GEOS-Chem Steering Committee Telecon
19 May 2021

Attending/Missing:
Amos Tai, **Andrea Molod**, **Andrew Schuh**, **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, **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**, **William Downs**,**Yanxu Zhang**, **Pam Wales**, **Yuxuan Wang**

1. **General updates, welcome to new members (Randall)**
    - Welcome to Andrew Schuh and Pam Wales!
    - Thank you to Emily Fischer (stepping down) for her contributions to the GCSC
    - Thank you to Will Downs (leaving in July)
    - Version 13.1 soon to be benchmarked
2. **GCST updates (Melissa)**
    - Released 13.0.0
        - Followed by 13.0.1 with a dry-run fix + restart file simulation date fix
        - Followed by 13.0.2 which fixes an issue where met fields were only read once per simulation
    - In final stages of 13.1.0 development
        - Includes HEMCO 3.0 release, documented in manuscript submitted by Haipeng Lin
            - Includes HEMCO intermediate grid feature
        - Includes fix to stratospheric water vapor boundary conditions at tropopause
        - GCAP 2.0 met fields
        - Vertical allocation for CEDS emissions
            - Diurnal scaling of Chinese power plants
        - KPP updates to speed up chemical solver
        - Several minor bug fixes and improvements in diagnostics
        - Initial modifications to allow GCHP adjoint
        - Updates to GMAO libraries in GCHP
        - Added logging files to GCHP
        - Added monthly diagnostics to GCHP
    - In future, GCST to send heads-up email to GCSC when benchmark is about to be circulated
    - Q: Primer on intermediate grid?
        - A: Allows choice of res for HEMCO.
        - Previously you would provide emissions at highest resolution possible which would be regridded to model grid.
        - Now you can specify higher resolution grid vs. model grid for emissions, which will then be regridded to model resolution
    - Q: Intermediate grid includes HEMCO extensions + gridded input files?
        - A: Yes
3. **KPP unification project (Bob)**

- From last newsletter:
    - Updating existing rate law functions to be more computationally efficient
    - Will go into 13.1.0
    - Speeds up chemistry by ~40%
- Mike Long working on sulfate mod
    - All chemistry in sulfate mod incorporated into KPP
    - Involves translating chemistry from sulfate mod, migrating rate law functions, adding work from Jonathan moch, and adding cloud fraction work from Chris Holmes to Sulfate Mod (already in gckpp_hetrates)
- Working on gckpp_hetrates
    - Moving rate law functions to KPP configuration file and cleaning them up
- Migrating specialty sims into KPP
    - Mercury code from Viral Shah
    - Unified carbon sim
- Updates to KPP itself
    - Will make KPP a submodule of GEOS-Chem
- Q: When updated KPP goes into GEOS-Chem, will the chemical mechanism remain the same?
    - A: Only new chemistry will be HMS chemistry (already slated for 13.3 anyway).
- May be able to go into 13.3
- Q: Will we still need to get bromine concentrations from archived data when doing Hg simulations?
    - A: Yes, should still need to read in oxidants
- Q: Porting other aerosols besides sulfate to KPP?
    - Complex SOA not portable to KPP
- FYI submodules clone into headless state which is not obvious. Maybe create a bash script that automatically checks out main branch at all levels
    - Will need to be careful about main branch when developing, but can definitely mention this issue in documentation
    - Checking out older tags may have no branch
- Concern regarding sulfate with gas phase chemistry: preventing aqueous chemistry from stiffening rest of chemistry. Adjustments may be necessary to prevent slowing down gas phase chemistry
- Q: Are we moving all chemistry discussed to consolidated solver? Could have one KPP for aqueous or gas phase etc.
    - A: Yes, moving to one KPP

4. Working Group updates & perspectives:

1. Aerosols (Becky, Colette, Jeff, Fangqun)

- HMS chemistry in 13.3.0
    - Sulfite and bisulfite react with dissolved formaldehyde to form HMS in clouds and fogs
    - HMS is removed by reacting with OH radical or OH-
    - New reactions in GEOS-Chem are in presentation
    - From Moch et al. 2020
- Blowing Snow Sea Salt Aerosol (SSA) Emissions (13.2 or 13.3?)
    - Produced from sublimation of wind-lofted salty snow on sea ice
    - Implemented in GEOS-Chem by Huang & Jaegle and Huang et al.
    - Sea ice age from Tschudi et al. over Arctic; minimum MERRA-2 sea ice over Antarctic

    - Should blowing snow emissions be turned on by default?
    - Should we separate the blowing snow and open ocean emissions as different tracers (currently lumped in together in HEMCO)?
    - Q: Resolution dependence of blowing snow emissions? Does Aerosol Working Group seek support for a grid-independent version of blowing snow?
        - A: Wind speed dependence is not linear, resolution is important.
        - Are currently being calculated as grid-independent emission.
            - Have been calculated for some years already, should extend this to all years that we have sea spray sea salt emissions
    - Q: Is there a reason this should be optional instead of required? Could just bundle it with existing emissions?
        - A: Should at least be on by default.
        - Makes sense to have it as a separate emission
    - Q: From a practical standpoint, are you using some independent monthly sea ice coverage source or is it from GEOS?
        - A: Coming from MERRA-2
    - Q: Where does sea ice age come from?
        - A: Separate input file
        - Q: Slide specifies where it comes from for Arctic, what about Antarctic?
            - A: Should be from same dataset but not totally sure
            - There are a few different versions of sea salt blowing snow parametrization floating around, so should meet and discuss
- Emerson et al. size-independent dry deposition (13.3)
    - Based on new size-independent measurements
    - Shifts dry deposition velocities in accumulation mode due to broadening of interception mode
    - Has relatively big impact in remote ocean locations, but comparing to Hammer et al. there is no large change over land in GEOS-Chem
- Additions of GC Wet Scavenging Options based on Luo et al. 2019 (12.7) and Luo et al. 2020 (13.2)
    - Rainout loss rate
        - In-cloud water content changed from fixed value of 0.1g/m3 to based on meteorology import
    - Washout coefficients
        - Use empirical washout coefficients and schemes for HNO3 and aerosols (2019)
        - Updated semi-empirical washout coefficient for aerosols (2020)
    - Rainout efficiencies
    - Cloud pH
        - The iterative calculation of cloud pH (Alexander et al. 2012) is updated to use Newton's method in order to arrive at a consistent result (Moch et al., 2020)
    - Aqueous phase chemistry in mixed cloud
        - Only occurs when T > 258K
    - Wet scavenging of SO2

        - Now is calculated with aqueous phase equilibrium for rainout, washout, and scavenging in convective updraft
    - Dry deposition of SO2
        - Changed minimum Vd of 0.2 cm/s over snow/ice to minimum of 0.01 cm/s over snow/ice and when T < 253K
    - Q: Is this going to be optional or default / required?
        - A: Currently optional. Need to discuss whether it should be optional or required
        - 2020 improved on / fixed some issues in 2019 and increased likelihood of becoming default
        - Should have offline discussion in Working Group about whether it should be optional or not
        - 13.2 will have benchmarks with this option enabled and disabled
    - Should include transport working group (and any others interested) in discussion about whether this should be optional or required.
    - Will send email to whole steering committee about discussion
        - Should probably defer this discussion until benchmarks have been run
- Brown Carbon from Fires
    - Fires are the largest source of BrC; BrC dominates uncertainty in the sign and magnitude of DRE of fires
    - Considerable uncertainty in initial absorption from different fires and how this evolves in the atmosphere (field observations generally consistent with a ~1 day photochemical bleaching)
    - Could be added to standard simulation (requires addition of 3 tracers) if sufficient interest
    - Q: Should there be a consequence on gas phases compounds at all?
        - A: Process is not well understood. Randall's group looked at OH impacts but Colette's group have been focusing on radiative effects
    - Q: Impact of brown carbon yield on organic landscape itself?
        - A: Higher black carbon content causes brown carbon to be browner
        - A bit tricky to implement. Have implemented BC:OA ratio in existing grid box
        - Existing parametrizations not quite sufficient
        - If people want capability, happy to share code
        - May be good to have as an option due to current interest in wildfires
        - Contact Colette & aerosol WG for further discussion
- Randall's group has upgraded hygroscopicity and added grid-independent dust
- Reach out with further followup

2. **Software Engineering (Lizzie, Melissa, Bob)**
    - SEWG consists of users and engineers interested in model software development.
    - Meet 2-3 times per year
    - Document projects (ongoing, completed, yet to begin) in public spreadsheet
    - Past meeting minutes available on SEWG wiki page

- Members are primarily grad students and programming staff with interests in software engineering and high-performance computing.
- All GEOS-Chem users interested in software development are encouraged to join
- Featured projects:
    - HEMCO 3.0 manuscript (Lin et al. 2021)
        - HEMCO interfaced with GCClassic, GCHP, GEOS, WRF-GC, CESM2
        - To be released with 13.1.0
    - Stretched-grid capability (Bindle et al. 2020)
        - Included in GCHP 13.0.0
        - Tutorial available at gchp.readthedocs.io
    - Profiling GCHP on multiple systems
        - Compute1 (WUSTL), Cannon (Harvard), AWS, York
        - To be included in AIST manuscript
- Ongoing projects
    - CESM-GC development
    - Consolidation of chemistry mechanisms with KPP
    - Migration of user manuals to RTD
    - Quality assurance (via automatic tests) for GCHP, GCClassic and GCPy
    - Profiling and performance improvements for GCHP and GCClassic
    - Modularization of GEOS-Chem - Step 1: Split off FAST-JX
    - Restructure HEMCO configuration file and convert to YAML
- Q: How extensible will consolidation of different chemistry mechanisms be? Will it be easy to add new specialty simulations? If you wanted to reduce the chemical mechanism would it be feasible?
    - A: As long as we have a description of mechanism, should be pretty easy to do in KPP
    - Would be appealing opportunity for people looking to simplify mechanism for longer simulations
        - Already being done - paper by Lu Shen about adaptive reduction of chemical mechanisms (13.3) - model chooses from 20 mechanisms locally
        - Q: Would that harness updates Bob mentions?
            - A: Does not benefit from Bob's work because it uses preexisting KPP mechanism as base, but point is capability is there in KPP to easily reduce mechanism
            - Paper will be migrated into new KPP framework

3. **Carbon Cycle (Kevin, Dylan J.)**
    - Joint CO-CO2-CH4 from Jenny's group is scheduled for release in 13.3.0 - will be submitted to GMD this week
    - Interest in expanding to CO-CO2-CH4 to include OCS following Kuai et al. 2015. Working with Elliott Campbell (UCSC) for updated emissions
    - Need to migrate CO-CO2-CH4 into GCHP
        - Working with GCHP team
        - Inclusion of observation operators for satellite measurements
    - Updates to bottom-up flux can be provided from CMS-Flux for CO2 through 2019
        - Challenge of supporting GC-Adjoint, GCClassic, and GCHP

- Merger of CO2 Adjoint branch with rain GCHP should be completed in May (Daven Henze)
- Q: There are various CH4 emissions going into standard model right?
    - A: Yes, need to meet about what these should be
- Q: Your OCS work - will you have consistent OCS and CO2 flux estimates available for running simulations?
    - A: OCS and CO2 estimates will not be quite self consistent, but they will be available for doing inversions once you have emissions in place. Use in adjoint will depend on adjoint development

Please share your presentations with the Steering Committee!

5. **Plans for versions 13.2 and 13.3 (Daniel)**
    - http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_model_development_priorities#13.2.0
    - NEI2016 inventory
    - Canopy Physics Model (will use MEGAN2 rather than MEGAN3 as MEGAN3 is not validated / mature)
    - Dust emissions from Meng et al.
    - Improved wet scavenging from Luo et al. 2020
    - Updated MODIS LAI product (to be used to recompute offline biogenic VOC emissions)
    - Updated Rn-222 emissions
    - Updated offline emissions
    - Climatologies for offline simulations for lightning NOx, volcano, open fire emissions
    - Trace metal simulation
    - GCHP advection to use total pressure and mixing ratio rather than dry
    - Add capability to GCHP to read mass fluxes for use in advection
    - Send email with any change requests
    - 13.3 (latter part of this year)
        - C2H4 and C2H2 chemistry
        - HMS chemistry
        - Blowing snow emissions of sea salt and sea salt bromide
        - Updated aerosol dry deposition
        - Adaptive chemical solver (as option)
        - Joint CO2-CO-Ch4-OCS Simulation
        - Should have aromatic chemistry ready
        - Should have updated KPP
        - Should have updated Hg simulation
    - Many priorities not assigned yet - contact Daniel and GCST if changes should be made
    - Q: Explicit plans for updating rate constants from 2020 JPL recommendation across model?
        - A: Don't know anyone doing this. Lee noticed non-negligible changes and may get someone to work on it
    - MEGAN
6. **Tropospheric ozone bias (Daniel)**
    - Prompted by paper from Xuan Wang which implemented a lot of halogen chemistry
    - Comparisons to ozonesonde profiles do not look good
    - Halogen chemistry is not directly responsible, as differences still show up when halogen chemistry is disabled

- Put in ox budget diagnostic in GCPy
- Large hit in 12.6 thanks to N2O5 uptake by clouds
- Some good news:
    - Strat-trop exchange is pretty good globally
    - Strat-trop exchange from 100hPA flux + residual in tropospheric budget agree very well
    - 10-year benchmark showed good stability (5-10% interannual variability in ox budget). Stratosphere in particular is stable
    - GEOS-FP and MERRA2 are consistent
    - GC Classic and GCHP are consistent
- Lightning increases ozone in tropics but biggest problem is in extratropical NH
- Could we have a problem with the distribution of STE? Seasonality of STE?
- Is there some PAN chemistry that needs to be restored?
- CO is too low at mid-latitudes - should we increase CO to increase ozone (though we'll need to be careful about OH)
- Currently testing if problem remains when GC chemical module is put into CESM
- Think it's a science problem rather than technical implementation problem
- Q: N2O5 went in and caused big change - did the lifetime of ozone change or was it only the source?
    - A: Lifetime and source both changed
- GCAP meteorology is now available for comparison
- Suggest further communication with Daniel about how to address this

7. **Cubed-sphere data archives for GCHP (Randall)**
    - GEOS-FP c720 (~12km) hourly advection archive began on March 11th and continues to be created
    - GEOS-IT hourly c180 full cubed-sphere archive for 2010-2020 should begin this summer and take several months to complete
    - Both being copied to ComputeCanada as well as MERRA2 c180 advection archive for 2017
    - Q: Any plans for being available on NASA machines?
        - A: Has been some discussion. Storage is a challenge.
        - WashU will likely be future repository for this data - expect to hear more about this transition in coming months
    - Q: How will we handle offline emissions for cubed-sphere meteorology?
        - A: TBD. Currently no pressing need to do so because c720 is just beginning, GEOS-IT is forthcoming.
        - Ultimately as community transitions to cubed-sphere, would make sense to transition offline emissions to same grid
8. **Containers, package manager, multinode cloud capability (Will)**
    - GCHP containers and Spack installation are stable
    - Containers have slight performance hit but are very good for quick setups of GCHP
    - Spack installation has been used successfully on several independent clusters
        - Please contact with any issues or additions to documentation
    - AWS runs at high core counts are currently non-functional due to an issue in Amazon fabric libraries
        - Should be resolved in the coming months
    - Initial performance results (using tweaks to allow high core counts) compare very well to non-cloud setups
9. **GCHP performance assessment (Liam, Lizzie)**

- 7-day timing tests with version 13.0.0
- Input bottleneck from previous versions of GCHP is now resolved
- Scaling significantly improved compared to v11-02c paper
- Model throughputs on the order of 150-200 days/day at c48 and c90 in 500-800 core range
- Generally seeing similar performance between Intel and GNU compilers
- Fancy interconnects (not gigabit ethernet) only really make a difference at >500 cores
- Q: Any benchmarking with recent AMD servers?
    - A: No. Have only ever run on Intel Xeon chips
- Q: If you were to run in a passive setup like a CH4 simulation, would scaling change at all / would absolute time cost change?
    - A: Probably would change in both ways due to differences in scaling between chemistry and transport

Ran out of time - general points of information from here on out. Follow up directly with people below with questions

10. **Dry vs total air advection (Lizzie, Seb)**
    - GCHP will have capability to use mass fluxes from GMAO to drive its advection
    - Fluxes are total air, not dry air
    - For consistency with that change, will update GCHP to use total air rather than dry air in advection
    - Longer question of why components of GEOS-Chem should remain in dry air
    - For the moment, only GCHP's advection will be in total air
11. **GMAO updates (Andrea, Christoph)**
    - Heads up about new GEOS-IT product - names of files and fields in files are totally different, so would be good to get a headstart on this
12. **Modularization of GEOS-Chem code (Daniel, Christoph, Lizzie)**
    - Postpone to next meeting
13. **GEOS-Chem website update (Lizzie)**
    - Harvard web designer will modify website to modernize it
    - Ideas or feedback regarding current website should be sent to Lizzie
        - Lizzie may create a shared document for ideas
        - Web designer is hoping for feedback and guidance going in

Thanks everyone! Scheduling of next meeting to come