GEOS-Chem Steering Committee Telecon
24 February 2021

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**

1. **General updates (Daniel)**
    - Hongyu stepping down from Transport Working Group co-chair
    - 13.0.0 release is impending
    - Latest newsletter (engineer's report) released
        - Last minute issues in 1-month benchmarks
        - GCHP updates
        - KPP performance improvements
        - More items and details in newsletter
    - GMAO now producing c720 hourly archive
        - Also c180 MERRA-2 data
2. **HEMCO 3.0 (Haipeng Lin)**
    - Paper soon to be submitted to GMD
    - Restructuring of code, implementation in other models
    - Abstract model-specific code to layers outside of HEMCO's core code
    - Prototype implemented in CESM2
    - Also being used at NOAA to serve emissions to upcoming UFS
    - HEMCO 3.0 will be included in GEOS-Chem 13.0.0
    - New intermediate grid functionality in GC 13.1 and beyond
    - No changes to input file (HEMCO_Config) structure
3. **Version 13.0 benchmark assessment (Daniel)**
    - 1-month and 1-year benchmarks approved
    - 10-year benchmark
        - Stratosphere in 10-year benchmark matches up well with 1-month benchmark
        - Large differences between GC Classic and GCHP, particularly in online emissions
            - Stems from difference in scaling factors

    a. **Using on-line or off-line emissions in benchmarks**
        - Should we use offline emissions in benchmarks?
        - GCHP recommends using offline emissions
        - Benchmark comparing offline emissions between GC Classic and GCHP revealed some differences between the two
        - Daniel recommends using offline in benchmarks for consistency between GC Classic and GCHP and so people know what sort of emissions are actually going into the model
        - Daniel recommends removing automatic scaling factors to eliminate extra layer of confusion / correction

        - Global correction factors currently occur during runs, when they should really be present in emissions files
        - Let people specify scaling factors for online emissions
    - Q: Which scaling factors are these?
        - For resolution dependent emissions (Dust, sea salt, biogenic VOCs, etc.)
    - Q: Are you separating this idea from scaling factors required for speciation?
    - Would be good to have scaling factors in config files rather than buried in code
    - Q: Is model less nimble for users if offline emissions are default?
        - When there is a new update, offline emissions need to be recalculated, redefined, redownloaded
            - We previously decided not to recompute offline emissions, but can recompute for benchmark year if needed
                - Would introduce step changes
    - Q: Could we run benchmark with offline emissions while calculating and saving online emissions so we can see that output as well without altering benchmark output?
    - Definitely want to preserve online emissions, document what they provide at different resolutions
    - Jintai's group was going to rerun biogenic emissions with new MODIS LAI fields
    - Perhaps possible to calculate new offline emissions automatically so that GCST can do it without contacting original inventory developer
    - Is part of the problem with using online scaling factors that it is currently a manual process to change them?
        - You have to change manually when resolution changes
        - Perhaps we should push for more resolution-aware online scaling factors
        - Implementing this ability would allow us to provide emissions to users at lower resolution (smaller files) and allow regridding to occur on their end
            - Possibly could have some of this regridding functionality in HEMCO standalone
    - Will discuss more before making changes, clearly need to clean up scaling factors currently in code
4. **Version 13.0 release (Melissa and GCST)**
    - Removed emissions inputs in input.geos (now all in HEMCO_Config.rc)
    - Improved documentation on ReadTheDocs and new run script samples
    - Various bug fixes
    - Ready to release 13.0.0 when current differences issues are fixed
5. **New GCST member Yanshun Li (Randall)**
    - Previous experience using GEOS-Chem
    - Taking over maintenance of meteorological archives
    - Welcome Yanshun!
    - Currently PhD student at WashU
6. **WRF-GC 2.0 (May)**
    - WRF-GC 1.0 released in 2019 (one domain)
    - Now can use nested grid simulations
    - Now has aerosol feedback including radiation and microphysics feedbacks
        - Developed partly from existing WRF-Chem feedback mechanisms
    - Have a GMD paper under review
    - Model downloadable from Github
7. **GCAP 2.0 (Lee)**

- Ready for public release
- Simulate any period of time for any grid that can use MERRA2, including exoplanet simulations
- Most code development in GISS model, so very few changes to GEOS-Chem code
    - Some changes to vertical grid pressures
- Archived fields for various past and future decades according to RCP scenarios
- Archived 180 simulation years that will be provided from Rochester U
- Processed CMIP6 emissions
- MERRA-driven simulations and GISS-driven simulations statistically identical
- Code publicly available on Lee's Github account
- Announcement to come in next week or so
- Manuscript will be submitted to GMD
- Q: Where does exoplanet atmosphere come from?
    - Comes from GISS; generalized to atmosphere for any rocky terrestrial planet
- Q: Have you done Mars?
    - It is not currently archived
- Q: When you were doing historical simulations, what did you do for surface variables like online dust?
    - Dust has been a nuisance because it is resolution and meteorology dependent
    - Some disagreement between different GISS and MERRA2 sims
    - Climate sensitive runs are driven online, calculated scaling factors in present day to match MERRA2 values
- GISS code will be made available for those who want to use it, but most users seem to want to use MERRA2 met fields
- Q: Will land cover maps be included in meteorological package?
    - Yes for paleo runs, for 1860 onward CMIP6 runs these haven't really been used
- Q: Will the emissions you processed be available for GC Classic as well?
    - Yes, they'll all be available for standard GC runs
    - Processed aircraft (3D) emissions to 47 levels and GISS vertical resolutions
    - Available at Rochester
    - HEMCO_Config lines / files will be provided
- Q: Is there anything you haven't done?
    - No
- Q: When you run with GCAP fields, which convection algorithm do you use?
    - As opposed to past where convection was changed to mimic convection in GISS, because GEOS-Chem uses code from NCAR model for convective transport, we use MERRA2-like convection fields with applied convection from GEOS-Chem as GEOS-Chem normally does.
    - Some differences between using different meteorologies

8. GMAO updates (Andrea, Christoph)

- Cubed-sphere archive
- FP change upcoming - upgrade related to fields in analysis
    - Q: Is there a way to find out specific date of update?
        - There's an email distribution list to get announcements that we can get you (Randall / someone else) signed up to

9. Working Group updates & perspectives:

a. Transport (Hongyu, Andrea)

- Improved wet scavenging from SUNY group's Luo et al. (GMD 2020)
    - Intended for version 13.2 to replace Luo et al. (GMD 2019)

- GEOS-Chem Rn-222 paper published (Zhang, B. et al. ACP 2021)
    - Implement new Rn-222 emissions as option in GC?
        - Currently being used as option in GEOS model at GMAO
        - Major difference is that new emissions considers spatial and temporally varying fluxes of Rn derived from soil radium measurements and soil models, as opposed to existing generally uniform emissions which use a temperature dependency
        - Improves Pb-210 simulations at high latitudes
        - Q: Is the new option used in GEOS present in the tracer gridded component?
            - Tracer gridded component has option for either new or old version
        - No real qualms to replacing existing scheme given it is so old
        - Would help compare better to observations and other models
        - Q: Is there any point to maintaining existing scheme in any form?
            - It is very simple and easy to interpret
            - New version is still quite new, so maybe use as an option rather than standard for awhile
            - But others feel that the existing scheme is so old it should be eliminated altogether in favor of newer, more accurate versions
            - Will add it to 13.2
- Stratosphere-troposphere exchange (STE) in GEOS-Chem
    - 7Be obs constraint: annually 23-27% of the 7Be in surface air at NH mid-latitudes is of stratospheric origin
    - STE in GC / MERRA2 looks OK in the mean (diff between GCC vs. GCHP, 4x5 TPCORE for GCC, c48 FV3 for GCHP)
    - Sensitivity of strat 7Be fraction to the location of tropopause (Liu et al., ACP 2016)
    - GC Starts archiving TROPPB (instead of TROPPT) for stratospheric tracer definition (to be consistent with the GEOS transport tracer)
    - Three existing tropopause pressures:
        - TROPPB: Tropopause pressure based on blended estimate (used in GEOS, not archived in GC)
        - TROPPT: Tropopause pressure based on thermal estimate (currently used in GC)
        - TROPPV: Tropopause pressure based on EPV estimate
    - Q: What is main benefit of blended vs. other estimates?
        - In the tropics, the thermal estimate is more accurate, while the higher latitudes are more accurately estimated by EPV estimate, so TROPPB may be best overall estimate
        - Almost no global model uses EPV estimate (it is invalid in tropics), so using that alone would make comparison harder
        - Thermal estimate has similar issues at poles
    - Q: What is our sensitivity to an accurate definition of tropopause pressure?
        - There is 5-10% difference in stratospheric 7Be fraction in surface air when tropopause location is shifted by one model layer
- Evaluation of benchmark radionuclide tracers with observations

        - Rn-Pb observational datasets & IDLcode for model-obs comparison sent to GCST & GMAO
        - Code for 7Be not ready, but strat 7Be fraction is a more useful diagnostic
    - Rediagnosis of RAS convection in GEOS-Chem
        - Work is finished and a manuscript is being finalized
        - It is working, recovering mass fluxes generated in a run at GC resolution. Issues in tracers more in tropics and subtropics than extratropics / polar latitudes.
        - Decision should be made if this should be the default behavior for users at specific resolutions when using FP data
    - A few things brought up by Daniel
        - Now that we have full GEOS transport tracer suite in GEOS-Chem benchmarks (have 2019 plots made that will be emailed out), how can we set up a procedure to compare these benchmarks to the on-line GEOS and to the GEOS-CTM?
            - Definitely issue with Rn emissions, possibly with SF6
            - GCST will look into installing the transport tracers as a gridded component in GCHP so that results can be exactly compared to GEOS and GEOS-CTM
            - More tracers available in GCHP
            - Have not done this with an FP simulation
        - GCC and GCHP have substantial differences in vertical transport, as induced by PBL venting of 222Rn (more venting in GCHP) and STE of 7Be and ozone (less leakage from strat and downwelling in GCHP). Some of that could reflect diff in resolution (4x5 GCC vs. c48 GCHP) but advection schemes are also different. Would be nice to understand this, or at least to know if GCHP is more consistent with on-line GEOS
        - Our model comparisons to ozonesonde vertical profiles over land suggest that PBL mixing in the model is too fast. Midday ozone profiles in PBL are flat in model but not in obs. CMAQ scheme has same problem. Might have to do with top-down vs. bottom-up mixing.

b. Stratosphere (Seb, Dylan, Susan)

- 13.0.0 stratospheric benchmark
    - Overall assessment: positive
    - Notable discrepancies remain
    - Transport
        - Evidence of excessive horizontal transport for long-lived species
        - Error greater in GCC than GCHP benchmark
        - Differences likely due to resolution (~2x)
        - Seen in multiple long-lived species
    - Water
        - “Stratospheric Monsoon”
        - Discovered some confusion over stratospheric water vapor setting - will be resolved in future GC version
        - Current stratosphere floods over time - work is needed to fix the boundary condition
            - Too much water is let through tropical tropopause
    - Chlorine

            - Most chlorine species seem low in GEOS-Chem compared to MLS
            - May be evidence of an emissions deficit
            - Possible issue in stratospheric clouds as seen in polar spring
        - Recommendations
            - Immediate
                - Water: Remove option to set init strat water vapor to meteorology
                - Long-lived species: Need GCHp age--of-air results to diagnose transport issues
                - Chlorine: Extend strat benchmark to include comparison to new GMI estimates of polar chlorine partitioning
            - Research actions (requests / suggestions)
                - Investigate resolution-dependency of stratospheric transport biases
                - Improve stratospheric water vapor boundary condition
            - Long term
                - If 47-layer full chemistry is tested by GC, would like to look at stratospheric results from that vs. other stratospheric benchmarking options
- Other strat updates
    - Near-term
        - Online methane fluxes
        - Mesospheric chemistry
        - Stratospheric chemistry in adjoint
    - Long-term
        - Strat adjustment for radiative forcing
        - Extended diagnostics for RRTMG
- Q: Isn't significant source of water vapor methane oxidation in strat - is flooding occurring even where this source is important?
    - The source is definitely there, but it looks like it's flooding because Seb has previously been able to resolve this issue by using stricter boundary condition on water vapor in long term simulations
- Q: Why can't we use that previous fix?
    - We could! Will do test
    - Issue is that it's not very flexible, as you are fixing certain quantities
    - Will look into options
- Q: For flooding maps, those were 72 layers? Would you expect it to be worse or similar at 47 levels?
    - Existing maps in 72 layers
    - Probably similar or worse at 47 levels

c. GCHP (Randall, Seb)

- Improved ease of building
    - New build system written in higher level language (CMake) that is easier to build
    - Spack package manager provides recipes for GCHP dependencies
        - Compiler, MPI, NetCDF libraries, CMake
        - Significantly streamlines system setup
        - Offers choice of compilers and MPI implementations

        - Enables single-line GCHP setup
    - GCHP containers for fast setup & running (ideal for casual users, testing, demos)
- New and Improved Capabilities
    - Updated MAPL eliminates I/O bottleneck
    - Improved testing (continuous integration build, runtime, and full chemistry)
    - Stretched-grid capability
    - GCPy supports stretched-grid capability
    - Mass flux ingestion and basic cubed-sphere online regridding on development branches
- Multiple Cubed-Sphere Advection Archives
    - Generated MERRA2 archive (hourly C180 (~50km) resolution) for 2017
    - Generation of GEOS-IT archive (hourly C180 resolution) for 2010-2020 in progress
    - Operational GEOS-FP archive (hourly C720 (~12 km) resolution) scheduled to begin this week
    - Avoids information loss and extra effort from unnecessary regridding; reduced advection error
- Answers to some FAQs
    - GCHP supports lat-lon output (e.g., useful for post-processing scripts that only work with LL data)
    - GCHP is faster than GC-Classic at 2x2.5
    - GCHP doesn't require fancy high-speed interconnects unless you're running >500 cores, or resolution >=C180
    - Ease of using GCHP has become similar to GC-Classic (e.g. some new PhD students are easily starting with GCHP rather than GC-Classic)
- Advances in Documentation
    - Youtube
    - ReadTheDocs
- Looking forward
    - Assess parallelization and performance
    - Support multi-node cloud capability
    - Continue working through minor issues (e.g. satellite diagnostic performance, subtleties in regridding and advection)
- Q: Is vertical resolution changed?
    - No, as far as known
- Q: How many cores required to beat GC Classic for 2x2.5 performance?
    - 1 node is approximately equal (tests done with 36 cores per node), faster with 2 and 3 nodes
- Issue with building using Spack for certain compilers at MAPL build step
    - Need more users to test on different setups
- Q: Who owns ReadTheDocs? Is it long-term dependable?
    - Should be, but regardless we have source code for documentation in open source language so this would not be huge issue
- Q: What are memory requirements for GCHP vs. GCC?
    - Memory leak fix
    - Need better estimates

Please share presentations with steering committee!

10. **Plans for versions 13.1-13.3 (Daniel)**
    a. Mostly communicated by email already
    b. Updates grouped into different versions depending on benchmarking requirements
11. **GEOS-Chem modularization beyond HEMCO (Christoph)**
    - Lots of duplication in different code pieces
    - How will we modularize different components while keeping GEOS-Chem independent?
    - Will go ahead with GOCART, GMI, strat chem modularization
    - Will move FAST-JX code to higher level in GEOS-Chem and try calling that from strat chem or GMI as proof on concept
    - More discussion in future committee meetings
12. **What to do (or not) about IGC9.5 (Daniel)**
    - Planning not to do anything
    - Will have IGC10 next year
    - Any feedback or comments, please email Daniel