GEOS-Chem Newsletter
Fall 2017 Edition

GEOS-Chem Support Team
07 September 2017

Table of contents

GEOS-Chem Asia Meeting

We are excited to announce that the **first regional GEOS-Chem Asia meeting (GCA1) will be held on May 21-23, 2018** at Nanjing University of Information Science and Technology (NUIST).

The international GEOS-Chem community has been gathering every two years at Harvard for International GEOS-Chem meetings (IGC) to share results and set directions for model development. The goal of GCA1 is to provide a supplementary venue for the Asian community to stay informed about model developments and initiate collaborations. GEOS-Chem users and the broader community outside Asia are also warmly invited to attend. We plan to conduct GCA meetings in alternate years with the flagship IGC meetings.

For more information, please visit **http://geos-chem.org/meetings/2018_GCA/**.

GEOS-Chem High Performance in the Standard Model

The first official benchmark of GEOS-Chem with the high performance option (GCHP) was performed as part of GEOS-Chem v11-02b benchmarking and received approval in July 2017. GCHP features the same science as GEOS-Chem using the standard "classic" capability (GCC) but operates on a cubed-sphere grid and is parallelized using a message-passing interface (MPI) implementation. GCHP improves upon GCC by (1) enabling more accurate transport through elimination of the polar singularity inherent to lat-lon grids, and (2) providing efficient scaling across multiple machines making finer resolution global simulations possible.

We encourage users to set up GCHP on their systems, join the GCHP Working Group, and provide feedback on user experience and model performance. The GEOS-Chem HP v11-02 wiki page lists version information as well as GCHP-specific features, bug fixes, and outstanding issues. Scientific updates from the community will continue to be implemented in the primary GEOS-Chem repository and documented on the GEOS-Chem v11-02 wiki page.

For more information on GCHP including tutorials and contact information, please see the GCHP homepage on the GEOS-Chem wiki.

News from the GEOS-Chem Steering Committee

Latest GCSC meeting minutes

The GEOS-Chem Steering Committee (GCSC) met on September 7, 2017. We invite you to read the meeting minutes.

The next GCSC meeting will take place on (date TBD).

New GCHP Working Group Co-Chair

Please join us in welcoming **Seb Eastham** (MIT) as a new GCSC member and co-chair of the GEOS-Chem High Performance (GCHP) Working Group, replacing **Mike Long** who is stepping down. Seb is taking on substantial leadership roles within GCHP (including connecting with NASA GMAO), is heavily involved in GCHP development, and has vision for future GCHP developments.

We would also like to take this opportunity to thank Mike on behalf of all of us for his service to the GCSC and his outstanding leadership of the GCHP development effort.

GEOS-Chem v11-02 development overview

The sections below describe in detail the various new features that have already been added to GEOS-Chem v11-02, as well as updates that are slated for the near future

NOTE: v11-02a, v11-02b, etc. denote 1-month benchmark simulations, which are designed to evaluate GEOS-Chem's performance at intermediate stages of development.

GEOS-Chem v11-02a

In this version, we fixed several issues that were brought to our attention by GEOS-Chem users after the public release of v11-01. We also added several structural updates to v11-02a, including support for the latest GNU Fortran Compiler versions, an update to HEMCO, and a fix for compressing netCDF output files. V11-02a was approved on 12 May 2017.

Please see the following links for complete information about the validation of v11-02a:

1. *Approval form for 1-month benchmark simulation v11-02a*
2. *Results for 1-year benchmark simulation v11-02a-Run0*
3. *Results for 1-year benchmark simulation v11-02a-Run1* (final version)

V11-02a Feature	Submitted by	Type
Features affecting the full-chemistry simulation:		
Update chemistry rate constants based on *JPL Publication 15-10*	Barron Henderson (US EPA), Mat Evans (U. York), & Oxidants and Chemistry WG	Science
Fixes to correct ALK4 lumping issue	Barron Henderson (US EPA)	Science
PAN updates (including emissions, deposition, species, chemistry)	Emily Fischer (CSU)	Science
Monthly mean NEI2011 emissions	GCST & Katie Travis (Harvard)	Science
Bug fixes in the GEOS-Chem sulfate module: • Fix error in production of SO4s and NITs in SEASALT_CHEM • Fix bug in CHEM_NIT • Fix for sulfate production in HET_DROP_CHEM • Fix bugs in sulfate chemistry routines	 Prasad Kasibhatla (Duke) Prasad Kasibhatla (Duke) Qianjie Chen (UW) Viral Shah (UW)	Bug fix
Fix bug in dry deposition aerodynamic resistance	Brian Boys (Dalhousie)	Bug fix
Fix acetone parameterization in hcox_seaflux_mod.F90	GCST	Bug fix
Bug fix in cos(SZA) for start of timestep	Lizzie Lundgren (GCST)	Bug fix
Include TOA pressure when calculating dry pressure edges	Seb Eastham (Harvard)	Science
Features not affecting the full-chemistry simulation:		
Implement ISORROPIA v2.0 as a Fortran module	Seb Eastham (Harvard) & GCST	Structural
Updates to the HEMCO emissions component: • Update to HEMCO v2.0.004 • Fixed bug in computation of local time in HCO_GetSunCos • Default US emissions to NEI2011 after 2013 • Read default DEP_RESERVOIR fields from file	Christoph Keller (NASA GMAO) Seb Eastham (Harvard) Jessica Morena (Dalhousie) Brian Boys (Dalhousie) & GCST	Structural & Bug fix
Updates to gain computational speedup: • Add simplified prod/loss families to KPP • Remove computational bottleneck in convection	Mike Long (Harvard) Bob Yantosca (GCST)	Structural & Bug fix

V11-02a Feature	Submitted by	Type
module		
Fixed typo in INIT_WINDOW	Bob Yantosca (GCST)	Bug fix
netCDF file I/O updates: • Enable data compression in netCDF-4 output files • Routine DO_ERR_OUT now returns a non-zero error code • HEMCO files now have an unlimited time dimension	Chris Holmes (Florida State) Andy Jacobson (NOAA) GCST	Bug fix & Structural
Makefile and build sequence updates: • Specifying NO_REDUCED=no now compiles GEOS-Chem for reduced grids • Removed the COMPILER variable from Makefile_header.mk	Jiawei Zhang (Harvard) GCST	Bug fix & Structural
Bug fixes for running UCX in ESMF environment	Christoph Keller (NASA GMAO)	Bug fix
Bug fixes for diagnostics: • Save out PM2.5 diagnostic at STP conditions • Bug fixes in convective mass flux diagnostic • Restore P(OH) in ND22 diagnostic • Make anthropogenic emissions diagnostics 3D • Fix ND65 bugs in tagged CO simulation • Fix bug in ND21 diagnostic indexing for dust species	Aaron van Donkelaar (Dalhousie) Jenny Fisher (U. Wollongong) GCST Jenny Fisher (U. Wollongong) Chris Holmes (Florida State)	Bug fix
Removal of obsolete variables: • Removed the NNPAR parameter from CMN_SIZE_mod.F • Removed obsolete variables NSOL and IDWETD • Removed obsolete fields of the Input_Opt object	GCST	Structural

GEOS-Chem v11-02b

GEOS-Chem v11-02b with and without the high performance option (GCHP) was approved on 16 Jun 2017. It contains several critical software updates for GCHP, as well as fixes for minor issues. GEOS-Chem v11-02b is the first benchmarked version of GCHP.

Please see the following links for complete information about the validation of v11-02b with and without the high performance option:

1. *Approval form for 1-month benchmark simulation v11-02b*
2. *Approval form for 1-month benchmark simulation v11-02b with high performance option (v11-02b-HP)*
3. *Results for 1-year standard benchmark simulation of v11-02b-HP Run0*
4. *Results for 1-year standard benchmark simulation of v11-02b-HP Run1* (uses offline archived lightning and dust emissions)
5. *Results for 1-year RnPbBe benchmark simulation of v11-02b-HP*

v11-02b Feature	Submitted by	Type
Features not affecting the full-chemistry simulation:		
Source code updates for high performance option (GCHP)	Seb Eastham (Harvard) Lizzie Lundgren (Harvard) Mike Long (Harvard) Jiawei Zhuang (Harvard) Bob Yantosca (Harvard)	Structural
Bug fixes for diagnostics: • Use FZ array to compute ND26 vertical flux diagnostic • Always write ND40 planeflight diagnostic when enabled	Ilya Stanevic (Toronto) Lee Murray (Rochester)	Bug fix
Write initial and final Ox mass to file when using the tagged O3 simulation	Bob Yantosca (GCST)	Structural
Convert CO2 emissions units using dry pressure used in advection	Meemong Lee (JPL)	Science
Add QFED emissions for 2014-2016	Christoph Keller (NASA GMAO)	Science

GEOS-Chem v11-02c

GEOS-Chem v11-02c introduces some long-awaited updates to the isoprene and SOA chemistry mechanisms, as well as fixes for minor issues and several structural updates. As of this writing, the v11-02c benchmarks are still awaiting final approval.

v11-02c Feature	Submitted by	Type
Features affecting the full-chemistry simulation:		
Enhance default GEOS-Chem simple SOA	Sal Farina (CSU) Aerosols Working Group Chairs	Science
Updates to isoprene and monoterpene chemistry	Katie Travis (MIT) Jenny Fisher (U. Wollongong) Eloïse Marais (U. Birmingham) Christopher Chan Miller (Harvard) Kelvin Bates (Caltech) Rebecca Schwantes(Caltech)	Science
Add aqueous isoprene uptake to SOA scheme	Eloise Marais (U. Birmingham)	Science
Carbon balance (fix C creation)	Sarah Safieddine (MIT)	Bug fix
Fix bugs for EOH and MGLY following implementation of PAN updates in v11-02a	Melissa Sulprizio (GCST)	Bug fix
Update HEMCO from v2.0.004 to v2.1.001	Christoph Keller (NASA GMAO)	Structural
Features not affecting the full-chemistry simulation:		
HEMCO updates: • Add a HEMCO-standalone run directory for benchmarking purposes • Now use YYYYMMDDhhmm for time stamp values • Add error trap in to avoid a segmentation fault when the DustGinoux extension is turned off	Christoph Keller GMAO) Andy Jacobson (NOAA) Paulo Tuccella (L'Aquila)	Structural
Fixes for several minor issues: • Bug fixes for the ND50 timeseries diagnostic • Fixed an incorrect format statement in input_mod.F • Add MERRA2 to #if and #elif statements where it had been omitted • Bug fixes for Hg emissions • Fix bug in species definitions for marine POA simulation	Chris Holmes (FSU) Chris Holmes (FSU) Jiawei Zhuang (Harvard) Amanda Giang (MIT) Katie Travis (MIT) Katie Travis(MIT)	Bug fix

• Fix diagnostic bugs in the SOA-SVPOA simulation		
Fixes for the TOMAS simulation: • Fixes for TOMAS simulation in v11-02c • Fix typo in wetscav_mod.F for TOMAS30 • Remove a couple of array temporaries and an out-of-bounds error	Sal Farina (CSU) Jack Kodros (CSU) Bob Yantosca (GCST)	Bug fix
Fix STE flux diagnostics and add to benchmark procedure	Melissa Sulprizio (GCST)	Bug fix & Benchmarks
Initial structural modifications for netCDF diagnostics: • Introduce Headers/State_Diag as a stub module (for now) • Add a registry object into State_Met, State_Diag, and State_Chm in order to obtain a pointer to any module variable (or slice) by looking up its name • Add new module Headers/registry_mod.F90 which contains derived types and routines for registering module variables.	Bob Yantosca (GCST)	Structural
Combine timestep settings in input.geos in a Timesteps menu	Melissa Sulprizio (GCST)	Structural
Update CO data used in 1-year benchmark plots	Jenny Fisher (U. Wollongong)	Benchmarks

GEOS-Chem v11-02d

This version will add a new halogen chemistry mechanism (cf. T. Sherwen et al, ACP, 16, 1161-1186, 2016) to GEOS-Chem. We will also remove support for the following met field products from v11-02d: GCAP (legacy 4^0 x 5^0 resolution data only), GEOS-4, GEOS-5, and MERRA.

v11-02d Feature	Submitted by	Type
Features affecting the full-chemistry simulation:		
Halogen chemistry updates	Tomás Sherwen (York) Johan Schmidt (Harvard) Oxidants and Chemistry WG	Science
Sulfur oxidation by reactive halogens	Qianjie Chen (UW)	Science
Sync GEOS-FP files on Harvard ftp with files at Dalhousie	GCST	Bug fix

v11-02d Feature	Submitted by	Type
Features not affecting the full-chemistry simulation:		
Update CH4 latitude bands for 2014-2016	Katie Travis (MIT)	Science
Remove support for GCAP, GEOS-4, MERRA, GEOS-5	GCST	Structural
Structural updates for netCDF diagnostics	GCST	Structural

GEOS-Chem v11-02e

In this version we will add more chemistry updates, including updates for stratospheric chemistry with UCX.

v11-02e Feature	Submtted by	Type
Features affecting the full-chemistry simulation:		
Update density of BC to 1.8 and add absorption enhancement factor in input.geos	Xuan Wang (MIT)	Science
Monthly mean surface methane distributions	Lee Murray (NASA GISS/LDEO)	Science
Remove initial stratospheric 2D mixing ratio option	Seb Eastham (Harvard)	Science
UCX stratospheric water boundary condition update	Chris Holmes (UC Irvine) Seb Eastham (Harvard)	Science
Metal catalyzed oxidation of SO2 (as a switch)	Becky Alexander (UW)	Science
Spatially varying OM/OC	Sajeev Philip (Dal/NASA Ames)	Science
Features not affecting the full-chemistry simulation:		
Radon flux diagnostic	GCST	Benchmarks

Priorities for future development

Beyond v11-02e, there are several updates that are currently listed as “in the pipeline” for inclusion into GEOS-Chem. The order of these updates has not been fully determined yet. For a list of these updates, please see the "in the pipeline" table of the GEOS-Chem v11-02 wiki page.

Emissions updates

Update to HEMCO v2.1

The Harvard/NASA Emsisions Component (HEMCO) was updated to **Version 2.1.001** in GEOS-Chem v11-02c. This new HEMCO version introduces three new features:

1. All internal timestamp variables have been changed to 8-byte floating-point precision (i.e. REAL*8) in order to be able to read netCDF time values in YYYYMMDDhhmm format;
2. Species-specific scale factors may now be applied across all inventories, categories, hierarchies, and extensions;
3. Mathematical expressions (such as "2.0 + SIN(HH)", where HH = the hour of the day) may now be used. (This feature, however, is not currently used in any of the standard simulations.)

We have also added a corresponding feature to the GEOS-Chem Unit Tester in v11-02c:

- We have added a run directory for the HEMCO standalone model to the GEOS-Chem Unit Tester for v11-02c and newer versions. GEOS-Chem users can drop their configuration file (HEMCO_Config.rc) into that directory and test their emission setup right away. This will also allow us to add HEMCO standalone runs to our standard benchmarking procedures.

For more information about these updates, please visit the following wiki pages:

1. Implementation of HEMCO in GEOS-Chem
2. *The HEMCO User's Guide*

Chemistry updates

New options for simulations with secondary organic aerosols (SOA)

The Aerosols Working Group decided on the following options for SOA in GEOS-Chem v11-02 and later. A quick summary of the SOA options is provided in the following table:

SOA option	Description
Option 1: **Simple SOA scheme**	Starting in GEOS-Chem v11-02, we will have an option for "simple" SOA that forms irreversibly. This option will allow GEOS-Chem users to get approximately the "correct" amount of global SOA without detailed chemistry. This scheme introduces two SOA-related tracers: **SOAP (SOA precursor)** and **SOAS ("simple" SOA in the particle phase)**. The emission of SOAP is tied directly to emissions of monoterpenes, isoprene, biomass burning CO, biofuel CO, and fossil fuel CO in HEMCO, and SOAP forms SOAS on a fixed timescale of 1 day. 50% of monoterpene and isoprene SOA is emitted directly as SOAS to reduce the average formation time for this SOA.

SOA option	Description
	The default yields specified in the HEMCO configuration file are: • Monoterpenes: 5% mass yield SOAP, 5% mass yield SOAS • Isoprene: 1.5% mass yield SOAP, 1.5% mass yield SOAS • Biomass burning and biofuel: 0.013 g SOAP/(g CO emitted) Kim et al., 2015 • Fossil fuel: 0.069 g SOAP/(g CO emitted) Kim et al., 2015 Each of the above yields may be adjusted in the HEMCO configuration.
Option 2: **Complex SOA scheme**	• **Default GEOS-Chem full-chemistry option** • Built on the Havala Pye VBS scheme • May be used with or without semi-volatile POA (default: no SVPOA) • Eloise Marais's isoprene aqueous uptake mechanism to be added to this (additional source of aqueous isoprene SOA, with new species identifying it as such, keeping existing SV isoprene SOA as well)

Option 3:
Combines Options 1 + 2
	• **Used in the benchmark simulations as of v11-02c**
	• This option is used in the GEOS-Chem benchmarks so that the community can validate both SOA mechanisms on a regular basis
	• Users may choose to use options 1+2, but are should be aware of the implications listed below
	  o This simulation will include *both* simple SOA (SOAP, SOAS) and complex SOA species (TSOA/G*, ISOA/G*, ASOA/G*)
	  o Expert users need to think about how/if to combine the complex and simple SOA species
	  o *Beginner users should not use this option to avoid confusion!!*

For complete information about these SOA options, please see *our wiki post entitled SOA schemes in v11-02 and later.*

You may specify the SOA options by setting flags in the AEROSOL MENU section of the input.geos file, starting with v11-02c.

To specify **Option 1**, make sure the simple SOA species (SOAP, SOAS) are defined in the Advected Species Menu and set the following switches in the Aerosol Menu:

```
Online COMPLEX SOA      : F
 => Semivolatile POA?   : F
 => Online Isoprene OA  : F
```

To specify **Option 2**, make sure the complex SOA species (MTPA, LIMO, MTPO, TSOA/G*, ISOA/G*, ASOA/G*) are defined in the Advected Species Menu and set the following switches in the Aerosol Menu:

```
Online COMPLEX SOA      : T
 => Semivolatile POA?   : F
 => Online Isoprene OA  : T
```

And to specify **Option 3,** make sure both the simple SOA and complex SOA species are defined in the Advected Species Menu and set the following switches in the Aerosol Menu:

```
Online COMPLEX SOA      : T
 => Semivolatile POA?   : F
 => Online Isoprene OA  : T
```

Halogen chemistry mechanism

In GEOS-Chem v11-02d, we plan on introducing the halogen chemistry scheme of Tomas Sherwen et al (cf. ACP, 16, 12239-12271, 2016) into the GEOS-Chem. From the abstract:

> *We present a simulation of the global present-day composition of the troposphere which includes the chemistry of halogens (Cl, Br, I). Building on previous work within the GEOS-Chem model we include emissions of inorganic iodine from the oceans, anthropogenic and biogenic sources of halogenated gases, gas phase chemistry, and a parameterised approach to heterogeneous halogen chemistry. Consistent with Schmidt et al. (2016) we do not include sea-salt debromination. Observations of halogen radicals (BrO, IO) are sparse but the model has some skill in reproducing these. Modelled IO shows both high and low biases when compared to different datasets, but BrO concentrations appear to be modelled low. Comparisons to the very sparse observations dataset of reactive Cl species suggest the model represents a lower limit of the impacts of these species, likely due to underestimates in emissions and therefore burdens. Inclusion of Cl, Br, and I results in a general improvement in simulation of ozone (O3) concentrations, except in polar regions where the model now underestimates O3 concentrations. Halogen chemistry reduces the global tropospheric O3 burden by 18.6 %, with the O3 lifetime reducing from 26 to 22 days. Global mean OH concentrations of 1.28 × 106 molecules cm−3 are 8.2 % lower than in a simulation without halogens, leading to an increase in the CH4 lifetime (10.8 w) due to OH oxidation from 7.47 to 8.28 years. Oxidation of CH4 by Cl is small (~ 2.1%) but Cl oxidation of other VOCs (ethane, acetone, and propane) can be significant (~ 15-27 %). Oxidation of VOCs by Br is smaller, representing 3.9 % of the loss of acetaldehyde and 0.9 % of the loss of formaldehyde.*

Met field data updates

Fixing an inconsistency in GEOS-FP met data at Harvard and Dalhousie for July 2013

We have recently identified an issue with the GEOS-FP met data files for July 5-31, 2013 that were stored on the Harvard shared data directory archive (ftp.as.harvard.edu), as described below:

Prasad Kasibhatla wrote:

> *I wanted to alert you about something you might know already. I have been trying to run Tomas Sherwen's halogen chemistry code here and was seeing some substantial differences in my output files compared to his, and I finally traced them to differences in the GEOS-FP 4x5 2013 *A3cld* met files between the Harvard (where I got my met files) and Dalhousie (where he got his met files) archives.*

Chi Li wrote:

> *I have retrieved the original GMAO GEOS-FP data for July, 2013, and generated the 4x5 A3cld data. I double checked the code and recompiled it, to guarantee that the new way of calculating CLOUD is included in the new processing.*
>
> *I read in "CLOUD", "OPTDEPTH" variables and compared the values. The differences were 0 everywhere and every time step when compared with the Dalhousie data for every day. Meanwhile when compared with the Harvard data, the maximum differences in OPTDEPTH could reach ~15 for July 5-31.*
>
> *So from my view I would say the Dalhousie archive should represent the more recent updates, at least for this month.*

Bob Yantosca wrote:

> *Odd – it seems like on our end, July 1-4 files were created on 2013-12-12, but July 5-31 were made on 2013-11-23 or thereabouts.. I am not sure what happened. Now I'm thinking that the Harvard files for...July 5-31…might not be correct.*
>
> *One thing – since we use July 2013 as our benchmarking year, this will affect the GC benchmarks.*

This inconsistency will be fixed in September 2017, and will be validated with benchmark simulations for v11-02d. The solution will be to recopy the "correct" files for dates July 5-31, 2013 from the Dalhousie archive to the Harvard archive.

****** As always, we recommend downloading all met fields from the Dalhousie shared data directory archive (rain.ucis.dal.ca) to avoid issues like this in the future. ******

De-supporting obsolete meteorological fields starting in v11-02d

We will remove support for the following met fields from GEOS-Chem v11-02d and later versions:

1. GCAP (legacy 4^0x 5^0 resolution data)
2. GEOS-4 (all resolutions)
3. GEOS-5 (all resolutions)
4. MERRA (all resolutions)

Discontinuing support for these old met fields in GEOS-Chem will bring the following benefits:

1. It will allow us to remove many lines of source code from the various GEOS-Chem modules, thus streamlining GEOS-Chem.
2. It will facilitate further GCHP development. GCHP cannot use these met obsolete met fields because they are stored as sequential unformatted binary files. This type of data cannot be read efficiently when running in high-performance computing environments.
3. We would also reclaim a substantial amount of disk space by not having to keep several decades of GEOS-4 and MERRA data online.
4. We would satisfy NASA/GMAO, who advises that we abandon GEOS-5 and MERRA in favor of GEOS-FP and/or MERRA-2.

While support for these obsolete met fields is being removed from the GEOS-Chem source code, **we would like to reassure everyone that the GEOS-5 and MERRA data will be preserved on the Dalhousie shared data archive (rain.ucis.dal.ca) for the foreseeable future**. So if your existing project requires that you continue using GEOS-5 or MERRA until the project's completion, you will still be able to access the entire GEOS-5 and MERRA data archives at Dalhousie.

Removing obsolete met field data from the Harvard archive (aka GcGrid)

We plan to upload a subset of the Harvard shared data archive (also known as "GcGrid") to Amazon Web Services (AWS). This will make it possible to run GEOS-Chem simulations on Amazon cloud computing resources. It will also make downloading GEOS-Chem met field and emission data more convenient and accessible.

Judit Flo-Gaya (Harvard IT) has been coordinating with AWS in preparation for this data migration. Given that GEOS-Chem v11-02 will remove support for obsolete met field products, we are planning only to migrate those data which the most recent GEOS-Chem model versions (i.e. v10-01 and later) can use. This will allow us to remove as much obsolete data (especially those in the obsolete "binary punch" format, which cannot be read efficiently in HPC environments) from the new Harvard data archive on AWS.

- *NOTE: we will still retain any data in "binary punch" format that is currently used by the GEOS-Chem adjoint model.*

We have prepared a summary spreadsheet of the data directories that we plan to migrate to AWS, and those which we plan to remove entirely. If you have any concerns, then please contact us at geos-chem-support@as.harvard.edu.

We have no firm timeline on when we expect the data migration to happen, other than to say that we believe it will occur before the end of 2017.

Structural updates

Archiving netCDF diagnostic output

GEOS-Chem v11-02 will contain structural updates to archive diagnostic quantities to netCDF output. Development of the netCDF diagnostic infrastructure is currently in progress. The existing diagnostics, which are archived to the "binary punch" file format, will be completely removed from the public release of v11-02, which is currently slated for late 2017 or early 2018. Binary file I/O cannot be done efficiently in high-performance computing environments.

We modeled the diagnostic structural updates on the History Component included in GCHP, specifically the MAPL History component developed by GMAO. The History Component requires a new configuration file (HISTORY.rc) that we designed for compatibility with both GEOS-Chem "Classic" and GCHP. The History Component will archive diagnostic output to COARDS-compliant netCDF-4 files. This format is easily read by several data processing packages, including **GCPy**, a Python package currently in development that will replace the IDL-based GAMAP.

GCST is working towards developing a new set of diagnostic names compatible with both GEOS-Chem "classic" and GCHP. This work is still in the beginning phase and will be documented on the GEOS-Chem v11-02 List of Diagnostics wiki page. GCST will send out a tentative list of diagnostics for comment once all constraints are identified.

We will continuously merge structural updates related to netCDF diagnostics into the GEOS-Chem v11-02 development stream as they are ready. NetCDF diagnostics will be fully functional in the GEOS-Chem v11-02 public release.

GCPy: A new Python visualization package for GEOS-Chem

Help us prioritize GCPy development by taking a short survey

(a message from the GCPy Development Team)

Dear GEOS-Chem Users,

The GEOS-Chem Support Team and various collaborators are currently developing **GCPy,** a Python-based toolkit for helping GEOS-Chem users tackle their research analyses using the free, powerful tools available in the modern scientific computing ecosystem.

Additionally, documentation for GCPy is being developed, and will feature many examples of how to carry out common analysis and visualization tasks using both GCPy and other tools. We hope that users throughout the GEOS-Chem community will not only find this useful, but will both learn new (hopefully easier!) ways to perform their common tasks and contribute new knowledge back to the community by publishing examples in this documentation.

At the current stage of development, we are actively seeking input from the GEOS-Chem community in order to determine where our development and documentation priorities should lie. To that end,

we have created a simple Google Form (that should take no longer than five minutes to complete) that aims to capture the following:

- The analysis tools that are currently being used by the GEOS-Chem community
- The difficulties experienced by GEOS-Chem users (e.g. parts of workflow requiring high compute/time cost), when carrying out analyses
- The types of analysis (e.g. specific plots, time series analyses, statistical analyses, re-gridding, etc.) that GEOS-Chem users would like to see documented as part of the GCPy project

The survey can be found here:

- **https://goo.gl/forms/GFPTFtE49ANW4LOp2**

and will be open until 2017/09/30, after which date we will analyze the responses and use them to directly inform our software development and documentation writing priorities. We would greatly appreciate you taking the time to submit a response to this survey, as the responses will help us to shape the initial GCPy project release to the needs of the GEOS-Chem community.

For those interested in an advance preview of the types of documentation that will be available, a sample tutorial and several shorter, worked example analyses can be found at the following locations:

- http://www.danielrothenberg.com/gcpy/tutorials/tutorials.html - tutorials
- http://www.danielrothenberg.com/gcpy/examples/index.html - worked examples

We've also included a *Getting Started with Scientific Python* guide aimed at helping users get up-and-running with GCPy as quickly as possible. We'd appreciate if you could give it a try and let us know how it worked for you!

Sincerely,

The GCPy Development Team:

Daniel Rothenberg (MIT)
Seb Eastham (MIT)
Killian Murphy (York)
Tomás Sherwen (York)
Jiawei Zhuang (Harvard)
and the **GEOS-Chem Support Team**

Cubed-sphere visualization tools

Jiawei Zhuang (Harvard) is also developing several extensions to GCPy that will allow users to analyze GCHP-produced data on the cubed-sphere grid. He writes:

> *I've built several data processing tools for my own research, but they are general enough and well-documented enough that every user can use them for:*

1. *Generate cube sphere to lat-lon (and vice-versa) remapping files for GCHP*
2. *Regrid GCHP output data to a desired grid*
3. *Visualize cubed-sphere data without regridding back to lat-lon.*

We had different pieces of software that could do those jobs before, but they were quite messy... I've made two python packages and users could in principle install them with one click. ***No additional software dependencies are required.***

1. *A package for cubedsphere data analysis and processing: https://github.com/JiaweiZhuang/cubedsphere*
2. *A "universal regridder" that should be able to handle most types of grids even the stretched-cubedsphere: https://github.com/JiaweiZhuang/xESMF*

The second one received quite a lot attention, and the ESMF team and NESII are very supportive for it.

My plan is to include these as optional dependencies in GCPy,

Conclusion

GEOS-Chem v11-02 will contain many new important chemistry updates, particularly involving the SOA and halogen species. Several new structural improvements—in particular, replacing diagnostic output in binary format with netCDF format—will also be added to this version.

Support for obsolete met fields will be removed from v11-02c. This will also allow us to migrate the Harvard "GcGrid" GEOS-Chem data archive to cloud-based storage.

GEOS-Chem v11-02b with the High-Performance Computing option has been validated with 1-month and 1-year benchmarks. We encourage interested users to take GCHP for a spin! Inclusion of diagnostics in GCHP output is in development and will be included in the v11-02 release.

Thank you for your continued support of GEOS-Chem! Please do not hesitate to contact us if you have any further questions or concerns.

Sincerely,

Bob Yantosca
with the GEOS-Chem Support Team
(Melissa, Lizzie, Chi, Yanko)