

**GEOS-Chem Steering Committee Telecon  
27 May 2020**

**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, William Downs (+ someone by phone)**

**1. Versions 12.8 and 12.9 releases (Daniel)**

- 12.8 released: isoprene chem, ozone deposition to ocean, wet dep algorithm (option)
- 12.8.1 released: bug fixes
- 12.9.0 on the way: updated halogen chemistry. Synthesis of different strands from over the years. Xuan will document this version in a paper starting in June. Also includes improved cloudwater pH, etc. (see wiki page). Will receive 1-month and 1-year benchmarks.
- Will be followed by 13.0: structural updates.

**2. Retiring Tropchem? (Daniel)**

- Problem with tropchem: not benchmarked, changes in standard have to be replicated in tropchem, extra work and leads to bugs
- GCST has addressed GCSC concerns
- Jeff's group is going to run some extra checks this week for TOMAS but initial concern has largely been alleviated.
- Will this impact our ability to run high resolution with FlexGrid?
  - No
- One concern is that it puts an onus on us to make sure the stratosphere is a reasonable boundary condition for the troposphere
  - Do we need to run a very long (10-20 year) simulation to test the strat-trop exchange in the 47L version?
  - Melissa is in the process of running a 1-year benchmark to compare 47L standard and tropchem to 72L standard. Also planning a 10-year benchmark for 13.0.0 so can potentially combine. Wouldn't need to retire tropchem earlier than that.
- It would be nice if we could work out why standard 47L is faster than tropchem, but if we can confirm that we are getting the same performance via the benchmarks then this probably shouldn't slow us down
- Could replace "tropchem" with same mechanism as standard but just confined to the troposphere. From tropopause up, we would have the same thing that we have now (saved production/loss from an older UCX run). This would get us to a point where we have one mechanism and more time to evaluate the 47L stratosphere.
  - We might get some performance hits from transporting some species in troposphere that are not used
  - Melissa can benchmark this version with other benchmark versions
  - Would also address some of the concerns about only running the adjoint with active tropospheric chemistry
  - Adopted!

### 3. Plans for version 13.0 (Lizzie)

- Purely structural update, largely to facilitate compatibility with ESMs
- HEMCO will move out of GEOS-Chem and alongside instead
- GEOS-Chem classic will have a new repository wrapper with GEOS-Chem and HEMCO as git submodules within it; also retiring unit tester and will create run directories from within the source code and will avoid version mismatch issues.
- GCHP will have a new wrapper repository. ESMF will be removed and dealt with separately which will significantly speed up compile time.
- Retiring carbon based units for VOCs; should make things more transparent
  - Q: What are we doing about lumped species? A: Most lumped species not in carbon units currently, and we have assumed molecular weights that we will use for any of these.
  - Q: What about emission inventories? A: Will still have to allow for the conversions to happen but will do explicitly within the HEMCO configuration files
- Will reduce the memory required for diagnostics by dynamically allocating arrays
- Retiring GNU make build system. Will streamline compilation and be faster
- Some structural updates within HEMCO (probably won't be noticeable to users)
- Q: Release candidate given the major structural issues? A: We do this with -rc versions in the github repository. Anyone can download these now with the caveat that we don't have full documentation. Could do it pre-release (usually do it at the beginning of benchmarking)
- Will be releasing YouTube videos for getting started with both classic and GCHP since it will be really different to what people are used to
- Benchmarking? Will have capability from 13.0 to have equivalent benchmarks for Classic and GCHP in GCPy. Comparison to observations still in IDL, discussions ongoing about which observations to port – not currently used for GCHP, but we could if we convert GCHP output to lat-lon.
- It would be worth us looking at whether we have the right observations in the benchmark (e.g. ATOm) – up to date? Do they give us what we need? Satellite observations besides total ozone columns? (but also need to be careful with satellite observations too)
  - Could be a research activity to build a set of benchmark observations. Lee has a student working on ATOm so could work on getting these data into the benchmark

### 4. GCPy Release (Bob, Will)

- Significant developments that expand usefulness
- Single level plots over any region, grid
- Zonal mean plots for both 47 and 72L and will allow arbitrary regridding
- Routines for benchmarking added
- Plotting now parallelized, much faster
- Creating comprehensive documentation, examples, videos
- Plan to make available via Anaconda Forge for easier installation via conda

### 5. Plan for remote GCE1 (Mat, Eloise)

- Remote GEOS-Chem Europe meeting to be held, Mat has circulated a rough schedule
- For presentations can use a Zoom webinar format
- For posters, may set up individual zoom rooms
- Some sort of random social where people are randomly allocated for 10 minute blocks (re-allocated each 10-minute session)
- Could be a trial run for IGC10 if we can't hold it in person in May

- Will have registration so that can circulate information e.g. for poster sessions, plus some idea of numbers
- Will need some rules around it for Zoom issues
- Could require registrants to commit to a certain number of hours (to avoid it being poorly attended, an anonymous meeting where people drop in and out and never a core group of people...)
- Webinars are kind of anonymous anyway; posters more of an experiment
- Could have a room for speakers after session for attendees to come in and talk to the speakers

#### 6. Cancellation of GCA2, looking ahead to IGC10 (Daniel)

- GCA2 cancelled – feeling from Chinese users was that in-person was important. GCA2 will be held in 2022
- IGC10 – planning for first week of May as usual. Had considered holding at Wash U (led by Randall) but given complications of COVID, plan to keep it at Harvard this year.

#### 7. AIST GCHP project update (Randall)

- Joint with Harvard (Daniel), MIT (Seb), GMAO
- About making GCHP more usable. Several updates happening in 13.0
- Progress towards a stretched grid simulation in GCHP
- Zhuang JAMES article showing efficient GCHP run on Amazon Cloud with efficient scaling at > 1000 cores
- Package manager on the way
- GCHP adjoint for CO2 in progress
- Q: is there a working version on the NASA Pleiades computer? A: not yet but maybe soon
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#### 8. WRF-GC update (May)

- Two-way nesting is now working: major development. Can run WRF-GC at various nested grids, May's group has demonstrated down to 9-km resolution.
- The two-way coupling (chemical feedback to meteorology) is also fully operational, and working within the nested-grid. We also made progress in making the lightning NOx emission work, which was not part of WRF-GC v1.0.
- All the necessary changes have been merged into GEOS-Chem v12.8.2.
- We are in the process of writing up a Part 2 paper, describing the chemical feedback. There is also recently a new paper published using WRF-GC to analyze the TROPOMI NO2 reduction during COVID-19. The model seems to be easy for new users to pick up.

#### 9. CESM-GC project update (Seb)

- CESM2.1 (current version) has been modified to build and run GEOS-Chem in place of CAM-chem. It is an option and builds from the standard code.
- Also have a version of HEMCO working in CESM and they work together. HEMCO can also feed CAM-chem, not just GEOS-Chem. Can allow online emission calculations at consistent resolution separate from run resolution.
- Now allows 3 different options for dry deposition parameterizations (to match GEOS-Chem method or CAM-chem/CLM methods). Some issues with entanglement of dry deposition and emissions.
- Convection & convective scavenging are the next big-ticket items on the list.
- Q: coupling with CLM? A: Has been a difficulty e.g. dry deposition fluxes because of a lot of hard coding in CESM. Trying to change this as much as possible. Trying to make everything flexible through an interface layer instead of direct communication. In long-run this will make it easier to

couple GEOS-Chem and CLM but it's not there yet.

#### 10. Stratospheric benchmarking needs (Dylan J., Susan, Seb)

- Have designed a procedure for comparison to satellite observations over a 12-month period (12-months of outputs regardless of spin-up time); 1 Dec – 30 Nov.
- For each major X.0.0 version change, want as long a spin-up as possible (minimum of 5, 10 better) Jan 2007 – Dec 2016. Will compare to the much less spun-up 1 year benchmarks. Should be done with MERRA-2 data.
- Same benchmark applied to 47L mechanism b/c of transport issues.
- Same requirements as 1-year benchmark but with one extra age of air tracer (may already be in transport tracer simulation)
- Will do full evaluation on 13.0.0, but preliminary evaluation (v11, MERRA-1, 10-year spin-up) shows some things we knew from the GMI simulation, but some things that are new
  - Too strong of horizontal mixing in lower stratosphere → bypassing Brewer Dobson with transport towards poles rather than higher altitude
  - Insufficient chlorine in mid and upper stratosphere
  - Insufficient ozone depletion in Antarctic ozone hole, insufficient denitrification
  - some of this due to 4x5 resolution issues
  - Note from Christoph: GEOS is showing loss of chlorine in stratosphere in ozone hole region, hoping that we can catch this issue with the benchmark (e.g. prod/loss terms)
- Q: Does GEOS-Chem stratosphere get ported to ESMs? A: yes if model includes stratosphere (e.g. CESM). Yes in WRF but model top is 50 hPa

#### 11. GEOS CTM and other GMAO updates (Andrea, Christoph)

- FP had a major update in Jan 2020. Some issues. If we use FP we have to be careful to use the right one.
- GEOS-CTM being benchmarked, some issues with radionuclides tracers. GEOS-CTM doesn't use the same emissions for radon, might need to run another simulation with the GEOS-Chem emissions too to make this comparable.
- Plots will be shared with GCSC

#### 12. What to do when simulation extends beyond range of input data (Lee)

- Lots of fields that don't extend to more recent periods (e.g. emissions, but also CH<sub>4</sub>, other chemical fields)
- Should the model stop gracefully and tell the user that fields are not for current time period? Or too heavy handed?
- Would also be good to compile a list of required input datasets that should be updated for each major release
- Q: is it possible to have a flag that defaults to "yes stop the model" but a user who knows what they are doing could turn it off? A: should be easy to do. Maybe should default to a climatology in those cases.
- General agreement

#### 13. Consistency of OH fields in off-line simulations (Jenny)

- Currently using 3 different versions in different offline simulations (v5, v7, v9). These are not just different magnitudes but also different seasonal cycles. We should at least be consistent
- Two possible future options suggested:
  - Lee has optimized OH fields that are about to be published, and we can include these as one option

- From 13.0.0 will be running the full 10-year benchmarks for the stratosphere, so we can save the OH for each year to give users year-specific OH as well as develop a climatology. This should probably become the default.
- Need to be careful when running CH<sub>4</sub> for inversions, don't want OH changing each version – but a user can change themselves to make sure they are using consistent versions.

#### **14. Unifying off-line simulations under KPP (Bob)**

- Funded EPA proposal to address our chemistry mechanism. First step to clean up and optimize KPP rates.
- A lot of code in offline simulations like sulfate\_mod, carbon\_mod that can be moved into KPP to standardize
- Carbon species (CO<sub>2</sub>, CH<sub>4</sub>, CO) can be brought into a single mechanism all being solved under KPP. Possibly other specialty simulations
- Work will start with 12.9

#### **15. Benchmarking new GEOS-FP convection (Melissa)**

- Jan 30 2020 – switch the GEOS-FP convection
- Jan 2020 have overlapping new and old schemes
- Melissa has run one-month benchmark simulations (chemistry, transport tracer) and will send out by the end of the week

#### **16. Tracking model performance (Melissa)**

- Deferred to next telecon

#### **17. HEMCO restructuring (Lizzie)**

- Deferred to next telecon

#### **18. Remote communications with users – clinics, WG meetings, videos (Daniel)**

- Deferred to next telecon