GEOS-Chem Newsletter, Fall 2014
28 Aug 2014

The GEOS-Chem Support Team
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The dates for IGC7 are now set!

We are pleased to announce that the 7th International GEOS-Chem Meeting (aka IGC7) will take place at Harvard University from May 4-7, 2015. You will find the latest information about the IGC7 meeting at our web site igc7.geos-chem.org.

As the meeting date draws closer, we will update the site with information about hotels, registration, and the list of oral and poster presentations.

We hope to see you in May 2015!

GEOS-Chem Steering Committee News

August 2014 GCSC telecon

Please take a moment to read the minutes from the August 28th GCSC telecon. The next GCSC telecon will take place in November or December 2014, date TBD.

List of New Developments and Narrative Description for v9-02

The GEOS-Chem Steering Committee has updated the *GEOS-Chem Narrative* and the *New GEOS-Chem Developments* web pages for GEOS-Chem v9-02. The *GEOS-Chem Narrative* provides a quick reference for papers to cite in describing the model. The *New GEOS-Chem Developments* lists updates of sufficient recent vintage—most of them for v9-02—that we recommend offering co-authorship to developers if they are significant for your paper.

We remind all GEOS-Chem users and developers to be generous in citations and co-authorships for GEOS-Chem developers. It is good practice and is key to our success as a community. See the *Credits and References* web page for more information.

GEOS-Chem website updates

We have updated the list of GEOS-Chem user groups

We have added the most recent GEOS-Chem user group information to the GEOS-Chem People and Projects page. If your user group information is missing or out-of-date, then please send an updated listing to the GEOS-Chem Support Team. We will be happy to add your listing to the page.

We have created new GEOS-Chem website URLs for your convenience

In order to make it easier to find certain commonly-viewed pages on the GEOS-Chem web site, we have added the following URLs:

http://people.geos-chem.org	Points to the GEOS-Chem People & Projects page
http://gcsc.geos-chem.org	Points to the GEOS-Chem Steering Committee page
http://igc6.geos-chem.org	Points to the page with presentations from IGC6 (May 2013)
http://igc7.geos-chem.org	Points to the IGC7 meeting page
http://manual.geos-chem.org	Points to the GEOS-Chem Online User's Guide
http://meeting.geos.chem.org	Points to the upcoming GEOS-Chem meeting page (currently IGC7)

We coordinate the list of GEOS-Chem publications with ResearcherID

Junwei Xu is now coordinating the GEOS-Chem publications list on ResearcherId. If you have any GEOS-Chem publications that you wish to add to the list, please contact Junwei at `jn231250[at]dal.ca`.

GEOS-Chem v10-01 development

Development timeline:

The table below lists some of the important features that have been added into GEOS-Chem v10-01. There have been a number of fixes, science updates (namely FAST-JX and UCX), and updates to improve computational performance.

Version	Date	Features
v10-01a	02/05/14	• Introduced a fix to reduce the dry deposition surface resistance when using the Olson 2001 land map.
v10-01b	03/06/14	• Corrected wrong molecular weights for PROPNN in input.geos file • Use MAP_A2A to regrid TOMS O3 data from 1x1 to other grids
v10-01c	05/29/14	• Introduced the UCX stratospheric-tropospheric chemical mechanism. | • See the 1-month and 1-year benchmarks done with UCX • Replaced FAST-J photolysis mechanism with FAST-JX • Added support for Tuning & Analysis Utilities (TAU) • Removed computational bottlenecks • Reduced memory footprint of the stratospheric chemistry module

		• Added several fixes for GEOS-Chem specialty simulations
v10-01d	06/03/14	• Corrected a typo in the chemical mechanism file globchem.dat • Corrected a parallelization error in the 0.5 x 0.666 nested-grid simulation • Corrected a minor bug in the ND44 dry deposition diagnostic • Implemented final recommendation for J(HAC) and J(PAN)
v10-01e	ongoing	• Incorporating the Harvard-NASA Emissions Component (HEMCO) • Removed many modules that were rendered obsolete by HEMCO

Harvard-NASA emissions component (HEMCO) update

Christoph Keller and the GEOS-Chem Support Team have been implementing the Harvard-NASA Emissions Component (HEMCO) into GEOS-Chem. We have many newsworthy items to report:

1. The journal article describing HEMCO has now been published in Geoscientific Model Development (aka GMD). The citation is:

   - C. A. Keller, M. S. Long, R. M. Yantosca, A. M. Da Silva, S. Pawson, and D. J. Jacob, *HEMCO v1.0: A versatile, ESMF-compliant component for calculating emissions in atmospheric models*, Geosci. Model Devel. , **7**, 1409-1417, 2014. [Link to Article]

2. As a condition to publishing in GMD, we agreed to make the HEMCO code publicly available as a stand-alone package independent of GEOS-Chem. Towards this end, we have created Git repositories for HEMCO and supporting files on the software development site GitHub.com. If you are interested in using the HEMCO standalone software, please see our HEMCO Installation Guide wiki page for complete installation instructions.

3. **GEOS-Chem users will NOT have to install HEMCO separately**. Starting with v10-01e, we are incorporating HEMCO directly into the GEOS-Chem source code directory structure. Furthermore, we use the "Git subtree" command to synchronize updates from the HEMCO code in GEOS-Chem with the master HEMCO repository on GitHub. This synchronization process, which will be transparent to most GEOS-Chem users, ensures that the same HEMCO version can be preserved between the GEOS-Chem source code and the HEMCO standalone code.

4. We have added the NCREGRID vertical regridding package (from the MESSY code base) to HEMCO. This will also allow HEMCO to directly ingest 3-D data sources that come from other models, or come on a regular pressure or altitude grid (e.g. volcanic emissions, aircraft emissions, etc.)

5. HEMCO has now rendered many of GEOS-Chem's legacy modules obsolete. We have now removed these modules from GEOS-Chem. For a complete list of removed modules, please see this listing.

6. HEMCO has "broken" most of the specialty simulations (i.e. Rn, Hg, Tagged CO, Tagged Ox, CH4, CO2, etc.). These simulations previously did their own file I/O, where emissions data would be read from binary file format. These simulations need to be modified so that the data I/O is done through HEMCO. This will allow HEMCO to keep track of the emissions in its

own data structure. Some specialty simulations will require some work to be made compatible with HEMCO, as they read many files from disk. We will work with the various specialty simulation user groups (Team Hg, Team TOMAS, etc) as we strive to re-establish this functionality.

Here is the current status of incorporation of HEMCO into GEOS-Chem.

Feature	**Status**
Full-chemistry simulations	Completed
SOA simulations	Completed
UCX simulations	Need to read UCX initial boundary conditions via HEMCO
Aerosol-only simulations	Need to reading global oxidant fields via HEMCO
CH4 simulation	Need to convert data files from binary (bpch) format to netCDF Need to replace legacy emissions routines w/ HEMCO Need to create a HEMCO configuration file for the CH4 simulation
CO (tagged) simulation	Need to create mask files used to define tagged CO regions Need to create a HEMCO configuration file for the CO simulation
CO2 simulation	Need to convert data files from binary (bpch) to netCDF format Need to read data files via HEMCO
Hg simulation	Need to convert data files from binary (bpch) to netCDF format Need to create mask files used to define tagged Hg regions Need to read data files via HEMCO
O3 (tagged) simulation	Need to convert data files from binary (bpch) to netCDF format Need to read O3 P/L files via HEMCO
POPs simulation	Nearly completed; validation & testing remain
Rn-Pb-Be simulation	Completed
TOMAS simulations	Need to track emissions of size-resolved dust with HEMCO Need to interface HEMCO w/ the TOMAS diagnostic outputs
Diagnostic archiving	HEMCO now tracks emissions data for the ND01, ND06, ND07, ND11, ND13, ND28, ND29, ND30, ND32, ND36, ND46, and ND63 time-averaged diagnostics.

While several important items have been completed, some work remains—especially to interface HEMCO with the various specialty simulations. Most of the remaining work involves preparing data files, and should progress very quickly.

GEOS-FP met field update

Available met data at Dalhousie and Harvard

GEOS-Chem Support Team member Junwei Xu has been archiving the GEOS-FP met fields on the `rain.ucis.dal.ca` server at Dalhousie University. You may now download GEOS-FP data from April 2012 thru August 2014 for the following horizontal grids:

- 4^o x 5^o global
- 2^o x 2.5^o global
- 0.25^o x 0.3125^o nested grids:
    a. CH: China (70^o E – 140^o E; 15^o N – 55^o N)
    b. EU: Europe (15^o W – 40^o E; 32.75^oN – 61.25^o N)
    c. NA: North America (130^o W – 60^o W; 9.75^oN – 60^o N)
    d. SE: Southeast Asia (75^o E – 130^o E; 10^o N – 30^o N)

We are also storing the 4^o x 5^o global, 2^o x 2.5^o global and 0.25^o x 0.3125^o NA nested-grid data on the `ftp.as.harvard.edu` server at Harvard University.

Archiving GEOS-FP data at 0.5^o x 0.625^o global resolution

The Nested Model Working Group, along with the Dalhousie University group, is planning to develop the degraded nested-grid capability over East Asia and North America. To facilitate this effort, Junwei Xu at has begun downscaling the GEOS-FP met data from its original 0.25^o x 0.3125^o resolution to 0.5^o x 0.625^o resolution. Downscaled met fields for July 2014 – present are available on the Dalhousie FTP server (`rain.ucis.dal.ca`).

Archiving data at 0.25^o x 0.3125^o global resolution

Paul Palmer's group at U. Edinburgh will take the lead on processing the GEOS-FP met data to the full 0.25^o x 0.3125^o global resolution for input into GEOS-Chem. The GEOS-Chem Support Team will provide technical assistance to Paul's group.

The advent of the new supercomputer (and mass-storage unit) in the UK has generated a lot of interest in being able to run GEOS-Chem not only at the 0.25^o x 0.3125^o nested grids, but also at the 0.25^o x 0.3125^o global grid. The current (OpenMP-enabled) GEOS-Chem can probably only support a simple simulation with a few tracers (i.e. CO2, CH4, Hg) with the global 0.25^o x 0.3125^o GEOS-FP met before running into a memory limit. But the global 0.25^o x 0.3125^o data would be available for use with the new ESMF/MPI standalone Grid-Independent GEOS-Chem (aka GIGC) that is currently being developed. This would allow us to evaluate the performance of the ESMF/MPI standalone GIGC at the full global resolution of the GEOS-FP met.

Paul's group at U. Edinburgh will collaborate with other GEOS-Chem groups in the UK on this effort. We should have some 0.25^o x 0.3125^o global data in place by the time the ESMF/MPI standalone GIGC code is ready for use later this year.

Jintai Lin's group at Peking University has also started to work on a global 0.25^o x 0.3125^o degree simulation, to be run with GIGC. Jintai writes:

> It is very likely that by Oct 1 I can secure thousands of computation cores on a supercomputer to do this global high-res simulation. I now have one month of global high-res GEOS-FP met data to work with, thanks to the generous help of Junwei Xu at Dalhousie. I also have come up with some ideas to, for example, alleviate/solve the transport problem in the polar areas. I feel it is a good idea for Paul's and my group to develop the modeling capability together, instead of repeating the efforts.

Grid-Independent GEOS-Chem (GIGC) update

The Chemistry Component of the Grid-Independent GEOS-Chem is very scalable

Mike Long has coupled the GEOS-Chem chemistry modules and HEMCO emission component with the NASA GEOS-5 GCM. (Read more about this in the following section.) He has run several test simulations using hundreds of CPUs of the NASA Discover supercomputer. Mike's findings demonstrate that the GEOS-Chem chemistry module scales extremely well with an increasing number of CPUs. This is encouraging news!

Mike's research will be presented in a journal article that will be submitted to Geoscientific Model Development very shortly.

The Grid-Independent GEOS-Chem is now running in the NASA GEOS-5 DAS!

Mike Long reports that the following milestones have been achieved in the effort to couple the Grid-Independent GEOS-Chem to the NASA GEOS-5 DAS:

1. The necessary source code updates for coupling GEOS-Chem v10-01d to the NASA GEOS-5 DAS have been added to our development repository (aka the "GC_Bleeding_Edge").

2. GEOS-Chem v10-01d + the Harvard-NASA emissions component (HEMCO) are now operational in the NASA GEOS-5 DAS.

3. Polishing up the "guts" of the coupling between GEOS-Chem and the NASA GEOS-5 DAS will be a priority in the near term. We need to clean up this coupling so that it can be made available to the public after our paper in GMD is published.

Christoph Keller and NASA Global Modeling and Assimilation Office (GMAO) personnel are currently performing a test simulation with GEOS-Chem v10-01d + HEMCO coupled to the NASA GEOS-5 DAS. Christoph writes:

> The GIGC-GEOS-DAS system is set up and being tested right now. This will let us assimilate ozone in the GEOS-5 system but with GEOS-Chem chemistry, which is a big step forward. We've also started to add NOx as an additional constituent to the assimilation system.

Eventually, the goal is to assimilate ozone and NOx jointly. We have identified the pieces of work that are required to achieve this, and will be working on this in the next months.

For the GIGC, I think going to a cubed-sphere should be considered high priority. This is especially important for the high-res simulations. We will need to obtain the grid areas from GEOS-5 instead of calculating them within GEOS-Chem and should also avoid the usage of grid edges wherever possible since those become somewhat arbitrary on a cubed sphere.

In addition, we need to add our convection code to the GIGC/GEOS-DAS. This is because the GEOS-5 convection currently doesn't include convective rainout, and if we want to capture that process (which we do), we need to use our own code.

The current GEOS-5 convection code will eventually be replaced by a component that also deals with rainout, and we can switch over to this component when that happens.

We are also working towards creating a new high-performance, ESMF-compatible GEOS-Chem

We are able to leverage the effort to couple GEOS-Chem with the NASA GEOS-5 DAS to create a new, ESMF/MPI compatible standalone GEOS-Chem CTM that will be able to run in high-performance computing environments on many more CPUs than is currently possible.

Mike Long writes:

- We have all the pieces for the stand-alone GIGC in place, and will be making big decisions and major leaps in the process this week (!!).

Bob Yantosca
on behalf of the entire GEOS-Chem Support Team
28 Aug 2014