GCST report to the GCSC
For the June 4th, 2018 telecon
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GCA1

The presentations from GCA1 will be posted on geos-chem.org this week.

v11-02 "release candidate"

The v11-02 "release candidate" 1 -year benchmark re-run is now complete. We are in the process of making up the plots and will post the results shortly..

This version contains all of the updates and fixes in v11-02f, PLUS:

- Uses the GEIA natural NH3 file at 4 x 5 resolution (1 x 1 was problematic)
- Avoid double-counting of ISOAAQ species in SOA diagnostics (i.e. only add ISOAAQ for simulations that use ComplexSOA)
- Updates for the Hg simulation:
    - Re-tuned Hg parameters (cf. Colin Thackray)
    - Bug fix: Change units of time steps from minutes to seconds in Hg code to match usage in the rest of GEOS-Chem
- Add clarifying comment for N2O5 + H2O rxn in KPP Standard.eqn file
- Add workaround for what appears to be a compiler bug in ifort 17.0.4 that causes a seg fault in the netCDF diagnostic module (state_diag_mod.F90)
- Bug fix: Enable nested-grid boundary condition output when netCDF diagnostics are turned on.
- Minor fixes for GCHP

We are currently finalizing the documentation for v11-02. We will announce that the v11-02 "release candidate" is ready for use once all of the documentation is complete,

v11-02 “testing” period and public release

GEOS-Chem users will have a “testing” period of approximately 4-6 weeks to test the v11-02 “release candidate” code. We will fix all bugs reported by users during this “testing” period.

We also received late word of several bugs and/or technical issues after the benchmarking of the v11-02f and v11-02 “release candidate” versions had begun. We will fix these issues during either during the “testing” period or early into the next version.

- RRTMG bug fix (Chris Holmes)
- Code updates to prevent HEMCO soil NOx error when using ifort 17 (Jenny Fisher)
- Correct missing Criegee intermediate rxn in Tropchem KPP mechansim (Xin Chen)
- Fix ARCTAS_SHIP scale factors in HEMCO configuration file (Barron Henderson)
- Fix error when distributing HEMCO emissions in the vertical (Sally Wang)
- Bug fix for liquid water content in KPP hetchem code (Jiayue Huang and Quanjie Chen)
- Bug fix in Flexchem: do not zero ACTA, EOH, HCOOH, this was a holdover from SMVGEAR (Katie Travis)
- Do not use both CEDS and GEIA NH3 biofuels together, to avoid double-counting (Eloise Marais)
- Disable Xiao emissions to avoid double-counting propane with CEDS (Christoph Keller)
- Fix bug grid offset bug in high-resolution MEGAN files at southern mid-latitudes

Priorities for further model development

We have updated the GEOS-Chem model development priorities wiki page with the latest status reports from GC developers.

Please note that “ready to go in” indicates that work by the developer is considered complete. However, GCST time to implement may vary significantly depending on the structural updates or reworking required for compatibility with the latest version.

GC in the Amazon Cloud

Jiawei Zhuang has created a tutorial that shows how you can run GEOS-Chem “Classic” (GCC) on the Amazon Web Services EC2 cloud computing platform. A copy of the GEOS-Chem “gcgrid” data directories has been synchronized to the Amazon S3 storage system and is available for use with your GEOS-Chem simulations.

Jiawei is also exploring how to run GCHP on the cloud. Currently, GCHP simulations using a single node are possible using the open-source GNU Fortran compiler. He writes:

> As you know, I've [gotten] GCHP running on the cloud. I got enthusiastic responses at [the recent] GCA1 [meeting], presumably because GCHP is so hard to set up from scratch, and it is quite amazing to be able to run the model immediately on cloud platforms.

Running multi-node GCHP simulations in the cloud will require more work. Nodes of a dedicated computer cluster are typically interconnected with the very fast Infiniband network. But in the Amazon cloud, nodes are usually connected with Ethernet, which is several orders of magnitude slower than Infiniband. This will make GCHP simulations that require multiple nodes run more slowly than on a dedicated cluster. Jiawei is looking into potential solutions for this.

Jiawei has also created a Python tutorial that illustrates how to analyze data generated by GEOS-Chem on the cloud.

GCHP

GCHP is currently up-to-date with GEOS-Chem v11-02e. GCHP v11-02, including all updates in v11-02f and the v11-02 candidate release, is currently being tested. GCHP v11-02 will additionally feature native resolution offline dust emissions developed by David Ridley (MIT) and lightning emissions developed by Sebastian Eastham (MIT), as well as a bug fix to improve performance when built with open-source GNU compiler GFortran.

We are continuing to collaborate with GMAO to improve GCHP performance and usability. Seb is spearheading the effort to acquire native resolution mass fluxes on the cubed sphere grid for input to GCHP. Lizzie Lundgren will be actively developing a shared GMAO MAPL repository to bring an updated version of MAPL into GCHP and feed our GEOS-Chem-specific updates back to GMAO. The new version of MAPL will include an improved I/O layer that we anticipate will speed up GCHP file I/O. Lizzie will also be working to remove the GMAO MAPL content included within GCHP that is not necessary for GCHP functionality.

GC embedded within GEOS-DAS

GCST member Lizzie Lundgren is currently collaborating with Christoph Keller on improving the development pipeline between GC and the NASA GEOS-DAS system. Right now the GC-to-GEOS-DAS interface is based off older code and is cumbersome to modify. The current phase of the work involves standardizing the GC-to-GEOS-DAS interface so that it will be consistent with the current v11 GCHP. In this way, any modifications that are made to the GCHP code base by GCST or GMAO will readily feed into both the GEOS-DAS system maintained by GMAO as well as GCHP maintained by GCST.

Ada Shaw, a graduate student at Harvard, will be interning at NASA/GMAO this summer. She will work closely with both Christoph and Lizzie.

Using the "Singularity Container" to simplify GEOS-Chem configuration

Jiawei Zhuang has been exploring the use of "Singularity Containers" as a way to easily export a given computer configuration. His work addresses the common difficulty that users encounter when initially setting up compilers, netCDF libraries, MPI libraries, etc for use with GEOS-Chem. GEOS-Chem users sometimes encounter system-dependent errors that the GCST cannot reproduce locally, particularly when using GCHP, which is very sensitive to environment setup.

Using Singularity containers may solve this issue. Any combination of compiler, netCDF libraries, and MPI built for either GCC or GCHP can be saved to a Singularity container. Any user with access to Singularity software on his or her system can simply load the container and replicate the pre-saved computational environment. Not only will this guarantee that GCC or GCHP will compile properly, but it will also ensure that simulation results generated by a user will be 100% bitwise identical to simulations performed by GCST. This will facilitate debugging and development.

Jiawei has successfully run both GEOS-Chem "Classic" and GCHP using Singularity. GCST will have more information about the use of Singularity Containers in the near future.

Proposed new numbering scheme for GC versions

In order to conform more closely to industry-standard software versioning protocol, we propose a new system for GEOS-Chem version labelling. Our proposal is based loosely on a system called Semantic Versioning.

We propose retiring use of letters and instead using 3 numbers of form **X.Y.Z** defined as follows:

- **X: Major version number:**
  - Analogous to previous "public" releases
- **Y: Benchmark number**
  - Denotes a collection of new features, analogous to previous lettered versions
- **Z: Bug fix number**
  - Denotes bug fixes that do not break backwards compatibility with run directories

X will change for each public release. Y will change whenever there is a 1-month benchmark (i.e. when a new set of features have been added). Most notably, Z will only change if backwards compatibility is preserved. This means all X.Y.0 run directories would be compatible with all X.Y.Z versions of GEOS-Chem.

We propose to apply this numbering as shown in the example below:

- This upcoming major release: **v11-02-final, aka 12.0.0**
    - 2 tags denote the transition from the old to the new numbering scheme
    - First benchmark after that: **12.1.0**
        - Fixed a bug identified during benchmark: **12.1.1**
        - Fixed a second bug: **12.1.2**
        - Fixed a third bug: **12.1.3**
        - ...etc...
    - Next benchmark of new features: **12.2.0**
        - Fixed a bug identified during benchmark: **12.2.1**
        - Fixed a second bug:: **12.2.2**
        - ...etc...
    - Next benchmark: **12.3.0**
        - Fixed a bug identified during benchmark: **12.3.1**
        - ...etc...
    - ...etc ...
    - Next release candidate: **12.N.0** (where N is yet to be determined)
- Next major release: **13.0.0**

We would only update the GC manual pages at each “major” release. But GC users would still be free to download any of the intermediate versions. We’ll also always keep the wiki up-to-date.

We seek feedback and approval from the GEOS-Chem Steering Committee regarding this proposed new numbering system for GEOS-Chem versioning. Please let us know if you have any questions or concerns.

Migration to Github as the source code repository

We are considering moving the GEOS-Chem source code repository from Bitbucket to GitHub. Switching to GitHub will make it much easier to assign a DOI to a particular GEOS-Chem version. For various technical reasons, this process is much more complicated when using other source code repository platforms than GitHub.

Thank you for your patience!

We would like to sincerely thank you for your patience and understanding during the v11-02 release process. We have been working hard to prepare this version and we truly appreciate your feedback and guidance

Bob, Lizzie, and Melissa