GEOS-Chem Year-End 2013 newsletter

GEOS-Chem Support Team

17 Dec 2013

(1) Ongoing GEOS-Chem Development

See the GEOS-Chem v9-02 wiki page for more details about individual features.

Since the last GCSC telecon, we have completed the following 1-month benchmarks:

GEOS-Chem v9-02q	
Update jv_spec.dat and jv_spec_aod.dat with better representation of OC growth with RH and correction to sulfate optics	D. Ridley (MIT)
Bug fix in jv_spec_aod.dat for dust optics	G. Curci (L'Aquila)
GEOS-Chem v9-02r	
Global simulations with "GEOS-FP" met fields FP = "forward processing"	GCST + SEAC4RS team
Nested simulations at ¼ degree resolution with GEOS-FP	GCST + SEAC4RS team
Hi-res emissions for ¼ degree nested simulations	Yuxuan Wang (Tsinghua) + GCST
Fix bug in CAC NH3 emission files	Wai-Ho Lo (Dalhousie)
Several minor bug fixes	GCST
Update molecular weight of sea salt tracers	Colette Heald (MIT)

We will release GEOS-Chem v9-02 pending the successful approval of the v9-02r benchmarks:

- The v9-02r 1-month benchmark with GEOS-5 met was approved on 14 Nov 2013
- The original v9-02r 1-month benchmark with GEOS-FP revealed several issues, and thus had to be withdrawn from consideration.
- We have just now (as of 13 Dec 2013) completed a new v9-02r 1-month benchmark with GEOS-FP. This is now before the GCSC for consideration.
- We will also perform a 1-year benchmark with GEOS-FP met prior to release.

We will list our findings from the benchmark simulations in the next section.

Several of the bug fixes mentioned in v9-02r corrected minor numerical issues that did not have much impact on the model results. Many of these bugs were detected with the new GEOS-Chem Unit Tester, which is mentioned in more detail below.

One important bug that was detected in v9-02r was that the MERRA and GEOS-FP relative humidity fields should have been multiplied by 100 in the code but weren't. The figure below illustrates this:

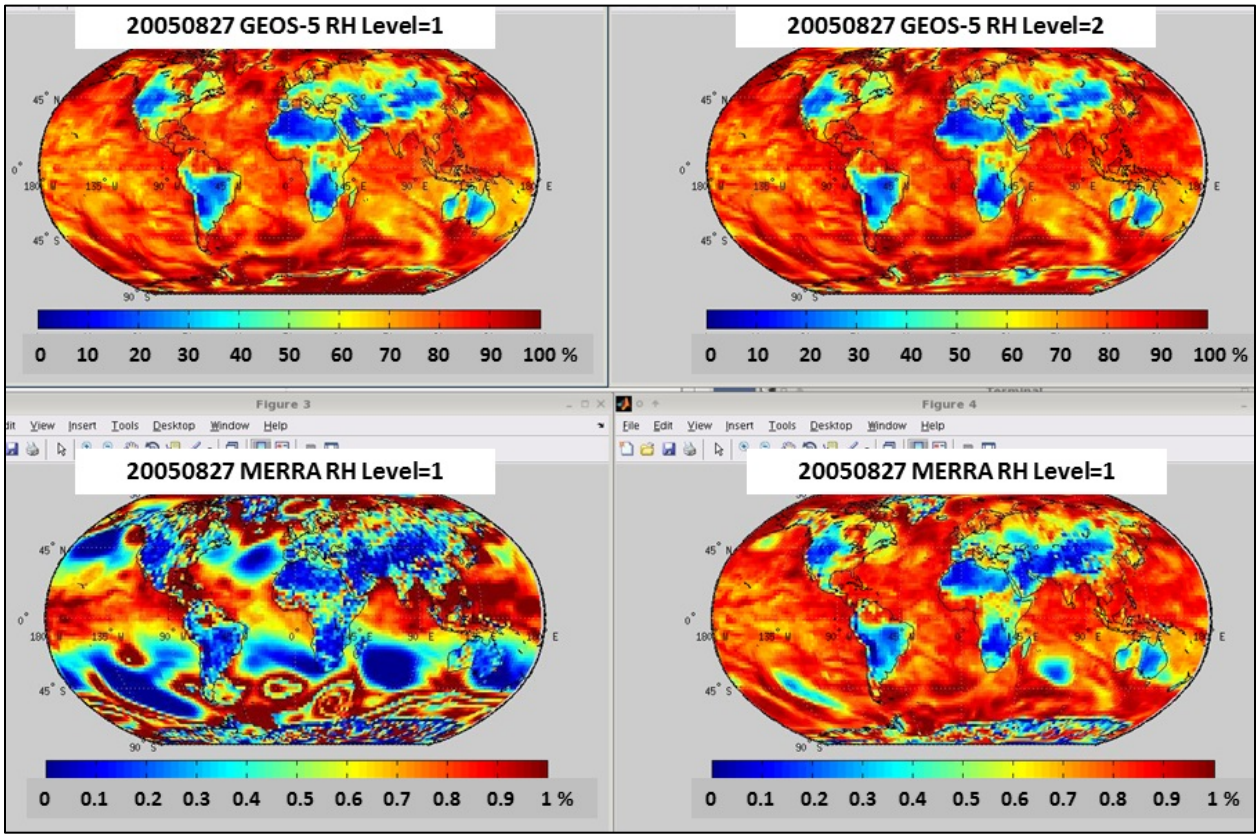


Figure: Comparison of GEOS-5 and MERRA relative humidity (RH) fields in the lowest two model layers, as saved out with the ND49 timeseries diagnostic. Note that while the GEOS-5 RH field goes from 0-100, the MERRA RH field only goes from 0-1. This is indicative of a unit conversion error within GEOS-Chem. Courtesy: Aaron van Donkelaar and Brian Boys (Dalhousie University).

For historical reasons, the GEOS-Chem code keeps relative humidity in percent. But the GEOS-5, GEOS-FP, and MERRA met fields contain relative humidity as a fraction. A unit conversion (multiplying RH by 100) is done in GEOS-Chem. For some reason, the corresponding unit conversion had not been applied to MERRA and GEOS-FP met fields. This issue has since been corrected in GEOS-Chem v9-02r.

NOTE: This bug was present in the GEOS-Chem SEAC4RS simulations that were done in summer 2013. This bug was fixed prior to the v9-02r GEOS-5 and v9-02r GEOS-FP 1-month benchmarks (which are discussed in Section 2).

(2) GEOS-Chem v9-02r benchmark results

We have performed the following 1-month benchmarks for v9-02r. Follow the links below to view the relevant benchmark approval forms for each version:

- v9-02r with GEOS-5 meteorology
- v9-02r with GEOS-FP meteorology

Here is a list of key similarities and differences between the two benchmark simulations:

Quantities	v9-02r GEOS-5	v9-02r GEOS-FP
Met fields	GEOS-5, July 2005, 4x5	GEOS-FP, July 2013, 4x5
GFED3 year	2005	2011 (last available)
Land map	Olson 1992 ½ degree	Olson 2001 ¼ degree
Column O3 for FAST-J	TOMS/SBUV monthly mean (with GEOS-5 column O3 where TOMS is missing)	GEOS-FP column O3 taken directly from met fields

We also note the following differences in emissions between the two simulations:

Quantities	Differences
Anthropogenic + Biofuel	The difference in simulation years (2005 vs. 2013) will cause the various anthropogenic and biofuel emissions inventories (BRAVO, EMEP, EPA/NEI, CAC) to yield slightly different totals. The simulation year is used to pick the base emissions year as well as the annual scale factors.
Biomass	The GFED3 base year (up to 2011, which is the last available) is tied to the simulation year. This will cause both v9-02r GEOS-5 and v9-02r GEOS-FP to have different biomass totals.
Biogenic	Biogenic emissions depend on several met field quantities (T, PAR), and thus will yield different totals in the two benchmark simulations.

Despite all of these differences, both benchmark simulations resulted in similar values for both mean OH and the methyl chloroform lifetime.

	v9-02r GEOS-5	v9-02r GEOS-FP	% difference
Mean OH (10^5 molec/cm3)	13.8467219229137	13.731733863556	-0.791
MCF lifetime (years)	4.4899	4.6673	3.951

This gives us some confidence that the GEOS-Chem w/ GEOS-FP met fields is performing adequately. Further testing will be done with a 1-year GEOS-FP benchmark.

(3) GEOS-FP met fields

Since the last GCSC telecon in September, the GCST has reprocessed the entire archive of GEOS-FP meteorology to correct several issues with the data files. These issues, and the corresponding solutions, are summarized in the following table.

Problem	Solution
GEOS-FP was formerly known as GEOS-5.7.2, which denoted the operational version GEOS-DAS used to create these data. When we regridded the GEOS-5.7.2 "raw" met data from 0.25^o x 0.3125^o resolution to the GEOS-Chem input grids, we created files named `GEOS572*.nc`. GMAO has recently updated the GEOS-DAS version, thus making the GEOS-5.7.2 nomenclature obsolete. Continuing to use the e `GEOS572` label in filenames may lead to confusion.	We have created a new GEOS-FP data archive for GEOS-Chem. We regridded from scratch the 0.25^o x 0.3125^o "raw" data files to the following GEOS-Chem grids: • 0.25 x 0.3125 China nested grid • 0.25 x 0.3125 Europe nested grid • 0.25 x 0.3125 N. America nested grid • 0.25 x 0.3125 SE Asia nested grid • 2 x 2.5 global • 4 x 5 global The new data files are named `GEOSFP*.nc`, in order to avoid any confusion.
The netCDF variable attributes in the old `GEOS572*.nc` files did not adhere to accepted standards. This prevents certain data analysis and visualization tools from being able to read and plot data in these files efficiently.	The new `GEOSFP*.nc` files now adhere to COARDS standards for netCDF file attributes.
The `GEOS572*.nc` files from our previous data archive contained multiple vertical dimensions per file (i.e. 73 level edges and 72 level centers). We have since discovered that the ESMF/MAPL libraries (which our stand-alone Grid-Independent GEOS-Chem relies on) cannot read netCDF files having more than one vertical dimension.	The new `GEOSFP*.nc` files only contain one vertical dimension per file. All met fields that are placed on level edges are now grouped together in the same file.
The `GEOS572*.nc` files did not contain the GMAO total column ozone field (TO3). This was an omission on our part.	The new `GEOSFP*.nc` files contain the GMAO column ozone field (TO3).

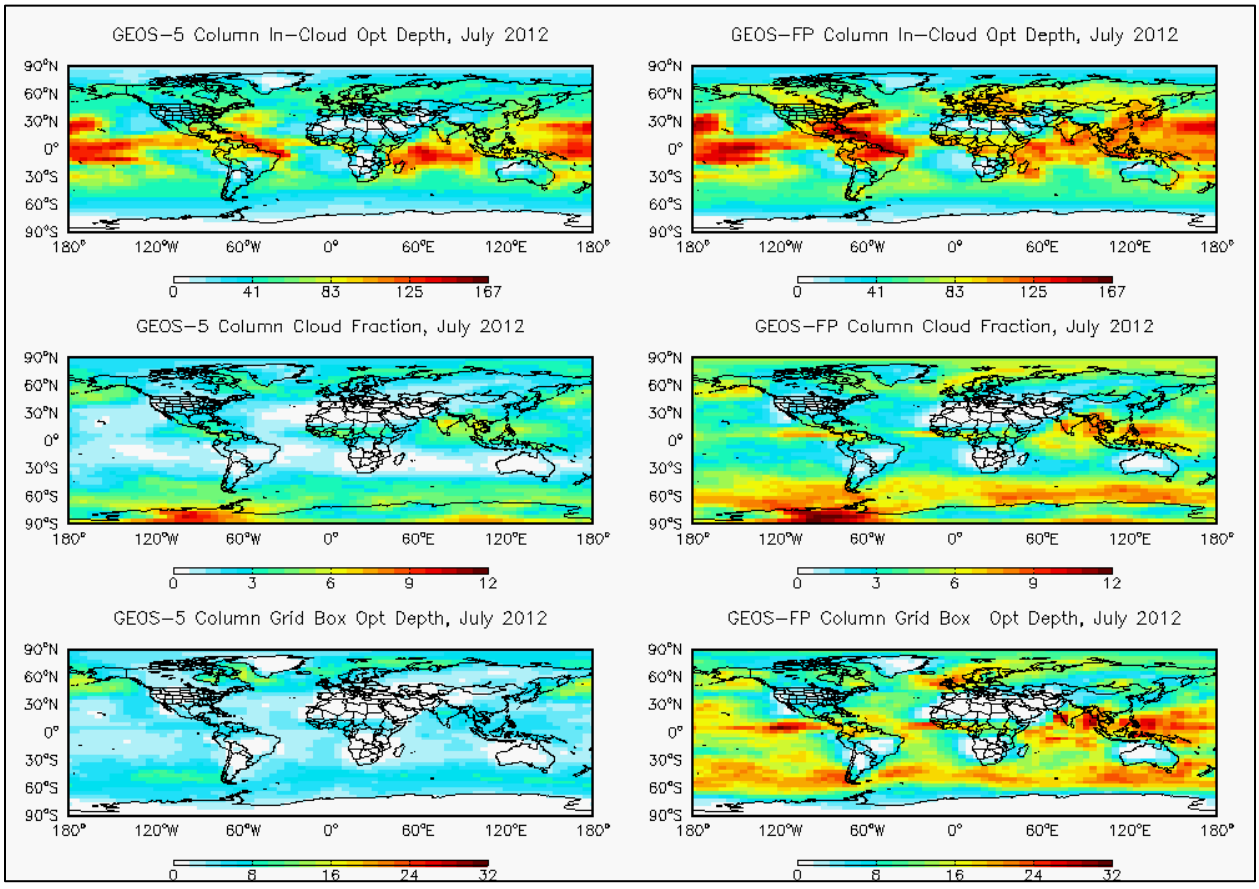
When we created the new GEOS-FP data archive (i.e. `GEOSFP*.nc` data files), we acted on a recommendation from GMAO to construct the 3-D cloud fraction field (named "`CLOUD`") from the anvil cloud fraction (`CFAN`) and large-scale cloud fraction (`CFLS`) as follows:

```
CLOUD = min( CFAN + CFLS, 1.0 )
```

instead of just reading `CLOUD` from the "raw" GEOS-FP data files. As we shall see in the plots below, this new formulation for `CLOUD` led directly to some anomalous behavior.

<u>Difference in GEOS-FP met: computed CLOUD field vs. CLOUD obtained from GEOS-FP raw data files:</u>

The following plot shows the in-cloud optical depth, column cloud fraction, and grid-box optical depth (i.e. cloud fraction * in-cloud optical depth) saved out from 1-month GEOS-Chem simulations done with both GEOS-5 and GEOS-FP meteorology for July 2012:



Here, the GEOS-FP cloud fraction (`CLOUD`) was computed as `min( CFAN + CFLS, 1.0)`, as described above. This results in much higher column cloud fractions as compared to GEOS-5. In turn, this causes the grid-box optical depths (which get fed into the FAST-J photolysis) to be much higher than in GEOS-5.

This difference plot (for 2013/08/01, 0 GMT) illustrates the difference in computing `CLOUD = min( CFAN + CFLS, 1.0 )` vs. taking the CLOUD field directly from the GEOS-FP met field archive.

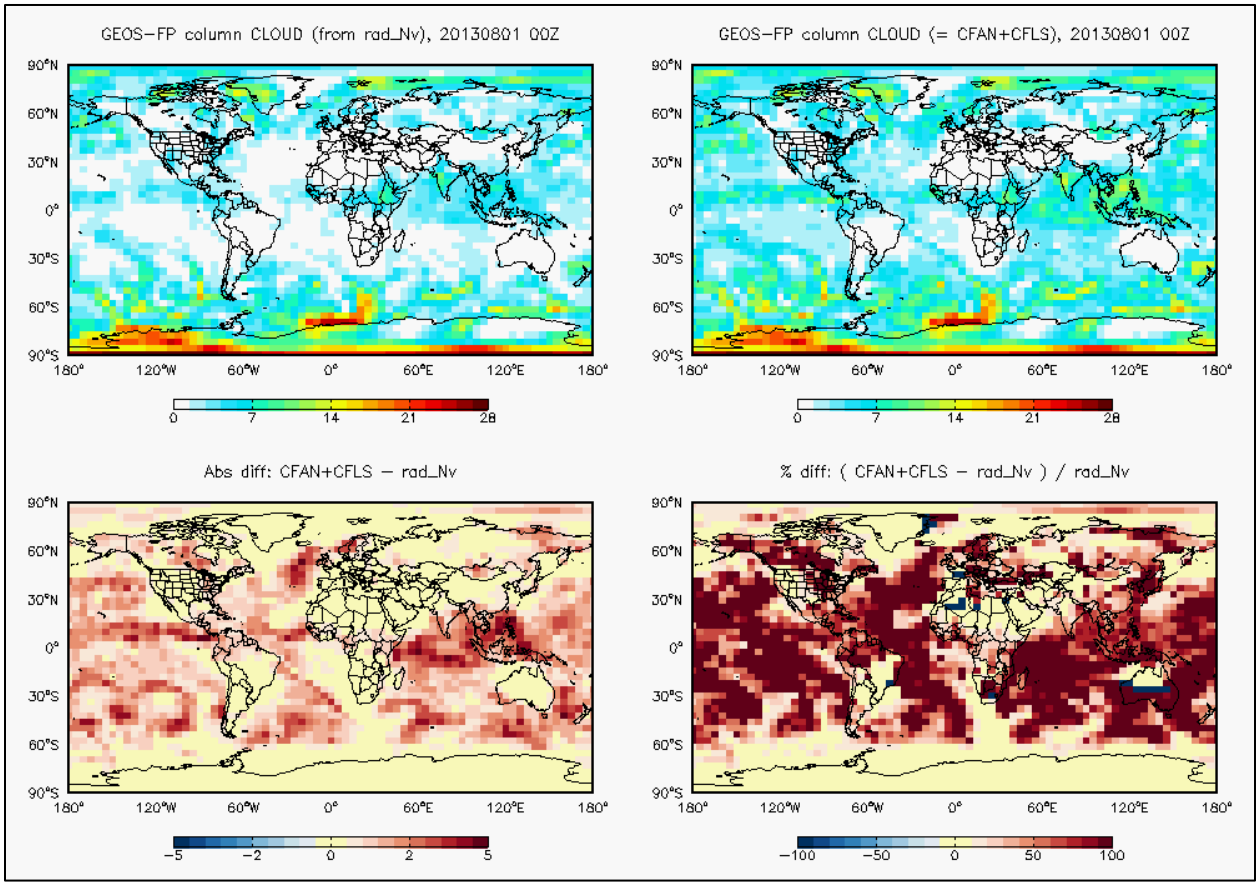


Figure: Top left panel: Column cloud fraction obtained by summing the GEOS-FP 4x5 `CLOUD` field in the vertical. `CLOUD` was taken directly from the 0.25 x 0.3125 GEOS-FP met archive and regridded to 4x5. Top right panel: Column cloud fraction obtained by summing the GEOS-FP 4x5 `CLOUD` field in the vertical, but in this case, `CLOUD` is computed as `min( CFAN + CFLS, 1.0)`. The bottom left and right panels show the absolute and percent difference plots respectively. The computed `CLOUD` field is biased high with respect to the `CLOUD` field that is taken directly from the GEOS-FP met archive.

Therefore, we now have decided that the `CLOUD = min( CFAN + CFLS, 1.0 )` is not a reliable approximation. We are now reprocessing the GEOS-FP data to correct this issue. The reprocessing only involved fixing one file per day per horizontal grid, so it should be a fairly quick process.

Difference in assimilated O3 columns: GEOS-FP vs. GEOS-5

Our GEOS-FP data archive for GEOS-Chem contains the assimilated total column ozone field (TO3). This TO3 field was also archived in our GEOS-5 data archive for GEOS-Chem. It appears at first glance that the GEOS-FP total column ozone is biased low with respect to GEOS-5.

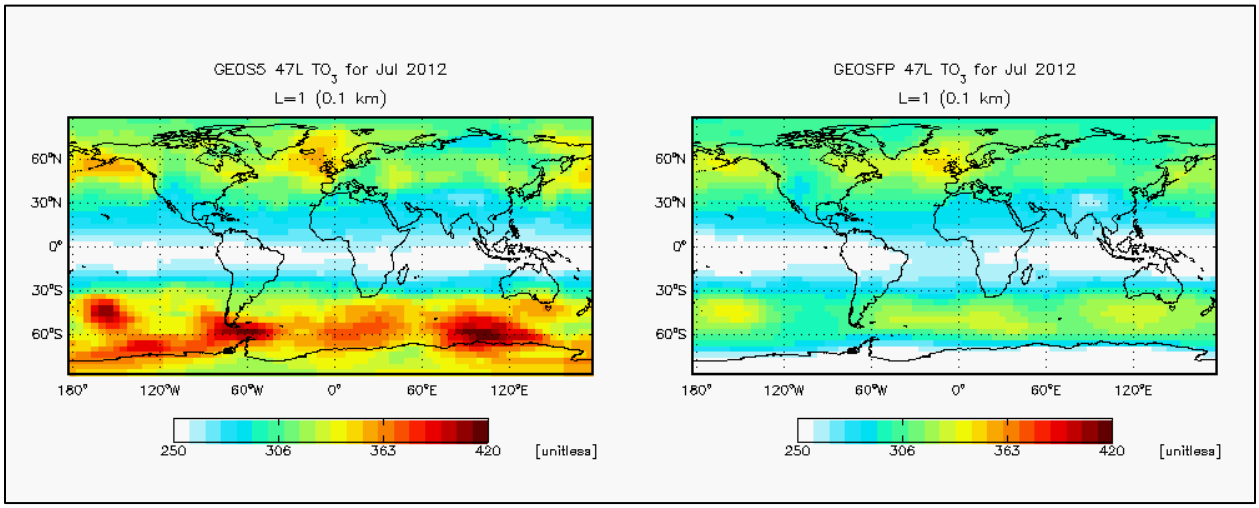


Figure: The left panel shows the GEOS-5 assimilated column ozone field (TO3), regridded to GEOS-Chem's 4^o x 5^o resolution. The right panel shows the corresponding TO3 field in the GEOS-FP data archive, also regridded to GEOS-Chem's 4^o x 5^o resolution. Both plots are on the same color scale. The GEOS-FP TO3 field appears to be lower than GEOS-5, especially in the southern midlatitudes.

By default, the standard GEOS-Chem simulation is set up to only use the column ozone from the GEOS-5 met fields only in locations where TOMS/SBUV ozone data does not exist. On the other hand, the standard GEOS-Chem simulation will use the GEOS-FP assimilated column ozone (TO3) field everywhere.

Sensitivity studies performed by Melissa Sulprizio suggest that the GEOS-FP assimilated TO3 column ozone field does not change J-values by a huge amount compared to using the TOMS/SBUV monthly mean O3. We are still investigating.

Variance of vertical pressure velocity (OMEGA)

The GEOS-Chem Transport Working Group has requested that we compute the variance of the vertical pressure velocity (OMEGA, units = Pa/s) when we create the GEOS-FP global 2x2.5 and 4x5 data files. We will start saving these out in 2014 after we return from winter break.

(4) GEOS-Chem Performance

Mat Evans and his group at York performed some scalability tests with GEOS-Chem (4^o x 5^o grid, GEOS-5 met, 1-month simulations). Their results are summarized in the plot below:

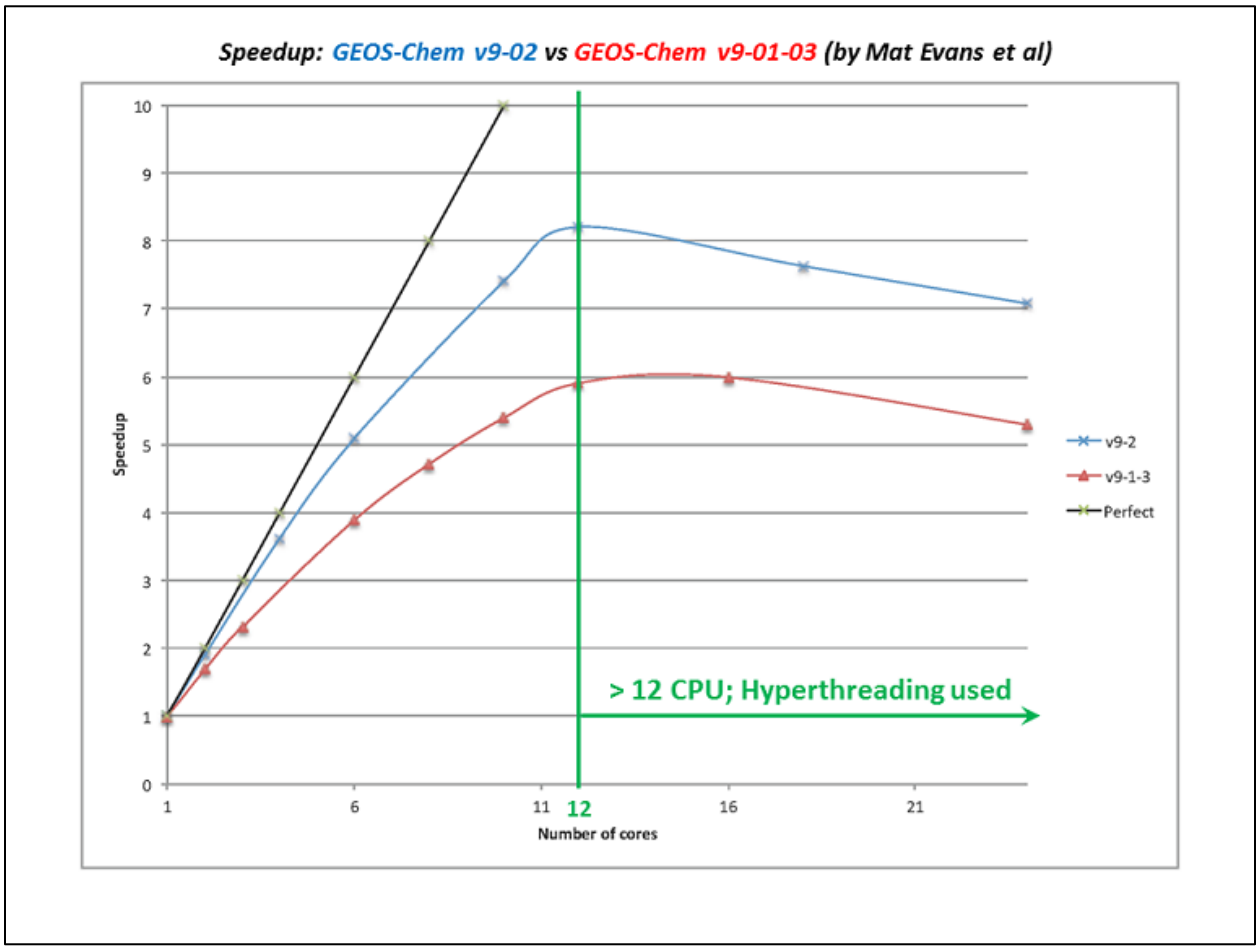


Figure: Speedup of GEOS-Chem v9-02 (blue line) vs. GEOS-Chem v9-01-03 (red line). The black line represents the "ideal" theoretical scalability. The departure from the "ideal" scalability represents (a) the presence of operations that occur only on a single computational core (i.e. disk I/O), and (b) system overhead. All tests were done on a computer with 12 computational cores (2 Xeon X5670 CPUs @ 2.93GHz with 6 computational cores per CPU). Hyperthreading (where each core behaves as if it were 2 cores) can be used to obtain up to 24 parallel threads of computation.

As you can see from the figure v9-02 is much closer to the expected ideal performance than v9-01-03. We believe that this improved performance reflects the removal of several computational bottlenecks from the GEOS-Chem source code (tested in v9-02k).

We also believe that OpenMP does not function as well when hyperthreading is used, thus leading to the turnover on the graph when more than 12 CPUs are used.

(5) Model development priorities for GEOS-Chem

The next version following GEOS-Chem v9-02 will more than likely be labeled GEOS-Chem v10-01. The change in version numbering will more than likely be necessitated by the updates of new features that will make GEOS-Chem differ significantly than previous versions.

The following items are now considered **Ready to go in**, and have already been delivered to the GEOS-Chem Support Team:

Item	Author(s)	Delivered to GCST when?
Acid uptake on dust aerosols	T. Duncan Fairlie (NASA/LARC)	Summer 2013
NEI 2008 emissions with hourly resolution	Katie Travis (Harvard)	Summer 2013. Also used in the SEAC4RS research G-C code.
Update to MEGAN2.1	Dylan Millet (U. Minnesota)	Summer 2013. Also used in the SEAC4RS research G-C code.
CO2 direct effect on isoprene emissions	Amos Tai (CUHK)	Nov 2013
PAN / Organics	Emily Fischer (Colo. State. U)	May 2013
Online GC radiative transfer (RRTMG)	David Ridley (MIT), Colette Heald (MIT)	Oct 2013
UCX strat chem mechanism: + Stratospheric chemistry + Stratospheric aerosols + FAST-JX photolysis	*UCX*: Sebastian Eastham (MIT); *FAST-JX*: Jingqiu Mao (Princeton)	Oct 2013
GIGC: Packaging ESMF/MAPL into the standard GEOS-Chem code	GCST, GMAO	Ongoing
Impaction scavenging for hydrophobic BC	Qiaoqiao Wang (Harvard, Max Planck Institute)	Nov 2013
Homogeneous IN removal	Qiaoqiao Wang	Nov 2013

The following updates are also listed as **Ready to go in**, but have not yet been officially received by the GEOS-Chem Support Team:

Item	Author(s)	Status
EDGAR 4.2 anthro emissions	Meng Li and Qiang Zhang (Tsinghua) Sajeev Philip (Dalhousie)	Currently in a research version of GEOS-Chem; more documentation and quantification needed
Improve temporal resolution of anthropogenic CO2 sources	Ray Nassar (Environment Canada)	
Replace CASA CO2 biosphere climatology with year-specific fluxes	Ray Nassar (Environment Canada) Dylan Jones (U. Toronto)	***Ray Nassar wrote:*** SiB Fluxes are available to replace the old CASA fluxes, courtesy of Janina Messerschmidt et al. New CASA fluxes would also be good, such that the user can select options in the input.geos file.
UNEP 2010 anthropogenic Hg emissions	Shaojie Song (MIT)	
Historical anthropogenic atmospheric emissions of Hg	Bess Corbitt (Harvard)	
Subsurface ocean Hg concentration update	Anne Soerensen (Harvard)	
NEI 2008 Hg emission inventory	Yanxu Zhang (Harvard)	
Arctic Hg cycling	Jenny Fisher (Wollongong)	Paper just published
Criegee intermediate	Dylan Millet (U. Minnesota)	Not used in G-C but has been used in the SEAC4RS research code.
VBS SOA option	Rokjin Park (Seoul Nat'l Univ.)	
Tagged sulfate and nitrate simulation	Becky Alexander (U. Washington)	
RRTMG radiative transfer code (integrated with APM)	Fangqun Yu (SUNY Albany)	
Interannual lightning	Lee Murray (Harvard)	Available for GEOS-4, but still needs to be implemented in GEOS-

(6) HEMCO: Harvard Emissions Component

Christoph Keller is working on the Harvard Emissions Component (HEMCO), as part of our Grid-Independent GEOS-Chem project. HEMCO can:

- Read emissions data from several different files,
- Calculate resultant emissions for various species as a combination or overlaying of both global and regional emissions inventories,
- Compute emissions that depend on local meteorological variables (temperature, pressure, incident radiation, etc.) via user-supplied extensions,
- Connect seamlessly to the Earth System Model Framework, and thus be integrated into the GEOS-5 data assimilation system, or within our ESMF stand-alone GEOS-Chem.

Christoph reports that HEMCO is mostly mature. He has implemented HEMCO into both a development version of GEOS-Chem and into the GEOS-5 GCM. Christoph is currently writing up a description of HEMCO for publication in the journal Geosience Model Development.

(7) Grid-Independent GEOS-Chem: ESMF standalone version (aka "SA-GIGC")

In addition to integrating the Grid-Independent GEOS-Chem (GIGC) into the GEOS-5/GCM, we are also working towards creating a standalone version of the GIGC (which we refer to as SA-GIGC) that will use ESMF/MAPL libraries to run with message-passing (MPI) parallelization. This will allow G-C to run on hundreds or thousands of CPUs. We are collaborating with Kevin Bowman and his team at JPL on this effort.

Here is an update on recent developments:

- Meemong Lee (JPL) is going to evaluate the TPCORE packages in the GEOS-CTM, GMI, and GEOS-Chem models to assess which is more accessible to us. She will also try to identify any potential problems that may crop up (i.e. serial-GC and SA-GIGC tpcore versions to be different.

- The framework for the transport is already included in the SA-GIGC. Some technical issues (i.e. a "haloing" problem) has not yet been resolved. Mike will place all of this code into the standard GEOS-Chem Git repository shortly.

- Christoph Keller and Mike Long are planning a "grand merge" of the GIGC code with the Harvard Emissions Component (HEMCO). This will bring the alluded to a 'grand-merge' of GIGC & HEMCO. This will bring the HEMCO into both the SA-GIGC and GEOS-5 GIGC development streams, which will facilitate testing.

(8) Grid-Independent GEOS-Chem: connecting with the GEOS-DAS

Christoph Keller has incorporated HEMCO into the GEOS-5 GCM and continues to test that interface.

Mike Long reports: “I'll start on porting in the dry deposition velocities from the GEOS5 land model [this week]. This will be the last major step for production/test simulations with the coupled system.”

(9) GEOS-Chem Unit Tester

We have found that G-C developers often send us code that has not been adequately debugged. In some cases, several months may elapse before an error is discovered. Then we have to send out a patch to the G-C user community, which is an inconvenience. Furthermore, some code submissions that we receive have only ever been tested on one type of met field (e.g. GEOS-5 but not MERRA or GCAP). Hidden errors may later manifest themselves when someone tries to run G-C with a different set of met fields.

We now have created a GEOS-Chem Unit Tester package that assists us in identifying several common GEOS-Chem bugs and coding errors. Our goal is to remove these bugs before starting the 1-month and 1-year benchmark simulations.

Using the GEOS-Chem Unit Tester, we have already identified and corrected several numerical issues in v9-02p, as shown on this wiki page.

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GEOS-Chem Support Team
geos-chem-support@as.harvard.edu