GEOS-Chem Steering Committee Telecon
4 November 2019

Attending/Missing**:**

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

1. **General update (Daniel)**
   - New member of support team at Harvard: Will Downs
   - NASA has funded a new AIST technology project led by Randall on GCHP development
2. **Engineer's report (Bob + GCST)**
   - New major release (v13) sometime in early 2020 to be consistent with GMAO updates
   - Moving GEOS-Chem run directory creation into source code
   - Changes to the way GCHP is structured (wrapper repository)
   - v13 will come out after v12.8
   - Most diagnostics have now been moved to netcdf except a few speciality sims & planeflight/satellite diagnostics
   - Now using continuous integration– any updates to github trigger automatic tests to ensure compilation – and continuous deployment which means a new container will be automatically created with each release
     - Q: Is expectation that we will all now use containers for installing GC on our systems? A: it is an option (e.g. for cloud, new systems), but not a requirement if you already have libraries installed
     - Q: Will it apply to GCHP as well? A: Probably in v13.0 (TBD – but will just be for one node); for now it is just ready for GC Classic
     - Q: how easy will v13.0 library builds be if not using container? A: Spack makes this relatively straightforward
     - Q: In China, cannot access Spack or containers; is there a way GCST can provide information on which MPI, intel, etc. versions should be used? A: GCST is aware of this. Best option would be to have a GCST member in China that can test/install/come up with optimal configuration. Ongoing conversation.
   - Starting with v12.7 we will have a GEOS-Chem "dry run" option that will print out all the files and check whether you need to download them, paired with a script to download
   - Migrating all support requests to Github; Lizzie will create some tutorials
   - 12.6.0 & 12.6.1 (bug fixes) out; 12.7.0 out soon followed by 12.8.0

3. **Aromatic chemistry status (Daniel, Jintai, Mat)**
   - Was going to go into 12.7 with SAPRC mechanism. Ran into some issues – but fundamentally SAPRC has a different approach to dealing with radicals than the rest of the GEOS-Chem mechanism. Concern about inconsistencies so started thinking RACM2 mechanism might be better for standard model. Currently testing RACM2 mechanism implementation – if it looks good it will go in to standard model.
   - SAPRC mechanism is available from Jintai for anyone interested.

4. **Halogen chemistry status (Mat)**

- Many parallel updates, we now have a stable version developed by Xuan Wang bringing together the different strands, it does not break ozone according to tests by Tomas Sherwen. We need to bring it into the standard model ASAP. It is not specifically documented in literature but it is a compilation of various published things so it is citable. Xuan will be writing a paper documenting this version. It is stable enough to go into the standard model now (currently slated for 12.9.0 but may change with timing of v13).

5. **Dealing with isoprene SOA in Kelvin's new mechanism (Daniel)**
   - Lots of interest in getting Kelvin's isoprene mechanism into standard model but it makes too much SOA from lots of low volatility products (research question, Kelvin is working on that). Plan for now is to use as isoprene precursors species only the ones previously identified by Eloise, keep her isoprene SOA scheme. If we do this, it should give us numbers that are comparable to standard model. We will evaluate against SE US which is where Eloise developed her mechanism. This approach will be citable as gas-phase isoprene chemistry from Bates, isoprene SOA from Marais (for now). Will eventually deal with those low volatility products.
   - Q: Are there other places in the world we can do evaluation besides just SE US? A: We need places where isoprene SOA is a reasonable contribution to SOA. If the goal is to reproduce Eloise's work then we will evaluate in same way. But there is a longer term issue here of monoterpene SOA being more important in many places.

6. **Aerosol-radiation interactions in GEOS-GC and CESM GC (Christoph, Seb)**
   - Tabled to next GCSC meeting when Christoph is available.

7. **HEMCO restructuring (Lizzie, Melissa)**
   - Coming out of CESM project but also consistent with GCHP needs
   - Will split up core routines to deal with I/O, regridding, and scale factors / masks separately
   - Won't impact GEOS-Chem classic in any way, purely structural
   - Might be some usability updates that come out of this that impact config files

8. **Reporting bug fixes (Lizzie, Jenny)**
   - Best way to communicate new bugs & fixes to users
   - Proposing a trial for the next quarter of using GitHub notifications for anyone who would like to be aware
   - Can customize notification settings for which bugs you want
   - Would get an email for each new bug but not subsequent (unless you set)
   - Can choose to get things via web or email and GCST has specific keywords in subject so that you can easily filter email
   - If user wants to follow a conversation because it is relevant, you can subscribe directly from the email
   - Lizzie will put together YouTube videos about all of this
   - Looking for people to trial and provide feedback

9. **Centralizing GEOS-Chem data (Randall)**
   - Current source of confusion that some files are stored at Harvard FTP, Dal FTP, Compute Canada
   - Centralizing everything to avoid errors and confusion
   - Compute Canada is currently the best place for this
   - Setting up a sync to make sure everything is up to date
   - Harvard & Dal FTPs being phased out

- Longer term setting up a repository at WashU – will be tested, could eventually be the primary repository, may be advantages to having two duplicated identical repositories, but there is time to work this out and we will decide as and when
- At the moment, Compute Canada is a 3-year grant (Dylan J is co-I), likely to be able to continue for some time

10. GCHP updates and benchmarks (Randall, Seb)
- Randall leading a just-funded NASA project to further develop GCHP with focus on accessibility. Enhancing connection with GMAO, performance and portability, cloud capability, archiving cube-sphere met.
- Liam Bindle has been making progress towards stretch grid capabilities
- Regularizing GCHP benchmarking – now minor version benchmarks
- A couple of bugs have crept in and are being resolved; one in particular had to do with a vertical coordinate – these are now getting caught more rapidly with additional benchmarking
- Working more and more with GMAO on reducing memory issues in GCHP (tracked to issue with MAPL, being diagnosed with their help). Also working to reduce the issues with multi-run and continuous run.

11. GCHP adjoint updates (Kevin, Daven)
- Need to get GCHP to run backwards in time – have made some progress in doing this. Emissions is a tricky component of this still being worked on.
- Conversations with Adjoint Center for Satellite Data Assimilation – working on public repository of data assimilation approaches. More explicitly linking adjoint GCHP with broader inverse modelling projects from this Center.

12. GEOS-Chem versions 12.7 and 12.8 (Daniel)
- 12.7.0: updated ozone deposition to ocean (Mat Evans), small alkyl nitrate chemistry (Jenny Fisher), methanol as part of chemical mechanism (Dylan Millet), optional updated nitric acid rainout and washout (Fanqun Yu). Likely ready within a couple of weeks.
    - Fanqun has evaluated updates in 12.6.0. In default, GEOS-Chem overpredicts nitrate everywhere they have looked by factor of 2-3. Sulfate looks fine except in Arctic & remote regions (too high). With updates, nitrate & ammonium look good everywhere, but sulfate underpredicted in US, Europe, but looks good in Arctic & remote regions. Sulfate underestimate occurs in winter. Working on that by focusing on SO2 chemistry. Chemistry in mixed-phase clouds has a large impact. Also looking at pH in clouds. Finding that they can bring underestimate down. Also some updates for cold clouds in upper troposphere which seems to help with comparison to ATom measurements. Hopefully will be able to circulate paper soon.
    - Hongyu's group did another run with Fangqun's update where they turned off ice scavenging and this fixed some issues with lifetimes of radionuclides – much closer to old runs.
    - Only a 1-month benchmark required because not many changes expected except rainout/washout which is optional.
- 12.8.0: updated isoprene chemistry and wet deposition parameterization for water soluble organics. This will get a 1-year benchmark
- 12.6.0 brought OH into a reasonable range
- 12.9.0: halogen chemistry (TBD with v13)
- Aromatic chemistry will go to head of the queue when it is ready.

13. GEOS-Chem town hall and clinic at AMS (Daniel)

- GC Town Hall Thursday at noon – general overview of model and recent updates. Geared both for non-GC users and GC users.
- GC clinic at Harvard on Friday (AMS ends Thursday) for all levels of users. Experimental – will see who shows up!

14. **Suggestion for rotating WG updates at telecons (Randall)**
- Suggesting a planned, rotating schedule with ~3 WG per telecon (= 1 update/WG/year). Would allow each group to develop substantive updates.
- WG Chairs could still speak at any GCSC call where updates are needed
- Would energize WG Chairs to try to get updates from their communities as only doing once per year

15. **Updates from GMAO and Working Groups (all)**
- Stratospheric Working Group (Dylan, Susan, Seb)
    - Seb was original developer of UCX, now officially co-chair of the WG
    - Stratospheric benchmarks needed to make sure that we don't mess up the stratosphere when we update the troposphere. Would be for annual benchmarks, compare to observations (in addition to comparisons between model versions). Seb has a Python package that will compare against column NO2, O3 from OMI plus several zonal mean species compared to MLS. Plan for first iteration with v12.7.
    - Q: how will we deal with different timescales & restart drifts? A: Seb would like a longer benchmark ideally to see how much drift in things like water vapour in stratosphere. But that will have to be done infrequently. Will need to work this out in consultation with support team. Could do 5-year simulation at 4x5 to keep it relatively quick. We will do this the next time we do a 1-year benchmark.
- GMAO (Andrea)
    - Will be posting transport tracer benchmark images for users to see (started with MERRA-2, will do GEOS-FP as well)
- Software Engineering Group (Lizzie)
    - Looking for people to get involved, especially if you have interested students – there are small projects they can be given that will be helpful to everyone.