also be used ito archive output at point locations. For more information about diagnostics in GEOS-Chem, please visit the *Guide to GEOS-Chem Diagnostics* on the GEOS-Chem wiki.

GEOS-Chem documentation updates

The GCST has been reorganizing the GEOS-Chem wiki in order to make it more readable and accessible. Here are some of the recent highlights:

- The wiki ***Main Page*** is now streamlined to contain much fewer links, with many of them now moved to the ***GEOS-Chem overview*** page.
- The GEOS-Chem Manual on the web (`manual.geos-chem.org`) now redirects to the new wiki guide ***Getting Started with GEOS-Chem***.
- There are several new easy-to-navigate GEOS-Chem Guides to assist you in finding information on important GEOS-Chem topics, such as compilers, netCDF, Git, and diagnostics. See the ***GEOS-Chem Guides* section** of the GEOS-Chem overview wiki page for a complete list.

- There is now a ***Recent Changes*** section on the ***Getting Started with GCHP page*** to help experienced users stay up-to-date with logistical changes for compiling and running GCHP. This section will be updated for every GCHP version and summaries per version release will be archived.

Use GitHub issue trackers to report bugs and ask questions

We encourage all GEOS-Chem users to begin using the GitHub issue trackers when reporting bugs or technical issues. Each repository on GitHub has its own issue tracker. Once an issue is posted, it and the ensuing conversation remain visible and searchable.

We also highly recommend watching the GEOS-Chem GithHub repositories so that you will receive an email when new releases are issued. This is a convenient way to stay aware of bug fixes and new issues as well.

For more information, please see *How can I make a support request?* on the GEOS-Chem wiki. Also be sure to review our checklist of items to include in any support request.

Ongoing GCHP Development

Speed improvements in GCHP 12.5.0

GCHP 12.5.0 uses MAPL version tag "gchp/v1.0.0" (released early 2019). The MAPL library, which is developed by NASA, is a wrapper for the Earth System Modeling Framework (ESMF), and handles not only I/O but also passing of data between components. **With this version update GCHP input speed executes roughly 3-4 times faster than previous versions!** This speed-up is due to parallelization within input read across one node, and the MAPL updates in this version are just the beginning of improvements to GCHP I/O bottlenecks.

GCHP 12.5.0 caveats

While we are encouraged by the speed improvements to GCHP in 12.5.0, a few issues remain open until the next MAPL update later this year.

- The 1-month GCHP benchmark shows a resolution-dependent positive surface ozone bias over the southern ocean in GCHP. The issue occurs in FV3 and is an open issue with GMAO. The issue is currently under investigation.
- There is a slow memory leak in GCHP 12.5.0 due to updates to MAPL ExtData. GMAO is aware of the issue and is working on a fix. The memory leak is more pronounced for long simulations and can result in a simulation crashing due to exceeding memory available. Breaking up long runs into smaller consecutive runs avoids the issue but we

find that doing so changes the output. The GCST is investigating single versus multi-run differences in both GCHP and GEOS-Chem Classic and are posting comparison plots on the Harvard ftp site.

- GCHP 12.5.0 uses online ESMF regridding weights rather than external tile files for regridding. Due to ESMF domain decomposition rules this can result in a MAPL error if an input grid is too coarse for a run's configured core count. We have seen this problem for 4°x5° input files when using >600 cores. All 4°x5° input files are therefore replaced with higher resolution files for GCHP 12.5.0 to avoid this issue. However, users may still run into problems if running with thousands of cores. This will be fixed in the next MAPL version update.

GCHP changes in the pipeline

Several major development updates to GCHP are slated for release in fall 2019. Updates include:

- Update to ESMF v8 public release
- Separation of ESMF from the GCHP repository and inclusion as an external module
- Replacement of GNU make with CMake for compilation
- Use of new GMAO public GitHub repositories as git submodules
- Restructuring of the GCHP repository to be a wrapper around GEOS-Chem, with GEOS-Chem at a git submodule within GCHP

The GCHP changes are necessary to keep pace with changes in the GMAO libraries upon which GCHP depends. They will enable ongoing inclusion of new MAPL developments that will improve GCHP performance and extend capabilities over time.

The GCST is looking for volunteer beta testers to try out the new version on their systems and provide feedback. If you are interested in becoming a beta tester please contact the GEOS-Chem Support Team.

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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