GEOS-Chem Support Team Report to GCSC
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NOTE: In the interest of time, we are submitting a much more simply formatted report. We plan to publish a much more detailed GEOS-Chem Newsletter at the time of the v11-02 provisional release in March.

V11-02d
- Approved on 2/12/18
  - Evaluation of halogen chemistry is ongoing by developers. Recommended fixes and updates will be included in v11-02e,f and v11-03.

- Features affecting the full-chemistry simulation:
  - Halogen chemistry updates (Tomas Sherwen et al.)
  - Sulfur oxidation by reactive halogens (Qianjie Chen)
  - Bug fixes
    - Het chem fixes for GLYX, MGLY, IEPOX, IMAE (Seb Eastham)
    - Reading the wrong optical properties file for UCX (Melissa Sulprizio)
    - Fix high P(Ox) and L(Ox) caused by IPMN reactions (Eloise Marais)

- Features not-affecting the full-chemistry simulation
  - CH4 latitude bands for 2014-2016 (Katie Travis)
    - To be replaced by monthly mean CH4 distributions in v11-02e
  - Removed support for GCAP-1, GEOS-4, MERRA, GEOS-5 (Melissa Sulprizio)
  - Timestamp HEMCO diagnostics output file with start time (Lizzie Lundgren)
  - Structural updates for netCDF diagnostics (Bob Yantosca + Lizzie Lundgren)

V11-02e
- In progress now

- This version will require the following benchmarks:
  - 1-month full-chemistry benchmark
  - 1-year full-chemistry benchmark
  - 1-year Rn-Pb-Be benchmark

- Features affecting the full-chemistry simulation:
  - Monthly mean surface methane distributions (Lee Murray)
  - UCX updates (Seb Eastham, Chris Holmes, Melissa Sulprizio)
  - Use monthly mean strat prod/loss from UCX instead of GMI (Melissa Sulprizio)
    - Prod/loss fields are saved out from 1-year v11-02d simulation; Will need to update fields at intervals specified by GCSC (e.g. every public release)
  - Metal catalyzed oxidation of SO2 as a switch - on by default (Viral Shah, Becky Alexander)

- - [SOA updates and fixes](#) (Sam Silva, Chemistry WG, Aerosols WG, Eloise Marais)
    - [Fix dust rainout settings to match BCPO](#) (Colette Heald)
    - [Fixes in gckpp_HetRates.F90 for halogen chemistry](#) (Lei Zhu, Seb Eastham)
    - [Sync GEOS-FP files on Harvard FTP with those at Dalhousie](#) (Melissa Sulprizio)
      - ***NOTE: GCST always recommends downloading met fields from Dalhousie and emissions data from Harvard***

- Features not affecting the full-chemistry simulation
  - [Spatially varying OM/OC ratios as a switch](#) - off by default (Sajeev Philip)
  - [Rn-Pb-Be simulation now uses 72 levels by default](#) (Melissa Sulprizio)
  - [ND49 timeseries diagnostic for 10m ozone](#) (Katie Travis)
  - [Bug fixes for ISORROPIA stable mode](#) (Jingyuan Shao, Shaojie Song)
  - [Change timestep input from minutes to seconds](#) (Lizzie Lundgren)
  - [Fixes for ND21 binary diagnostics](#) (Lizzie Lundgren)

V11-02f
- This version will require the following benchmarks:
  - 1-month full-chemistry benchmark
  - 1-year full-chemistry benchmarks
    - Run0 using 2013 GEOS-FP meteorology
    - Run1 using 2016 GEOS-FP meteorology
  - 1-year Rn-Pb-Be benchmark using 2016 GEOS-FP meteorology
  - NOTE: The 2016 benchmarks will be used for comparison with GCHP, comparison of netCDF and binary diagnostics, and as reference in future benchmarks. We will use 2016 GEOS-FP meteorology for all benchmarks starting in v11-03.

- Features affecting the full-chemistry simulation
  - [Use global 0.25 x 0.25 files for MEGAN and MODIS](#) (Jenny Fisher, Eloise Marais, Dylan Millet)
  - [Update HEMCO from v2.1.001 to v2.1.005](#) (Christoph Keller)
  - Many new emissions inventories, [see wiki for details](#)

- Features not affecting the full-chemistry simulation
  - [Updated CH4 simulation](#)(Bram Maasakers, Melissa Sulprizio)
  - [Updated Tagged CO simulation](#) (Jenny Fisher)
  - [Updates to Hg chemistry from Horowitz et al (2017)](#) (Hannah Horowitz, Colin Thackray, Rebecca Stern)

Provisional Release
- We will issue the v11-02 provisional release after approval of v11-02f
  - There will be a provisional period of 4-6 weeks in which users can submit bug fixes etc. before the v11-02 public release is announced.

GCHP

- GCHP continues to be up-to-date with GEOS-Chem "classic" (GCC) and v11-02d is now available as the master branch.

- GCHP v11-02e will feature expanded netCDF diagnostics, including all benchmark diagnostics.

- The GCHP benchmark will be performed with v11-02f and will require a 1-month full-chemistry benchmark, a 1-year full-chemistry benchmark, and a 1-year RnPbBe benchmark.

- The GCHP benchmark simulations will be run with C48 cubed sphere resolution (~2x2.5) using 0.25x0.3125 GEOS-FP meteorology fields for 2016.

- We plan on using archived offline 2x2.5 emissions developed by Sebastian Eastham for lightning NOx (NO), dust (DST1-4), sea salt (SALA, SALC, and Br2), and sea salt flux (ACET, ALD2, and DMS) in all GCHP full-chemistry benchmark simulations to reduce differences with GEOS-Chem classic that are due to grid-dependent emissions.

- The offline emissions will also be used in a custom GCC 1-month run to further minimize these differences.

NetCDF diagnostics

- All of the diagnostics required for benchmarking GEOS-Chem will be available in netCDF format in both GEOS-Chem "Classic" and GCHP configurations, for the v11-02 public release.

- While the netCDF diagnostics are functional, we shall nevertheless consider them to be as "beta" for the v11-02 public release. This means that the bpch diagnostics will be activated by default, unless the user specifies otherwise during compilation. This is for the following reasons:

  - Not all possible bpch diagnostics have been ported to netCDF yet. For example, most of the specialty simulation diagnostics (except for Rn-Pb-Be, which is used for benchmarking) will only be available in bpch for v11-02.

  - Several "specialty diagnostics" (e.g. satellite timeseries) are not able to be replicated for GCHP at the moment, which is constrained by the MAPL diagnostic I/O module. These specialty diagnostics will remain as bpch-only options for GEOS-Chem "Classic" in v11-02.

  - Benchmark scripts using the new python package GCPy are in development and will not be complete in time for the v11-02 benchmark. We will therefore use our IDL/GAMAP benchmark plotting software to create the v11-02 GEOS-Chem

"Classic" 1-month and 1-year plots. However, the GCHP benchmark will use GCPy and the cubed-sphere and xESMF python packages developed by Jiawei Zhuang in combination with IDL/GAMAP. We will also compare GEOS-Chem "Classic" binary and netCDF diagnostics using GCPy. We plan to transition completely from IDL to python for the v11-03 release benchmark.

- Validation of the netCDF diagnostics has been proceeding throughout v11-02c, v11-02d, v11-02e, and v11-02f.:

  ○ We plan on releasing comparing plots of netCDF and binary diagnostics as part of the v11-02 public release benchmark.

  ○ NOTE: For several diagnostics, the bpch diagnostic output will not exactly match the netCDF diagnostic output. Many of the bpch diagnostics are updated once per chemistry timestep (usually 20 minutes), but the netCDF diagnostics (in both GEOS-Chem "Classic" and GCHP) will be updated once per "heartbeat" timestep (usually 10 minutes). This discrepancy in update time will cause differences greater than are to be expected from numerical noise/roundoff error alone. We will just have to live with this.

- NetCDF diagnostic output will be configured for a set of default file collections.

  ○ A collection is a series of netCDF files that contain one or more diagnostic quantities. For example, there is a dry deposition collection in which all dry deposition diagnostics are calculated at a user-configured frequency ("frequency") and output to a file at another user-configured frequency ("duration"). Each collection has a single output metric ("mode") that can either be instantaneous or time-averaged.

  ○ Collections, including diagnostic names and user-configured settings, are defined by the user in the HISTORY.rc file. The GEOS-Chem Unit Tester for v11-02 will contain a unique HISTORY.rc file for each possible GEOS-Chem simulation. Please note that not all specialty simulations will have a full set of netCDF diagnostics available in the v11-02 public release.

  ○ Grouping diagnostics into collections has several advantages, namely:

    ■ It prevents any single file from becoming too large and unwieldy;

    ■ It makes it easier to exclude diagnostic output that is not relevant to a simulation (i.e. don't print out SOA diagnostics if you're doing a Rn-Pb-Be simulation, etc.)

    ■ It mimics how many other ESMs (e.g. GEOS-DAS) archive diagnostic output.

- ○ Our default list of netCDF diagnostic collections are as follows:

    - ■ SpeciesConc: Species concentration (cf. ND45)
    - ■ AerosolMass: Aerosol, SOA, and PM2.5 mass (cf. ND42)
    - ■ Aerosols: Aerosol mass, radius, optical depth etc. (cf. ND21)
    - ■ CloudConvFlux: Cloud convective flux (cf. ND14)
    - ■ ConcAfterChem: Concentrations after chemistry (cf. ND43)
    - ■ DryDep: Drydep frequency and velocity (cf. ND44)
    - ■ JValues: Instantaneous J-values
    - ■ JValuesLocalNoon: J-values at local solar noon (cf. ND22)
    - ■ LevelEdgeDiags: For diagnostics defined on level edges
    - ■ ProdLoss: Chemical production and loss (cf. ND65)
    - ■ StateChm: Archives fields of State_Chm object
    - ■ StateMet: Archives fields of State_Met object
    - ■ WetLossConv: Loss of soluble species in convection (cf. ND38)
    - ■ WetLossLS: Loss of soluble species in wet deposition (cf. ND39)

  - ○ GEOS-Chem users will have complete freedom to easily turn off these collections and create their own custom collections within the HISTORY.rc file. Custom collections may include any combination of existing diagnostics and user-defined diagnostics, instantaneous or time-averaged, and archived at any frequency and duration down to the dynamic timestep. Documentation on how to do this will be available at the v11-02 release.

- We have created a table on the GEOS-Chem wiki that maps each existing bpch diagnostic to the new netCDF equivalent. See the wiki page: *List of diagnostics archived to bpch format*. We are also updating its sister page, *List of diagnostics archived to netCDF format*, which will serve as an easy reference for what netcdf diagnostics are available for archiving as well as a full description of the naming conventions used.

- Due to time constraints, we have only implemented existing binary diagnostics in netCDF. New diagnostics, such as the flux diagnostics submitted by Chris Holmes, will be a high-priority item for v11-03.

- Diagnostics for emissions and other quantities computed by HEMCO will be handled by HEMCO separately from the new netCDF diagnostics. This preserves how HEMCO functions in GCHP mode, and also when using HEMCO in standalone mode.

  - ○ You can specify which HEMCO diagnostic quantities will be archived by modifying the HEMCO_Diagn.rc file as described in *The HEMCO User's Guide* on the wiki.

- ○ The GCST will provide a `HEMCO_Diagn.rc` file customized for each GEOS-Chem simulation. This will ship with the GEOS-Chem Unit Tester (from which you can generate run directories).

- ○ By default, HEMCO diagnostic output will be to archived files named `HEMCO_diagnostics.YYYYMMDDhhmm.nc`. You can change the name in the HEMCO_Config.rc file.

- ○ HEMCO diagnostics should not be included in the `HISTORY.rc` for GCC but should be included for output by GCHP.


Other structural modifications
- ● NASA/GMAO requested that GEOS-Chem timesteps be in seconds instead of integral minutes. This will allow GEOS-Chem to use the GEOS-DAS dynamic timestep of 450 seconds (7.5 minutes). Lizzie Lundgren made the appropriate changes in v11-02e.

- ● Bob Yantosca and Lizzie Lundgren modified many GEOS-Chem routines in order to prevent simulations from exiting from the point in the code where a fatal error occurs. Instead, an error code will propagate all the way up to the main program level, where GEOS-Chem can be terminated gracefully. We have also improved the error messages to be less cryptic and more descriptive. We made these modifications primarily to prevent GCHP simulations from terminating on one node while continuing to execute on other nodes. We will continue adding in this functionality into the v11-02 public release and v11-03.

- ● Melissa Sulprizio made initial changes to remove unnecessary C-preprocessor switches in v11-02e. In that version, the `#if defined( UCX )` CPP switches have been replaced with the logical switch `Input_Opt%LUCX`, allowing users to switch between tropchem and UCX-based mechanisms without having to recompile GEOS-Chem. In addition, the input.geos file is now read at the very start of GEOS-Chem. This will eventually facilitate removal of #ifdefs for `ESMF_`, `EXTERNAL_GRID`, and `EXTERNAL_FORCING` by GCHP developers in a move to reduce or eliminate GCHP-specific code. These changes are purely structural and should have no impact on the average user.

Performance
- ● In general, GEOS-Chem "Classic" simulations (using OpenMP serial parallelization) scale as expected when adding additional CPUs. Adding more CPUs will always make the simulation go faster, but the improvement increases "asymptotically". This is due to the extra CPUs incurring computational overhead when communicating with memory. See figure below:

Scalability plot
1-month GEOS-Chem "Classic" simulations
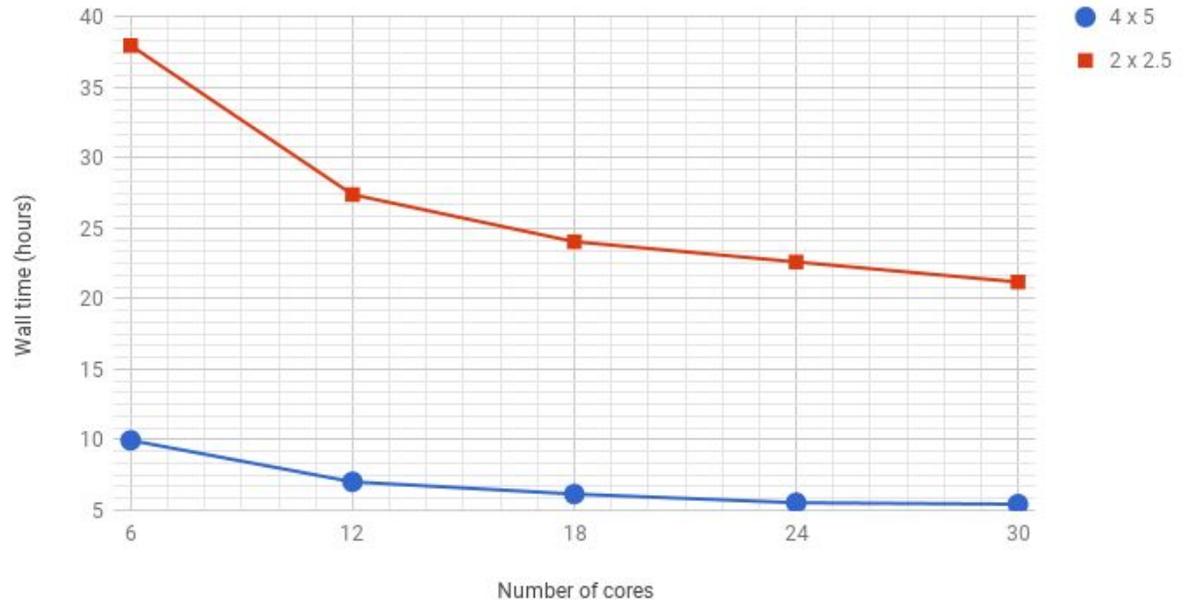
- Our preliminary analysis also has indicated that the gas-phase chemistry (FlexChem) scales very well, but convection and wet deposition scale much less well. We will investigate how these bottlenecks can be improved in v11-03.

- Seb's GCHP paper goes into more detail about the performance of GEOS-Chem "Classic" and GCHP -- he will discuss further.

GCPy Python package
- The GCPy package is in development but we welcome users to download it and follow the example Jupyter Notebooks to get started and contribute.
- GCPy can be downloaded from: https://bitbucket.org/gcst/gcpy/
- Users interested in using python with GCHP output should contact Lizzie Lundgren for more information.