GEOS-Chem Newsletter
Winter 2016 Edition

GEOS-Chem Support Team
03 Feb 2016

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GEOS-Chem v11-01 Development Overview

GEOS-Chem v11-01 development continues to proceed at a rapid pace. In the last few months, we have invested a lot of effort towards streamlining the code and removing inefficiencies and inconsistencies left over from legacy routines. This will facilitate the implementation of the FlexChem chemical solver package, which is currently slated to be added in GEOS-Chem v11-01g.

GEOS-Chem v11-01e

GEOS-Chem v11-01e was approved on 04 Jan 2016. This version included several structural updates and bug fixes, notably Phase 2 of the GEOS-Chem Species Database (removing inconsistencies and standardizing Henry's law functions), and Phase 1 of the Tracer Units implementation. You can read more about these updates in the table below.

v11-01e Feature	Type	Submitted by
Update HEMCO from version 1.1.005 to version 1.1.016	Structural	Christoph Keller (Harvard)

Speed up GEOS-FP and MERRA-2 met field input by only opening each netCDF file once per day	Structural	Bob Yantosca (GCST)
Bug fixes for Arctic Hg updates in v11-01c	Bug Fix	Jenny Fisher (Wollongong)
Bug fix to update air quantities after specific humidity is updated in non-local PBL mixing	Bug fix	Lizzie Lundgren (GCST)
Tracer Units Phase 1: Initial implementation of area-independent tracer units	Structural	Lizzie Lundgren (GCST)
Modifications for running nested grid simulations with MERRA2	Structural	Melissa Sulprizio (GCST)
Species Database Phase 2a: • Remove inconsistencies in the definitions of physical properties of GEOS-Chem species; • Use proper molecular weights for sea salt aerosols in the dry deposition module; • Give SO4s and NITs the same molecular weight as SALC; • Define molecular weight fields of the Input_Opt object from the species database	Structural	Bob Yantosca (GCST)
Species Database Phase 2b: • Update the wetdep module to use the same Henry's law functions as are used in HEMCO, for consistency's sake	Structural	Bob Yantosca (GCST)

GEOS-Chem v11-01f

GEOS-Chem v11-01f is currently in development. This internal version will add more structural updates and bug fixes, mostly to pave the way for the implementation of FlexChem, which is currently slated for v11-01g.

To facilite a smooth transition to FlexChem, we have postponed further chemistry updates until after FlexChem is integrated into GEOS-Chem. Validation of FlexChem will require difference-testing the new FlexChem/KPP chemical solver against a "frozen" version of GEOS-Chem using the existing SMVGEAR solver. Adding new chemical reactions into GEOS-Chem at this time would complicate this validation process.

A complete list of updates and bug fixes planned for v11-01f is in the table below.

v11-01f Feature	Type	Submitted by	Status
Add a script (NcdfUtil/perl/isCoards) to determine if a netCDF file is COARDS-compliant	Structural	Bob Yantosca (GCST)	Completed 06 Jan 2016
Bug fixes for hydrophobic aerosol properties	Bug fix	Seb Eastham (Harvard)	Completed 06 Jan 2016

[Use an updated EMEP mask file to prevent zero emissions at 30 N for 2° x 2.5° or higher resolutions](#)	Bug fix	Eloise Marais (Harvard)	Completed 06 Jan 2016
[Correct too-high emissions of Hg2 over China and EU](#)	Bug fix	Amanda Giang (MIT)	Completed 06 Jan 2016
[Fix typo in HEMCO extension module hcox_gc_RnPbBe_mod.F90](#)	Bug fix	Mat Evans (U. York)	Completed 08 Jan 2016
[Fix syntax error in globchem.dat for the MOBA + OH —> MOBAOO reaction rate](#)	Bug fix	Will Porter (MIT)	Completed 08 Jan 2016
[Fix bug in reaction ISNOOA + NO2 --> PMN in globchem.dat](#)	Bug fix	Mike Long (Harvard)	Completed 26 Jan 2016
[Fix an emissions error in the SOA-SVPOA simulation](#)	Bug fix	Prasad Kasibhatla Melissa Sulprizio ([GCST](#))	Completed 11 Jan 2016
[Consistent physical parameter values throughout GEOS-Chem](#)	Structural	Lizzie Lundgren ([GCST](#))	Completed 12 Jan 2016
Drive full-chemistry simulations with MERRA2 met fields	Structural	Melissa Sulprizio ([GCST](#))	In progress
NetCDF Output Phase 1: Convert restart file from bpch to netCDF format	Structural	[GCST](#)	In progress
[Add further fixes for compiling GEOS-Chem with PGI Fortran](#)	Structural	Bob Yantosca ([GCST](#))	Completed 27 Jan 2016

In the Pipeline

As previously discussed, FlexChem will be introduced in GEOS-Chem v11-01g. Several chemistry updates are currently slated for GEOS-Chem v11-01h, as listed below.

v11-01h Feature	Type	Submitted by	Status
[PAN updates](#)	Science	Emily Fischer (CSU)	Delivered to GCST, partially implemented into development code
[Monthly mean surface methane distributions](#)	Science	Lee Murray (NASA GISS/LDEO)	Awaiting code from developer
[Ocean ammonia emission inventory](#)	Science	Fabien Paulot (NOAA/GFDL)	Delivered to GCST
[Temporary fix to remove SO2 scavenging in convective updrafts](#)	Science	Duncan Fairlie (NASA/LARC)	Delivered to GCST
[Update density of BC to 1.8 and add absorption enhancement factor in input.geos](#)	Science	Xuan Wang (MIT)	Delivered to GCST

Details for Structural Updates

Consistent Values for Physical Constants

In GEOS-Chem v11-01e and prior versions, physical parameters (e.g. universal gas constant) are defined in multiple locations within GEOS-Chem. In some cases, the parameters are defined with different values or precisions. In an effort to improve accuracy, consistency, and transparency within GEOS-Chem, v11-01f introduces usage of a single set of global parameters everywhere in `GeosCore`. A complete summary of updates is described [on the *Physical Constants* wiki page](#).

Area-independent Tracer Units

In [GEOS-Chem v10-01](#) and prior versions, GEOS-Chem tracer units are converted between molar mixing ratio (`v/v`) and mass per grid box (`kg`) throughout `main.F`. The conversion between (`v/v`) and (`kg`) inherently requires knowledge of grid area, which is incompatible with the grid-independent high-performance GEOS-Chem (aka "GEOS-Chem HP"). Furthermore, the switch between units is confusing and inconsistently documented.

In order to achieve grid-independence and bring greater clarity to GEOS-Chem, the GEOS-Chem Support Team is working towards implementing [consistent area-independent tracer units](#) throughout the model. Because this project touches nearly all parts of GEOS-Chem and is being conducted concurrently with several other development projects, we are working towards these goals in distinct phases. Phase 1 of this process was completed in v11-01e (approved 04 Jan 2016). Lizzie Lundgren (GCST) is leading this project and is documenting progress on the [*GEOS-Chem Tracer Units* wiki page.](#)

Correction of Inconsistent Molecular Weight Definitions

During the implementation of the [GEOS-Chem species database](#), we discovered many inconsistent molecular weight definitions for GEOS-Chem tracers. In particular, several tracers used a different molecular weight in the dry deposition module than in other areas of GEOS-Chem. We attribute many of these discrepancies to legacy code.

For some tracers the differences were minor, only involving the addition of extra decimal places. For example, the molecular weight of species MTPO was listed as 136 g/mol in the dry deposition module (`GeosCore/drydep_mod.F`), but should have been 136.23 g/mol. A few tracers, on the other hand, were using completely wrong molecular weights. The SO4s tracer (sulfate on sea salt aerosol) should have had a molecular weight of 31.4 g/mol, but was using 36 g/mol in dry deposition and 64 g/mol elsewhere.

We removed all such inconsistencies during Phase 2 of the GEOS-Chem Species Database implementation, which was completed in v11-01e (approved 04 Jan 2016). Bob Yantosca (GCST) has compiled a [table on the GEOS-Chem wiki](#) listing the affected tracers.

Implementation of Consistent Henry's Law Functions

When HEMCO was introduced in GEOS-Chem v10-01, it added a new module (`GeosUtil/henry_mod.F`) containing functions `CALC_KH` and `CALC_HEFF`. These functions

compute the dimensionless Henry's law liquid/gas constant, accounting for the pH of water. HEMCO uses these functions to compute the sea-air exchange of species such as dimethyl sulfide (DMS) and acetone (ACET).

The GEOS-Chem wet deposition module (`GeosUtil/wetscav_mod.F`) also computes the dimensionless Henry's law liquid/gas constant, but with a different function (`COMPUTE_L2G`). This function used a slightly different value for the gas constant R than the newer functions `CALC_KH` and `CALC_HEFF`, and could not take into account the pH of water.

During Phase 2 of the GEOS-Chem Species Database implementation, [we updated the wet deposition module so that it calls the newer functions `CALC_KH` and `CALC_HEFF`](#) from `GeosUtil/henry_mod.F`. This will ensure that the Henry's law computations are done consistently throughout GEOS-Chem.

This update was added in v11-01e (approved 04 Jan 2016).

HEMCO Base Version Update to v1.1.016

Christoph Keller (GMAO, formerly Harvard) recently made several updates to the HEMCO emissions component.   In GEOS-Chem v11-01e, we updated HEMCO from v1.1.005 to v1.1.016. For a list of individual features included in this new HEMCO version, please see [this post on our *Implementation of HEMCO in GEOS-Chem* wiki page](#).

Compatibility with the PGI compiler (pgfortran)

Bob Yantosca (GCST) has [added several updates to v11-01f](#) for compatibility with the Portland Group International Fortran compiler (aka `pgfortran`). For more information, please see [our *PGI compiler* wiki page](#).
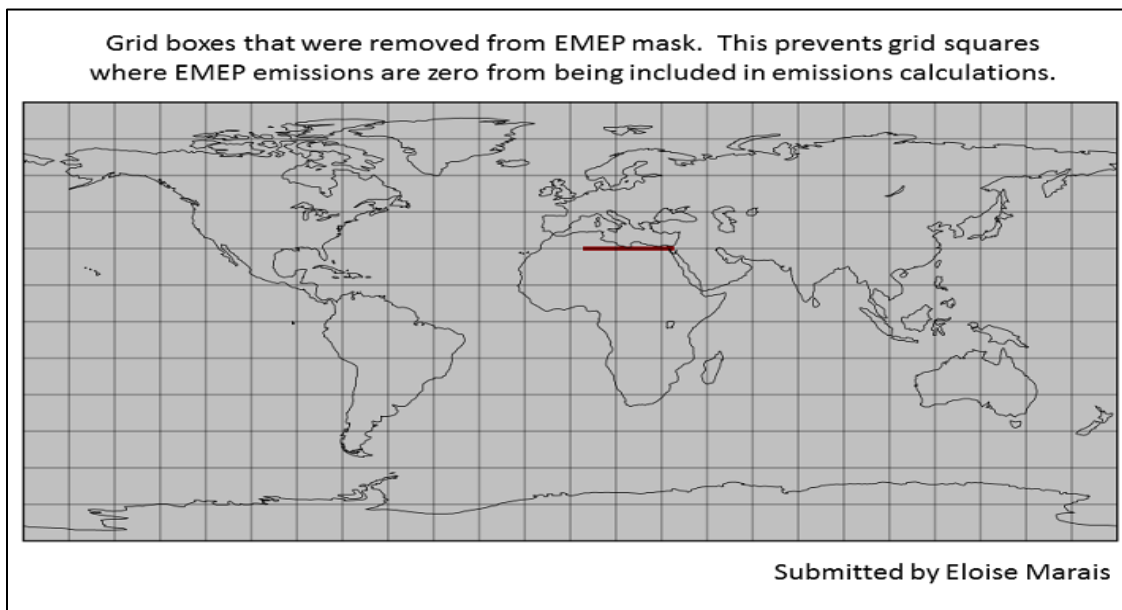

Details for Notable Emissions Fixes

EMEP Emissions Mask File Bug Fix used by HEMCO

Eloise Marais (Harvard) pointed out a bug in EMEP emissions mask file used by HEMCO. She wrote:

> *Anthropogenic emissions are zero where the EMEP and EDGAR emissions coincide at 30 degrees North (using [GEOS-Chem v10-01](#)). This is because the EMEP mask extends to gridsquares where EMEP emissions are zero. Anthropogenic emissions are relatively low there, so this issue only shows up when NOx emissions are plotted on a log scale.*

> *My quick fix is to shift the minimum latitude of the EMEP mask up by 1 degree latitude (so starting at 31 deg N instead of 30 deg N), in an updated mask file*

*EMEP_mask.geos.1x1.20151222.nc. (The boxes that were removed show up as **RED** in the plot below.)*

Grid boxes that were removed from EMEP mask. This prevents grid squares where EMEP emissions are zero from being included in emissions calculations.

Submitted by Eloise Marais

This issue will be resolved in GEOS-Chem v11-01f. We have added the new mask file EMEP_mask.geos.1x1.20151222.nc to the HEMCO data directory path on the GcGrid server. We have also updated the relevant HEMCO configuration files in the GEOS-Chem so that this mask file will be read by default. The original EMEP mask file shall be preserved on the GcGrid server, so that it can be used for simulations requiring backwards compatibility.

Details for Notable Chemistry Fixes

Bug Fixes for Hydrophobic Aerosol Properties

Sebastian Eastham (Harvard) identified several bugs where hydrophobic aerosol properties are defined in module GeosCore/aerosol_mod.F. Please see this post on our *Mineral Dust Aerosols* wiki page for more information. These bugs will be fixed in GEOS-Chem v11-01f.

Typo Fix in ISONOA + NO2 → PMN Reaction Specification

As described in this wiki post, Mike Long (Harvard) discovered a syntax error in the reaction rate for ISNOOA + NO2 → PMN as specified in the globchem.dat chemistry mechanism file. This error caused concentrations of PMN to be smaller than they should have been by a factor of 10^{15}. The fix is simply to add a missing "M" character (as shown in **green**) to this reaction in globchem.dat:

```
A  442 9.00E-28  8.9E+00      0 1 P   0.60     0.    0.
        7.70E-12  0.2E+00      0 0     0.00     0.    0.
```

```
      ISNOOA          +      NO2                      M
```

We have added this fix to the relevant `globchem.dat` files that ship with the GEOS-Chem unit tester for v11-01f.

Typo Fix in MOBA + OH → MOBAOO Reaction Specification

Will Porter (MIT) wrote:

> *I wanted to pass on what I believe is a small error in the default GEOS-Chem v9-02 `globchem.dat` file. The first line of the MOBA + OH —> MOBAOO reaction reads:*

```
   A 999 2.79E-11   0.0E+00    380 0     0.00     0.    0.
```

> *However, there is only one space between the "A" and the "999", resulting in (I believe) an incorrect parsing of the following numerical value, as evidenced in the `smv2.log` file:*

```
   388 7.9E-12    0.00    380 .00 MOBA  +OH    +      =1.0MOBAOO
```

> *(NOTE: Instead of 2.79e-11 we get 7.9e-12.)*

> *My tests seem to show that the impact on surface O3 is minimal, but anyone interested in this particular species ("5C acid from isoprene"), or isoprene chemistry in general, will likely be very interested in having it fixed! Over the US, correcting `globchem.dat` reduces average MOBA levels by around 2-6%. I've attached plots of base surface MOBA using a nested NA run (2010-2011), along with absolute change and percent change using a corrected `globchem.dat` file.*
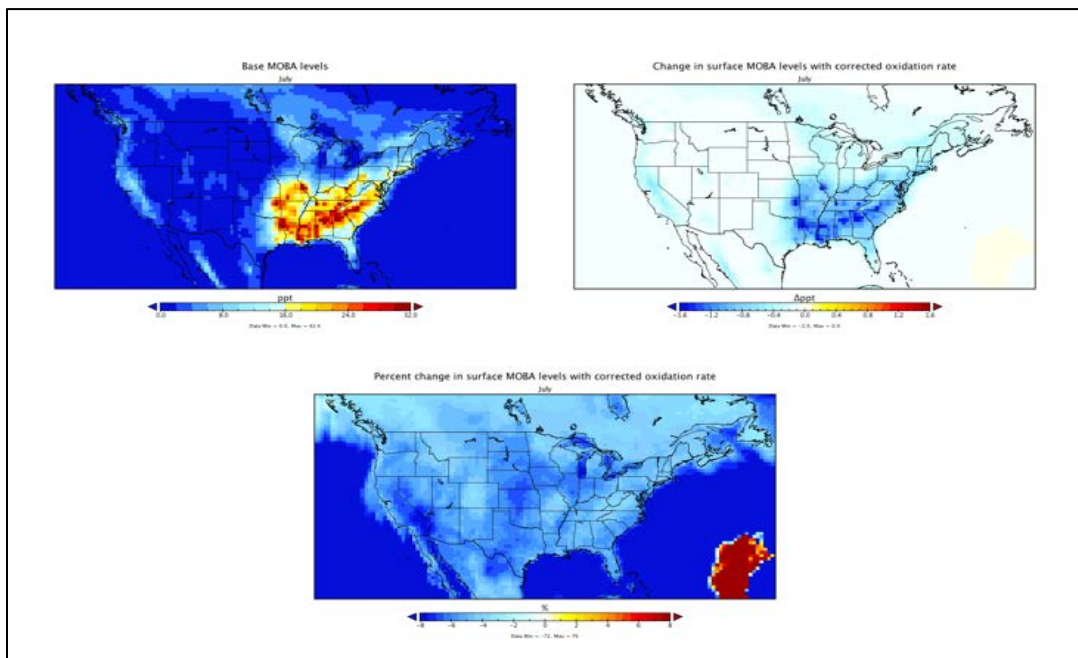
7

We have added this fix to the relevant `globchem.dat` files that ship with the GEOS-Chem unit tester for v11-01f.

Bug Fixes for the SOA-SVPOA Simulation

Prasad Kasibhatla (Duke) wrote:

> *It looks like there are some problems in the implementation of the semi-volatile POA option in v10-01. I ran 2 one month simulations (2009 July) using GEOS-5 meteorology and out-of-the-box set up of v10-01 (using run directories created by `gcCopyRunDirs`) - one simulation used the traditional nonvolatile POA option and the other (with the same executable) used the semivolatile POA option.*

> *Attached are plots from the restart file after 1 month of simulation. OCPI and OCPO are from the traditional nonvolatile POA run, and the remainder [are] from the semivolatile POA run. The OCPI and OCPO plots from the traditional nonvolatile POA run are as expected, but the plots from the semivolatile POA run are not.*

> *Looking at the code (`GeosCore/carbon_mod.F`) it looks like one problem is that SVOC emissions are allocated to POG1 and POA1, instead of to POG1 and POG2 as they should be in the semivolatile POA simulation. But the patterns seen in the some of the plots from the semivolatile POA simulation suggest other problems as well.*

Melissa Sulprizio (GCST) ultimately traced this bug back to GEOS-Chem v10-01, when the legacy SOA-SVPOA emissions routines were replaced by the HEMCO emissions component. For more information on how this bug was corrected, please see this post on our *Secondary Organic Aerosols* wiki page.

New Tools for GEOS-Chem Users

Determine if NetCDF Files are in Proper Format for HEMCO

The GEOS-Chem Support Team has created a script named `isCoards` that will let you easily determine if a netCDF file adheres to the COARDS standard. This is particularly useful since all netCDF data files read by HEMCO must be COARDS-compliant.

You may obtain this script from our NcdfUtilities repository. We also recommend that you copy `isCoards` into a folder that is in your search path (such as `~/bin`) so that it will be available to you in whatever directory you are working in.

```
git clone https://bitbucket.org/gcst/ncdfutilities NcdfUtil

cp NcdfUtil/perl/isCoards ~/bin
```

Starting with [GEOS-Chem v11-01](#), `isCoards` will also be added to the `NcdfUtil/perl` subfolder of the GEOS-Chem source code directory. The `isCoards` script will give you detailed output of which elements of a netCDF file are COARDS-compliant and which are not. For more information, please see [this post on our *Preparing data files for use with HEMCO* wiki page](#).

Ongoing GEOS-Chem Development Projects

MERRA-2 Update

As of v11-01c, GEOS-Chem can now be driven by the NASA/GMAO MERRA-2 meteorological reanalysis data product. MERRA-2 is a long-term reanalysis (30+ years of data) created with version 5.12.4 of the NASA GEOS-5 Data Assimilation System. Several GEOS-Chem specialty simulations (including Radon, Mercury, POPs, Tagged O3, and CH4) can already use the MERRA-2 meteorology.

Junwei Xu (GCST) is in the initial phases of processing MERRA-2 met fields for the entire coverage period (1980–present). The MERRA-2 met fields will be available on the global 4°x5° and 2°x2.5° grids and on the nested Asia, Europe, and North America grids at 0.5°x0.625° resolution. The nested China/SE Asia grid for MERRA-2 is now referred to as the nested Asia grid since this domain has been expanded to include India and Japan (10°S–55°N, 60°E–150°E). Processing the MERRA-2 met fields will likely take several weeks.

Melissa Sulprizio (GCST) is currently working on adding compatibility for MERRA-2 into the full-chemistry simulations (benchmark, UCX, SOA-SVPOA, tropchem, etc.). She is computing meteorology-dependent scale factors for dust and lightning emissions based on MERRA-2 meteorology for the years 2009-2014. These factors will be updated for the entire MERRA-2 coverage period when the processed data are available. We anticipate that these modifications will be ready for v11-01f.

FlexChem Update

Mike Long (Harvard) and Melissa Sulprizio (GCST) are currently adding the new FlexChem chemical solver package into GEOS-Chem. This will finally allow us to remove the legacy SMVGEAR code from GEOS-Chem. FlexChem, which uses the faster KPP solver, should also be much more computationally efficient than SMVGEAR.

To date, Mike and Melissa have fully implemented the "tropchem" simulation (i.e. troposphere-only) into FlexChem. Much of this work involved converting the SMVGEAR `globchem.dat` mechanism input file into the KPP master equation file format, and then making sure that photolysis and heterogeneous chemistry rates were correctly passed into the KPP solver. Mike and Melissa are currently repeating this work for the other chemical mechanisms (e.g. "benchmark", "SOA-SVPOA", etc.).

Complete integration of FlexChem into GEOS-Chem will require additional structural modifications, mostly to change how tracers and species are indexed. Mike Long writes:

> *The intent is to completely deprecate [legacy GEOS-Chem module]* `tracerid_mod.F`. *The end result will include these properties:*
>
> 1) *All species identification and initialization will flow from KPP (specifically* `gckpp_Monitor.F90`) *instead of from* `tracerid_mod.F`:
>
>   a. *In KPP, all species are automatically assigned integer index values PRIOR to runtime. And they can be accessed simply through the variable* `ind_<SPC_NAME>`. *For example,* `ind_OH` *is the index value for species "OH".*
>
>   b. *There is a species name (string) vector* `SPC_NAMES(NSPEC)` *where* `SPC_NAMES(ind_OH) = "OH"`.
>
> 2) *The interface between KPP and GEOS-Chem will route through the* [GEOS-Chem species database](#).
>
>   a. *The result should yield, within GEOS-Chem, access to species and tracer fields via* `State_Chm%Species(ind_OH)` *where* `ind_OH` *is from KPP.*
>
>   b. *(While it may not happen yet), we would like to get rid of* `State_Chm%Tracers` *completely, and use the species database's designation of* `is_Advected`.
>
> 3) *For specialty simulations that DON'T use KPP, we declare the appropriate index and character structures within their controlling modules.*
>
>   a. *e.g.* `mercury_mod.F` *would include* `ind_Hg0, ind_Hg2,` *and any other necessary indices.*
>
>   b. *It would also include a* `SPC_NAMES` *declaration. This preserves the functionality of all the general structures.*
>
> 4) *HOPEFULLY: in the process, we can purge the remainder of vectorization (i.e. big 1-D arrays) in FlexChem. Specifically the use of* `CSPEC` *and the looping variables (*`KTLPPP, JLOOP,` *etc.). Melissa has already done quite a bit of this.*

Interfacing to the NASA GEOS-5 Data Assimilation System

Mike Long (Harvard) writes:

> *GEOS-Chem is currently running within the GEOS-5 DAS on the c360 cubed-sphere grid. This is equivalent to 25 km (~ 0.25°) horizontal resolution.*

We evaluated the output of the coupled GEOS-Chem/GEOS-5 DAS against GEOS-Chem output for the month of January. The coupled system passed the evaluation. Profiles were better with GEOS-5 (exact replay) on the c360 grid.

We are now finishing up a 1-year run with the coupled system on the c360 grid, and will evaluate those results shortly. Lu Hu (Harvard) is comparing the results from the coupled system for the month of July against GEOS-Chem output. If the coupled system passes this evaluation, we will start a run on the c720 grid, which is equivalent to 12 km (~ 1/8°) horizontal resolution.

Outputting GEOS-Chem Data in NetCDF Format

The [HEMCO emissions component](#) can save diagnostic output (time-averaged or instantaneous) as well as end-of-run restart information to netCDF files. Currently, this feature is only used for data that is read from disk and/or processed by HEMCO.

The GEOS-Chem Support Team is currently leveraging HEMCO's very useful diagnostic capabilities in order to remove all ["binary punch file" output](#) from GEOS-Chem. This work has started in v11-01f and will likely continue into future internal versions.

Migrating to netCDF format will bring the following benefits: (1) Using HEMCO's diagnostic archival functions will ensure that all quantities will be archived consistently throughout GEOS-Chem; (2) Use of netCDF output will facilitate further GEOS-Chem "HP" development, since binary files cannot be written efficiently in high-performance computing (HPC) environments, and; (3) GEOS-Chem users will have more options for visualizing GEOS-Chem output. Many free and open-source software packages (e.g. [Python tools](#)) are compatible with netCDF format.

This work will be done in two phases:

1) Converting GEOS-Chem tracer restart files from "binary punch" format to netCDF format, and;
2) Converting all GEOS-Chem diagnostic outputs from "binary punch" format to netCDF format.

In order to facilitate testing, there will be a transition period in which both "binary punch" and netCDF output formats will be available. We envision that the public release of GEOS-Chem v11-01 will contain both binary and netCDF output options. For the time being, the default option will be to write out diagnostics to binary output. To select netCDF output, you can compile GEOS-Chem with the NETCDF=yes option.

GEOS-Chem "HP" update

Our high-performance computing version of GEOS-Chem (aka GEOS-Chem HP, or GCHP) currently uses the v10-01 "public release" of GEOS-Chem. Since the v10-01 release (June

2015), many important updates have been made to GEOS-Chem (as listed in the previous sections above.

Matt Yannetti is currently working on bringing GCHP up-to-date with the current development version v11-01. He plans on doing this in an incremental fashion: first updating GCHP first from v10-01 "public" to v11-01a, then to v11-01b, and so on. This will allow Matt to debug GCHP for each intermediate GEOS-Chem version. The work is ongoing.

Seb Eastham (Harvard) & Jiawei Zhuang (PKU) are debugging a divergence conservation bug in the Cubed-Sphere FVDycore used by GCHP. This work is ongoing and has considerably slowed the validation of the chemistry.

Matt Yannetti and Michael Long (Harvard) have been working to create software modules for the ESMF and NASA's MAPL libraries. Once complete, work will begin to remove these libraries from with the GCHP source.

Proposed GEOS-Chem Updates

Optimal Transport and Chemistry Timestep Settings

Sajeev Phillip and Randall Martin (Dalhousie) recommend the following default GEOS-Chem timestep durations for future GC simulations when sufficient CPU resources are available.

> *[Philip et al.](#) (submitted) examines the sensitivity of GEOS-Chem simulations to the duration of chemical and transport operators. Based on that study, we recommend chemical timesteps of 20 minutes and transport timesteps of 10 minutes for simulations when sufficient CPU resources are available. Fine horizontal resolution should take priority over fine temporal resolution. In some cases, it may be beneficial to use coarser timesteps for initial simulations, and the recommended resolution (C20T10) for final simulations. We encourage specification in publications of the duration of operators due to their effects on simulation accuracy.*

On 03 Feb 2016, the GEOS-Chem Steering Committee gave final approval to use these optimal timestep settings in the default run directories that ship with GEOS-Chem. This update will be made starting in internal version v11-01f, and in all future versions (including the v11-01 public release).

Conversion of Existing Chemistry Mechanisms into KPP format for FlexChem

At present, GEOS-Chem can use the following "full-chemistry" mechanisms:

Mechanism	Description	Vertical grid	Solvers
tropchem	From the surface to the tropopause: • NOx-Ox-hydrocarbon-aerosol species • PLUS bromine species • PLUS Methyl peroxy nitrate chemistry From the tropopause to the top of the atmosphere: • Ozone: **LINOZ** stratospheric ozone chemistry • All other species: **GMI** stratopsheric chemistry (archived P/L rates)	47 levels 72 levels	SMVGEAR KPP
UCX	From the surface to the stratopause: • All of the species in the **tropchem** mechanism • PLUS online stratospheric chemistry • PLUS long-lived species such as N2O, CH4, OCS, CFCs, HCFCs, and halons From the stratopause to the top of the atmosphere: • Ozone: **LINOZ** stratospheric ozone chemistry • All other species: **GMI** stratopsheric chemistry (archived P/L rates)	72 levels only	KPP
SOA	From the surface to the tropopause: • All of the species in the **tropchem** mechanism • PLUS SOA species • PLUS Semi-volatile primary organic aerosol (OPTIONAL) From the tropopause to the top of the atmosphere: • Ozone: **LINOZ** stratospheric ozone chemistry • All other species: **GMI** stratopsheric chemistry (archived P/L rates)	47 levels 72 levels	SMVGEAR KPP
benchmark	From the surface to the stratopause: • All of the species in the **tropchem** mechanism • PLUS all of the species in the **UCX** mechanism • PLUS all of the species in the **SOA** mechanism From the stratopause to the top of the atmosphere: • Ozone: **LINOZ** stratospheric ozone chemistry • All other species: GMI stratopsheric chemistry (archived P/L rates)	72 levels only	KPP

As part of the FlexChem implementation, Mike Long (Harvard) and Melissa Sulprizio (GCST) are converting the "standard" mechanisms listed above from SMVGEAR input format into KPP input format.   These "standard" mechanisms will be preprocessed with the newer KPPA (Kinetic Pre Processor—Accelerated) version of KPP (cf. John Linford, ParaTools Inc.), which can produce highly-optimized Fortran source that can be directly compiled into GEOS-Chem.

We will also give GEOS-Chem users the option to create custom chemical mechanisms with the free and open-source version of KPP.   Users will be able to modify the KPP equation and species files as they wish. These specifications will be compiled into the GEOS-Chem executable as part of the build process.

Please send feedback to the GEOS-Chem Support Team at
 `geos-chem-support@as.harvard.edu`.

Conclusion

We are currently working on several open lines of GEOS-Chem development simultaneously. Our highest priority is to bring the new FlexChem chemistry solver into GEOS-Chem. FlexChem will facilitate GEOS-Chem simulations at high-resolution, not only with our current nested model capability, but also with our high-performance GEOS-Chem "HP" model.

But before FlexChem can be completely integrated into GEOS-Chem, a significant amount of structural programming (e.g. removing legacy module `tracerid_mod.F` so that we can use tracer indices generated automatically by KPP) has to be done first. We will strive to complete this work in the upcoming weeks. We ask for your patience during this process.

Thank you for your continued support of GEOS-Chem!

Sincerely,

Bob Yantosca
with the GEOS-Chem Support Team
(Melissa, Matt, Lizzie, Mike, Junwei, Yanko)