GEOS-Chem

Winter 2021 Newsletter

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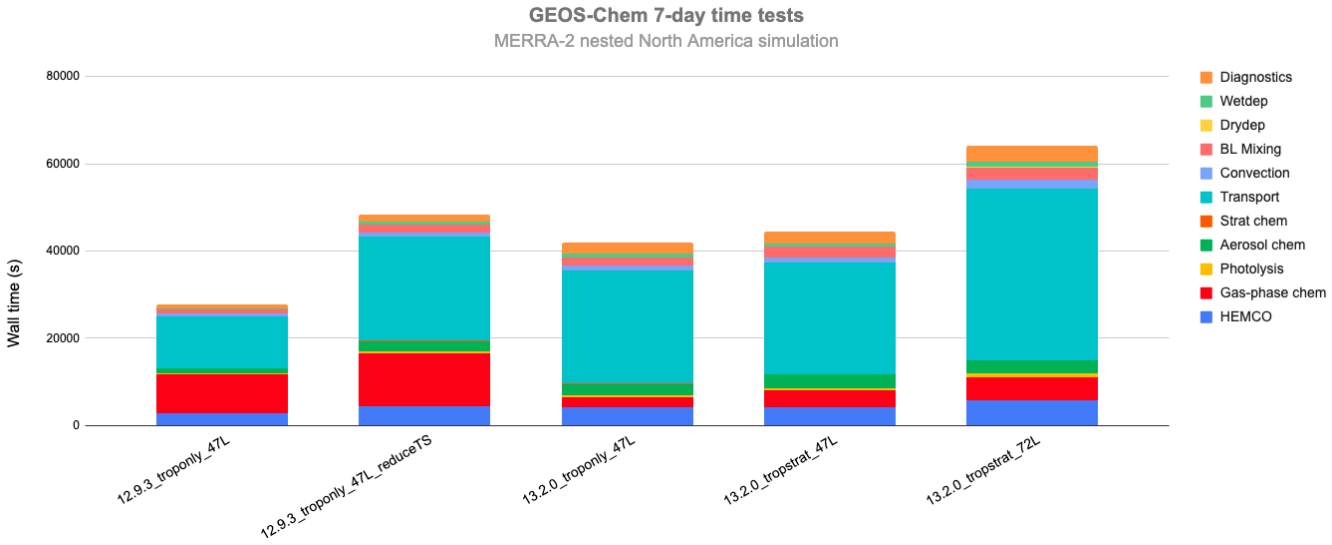
1. Featured News

1.1 Speeding up nested-grid simulations with choice of timesteps

Several GEOS-Chem users had reported that their nested-grid simulations (especially those using the full-chemistry mechanism) were taking an inordinately long amount of time to complete. GCST member **Melissa Sulprizio** recently performed a set of experiments in order to identify the bottleneck.

Melissa wrote:

> My 7-day nested-grid timing test simulations comparing GEOS-Chem 12.9.3 with 13.2.0 seem to confirm that the culprit is in the reduced timesteps. I used the 0.5x0.625 nested North America grid and MERRA-2 meteorology for 2019/07/01-2019/07/07. I used ifort 19.0.5 and all 48 CPUs on 1 Intel Cascade Lake node.



For full timing test results see [this Google Sheet](#).

The leftmost stacked bar is for the default troponly nested-grid simulation in 12.9.3, which used transport/chemistry timesteps of 10/20 minutes (600/1200 s). I ran the same simulation with the 5/10 minute (300/600 s) timesteps used in GEOS-Chem 13 nested-grid simulations. In that simulation (12.9.3_tropchem_47L_reduceTS) we can see similar timing results to the 13.2.0_troponly_47L and 13.2.0_tropstrat_47L simulations (troponly = tropospheric chemistry only; tropstrat = tropospheric + stratospheric chemistry; 47L = GEOS-Chem ran with 47 vertical levels). In fact, the 13.2.0_troponly_47L simulation is faster than the comparable 12.9.3_troponly_47L_reduceTS simulation due to improvements and bug fixes in the gas-phase chemistry routines that have been implemented since 12.9.3.

I would therefore recommend that users revert to the 10/20 minute (600/1200 s) timesteps in input.geos for MERRA-2 nested-grid simulations if they are looking to improve run

time. I will follow up with the Nested Model Co-Chairs to make sure they are on board with this recommendation and, if so, we can implement this fix in GEOS-Chem 13.3.0.

See the full discussion here: https://github.com/geoschem/geos-chem/discussions/875.

As a result of Melissa's investigation, in GEOS-Chem 13.3.1 and later versions, full-chemistry nested-grid simulations running on the 0.5º x 0.625º grids will use a transport timestep of 600 seconds and a chemistry timestep of 1200 seconds by default.

1.2 Retirement of GEOS-Chem data servers

We invite you to begin downloading data from **http://geoschemdata.wustl.edu**, which is the new GEOS-Chem data server at Washington University in St. Louis (WashU). If you have access to Globus, you may also download data from the **GEOS-Chem data (WashU)** endpoint. Either way, you will get lightning-fast data download speeds.

With the WashU data server having come online, we will retire the following data servers:

- **Harvard:** http://ftp.as.harvard.edu/gcgrid/data/ExtData/.
- **ComputeCanada:** https://geoschemdata.computecanada.ca
    - NOTE: This link will start redirecting to the WashU server soon.

1.3 New GEOS-Chem website

Please take a moment to view our new GEOS-Chem website, which is now online at **geos-chem.org**. In particular we would like to thank Harvard web designer Vittorio Bucchieri, who spent many hours porting the site to a new platform while trying to preserve its functionality and user experience.

We appreciate your feedback and your vision for the GEOS-Chem website! Please send your thoughts to us at geos-chem-support@g.harvard.edu.

2. List of recent GEOS-Chem publications

Here is a list of the most recent GEOS-Chem publications. For the complete list (with links to each article), please visit our GEOS-Chem Publications Page on Google Scholar.

The Google Scholar page is generously maintained by GEOS-Chem user **Gongda Lu**. If you find that any of your GEOS-Chem co-authored papers are missing from the Scholar page, please email Gongda (**gxl642@student.bham.ac.uk**) with the title of the publication.

- *Exposure and dose assessment of school children to air pollutants in a tropical coastal-urban area*, YKL Kitagawa, P Kumar, ES Galvão, JM Santos, NC Reis Jr, Science of The Total Environment, 803, 149747, 2022.

- *Exploring dust heterogeneous chemistry over China: Insights from field observation and GEOS-Chem simulation*, R Tian, X Ma, T Sha, X Pan, Z Wang, Science of The Total Environment, 798, 149307, 2021.

- *The added value of satellite observations of methane for understanding the contemporary methane budget*. PI Palmer, L Feng, MF Lunt, RJ Parker, H Bösch, X Lan, A Lorente, ... Philosophical Transactions of the Royal Society, A 379 (2210), 20210106, 2021.

- *Tropospheric NO2 and O3 response to COVID-19 lockdown restrictions at the national and urban scales in Germany*, V Balamurugan, J Chen, Z Qu, X Bi, J Gensheimer, A Shekhar, … Journal of Geophysical Research: Atmospheres, 126 (19), e2021JD035440, 2021.

- *Gas-Phase Oxidation Rates and Products of 1, 2-Dihydroxy Isoprene*, KH Bates, JD Cope, TB Nguyen, Environmental Science & Technology, 2021.

- *Trifluoroacetic acid deposition from emissions of HFO-1234yf in India, China, and the Middle East*, LM David, M Barth, L Höglund-Isaksson, P Purohit, GJM Velders, S Glaser, …, Atmospheric Chemistry and Physics, 21 (19), 14833-14849, 2021.

- *Grid-stretching capabilaty for the GEOS-Chem 13.0. 0 atmospheric chemistry model*, L Bindle, RV Martin, MJ Cooper, EW Lundgren, SD Eastham, BM Auer, …, Geoscientific Model Development, 14 (10), 5977-5997, 2021.

- *Health Burden and economic impacts attributed to PM2. 5 and O3 in china from 2010 to 2050 under different representative concentration pathway scenarios*, Y Wang, J Hu, J Zhu, J Li, M Qin, H Liao, K Chen, M Wang, Resources, Conservation and Recycling, 173, 105731, 2021.

- *UK ammonia emissions estimated with satellite observations and GEOS‐Chem*, EA Marais, AK Pandey, M Van Damme, L Clarisse, PF Coheur, … Journal of Geophysical Research: Atmospheres, e2021JD035237, 2021.

- *Harmonized Emissions Component (HEMCO) 3.0 as a versatile emissions component for atmospheric models: application in the GEOS-Chem, NASA GEOS, WRF-GC, CESM2, NOAA GEFS-Aerosol* …, H Lin, DJ Jacob, EW Lundgren, MP Sulprizio, CA Keller, TM Fritz, …, Geoscientific Model Development, 14 (9), 5487-5506, 2021.

- *Risk and burden of hospital admissions associated with wildfire-related PM2.5 in Brazil, 2000–15: a nationwide time-series study*, T Ye, Y Guo, G Chen, X Yue, R Xu, MSZS Coêlho, PHN Saldiva, Q Zhao, …, The Lancet Planetary Health, 5 (9), e599-e607, 2021.

- *Understanding Sources of Atmospheric Hydrogen Chloride in Coastal Spring and Continental Winter*, AA Angelucci, TC Furlani, X Wang, DJ Jacob, TC VandenBoer, CJ Young, ACS Earth and Space Chemistry, 2021.

3. GEOS-Chem Version Releases

Since our last newsletter, the following GEOS-Chem versions have been released:

3.1 GEOS-Chem 13.3.0

Release Date: 15 Nov 2021

GEOS-Chem 13.3.0 contains the following updates:

- Gas-phase chemistry updates:
  - Update of aromatic VOC chemistry
  - Addition of C2H2 and C2H4 chemistry
  - Addition of CH3O2 + OH reaction
  - Addition of HMS chemistry
- Heterogeneous chemistry updates:
  - Cleaning up het chem reaction rate computations for clarity and efficiency
  - Updates to IONO2 hydrolysis reaction following Wang et al. (2021)
  - Revise gamma(N2O5) computation; cap A at 3.2e-8
  - Fixed typo in routine CloudHet
  - Fixed typos in ClNO2 hetchem reactions: HNO2 should be a product, not HNO3
  - Add better error trap criteria to prevent reaction rate computations from blowing up
- Emissions updates:
  - Add option to use NEI2016 emissions over the US (turned off by default)
  - Avoid double counting of acetone source from monoterpenes when using online MEGAN
  - Update volcano emissions to May 2020 and add climatology
  - Updated offline dust emissions from Meng et al. (2021)
    - NOTE: benchmark simulations use online dust emissions instead
  - Send all HEMCO error messages to GEOS-Chem log
- Other updates:
  - Updated aerosol dry deposition
  - The ObsPack diagnostic can now use the ?ADV? Wildcard
- Features only affecting GCHP:
  - Include thread number in GEOS-Chem and HEMCO error messages
  - GCHP Adjoint updates

Please see the following pages for details on these updates, including benchmarks:

- 13.3.0 wiki page
- 13.1.0 Github milestone for geoschem/geos-chem
- 13.1.0 Github milestone for geoschem/GCHP
- 3.2.0 Github milestone for geoschem/HEMCO

3.2 GEOS-Chem 13.3.1

Release Date: 15 Nov 2021

GEOS-Chem 13.3.1 contains fixes for minor issues that were discovered during the 13.3.0 benchmarking process:

- Diagnostic fixes:
    - Fix incorrect units in ProdLoss diagnostic output
    - Bug fix: Remove second underscore from State_Chm Hg simulation fields
    - Remove duplicate unit conversion from kg/kg dry to v/v dry in planeflight_mod.F90
    - Now allow GEOS-Chem Classic History collection names to contain an underscore
- Other updates and fixes:
    - Stop gracefully if the chemical solver fails to converge to a solution twice in a row
        - Also print out concentrations and reaction rates at the affected grid box, which can aid in debugging the problem
    - Fix call to timers in fullchem_mod.F90
    - Use default timesteps (transport=600s, chemistry=1200s) for nested-grid simulations using 0.5° x 0.625° grids
        - EXCEPTION: CH4 simulations at 0.5° x 0.625° will still use transport=300s, chemistry=600s timesteps
    - Fix incorrect file path in TOMAS routine YuIMN_Code.F90
- GCHP updates and fixes:
    - Fix incorrect file timestamp with freq=1hr and duration=24hr
    - The cleanRunDir.sh script now removes additional log files produced by GCHP

Please see the following pages for details on these updates:

- 13.3.1 wiki page
- 13.3.1 Github milestone for geoschem/geos-chem
- 13.3.1 Github milestone for geoschem/GCHP
- 3.2.1 Github milestone for geoschem/HEMCO

3.3 GEOS-Chem 13.3.2

***** THIS IS THE CURRENT STABLE GEOS-CHEM VERSION *****

Release Date: 18 Nov 2021

GEOS-Chem 13.3.2 a bug fix for GCHP::

- Fixed incorrect file path to OFFLINE_DUST emissions in ExtData.rc
    - NOTE: This will not change any benchmark results, as GCHP benchmarks use the online dust emissions.

Please see the following pages for details on these updates:

- 13.3.2 wiki page
- 13.3.2 Github milestone for geoschem/geos-chem

If you are considering updating your GEOS-Chem version, please download 13.3.2 instead of 13.3.0. This will make sure that you will have the most up-to-date bug fixes.

4. Model development priorities

The GEOS-Chem Steering Committee regularly prioritizes science updates for inclusion into GEOS-Chem. Please view our Model Development Priorities wiki page to view a list of prioritized updates.

We have already started work on several of these updates, which we hope to include in GEOS-Chem 13.4.0 (to be released in late February or early March 2022).

5. Ongoing Development

5.1 Updates on GCHP with Amazon Web Services (AWS)

GCST members **Liam Bindle** and **Lucas Estrada** are working on running GCHP with Amazon Web Services (AWS). We have successfully tested simulations on AWS with up to 1044 cores and C180 resolution (higher values not tested). We are aware of an outstanding issue where simulations hang if too many output variables are requested, but the threshold for "hanging" is higher than generally required for scientific simulations (30-100 output variables is the threshold). This means that AWS, today, is a feasible platform for conducting scientific GCHP simulations.

We are also working to establish an efficient workflow for running GEOS-Chem simulations on AWS. The goal is to reduce GCST hours spent on manually testing pull requests and structural updates, by creating an automatic pipeline that can initiate, execute, and plot the results of test simulations. In addition to reducing human hours spent on testing, the tooling is broadly applicable to facilitating the use of GEOS-Chem on AWS. Specifically, automatically synchronizing GEOS-Chem input data according to simulation period, GEOS-Chem version, and meteorology, and a suite of conveniently available AMIs and Docker/Singularity images with pre-built GEOS-Chem dependencies.

5.2 Kinetic PreProcessor (KPP) updates

The GEOS-Chem Support Team has taken over further development of the KineticPreProcessor (KPP), which translates a chemical mechanism specification from text format to highly-optimized Fortran source code that can be directly added to atmospheric models such as GEOS-Chem.

This work has advanced along the following fronts:

5.2.1 Consolidation of divergent branches of development

GCST members **Bob Yantosca** and **Lucas Estrada** have created a new Github repository for KPP at https://github.com/KineticPreProcessor/KPP and are working on merging prior KPP lines of development into the main branch of this repository.. The current KPP repository (https://github.com/geoschem/KPP) will eventually be retired.

5.2.2 Implementation of continuous integration testing

Lucas and Bob have created a Microsoft Azure pipeline for continuous integration. This pipeline runs a suite of tests whenever a commit is pushed to the KPP Github repository. Each individual test in the suite (1) uses KPP to generate source code files for solving an example mechanism; (2) compiles this code (plus a driver program) into an executable; and (3) runs the executable in order to integrate the chemistry mechanism forward by a short amount of time. These tests are designed to identify source code modifications that would break existing functionality.

5.2.3 Adding an adaptive solver capability

GCST member **Mike Long** and Harvard graduate student **Haipeng Lin** have been working on introducing an adaptive solver capability within KPP. They have found that it is possible to subset any chemistry mechanism to remove “slow-reacting” species from the Jacobian matrix for each grid box and on each chemistry timestep. This method, which can potentially speed up the forward integration step by approximately 50%, is based on Shen et al [2020] with more flexible implementation.

The adaptive solver capability in KPP is currently undergoing validation. We hope to be able to bring it into GEOS-Chem in the near future.

5.3 Replacing FAST-JX with Cloud-J

GCST member **Lizzie Lundgren** is working to replace FAST-JX with Cloud-J in GEOS-Chem. Developed by **Michael Prather** (UC Irvine), Cloud-J is a multi-scattering eight-stream radiative transfer model for solar radiation that improves on FAST-JX. As part of this work Cloud-J is now developed under Git version control, the Cloud-J standalone model is available on GitHub at https://github.com/geoschem/cloud-j, and users may now build the model with CMake. Work to implement Cloud-J as an alternative to FAST-JX within GEOS-Chem is in progress. Validation will be done prior to removing FAST-JX from the model. For more information about this work, please see GEOS-Chem GitHub Issue #953.

5.4 Separating 4D species array into vector of 3D arrays

GCST member **Lizzie Lundgren** is working on a structural update to store concentrations in one 3D array per species, with access to all concentration arrays via 1D species vector. Currently species concentrations are stored in a 4D array called State_Chm%Species which is allocated with dimensions State_Grid%NX, State_Grid%NY, State_Grid%NZ, and State_Chm%nSpecies.

The motivation of this update is to reduce the memory footprint for GCHP and for GEOS-Chem run within GEOS by making the species concentration containers the same size as those stored in the MAPL internal state. Having them the same size would allow (1) pointing the new 3D concentration arrays to the internal state and (2) avoidance of allocating and copying 3D concentration arrays to contain duplicate information.

We propose to issue this update as part of a GEOS-Chem 14.0.0 major release. It will require changes to the code throughout the model due to the extensive use of State_Chm%Species and will therefore likely cause conflicts when merging with separate lines of development.

6. Steering Committee News

The GEOS-Chem Steering Committee met on 17 November 2021. We invite you to read the meeting minutes as well as the following related presentations:

- Update from the Adjoint Model and Data Assimilation Working Group
- Update from the Emission and Deposition Working Group
- GCST Update: Tools for the Amazon Web Services Cloud Computing Platform
- GCST Update: Direct Reading of GMAO Meteorological Data into GEOS-Chem

7. GCST Winter Holiday Break Schedule

Please be advised that the GEOS-Chem Support Team will be on holiday break starting on Monday, December 20th, 2021 and returning on Monday, January 3, 2022.

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

The GEOS-Chem Support Team:
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