

GEOS-Chem Steering Committee Telecon

3 Sept 2020

Attending/Missing:

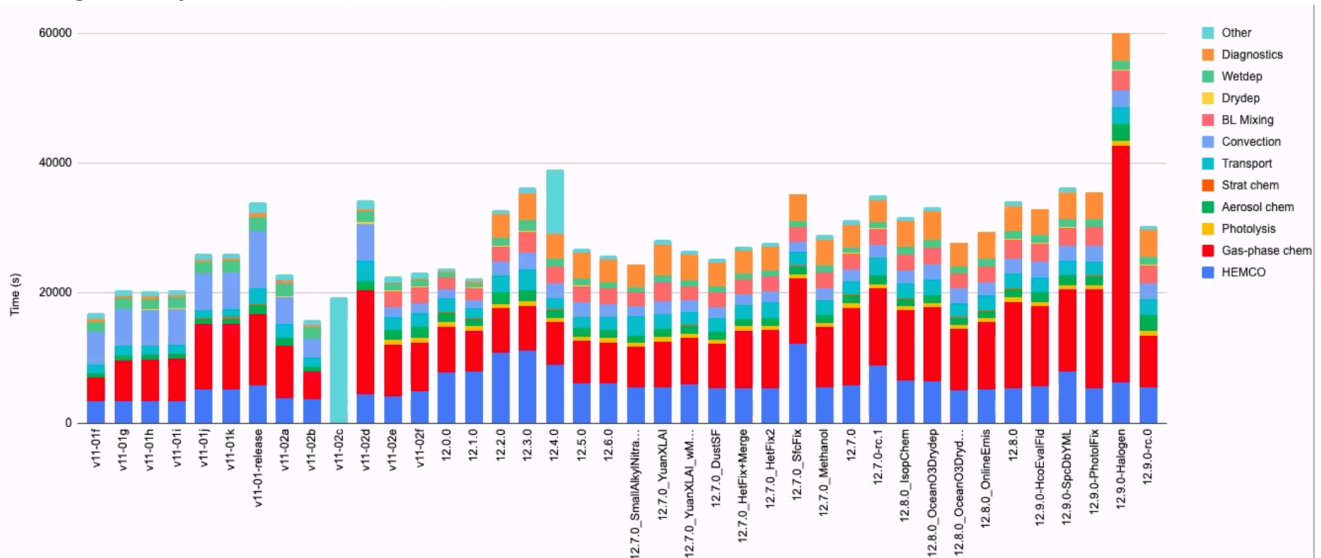
Amos Tai, Andrea Molod, Barron Henderson, Becky Alexander, Bob Yantosca, Chris Holmes, Christoph Keller, Colette Heald, Daniel Jacob, Daven Henze, Dylan Jones, Dylan Millet, Eloise Marais, Emily Fischer, Fangqun Yu, Hong Liao, Hongyu Liu, Jeff Geddes, Jeff Pierce, Jenny Fisher, Jingqiu Mao, Jintai Lin, Jun Wang, Kevin Bowman, Lee Murray, Liam Bindle, Lin Zhang, Lizzie Lundgren, Lu Hu, Mathew Evans, Tzung-May Fu, Melissa Sulprizio, Prasad Kasibhatla, Randall Martin, Sebastian Eastham, Susan Strahan, William Downs, Yanxu Zhang, Yuxuan Wang

Update from Daniel: Current version 12.9 has chemistry in a place where we're happy with it, stable template for 13.0 which will have major structural updates

1. GCE1 report (Eloise, Mat)

- Exceeded expectations; 150 registrants, with 40-50 people per session
- Feedback: people advocated for longer talks, but not great for Zoom
- Most enjoyed keynote talks (non GEOS-Chem speakers)
- Networking session was not successful
- Q&A, only a handful of people and not younger scientists
- Most people want to see it every other year alternating with international meeting
- Videos are available on GEOS-Chem website, will be distributed

2. Tracking model performance (Melissa)



- GEOS-Chem performance had indeed gotten worse from version to version; biggest offenders were HEMCO and gas-phase chem
- The HEMCO problem is transient
- We were able to greatly improve performance by cleaning up heterogeneous chemistry

3. Corrected GEOS-FP fields (Melissa)

- Jan 30 2020: switch from GEOS5.22 to GEOS5.25 – updated radiation scheme and convection scheme
- April 7 2020: GMAO addressed some bugs in the system

- Andrea recommended we use 5.22 fields until April 7th (instead of buggy 5.25)
- Jun Meng is in final stages of processing this and will transfer to ComputeCanada, will replace original fields and everyone should replace those. Email to users next week.
- Q: what about studies running over e.g. COVID period?
 - 5.22 stopped June 1
 - Consensus: make 5.22 available to interested users for full overlap, will switch default to 5.25 from end of April for consistency

4. Version 13.0 update and schedule (Melissa)

- GCST working on 13.0.0 – major version change
- Updates to classic and GCHP
- Structural updates mostly implemented, working on retiring carbon-based units and emission updates for specialty sims
- 13.0-alpha.10 for GCHP released already
- Hoping to wrap up development by end Sept, basic documentation in place (significant changes to downloading, creating run directories)
- 1-month benchmarking to start end Sept, to be followed by 10-year benchmark for strat; end of that for 1-year benchmark.
- 10-year benchmark will take ~30 days
- In interim: soft release to community (e.g. release candidate) to identify & fix bugs, etc.
- Has updated MAPL in GCHP, so should fix some memory issues, etc. Andrea has seen substantial difference in GEOS-CTM with MAPL update

5. Memory reduction for diagnostic arrays (Bob)

- HISTORY diagnostics: currently full arrays allocated, even if you're only using e.g. one species. Especially problematic in ESMs
- Can now use reaction rate diagnostic (it was impractical before b/c used ALL reactions)

6. "Metrics" collection (Bob)

- Diagnostics in log file e.g. global mean OH problematic in GCHP b/c we need a gridded diagnostic
- Working on a metrics collection for things like total air mass in each column, total OH in each column individually to be saved to output diagnostics
- Python script provided in run directories will allow us to print those diagnostics after the run
- Working in Classic, hitting a technical issue in GCHP; planning to change units to avoid overflow issues
- Q: How does it differ from the ConcAfterChem diagnostic? A: Could do that, but trying to replicate prior code for consistency. A difference may be the air mass weighting.

7. Stretched-grid capability in version 13.0 (Liam)

- Multi-scale grid for GCHP
- Transform done for cube-sphere to get finer resolution in region of interest
- Inherent 2-way coupling, smooth transition between coarse and fine grids
- Easy to specify in configuration file (stretch factor, center lat/lon)
- Have to regrid restart file to stretch grid, tool going into GCPy for that
- Will be in GCHP v13 but already working and tested so anyone can reach out to Liam to start now
- Manuscript in progress that contains guidance on choosing stretch factor parameter
- Q: can we choose multiple regions? A: only one region at a time (would be a lot of work to generalize to multiple regions)
 - Note that two way coupling is available in GEOS-Chem classic, can run multiple regions that way

- Q: are there any mass conservation issues? A: haven't explicitly checked for that but nothing noticeable in benchmarks
 - Might be worth checking on this for long-lived GHGs, different time scale than usually tested
 - Should do transport benchmark with inert tracer to test for this
- Q: what is range of stretch factor? A: 1 = normal cube sphere @c24(?); have tested up to a factor of 10 which gives very high res
- Q: calculation cost? A: overhead pretty minimal, about 20% of base simulation cost; much more efficient than moving to global high resolution
- Q: will changing stretch factor change domain size? A: yes – higher stretch factor → narrower domains; guidance in manuscript
- Q: timestep? A: no additional things that are done automatically; Liam has been doing this manually but left up to user

8. GCPy release in version 13.0 (Will)

- GCPy 1.0 first official release
- Easy installation through conda forge in formats for users and users/developers
- Extensive, up-to-date documentation included example scripts, videos, wiki on GCPy github repository
- Support for stretched-grid regridding
- Already includes spatial plotting (single level, zonal mean, regional, global, cube sphere, lat-lon)
- Q: will it come with a doi? A: we can add one like we do for GEOS-Chem versions (should also do for standalone HEMCO)

9. RRTMG in version 13.0 (Colette)

- Has been an option in GEOS-Chem for some time using bpch diagnostics
- Jonathan Moch found some issues with netcdf diagnostics
- Seb found some issues with implementation plus a bug
- Lizzie has been trying to fix all the issues to work properly in netcdf diagnostics
- V13 will retain both bpch and netcdf for last iteration
- Will be in both Classic and GCHP
- Not included in the benchmark simulation

10. Benchmarking (Randall)

- Process is good, objectives have not been documented
- Opportunity to consider these objectives
- Randall & Daniel have drafted a few ideas:

Benchmarking supports the maintenance of GEOS-Chem as a robust state-of-the-science facility with a nimble grass-roots approach and strong version control. Benchmarking has main objectives:

- 1) Document the standard recommended GEOS-Chem model configuration, and the expected characteristics of that configuration.
 - 2) Support version control through traceability, and by confirming the accurate implementation of model developments submitted by the community.
 - 3) Track the evolution of the model over the years
 - 4) Promote scientific transparency of GEOS-Chem
- Update “accurate implementation” to “expected behaviours”
 - “standard recommendation” – most users don't run with all chemistry; offline vs. online emissions, two SOA schemes... “the default” instead? But defaults are not what are in benchmarks. “a standard configuration with frequently used features?” add something about user should choose most

appropriate configuration

11. AIST GCHP project update (Randall)

- Seb has made progress on directly reading in cube sphere data to eliminate pre-processing data
- Christoph has made available full year of native MERRA-2 data
- GCST updates easier for implementing GMAO updates in GCHP
- Package manager will make it easier to document updates

12. Notification and record of GEOS-Chem publications (Randall)

- Paul Palmer expressed interest in new GEOS-Chem publications
- Used to track via Web of Science but switch to Publons broke this
- Can Google Scholar help do this with GEOS-Chem group?
- Monthly or quarterly digest?
- Go into newsletter?
- If a listserve or other similar group like github issue, user can configure own frequency
- <https://umd.libanswers.com/faq/125299>

13. GMAO updates (Andrea)

- Nothing to update

14. NEI16 updates and vertical allocation in CEDS (Barron)

- Have some benchmarks, things are performing well, will be distributed soon
- Other models like CMAQ provide sector-based representative vertical allocation for anthropogenic emissions
- Current version of GEOS-Chem – CEDS doesn't have vertical allocation, but NEI11 (and eventually NEI16) does
- Currently use 3 levels, look at stack height but don't do full plume rise
- For NEI16, Barron has been using the CMAQ hemispheric representative vertical allocation
- Should we do this for other anthropogenic inventories like CEDS, others? HEMCO offers three distinct ways to do that (static file read once, inventories apply their own)
 - Example: NEI16 was originally using 29 layers daily → lots of extra file i/o
 - Has implications for surface concentrations (e.g. at night, diff between surface layer vs above PBL)
- Barron has this for 9 sectors (e.g. power, oil & gas, etc.)
- Jintai has been thinking about implementing a 20-m surface layer within first model layer that could help with a lot of things including emissions, nighttime simulations, ozone simulations
 - Not sure about difficulty of that
 - Would be very valuable!
 - "pseudo layer" near surface? But difficult to downgrade resolution
 - Sometime next year GEOS-FP will have many more vertical layers, extra near surface
- For now makes sense to apply Barron's sector-specific allocation

15. GC-YIBs and new ecophysiology module (Amos)

- Xu Yue – GC-YIBs coupled biosphere/ecosystem model with GEOS-Chem
- Available to community at MERRA2 native plus standard GEOS-Chem Classic global resolutions
- All input data hosted at NUIST
- New ecophysiology module from Amos's group – not fully fledged biosphere model, just most important processes implemented directly in GEOS-Chem. LAI, canopy height are not dynamically simulated

- Biggest difference is time scales. Multi-decadal co-evolution should use GC-YIBs; shorter time scales can use ecophysiology module (don't need to simulate full carbon cycle)
- Ecophysiology module mature but not yet published, can share now
- To be hosted at CUHK, they will be responsible for making sure it stays up to date with versions of GEOS-Chem
- Not very clean to couple at moment – one would get full coupled code from CUHK, maybe a bit behind standard GC

16. Review of model development priorities (Daniel, all)

- All to look at priorities, see what needs to be cleaned up, prioritized, etc.
- Need this ready post 13.0 for 13.1
- Will be important activity at next SC meeting

17. IGC10 planning (Daniel)

- Still planning on in-person meeting week of May 3-7 at Harvard
- Daniel has started to raise some money for this
- If cannot have physical meeting should move to May 2022
- Might need to think about hybrid models, including for working group meetings

For next GCSC meeting – by email to Randall:

- Welcome volunteers for working groups that would like to provide WG updates at next GCSC – can rotate
- Welcome suggestions for GCSC meetings