GEOS-Chem Steering Committee Telecon

17 November 2021

Attending/Missing:

Amos Tai, **Andrea Molod, Andrew Schuh, Barron Henderson, Becky Alexander, Bob Yantosca,** Chris Holmes, **Christoph Keller, Daniel Jacob, Daven Henze, Dylan Jones, Dylan Millet, Eloise Marais, 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, Lucas Estrada,** Mathew Evans, **Tzung-May Fu,** Melissa Sulprizio**, Prasad Kasibhatla, Pam Wales, Randall Martin, Sebastian Eastham,Yanxu Zhang,** Yuxuan Wang

1. General updates (Randall)
   - Compute Canada site is being retired. Everyone should switch to WUSTL endpoint.

2. Version 13.3.0 status (Bob)
   - 13.3.0 and 13.3.1 released
   - chemistry updates are the biggest changes
     - HMS chemistry
     - Update of aromatic VOC chemistry
     - Addition of C2H2 and C2H4 chemistry
     - Addition of CH3O2 + OH reaction
     - Updates to IONO2 hydrolysis reaction
     - Revise N2O5 computation
     - Emissions -- fixed double counting acetone in MEGAN
     - Updated volcano emissions from Christoph. 13.3.0 benchmark used new volcanic eruptive/non-eruptive data for 2019 but 2019 eruptions led to confusing changes relative to 13.2.0. Will return to non-eruptive climatology (no eruptions) in 13.4.0 benchmark
     - Updated offline dust emissions
   - 13.3.1 includes minor diagnostic issues and bugfixes
   - Full chem nested simulations will by default use a larger time step for better performance

3. Plans for version 13.4.0 and beyond (Daniel)
   - 13.3
     - Bugfix to cloud entrainment in 13.3.0 increased NO_x and ozone in most places, but also increased BrO because of less HOBr+S(IV) and more HOBr + Br-/Cl-.

and that causes ozone depletion at high latitudes in winter/spring. Would like to decrease BrO but that is a scientific problem.

- Becky Alexander: looking into and have some ideas that may help. Will be a timeline of several months

- 13.4 outlook
  - Nothing that will affect standard chemistry much, but new Hg chemistry will change that simulation.
  - Most changes will be structural, including streamlining and merging of sulfate chemistry into KPP
- Beyond 13.4
  - Not very much. We are hoping the community will let us know if there are any additional priorities out there.
  - Eloise: Code update that takes satellite data and puts it into ND51 format, which would replace bpunch
    - Lee Murray: we can retire timeseries punch diagnostics using obspack diagnostic
  - Jenny Fisher: what is the process for updating the tables?
    - Send updates to the GCST and cc the working group
    - Working group lists are not as up to date as we would like. Use general GC email list if it is something important

4. StateChem and GEOS-Chem versioning (Lizzie)

- We have a proposal to do a no diff structural update. This update would split the 4d species concentration array into 1d vector array with a pointer to a 3d concentrations array
- The motivation for this change is so that GEOS can point to the MAPL internal state. We do not need the species concentration array for this, so splitting the array simplifies things
- The update will benefit memory and potentially have time savings as well
- This would be a breaking change that will cause many merge conflicts for others code and pull requests. The update would warrant version 14.0. This will not occur until after 13.4.
- What do people think? Everyone okay with this?
- Eloise: Is it possible to output specific levels?
- Lizzie: you can already do so in both GCHP and GCC
- This update will not affect the model output
- Will the switch complicate users' lives? No, it shouldn't. Should be more logical with more descriptive naming conventions

5.   Working Group updates & perspectives:

a.   Adjoint Model and Data Assimilation (Daven)

[*See accompanying slides for more detail](#)

- GCHP Adjoint
  - Framework for GCHP adjoint model is now in the forward model repo
  - Can have an easier platform for people to jump in on development and testing
  - Prioritized getting it into the standard code and now they are working on refining and turning features back on
  - Please contact Daven if you would like to test or develop the adjoint
- GCC Adjoint:
  - UCX update courtesy of MIT folks
    - Includes stratospheric processes enabling evaluation of sensitivities
    - Will soon be released into new version
- In the pipeline
  - Sector based inversion framework
  - Simplified SOA
  - New nested domains for central South America
  - Methane code development
- Emissions:
  - Top down emissions are available and published
  - MACE inventory for black carbon and dust
  - VOC emissions
  - Global NOx emissions inventories
  - CO2:
    - CMS-Flux product using 4D var simulation product

- Questions:
  - Eloise: Why is bidirectional ammonia only in the adjoint and not in the standard model?
    - No good reason mostly a lack of momentum -- slightly more effort involved
    - Randall: Having it in the adjoint will increase momentum for including in standard model to promote consistency with adjoint
- Lee: What version is GCC adjoint available in?
  - UCX update brings it to version 10
- Lee: Old format but using UCX?
  - Using version 36. The effort to update scaling emissions through hemco has been poured into GCHP updates

b.   Emissions and Deposition (Eloise, Jintai, Dylan M.)

Dylan:

- Recent emission updates:
    - Offline dust emissions
    - NEI 2016 emissions as an option
    - Volcano emissions (Christoph)
    - CEDS v2 emissions through 2019
    - LAI 2000-2019
    - sea salt and sea salt bromide
    - Offline BVOC and soil NOx emission data reprocessed with new MODIS LAI data to September 2020
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- In Progress
    - Climatologies for fires, lightning
    - Updated Rn-222 emissions
- To be prioritized:
    - Updated canopy physics for BVOC. Standard model uses offline BVOC, so hasn't been prioritized
    - Future fire and dust emissions
    - Methane updates for canada and global for oil, gas, and coal
- Upcoming:
    - Aircraft emissions from 1990 to 2019
        - HEMCO extension to process AEIC emission inventory to include plume-scale effects
    - Updated APEI anthropogenic emissions for Canada
    - Emissions for rocket emissions and re-entry ablation in 2019
- Additional thoughts:
    - Should lightning produced oxidants go in? We should implement plumbing so that people can test it and decide
        - Lee: Lightning oxidants: disagrees mechanism is well understood -- he will connect with Jingqiu on it
    - MEGAN3 : Should it go into the standard model? It is better for land cover and more robust for BVOC, but could exacerbate existing biases.
    - New Soil NOx -- specifically tested over central us
- Randall: where do fire climatologies come from?
- Daniel: 10yr avg with the same time period we did the benchmark for (2010-2019)
- Daniel: Colette was saying we shouldn't use MEGAN3?
    - Dylan: We have the code and we should implement it. If concerned about magnitude we can adjust scaling. IN favor of putting code in there. Sam is taking a job at USC and has delivered code

- - Dylan: We should prioritize this.
  - Jenny: MEGAN3 has updates for parts of the world that are neglected
  - Randall: May make sense to implement in version 13 before v14 breaks compatibility with existing pull request
  - Daniel: Is there a paper for MEGAN3:
  - Dylan: Papers have come out
  - Jenny: Are there different implementations of MEGAN3?
  - Dylan: Unclear, but possibly several different versions

6.   Outcomes from SF6 Transport WG meeting (Andrew)

- Updates from SF6
  - Take GCHP and enter into SF6 comparison study with a bunch of other CTMs with a long runtime protocol: 20 years. There are a lot of bottlenecks for GCHP.
    - Issue with existence of met files for that long of a time period
  - A preliminary step is testing runs of c90 and c180 for 1 year to test effect on SF6 and see which resolution makes sense for the official test
  - The sensitivity test has been slow coming and is likely to happen in the new year rather than this year.
  - Seb is a key component to making this happen
  - We are expecting more mass fluxes in the future but unsure when that will happen
- Questions:
- Daniel: Why do we need 20 years?
  - Stratosphere
- Need to wait for SF6 emission inventory update -- probably not till early/mid next year

7.   GMAO update (Christoph, Andrea, Pam)

Christoph:
- GEOS IT is on schedule but will take a while
- We have been looking at stratospheric chemistry in GCC and see some strange behavior in chlorine
  - Pam is taking stratospheric mechanism apart
  - Andrea: Attempting to disentangle whether chlorine is from GEOS-CF or GCC.
  - Pam: vertical transport is an issue and the upcoming GEOS-IT will have this bug. Transport is too quick. There is a partial fix and the following version will have the fix -- vertical remapping was doing too much diffusion.

8.   Direct reading of GMAO meteorological data (Liam, Seb)

*See accompanying slides for more detail
Liam:

- We would like to drive GCHP with meteorological data directly from GMAO. Currently we do some preprocessing and then it is served via the wustl endpoint.
- The issue is using new met products is difficult because the the preprocessing code is difficult to work with and updating the preprocessing to accept different formats is a lot of work
- Reading directly from meteorology is an option. The preprocessor output is not that different from the original data and the processing can be easily done online: vertical flipping, albedo, and optical cloud calculation
- Reading native meteorology data will be added as an option in 13.4, but by default will still use the preprocessed data
- The outcome is that it will be easy to work with alternative meteorology products and this opens up the possibility for near real time simulations
- It could also be extended for GCC

Questions:
- May: where is the native met processing code going to be located?
  - Liam: Will be included in the environment component of the official repo. In between where we read in data and HEMCO
  - May: WRF-GC has something similar -- may be useful to think about where code is put to be consistent.
- GHGSat folks are doing near real time simulations now with unprocessed GEOS data
- Andrea: Have you tested it with GEOS-FP?
  - Liam: Yes, and it runs successfully. Although not extensively tested.

9. Using total air mass fluxes for advection (Seb, Liam)

Seb:
- We have code that ingests air mass fluxes into GCHP to reduce influence of pressure fixer
- Liam pushed it through to a PR
- It does seem to work and reduces spurious vertical motions
- Testing using GEOS-IT data and transport tracer simulation to see what the difference is in distribution of SF6

Questions:
- Becky: Wondering if this influences cross-tropopause ozone fluxes?
  - Seb there is some effect and it should be looked into. Intending to do fullchem simulations soon
- Andrea: Why does it eliminate the pressure fixer issue?
  - Won't completely remove it because of precipitation but effect will be much slower.
- Lee: What does this mean for archiving of 4d wind fields?
  - Seb: Continue to archive for diagnostics
  - Seb: There are two sticking points: regridding and GCClassic
  - Daniel: mass fluxes are only on cubesphere

- ○ Lee: no way to get it archived for rectilinear grid?
- ○ Seb:It is an open problem

10. Tools for the cloud (Liam, Lucas)

*See accompanying slides for more detail

Liam:
- We are working on streamlining GC testing, including PRs and structural updates. To this end we are developing automated pipelines on AWS to initiate, execute, and plot the results of test simulations
- This will involve an automated solution for building environments, a method of keeping the data repository up to date, and infrastructure to actually run the simulations
- We will be using EC2 image builder to create amis and images for docker and singularity. This is a solution that greatly simplifies and automates the creation of pre built environments
- BashDataCatalog: A new tool Liam is creating to automatically get new data using collections and catalogs. This tool greatly simplifies fetching data and retrieving missing files

Lucas:
- Using the tools Liam describes, we are working on creating a method to automatically run benchmark simulations on the cloud. This could eventually lead to running simulations on the cloud with little manual intervention.
- We will be using AWS Batch to manage the launch and termination of EC2 instances deployed with the docker image created by EC2 image builder.
- The run directory, output directory, and benchmark plots will be uploaded to s3. These steps will be separated into three distinct AWS Batch runs.
- All of the AWS infrastructure is being managed with Terraform, an infrastructure as code (IaC), which aids in configuration, documentation, and predictability of the infrastructure.

11. Testing Hg updates in version 13.3 (Yanxu)

- Benchmarking Hg for 13.3. It has not been benchmarked since 12.9
- Issues: concentration is much lower over land, emissions are not properly read
- We are modernizing the benchmark scripts, which are from v11
- Upgrading them to read nc4 files rather than bpunch files

12. KPP project (Bob)

- KPP updates are in the newsletter -- won't say more to save time.

13. Nested model issues in version 13 series (Yuxuan, Bob)

Bob:
- Increasing timesteps speeds up fullchem simulations

- A lot of users are using tropchem but that is not recommended

14. GEOS-Chem website update (Lucas)

- The People and Projects map is back
- We removed the Harvard-specific branding
- Greater prominence of citation and new developments information
- Adjusted mobile display of meetings menu
- Small cosmetic updates (font and coloring)
- We are happy to continue to receive more feedback

15. Retiring gcgrid data access on Harvard ftp server (Daniel)

- Retiring gcgrid ftp server at Harvard over the next few months. Don't think anyone is using it and Harvard wants to start charging us

16. IGC10 planning (Daniel)

- Dead set on in person meeting in May
- Harvard is willing to host it with restrictions and caveats depending on the covid situation at that time
- We need an in person meeting and know that many will not be able to come, but maybe we can make it hybrid
- Randall: Enthusiastic about in person meeting