GEOS-Chem Newsletter, Fall 2018

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GEOS-Chem 12 release series

Released versions

The GEOS-Chem 12 versions listed below have already been released. These are the first versions to use our new purely-numeric version numbering system.

GEOS-Chem 12.0.0

Release date: 10 Aug 2018
DOI 10.5281/zenodo.1343547

GEOS-Chem 12.0.0 (aka "v11-02-final" in the old numbering system) is the first release in the GEOS-Chem 12 series. It contains fixes for several user-reported issues that were identified during the v11-02-release-candidate evaluation period.

Highlights:

- Avoid double-counting of trash-burning emissions
- Update to HEMCO 2.1.007 to fix several minor issues
- Add fixes for bugs in heterogeneous chemistry
- Add fixes for bugs in stratospheric chemistry
- Add fix for the scale factor for ARCTAS_SHIP emissions
- Add fixes for the DICE-Africa emissions inventory entries in the HEMCO configuration file
- Add GFED 4.1 data for 2015 and 2016
- Add QFED v2.5r1 biomass burning data (optional)
- Updated the two-way-nesting option up-to-date
- Several other fixes for minor issues

For a complete description of this version, please see:

- GEOS-Chem 12.0.0 (subsection of the *GEOS-Chem 12* wiki page)

GEOS-Chem 12.0.1

****** THIS IS THE CURRENT STABLE VERSION OF GEOS-CHEM ******
Release date: 24 Aug 2018
DOI: 10.5281/zenodo.1403144

GEOS-Chem 12.0.1 contains minor fixes that users reported after the release of 12.0.0.

Highlights:

- Added compatibility for GNU Fortran 8.2
- Added compatibility for Intel Fortran 18
- Added fix to restore compatibility for GCHP with GNU Fortran 6+
- Fixed minor issues in diagnostics
- Added updates for the Hg simulation

For a complete description of this version, please see

- GEOS-Chem 12.0.1 (subsection of the GEOS-Chem 12 wiki page)

Performance

GEOS-Chem "Classic"

Bob Yantosca ran a series of timing tests with GEOS-Chem "Classic" 12.0.0 to evaluate its performance. For a complete analysis of these timing results, please see:

- Table of 7-day timing tests with GEOS-Chem 12.0.0
- Graphs from 7-day timing tests with GEOS-Chem 12.0.0
- Presentation: *GEOS-Chem "Classic" 12.0.0 timing results* by Bob Yantosca

GCHP

Lizzie Lundgren has set up a corresponding timing test wiki page for GCHP. We invite you to view timing results for 12.0.1 and to for users to submit their own GCHP timing results here:

- GCHP timing tests

Ongoing GEOS-Chem Development

New GEOS-Chem code and data submission guidelines

We are introducing new guidelines for developers to follow when submitting source code or data updates to the GEOS-Chem Support Team. We now ask that users fill out an update submission form to ensure all required information is included. For more details, please see these instructions on the GEOS-Chem wiki.

Version in development now: GEOS-Chem 12.1.0

This version is currently in development, and will include the following features:

- FlexGrid Stage 1: Use HEMCO to read met fields
- AFCID emissions inventory (anthropogenic PM2.5 from dust)
- Updates to eliminate differences between single and multi-segmented GEOS-Chem runs
- Updates and fixes for the CEDS emissions inventory
- Add explicit unit conversions into the HEMCO configuration file
- Fix mass conservation in non-local PBL mixing
- Budget diagnostics defined as change in column mass across individual components
- Add support for continuous integration (i.e. test commits as they are pushed to Github)
- Structural updates to facilitate interfacing GEOS-Chem into WRF
- Structural updates to facilitate interfacing GEOS-Chem into GEOS-5

For a complete description of this version, please see:

- GEOS-Chem 12.1.0 (subsection of the GEOS-Chem 12 wiki page)

Model Development Priorities

The GEOS-Chem Steering Committee has prioritized several updates that will be added into versions following 12.1.0. You can read more about them here:

- Updates to be added into GEOS-Chem 12.2.0
- Updates to be added into GEOS-Chem 12.3.0

In addition, several more features have been identified as priorities for GEOS-Chem, but have not yet been assigned to a specific version:

- Ready to go in
- Almost there (less than 6 months away)
- Over the horizion (6-12 months away)
- Longer term (12-24 months away)

We invite you to review these list of proposed features. If you would like to “champion” a particular feature for inclusion into GEOS-Chem, then please contact the relevant GEOS-Chem Working Group(s).

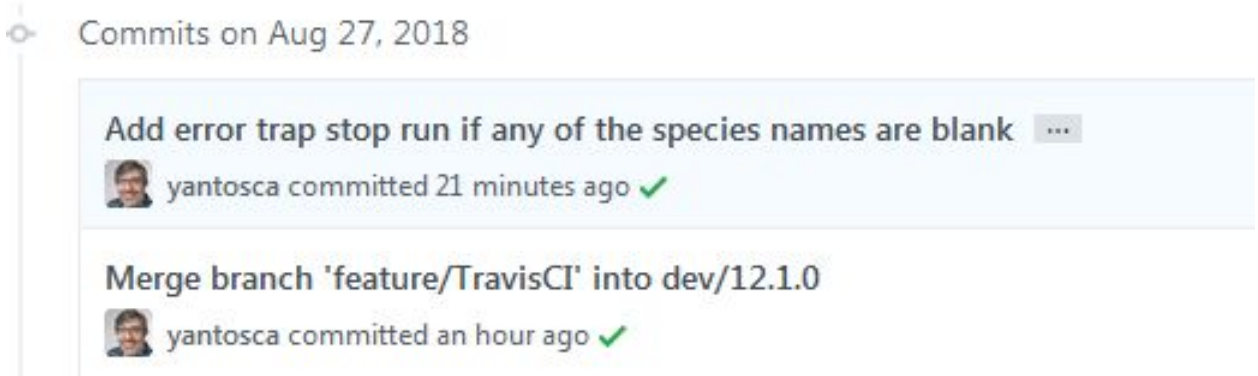
Continuous integration with TravisCI

We have now linked the GEOS-Chem Github repository to the continuous integration tool TravisCI. Each time a commit is pushed to the repository, TravisCI will perform a test to ensure that the commit will not "break" GEOS_Chem. Right now, TravisCI only compiles GEOS-Chem, but we will eventually implement compile-and-run tests in the near future.

You can see the TravisCI status page for GEOS-Chem here:

- https://travis-ci.com/geoschem/geos-chem/builds

Also, if you navigate to the "commits" page of the GEOS-Chem Github repository, you will see a green checkmark next to each commit that was checked by TravisCI and passed:



As of this writing, TravisCI is only operational with the GEOS-Chem 12.1.0 development branch. When GEOS-Chem 12.1.0 is released, then commits pushed to any branch of the GEOS-Chem Github repository will be checked by TravisCI.

Structural updates for interfacing GEOS-Chem into WRF

Haipeng Lin (working with Prof. Tzung-May Fu at Peking University) has begun to make structural changes in order to facilitate interfacing GEOS-Chem into WRF. Several of Haipeng's initial updates have been added "under-the-hood" into GEOS-Chem 12.0.0 and GEOS-Chem 12.0.1.

Much of this work involves moving arrays out of modules and into the state variables (State_Met, State_Chm, and State_Diag). This is necessary because WRF needs to be able to dynamically resize arrays from the global grid dimensions to the regional grid dimensions on each node of a distributed-memory computing environment. Even though GEOS-Chem currently passes most global quantities via the state variables, there remains a significant amount of legacy and/or 3rd-party code where arrays are passed from one module to another via USE statements.

The necessary structural updates will impact several areas of GEOS-Chem, especially in the aerosol, SOA, and microphysics modules. We believe that the necessary updates can be made "under-the-hood" in a way that will minimize disruption to GEOS-Chem users.

Other GEOS-Chem news

Proposed updates to benchmark plots

The GEOS-Chem Steering Committee is discussing how the plots from the 1-month and 1-year benchmark simulations can be more easily presented online. We will post more information about this shortly.

The GEOS-Chem Support Team will soon begin the process of migrating the benchmark plotting code from IDL (which is proprietary) to Python (which is free and open-source). This will improve the portability of the plotting code while also making it easier to maintain and update. It will also allow us to finally retire the "binary punch" diagnostic output that is now replicated as netCDF output. The new benchmarking suite in python will include support for handling GCHP output on the cubed sphere grid.

GCHP update

GCHP is compatible with 12.0.1 and validation is in progress. Please see the following resources for more information about the latest version of GCHP:

- GCHP version history
- GCHP Online User Manual
- GCHP Home Wiki Page

Lizzie Lundgren has also compiled a handy guide of items that need to be changed in GCHP when making updates to GEOS-Chem Classic. We encourage all GEOS-Chem developers to review this list to ensure compatibility of their updates with GCHP. For more information, please see:

- GCHP updates required with GEOS-Chem Classic Updates (on GEOS-Chem wiki)

As always, if you or someone you know is working on a project using GCHP, please help us collect the project information in the GCHP projects list. Please contact the GEOS-Chem Support Team with questions.

Running GEOS-Chem in the Amazon cloud

Jiawei Zhuang has created a tutorial that shows how you can run GEOS-Chem "Classic" (GCC) on the Amazon Web Services EC2 cloud computing platform. A copy of the GEOS-Chem "gcgrid" data directories has been synchronized to the Amazon S3 storage system and is available for use with your GEOS-Chem simulations.

IGC9 will take place in May 2019!

IGC9 will be held at Harvard on May 6-9, 2019, with model clinics and Young Scientists' social on May 5. Registration will open up in December. More information will be posted to the IGC9 website at a later date. For now, mark your calendars, and see you in May!

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

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