GEOS-Chem Steering Committee Telecon

18 November 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**

1. **General updates (Randall, Daniel)**
   - 13.0.0 imminent
   - Includes stable parallel GCHP, CEDS updates, GCPy, various other updates
   - Thank you to Jenny for her notetaking
   - New notetaker: Will Downs
   - 1-month benchmark is approved, other benchmarks are proceeding
2. **v13.0 release (Melissa)**
   - 1-year benchmarks in progress for GC Classic, GCHP
   - First official 1-year GCHP benchmark
   - Updated benchmark year to 2019, met fields to 2019 MERRA2 from 2016 GEOS-FP
   - Will send out release candidate to community once 1-year benchmarks are approved
   - Will release tutorial videos for 13.0.0 + GCPy
   - Release candidate will be out for about a month before 10-year benchmark completes
   - Will send SC plots from the 10-year benchmark
   - Then will officially release 13.0.0: either end of year or early January
3. **GEOS-Chem integration tests in v13.0 (Bob)**
   - Automated testing for GEOS-Chem with various simulation types, build flags
   - Compile GC Classic code with different extensions:
     - No extras
     - APM on
     - BPCH diagnostics on
     - RRTMG on
     - TOMAS on
   - Run GEOS-Chem and GCHP with different Meteorology, grid resolutions, simulation types (fullchem, benchmark, Transport Tracers)
   - Q: How do you judge whether it's working: crashes or something else?

    - A: Mostly whether it crashes
- Q: What does ctm mean in GCHPctm? Is it the same as GCHP?
    - A: Basically the same, wrapper is called GCHPctm because 13.0.0 separates out GEOS-Chem and HEMCO as submodules. Credit to Lizzie for developing this new setup and its ease-of-build capabilities.
    - Will still call it GCHP verbally, but name GCHP was already taken on Github by pre-13.0 GCHP

4. New documentation platform, Read the Docs (Liam)

- New approach for hosting technical user guides for GCHP
- Will eventually use it for GC Classic and HEMCO
- ReadTheDocs is fairly ubiquitous in software documentation
- Advantages: versioned documentation, easier to maintain as code is updated
- Available in all countries
- Small advertisement is included on all free ReadTheDocs pages
- GCHP docs will be ready for 13.0.0 release, other docs will come later
- Q: Is it ready now (GCHP docs)?
    - A: Still a pre-release and still working on it, but it's the most up-to-date documentation
- Q: Demonstration of how it's integrated in code?
    - A: Written in reStructuredText (.rst), is included in Github repositories
- Not all documentation will be on RTD, but all technical documentation will be on RTD
- Q: For only GCHP, not GC Classic?
    - A: Currently just GCHP, will eventually have technical documentation for GC Classic on it as well.
    - Will keep Wiki and RTD docs parallel for a bit with technical documentation, then phase-out Wiki technical documentation
- Q: Will use auto API documentation capabilities?
    - A: Not planned right now due to scope of work required, but possible in future

5. Stretched Grid in v13.0 (Liam)

- RTD has info on defining stretched-grid parameters, running GCHP in stretched-grid format
- Manuscript almost ready
- Ran mass conservation tests for stretched-grid, no unexpected issues
- Q: What met fields do you need to run stretched-grid? Do you need global gridded met fields?
    - A: need global met fields, ideally at resolution of target face
- Q: First-time user guide for tuning parameters?
    - A: Online tool allows experimentation, but manuscript will provide additional details
- Q: Can you provide a stretched-grid verification example?
    - A: Yes, will add one for users to verify their results against for test regions

- Q: What is the scientific implication of sacrificing resolution on opposite side of world from stretched-grid target region?
    - A: Ongoing area of research which types of species are most vulnerable, what lowest tolerable grid resolution is
    - Perhaps add tool for showing what lowest associated resolution is with a set of input parameters. There is some guidance for this already
- Manuscript will provide extra clarity
- Manuscript is likely ready within weeks
- Q: Stretched-grid only usable with GCHP?
    - A: Yes, GC Classic will continue to support FlexGrid for similar use cases

6. Transport tracer suite (Andrea, Hongyu)

- Running TT sim using GEOSctm to produce tracer fields at MERRA2 resolution for MERRA2 time period
- Want to get them done for 1-year benchmark period
- Want to be able to compare this output to other runs
- Q: This is a gridded component? Should use same gridded component for GCHP?
    - A: For GMAO it is.
    - Work is ongoing for implementing same gridded component in GCHP for 1-to-1 comparisons.
    - Can also do comparisons with existing tracer capabilities implemented in GC Classic and GCHP
    - Rn emission is different right now in GEOSctm vs. GEOS-Chem options, but is being rerun with same emissions as GEOS-Chem for the GEOS-Chem benchmark period
- Hongyu uses IDL code to produce plots, GCST can use IDL themselves to generate the comparison plots

7. Other GMAO updates (Andrea, Christoph)

- Next reanalysis to do will be R21C Modern Era Reanalysis (EOS period)
- Transport characteristics (tropospheric and stratospheric) in system will be evaluated before release of reanalysis product
- Q: Rough release timing?
    - A: Starting creation next July, probably initially available near the end of 2021
- Q: In addition to transport modifications, other expected changes?
    - A: Fleshing out details.
    - Two parts: met reanalysis at higher res than MERRA2 (likely 12km horizontal, higher vertical resolution than currently), chemical reanalysis

8. Working Group updates & perspectives:

- Testing this new structure for giving updates for different working groups at different GCSC meetings
- Each working group expected to speak for ~5 minutes
  a. **Adjoint Model and Data Assimilation (Daven, Jun)**
    - Irene Dedoussi submitting paper on UCX adjoint
    - Colin Lee working on GCHP adjoint
    - He has worked on CO2 simulation in GCHP
    - GCHP 13.0.0 CO2 adjoint exists as its own switch within GCHP repo r in hopes of facilitating easier maintenance and future development of adjoint
    - Will issue pull request to GCST for incorporating these developments into core GCHPctm repo
    - Includes sensitivities for initial conditions, emissions through HEMCO
    - Tracking an existing unit conversion issue before submitting PR
    - Wiki page for adjoint needs to be updated, currently only updated to 2019
    - Feel free to update this page if you are using the adjoint
    - Many existing projects focus on bottom-up emissions changes
    - Will likely create a specific section of Wiki page for emissions
    - Feel free to add links / DOI to your own projects on the Wiki page
    - Q: Does ability to write out satellite output from runs work yet?
      - A: Will be in 13.0.0 as part of MAPL updates from GMAO (not ND51 but equivalent)
    - Q: Is adjoint chemistry up-to-date with forward model?
      - A: Currently up-to-date for CO2 sim in GCHP
      - Including adjoint in main GCHP repo should help keep chemistry from becoming progressively outdated in adjoint
    - Q: Isn't there a project running to integrate specialty chemical mechanisms into KPP?
      - A: Yes, Bob is working on this, should further help to keep chemistry up-to-date in adjoint
  b. **Chemistry (Mat, Barron, Lu, Jingqiu)**
    - Surveyed community to get info on what people are up to
    - Update from Kevin Bates focuses on C2H2/4 chemistry
      - Paper in revisions
      - Update should be ready for community in ~6 months
    - Update to aromatics
      - Update should be ready for community in ~6-12 months
    - Jonathan Moch sulfate update
      - Submitted to GCST

- UC Riverside working on DMS emission and oxidation scheme
- Jenny: Student putting H2 chemistry into model
    - ~6 months from readiness
    - Christopher Holmes also has H2 chemistry ready to put in, Jenny and Chris to touch base
- Q: Have UCX do chemistry to model top rather than switch to linear scheme above stratopause?
    - A: GMI has implemented this
    - Want to look at performance implications (not currently any significant ones noticed)
    - Christoph: Already running GCHP in this way at GMAO because it already exists in MAPL/ESMF, but may need to do some extra Br/Cl mass conservation scheme
- Bromine concentrations are lower in 1-month benchmark than in 12.9.0 because of bug fixes to heterogeneous chemistry
    - Paper from Xuan Wang will include these changes

c. Emissions and Deposition (Emily, Jintai, Eloise, Dylan M.)

- Updated default anthropogenic emission inv is CEDS GBD-MAPS
- Retire use of carbon emissions for VOCs. Use compound molecular weight by default
- On horizon:
    - China: update to MEIC
    - China: diurnal variability of power plant emissions
    - US: NEI 2016
    - Africa: charcoal production and use emissions
    - Vertically resolve anthropogenic emissions
    - MEGAN3 + updated canopy treatment
- Concerns, issues, considerations
    - Future emissions: RCP still best to use?
    - Aircraft from 2005 - how to deal with becoming more outdated?
        - Updated inventory does exist, but has licensing issues
        - Scaling factors to 2005 inventory should be implementable
        - Talk to Seb if you need actual updated inventory
    - Natural NH3 emissions not from seabirds is from 1997. Still appropriate?
    - Ongoing issues with alkane emissions and chemistry
    - Incorporate lessons/findings from major fire-focused field campaigns
    - Ocean exchange/emissions summary needs to be conducted
    - Recently updated EDGAR?

        - NH3 bidirectional flux: should it be in the standard version of model?
        - How to represent emissions due to pandemic lockdowns?
        - Neaten up WG wiki
        - Recommended inventories table needs to be updated to match benchmark
        - What's the best approach to update other aspects of the model that rely on emissions (complex and simple SOA schemes)?
    - Post these Qs as Github issues to keep them public and up-to-date
    - Q: Are up-to-date NEI 2016 emissions already published?
        - Available from a couple different sources right now
        - Look good but not included in a publication yet
        - Probably to go in version 13.1

9. GEOS-Chem publication website (Eloise)

- Gongda Lu developing Google Scholar page
- Likely ready in early December
- Track papers using GEOS-Chem
- Contact: geos.chem.publications@gmail.com
- Will send email to community when page is public
- Community can track updates by clicking the FOLLOW button on the page
- Google access limitations in China may be an issue. This is being looked into.
- Q: Does it look for GEOS-Chem in title of abstract?
    - A: Some of it is from titles, some of it is searched for manually in bodies of papers
    - Consistent with previous Google Scholar GEOS-Chem lists
- Q: Does it need to be manually maintained?
    - A: Mostly only for eliminating redundant entries
- Q: If you want to submit your own publication to list, can you do it yourself or need to send to Gongda?
    - A: Probably need to send to Gongda

10. GCPy (Will)

- A beta of version 1.0.0 is now available on conda-forge
- New documentation is up on ReadTheDocs
- Documentation includes installation steps for users and devs, usage examples, and details of the primary plotting, tabling, and regridding functions of GCPy
- Added ability to regrid between stretched-grid, standard cubed-sphere, and lat/lon
- Can also now regrid between arbitrary vertical grids
- Lots of additions to benchmark plotting and tabling
- Official release of 1.0.0 will coincide with release candidate of 13.0.0
- Q: Are there expected dependency conflicts?

    - A: Have set minimum requirements for dependencies, which are handled by conda and also documented in environment files in GCPy repo
- Q: Is there a plan for supporting post-Python 3.8?
    - A: 3.6-3.8 work right now, 3.9 doesn't work but will look into maintaining it

11. Package manager & containers (Will, Liam)

- Spack allows streamlined installation of requisite libraries for GCHP
- Tested GCHP with Spack-built MPI implementations of OpenMPI, Intel MPI, MVAPICH2
- Instructions up for using OpenMPI and IntelMPI with gfortran
- Will add instructions for MVAPICH2 and intel compilers
- May add GCHP to the Spack repository of packages, requires updating ESMF in Spack
- Set up CI pipeline to automatically build and deploy GCHP docker containers
- Can be used directly with Singularity
- Containers include built source code and requisite libraries
- Investigating best usage practices for containers
- Good for small tests and demonstrations, eliminate need for some libraries on host
- Can run on multiple nodes with minimal interference, but performance may not be adequate for widespread use

12. Cubed-sphere archive (Christoph, Liam)

- Have entire system for generating cubed-sphere archive
- Lizzie generated archive for 1-year time period
- Archive transferred to WashU servers
- Now have full year of cubed-sphere meteorological archive

13. Request for review of GEOS-Chem development priorities (Randall, Daniel)

- Please look at the list and send feedback to Randall / Daniel
- Need to think about what to put into 13.1.0

14. IGC10 planning (Daniel)

- Have reached out to different agencies for funding
- Target is May, but can we postpone to September if not feasible if not wanting to wait until 2022?
- IGAC also postponed to September virtually
- September is the start of semester for many, maybe do earlier?
- Very hard to travel first week of semester, maybe later in September works?
- May want to allow some people virtually, because some countries / people may not be able to travel
- Worth having virtual working group meetings in the interim?
- Daniel has a few thousand dollars from GCE funds to forward on, possibly to IGC, possibly to website update

15. GCSC meeting minutes (Randall)

- If anyone wants to volunteer to take minutes next time, please reach out to Daniel or Randall