GEOS-Chem Newsletter, Spring 2015
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IGC7 information

The 7th International GEOS-Chem Meeting (IGC7) will take place from May 4-7, 2015 at Harvard University. Please see the meeting website igc7.geos-chem.org for the latest information.

In particular:

- Registration for IGC7 closed on March 1, 2015.
- IGC7 lodging information has now been posted.

We hope to see you in May 2015!

GEOS-Chem v10-01 status

Our goal is to release GEOS-Chem v10-01 prior to IGC7. Here is a update of what we have accomplished to date.

GEOS-Chem v10-01f

GEOS-Chem v10-01f, which contained the features listed below, was approved on 13 Jan 2015.

Feature	Type	Submitted by
Two-way coupling between global and nested GEOS-Chem models	Science	Jintai Lin (Peking U.) Yingying Yan (Peking U.)
Update ALD2 photolysis in FAST-JX v7.0	Science	Jingqiu Mao (Princeton), Sebastian Eastham (MIT)
Read 2D data for individual NOx species in ucx_mod.F	Bug fix	Sebastian Eastham (MIT)
Bug fixes and updates for tagged CO simulation	Bug fix	Jenny Fisher (U. Wollongong)
Bug fixes for scavenging by co-condensation	Bug fix	Duncan Fairlie (NASA LaRC)
Correct bugs in stratospheric Bry data	Bug fix	Johan Schmidt (Harvard)
Introduction of flexible precision into GEOS-Chem	Structural	GEOS-Chem Support Team
Updates for 0.25° x 0.3125° China nested grid with GEOS-FP meteorology	Structural	Yuxuan Wang (Tsinghua/Galveston)
Additional minor updates to HEMCO	Structural	Christoph Keller (Harvard)

The stratospheric Br_y data is now read into GEOS-Chem via HEMCO.

GEOS-Chem v10-01g

GEOS-Chem v10-01g contained only bug fixes and other structural updates that did not affect the chemistry output. As such, we did not perform a benchmark on v10-01g. These updates will be validated by the benchmarks for the next version, v10-01h.

Feature	Type	Submitted by
Add fix to prevent a segmentation fault in HEMCO when emissions are turned off	Bug fix	Christoph Keller (Harvard)
Bug fix in planeflight diagnostic when using short chemistry timesteps	Bug fix	Luke Schiferl (MIT)
Fix calculation of WETLOSS for non-aerosol tracers in DO_MERRA_CONVECTION and DO_WASHOUT_ONLY	Bug fix	Carey Friedman (MIT)
Make the netCDF library linking process more portable	Structural	Bob Yantosca (Harvard)

GEOS-Chem v10-01h

GEOS-Chem v10-01h will add many new types of emissions to GEOS-Chem. These emissions are being implemented via the HEMCO emissions component.

Feature	Type	Submitted by
FINN biomass burning emissions (optional inventory implemented via HEMCO)	Science	Jenny Fisher (U. Wollongong) Min Huang (JPL)
Add Guenther et al (2012) updates to MEGAN2.1 biogenic emissions (implemented via HEMCO)	Science	Dylan Millet (U. Minnesota)
Updates to ship NOx chemistry, includes: Fix for high O3 values of dry deposition	Science & Bug fix	Chris Holmes (UC Irvine) Geert Vinken (Eindhoven)
MASAGE NH3 agricultural emissions (implemented via HEMCO)	Science	Fabien Paulot (Harvard)
Replace EDGARv3 with EDGAR v4.2 anthropogenic emissions (implemented via HEMCO)	Science	Meng Li and Qiang Zhang (Tsinghua) Sajeev Philip (Dalhousie)
HTAP emissions (optional inventory implemented via HEMCO)	Science	Qiang Zhang (Tsinghua U.)
MIX Asian emissions (implemented via HEMCO)	Science	Qiang Zhang (Tsinghua U.)
NEI 2008 emissions with hourly resolution (implemented via HEMCO)	Science	Katie Travis (Harvard)
NEI 2011 emissions with hourly resolution (implemented via HEMCO)	Science	Katie Travis (Harvard)
Update EMEP emissions for 2008-2010 (implemented via HEMCO)	Science	Aaron van Donkelaar (Dalhousie)
Update OTD/LIS factors for GEOS-FP through October 2014 (implemented via HEMCO)	Science	Lee Murray (Columbia)

NEI 2008 Hg emission inventory (implemented via HEMCO)	Science	Yanxu Zhang (Harvard)
UNEP 2010 anthropogenic Hg emissions (implemented via HEMCO)	Science	Shaojie Song (MIT)
Re-implement RCP future emission scenarios via HEMCO	Structural	Christoph Keller (Harvard)
Split AEROCOM volcanic emissions back into eruptive and degassing (implemented via HEMCO)	Structural	Christoph Keller (Harvard)
Additional updates to HEMCO	Structural	Christoph Keller (Harvard)

Most of these emissions are already in place in our development code. We are still preparing data files for a few inventories. In many instances we have had to convert the existing data into COARDS-compliant netCDF format for compatibility with HEMCO. We have also been busy preparing the relevant documentation.

GEOS-Chem v10-01h contains some important updates in order to make HEMCO more user friendly. We have added a section near the top of the HEMCO configuration file that allows you to turn emissions on or off with a simple switch, instead of having to manually comment out many individual lines of code. You will see this text:

```
# ExtNr ExtName           on/off  Species
0       Base              : on    *
    --> AEIC              :       true
    --> BIOFUEL           :       true
    --> BOND              :       true
    --> BOND_BIOMASS      :       false
    --> BRAVO             :       true
    --> CAC               :       true
    --> C2H6              :       true
    --> EDGAR             :       true
    --> EMEP              :       true
    --> GEIA              :       true
    --> LIANG_BROMOCARB   :       true
    --> NEI2005           :       true
    --> RETRO             :       true
    --> SHIP              :       true
    --> SHIPNO_BASE       :       false
    --> STREETS           :       true
    --> VOLCANO           :       true
```

By setting the option to either true or false, you can enable or disable a specific set of emissions.

In addition, HEMCO can now read non-emissions data sets, such as the GMI stratospheric production and loss rates. These data sets will always be read by HEMCO, even if you decide to switch emissions off completely.

We should be able to start benchmarking this v10-01h within 1-2 weeks (by early March).

GEOS-Chem v10-01i

The following features are being held over to GEOS-Chem v10-01i.

Feature	Type	Submitted by
Online Radiative Transfer in GEOS-Chem	Science	David Ridley (MIT), Colette Heald (MIT)
Improve temporal resolution of anthropogenic CO2 sources	Science	Ray Nassar (Env. Canada)
Replace CASA CO2 biosphere climatology with year-specific fluxes	Science	Ray Nassar (Env. Canada) Dylan Jones (U. Toronto)

Due to technical issues with the RRTMG radiative transfer code, we have had to delay its implementation. David Ridley (MIT) is currently working on making RRTMG compatible with the FAST-JX photolysis code that was introduced in v10-01a. He expects to have a fix shortly.

Our goal is to proceed to the benchmarking of v10-01h, and then add the RRTMG fix soon afterwards. If there is a significant further delay, we will add RRTMG into the next major release of GEOS-Chem.

Ray Nassar expects to have the CO2 updates ready before IGC7. These updates do not affect the full-chemistry simulation, so they can be added just before the public release.

Updates still "in the pipeline" for GEOS-Chem v10-01

The following features will be likely implemented in the GEOS-Chem version following v10-01:

Feature	Type	Submitted by
Historical anthropogenic atmospheric emissions of Hg	Science	Bess Corbitt (Harvard)
PAN / Organics	Science	Emily Fischer (CSU)
CO2 direct effect on isoprene emissions	Science	Amos Tai (CUHK)
Arctic Hg cycling	Science	Jenny Fisher (U. Wollongong)
Criegee intermediate	Science	Dylan Millet (U. Minnesota)
Impaction scavenging for hydrophobic BC	Science	Qiaoqiao Wang (MPI)
Homogeneous IN removal	Science	Qiaoqiao Wang (MPI)
Acid uptake on dust aerosols	Science	T. Duncan Fairlie (NASA/LARC)
Subsurface ocean Hg concentration update	Science	Anne Soerensen (formerly Harvard)
RRTMG radiative transfer code in APM aerosol microphysics	Science	Fangqun Yu (SUNY Albany)
Interannual lightning	Science	Lee Murray (Harvard)
Updates to PAH code	Science	Carey Friedman (MIT) Helen Amos (Harvard)
Improved dust size distribution scheme	Science	Li Zhang (Colorado U.) Daven Henze (Colorado U.)

Script to facilitate downloading HEMCO data files

The HEMCO emissions component reads emissions and other types of atmospheric data (e.g. concentrations, production and loss rates, etc.) from COARDS-compliant netCDF files. Many of the emissions data sets used in GEOS-Chem prior to v10-01 were archived in the binary punch data format. This data format is not compatible with HEMCO. This means that GEOS-Chem user groups will have to download a new collection of netCDF data files for GEOS-Chem v10-01.

In order to make the data download process easier, we have created a script that will let user groups pick and choose which HEMCO emissions data sets to download. We supply the script with a "standard GEOS-Chem emissions configuration"—that is, the set of emissions inventories that we use to perform the GEOS-Chem benchmark simulations. But if user groups decide that they do not want to download a particular inventory, they can tell the script omit that particular inventory. (For example, those user groups who only run specialty simulations like Hg, CO2, or CH4 may not want to download a large "full-chemistry" data set like NEI2011, in order to save disk space.)

For instructions on how to use this data download script (which is named **hemco_data_download**), please see our *Downloading the HEMCO data directories* wiki post.

Updating the documentation for GEOS-Chem v10-01

We have been updating the GEOS-Chem wiki pages to remove outdated information, especially pertaining to the emissions data. Many emissions inventories have been updated to new versions, and files have been converted from binary to netCDF file format. Some new emissions inventories that have never before been included in GEOS-Chem are now being added. We have created a wiki page named *HEMCO data directories* that describes completely all of the emission inventories and other data sets that currently can be used with HEMCO.

Many existing posts on the GEOS-Chem wiki now refer to code that has been removed from GEOS_Chem v10-01. To reduce confusion, we have added text to denote obsolete wiki entries. We have also split up long wiki pages describing many different types of emissions into several shorter pages.

We are also working on rewriting the GEOS-Chem user manual for v10-01. This process is ongoing. Because there are many new updates in v10-01, we have to rewrite a lot of material.

Other fundamental software development efforts

We are adding a flexible precision definition into GEOS-Chem

Flexible precision is a language feature that was introduced in Fortran-90. It allows you to define GEOS-Chem's floating-point variables with 4 bytes (aka REAL*4) or with 8 bytes (aka REAL*8) when you compile the code. We invite you to read our *Flexible precision in GEOS-Chem* wiki page to learn more about the specifics involved.

The ability to switch between 4-byte and 8-byte precision in GEOS-Chem will have tremendous benefits. By using 4-byte precision, we will be able to reduce GEOS-Chem's memory footprint

dramatically. This will facilitate running GEOS-Chem at very fine resolution in high-performance computing environments. It will also reduce the amount of memory required to run the current nested-grid simulations.

GEOS-Chem Support Team member Matt Yannetti has been spearheading the effort to add flexible precision into GEOS-Chem. He has brought many of the necessary source code updates into GEOS-Chem v10-01f and higher versions. Matt is currently investigating the numerical differences in the output when switching from 4-byte to 8-byte precision. His work indicates that most modules of GEOS-Chem (with the exception of TPCORE transport) are relatively insensitive to the precision change. The work is ongoing.

Flexible precision will likely be declared an "official" GEOS-Chem option in the release following GEOS-Chem v10-01.

Correcting inaccuracies in the computation of air mass and related quantities

The current method of converting tracer units from vol/vol to kg in GEOS-Chem uses the air mass in a grid box and the molecular weight of dry air. This algorithm assumes that the surface pressure (which we obtain from the GEOS met data archive) is based on dry air content. But more recent versions of the GEOS met data products—which are used to drive GEOS-Chem—now account for water vapor in the computation of surface pressure, thus rendering this assumption invalid.

GEOS-Chem Support Team member Lizzie Lundgren is working to correct this situation and similar instances of dry air assumptions in GEOS-Chem. She is implementing the following solutions:

1. Grid box dry air partial pressure-edge and pressure-center arrays are now computed in GEOS-Chem. Input moist air pressures remain available for use.
2. Air mass is now computed with respect to dry air only.
3. Box height is now computed using the hypsometric equation with water vapor taken into account.
4. Both moist and dry air densities are now computed using the partial pressures of dry air and water vapor in the ideal gas law.
5. The computations of relative humidity (only necessary if using GEOS-4 or GCAP meteorology in GEOS-Chem) and water vapor volume mixing ratio were previously calculated by approximating the specific humidity (mass water / mass total air) as mass water per dry air. Both computations have been updated to take into account the more precise definition of specific humidity.

We will post this information on the GEOS-Chem wiki very shortly. We expect to introduce this fix into the version that follows GEOS-Chem v10-01.

Making units consistent throughout GEOS-Chem

GEOS-Chem has traditionally carried tracers in units of kg, and then has converted them to v/v mixing ratio and molec/cm3 in other areas of the code as needed. But these unit conversions rely upon the surface area of each grid cell. GEOS-Chem currently computes surface areas assuming a Cartesian grid. On the other hand, the latest generation of Earth System Models—including NASA's GEOS-5 GCM—often use cubed-sphere grids. This renders the assumption of a Cartesian grid invalid.

We are planning to recode GEOS-Chem such that tracer and species concentrations are carried in molar units, such as [mol gas/mol air]. This will:

- Remove the burden of having to know what the surface area of each grid box is,
- Remove several commonly-repeated multiplications and divisions, thus increasing computational efficiency,
- Facilitate coupling GEOS-Chem with the GEOS-5 GCM and other Earth System Models

Lizzie Lundgren is currently leading the effort to make the units consistent throughout GEOS-Chem. She writes:

> There will be two phases to this work. First, we will remove the existing conversions between kg and v/v. Second, we will assess and update all other places in GEOS-Chem that are area-dependent, such as where some air density is calculated as air mass divided by volume rather than using the available air density quantity calculated from the ideal gas law.

We expect to introduce this change into the version that follows GEOS-Chem v10-01.

Migrating diagnostics from binary output to netCDF output

For many years, GEOS-Chem has saved diagnostic output to binary punch file format—that is, unformatted Fortran binary output with standardized data fields. But binary files cannot be read efficiently in distributed high-performance computing environments. Therefore, we have begun to recode GEOS-Chem so that diagnostic outputs can be saved to COARDS-compliant netCDF files.

Christoph Keller has modified HEMCO so that we can use HEMCO's internal data structure to archive diagnostic output for any GEOS-Chem quantity. We have opened a new branch of development into which we are placing these modifications. We envision that netCDF diagnostic output will be standardized in the version of GEOS-Chem that immediately follows v10-01.

Implementation of Flexchem with KPPA solver into GEOS-Chem

John Linford (ParaTools, Inc.) and Mike Long have been working towards the implementation of KPP-Accelerated (KPPA) into GEOS-Chem. KPPA is a newer, faster version of the previous KPP chemical solver software. Preliminary tests show significant speedup (50-70%) over the existing SMVGEAR chemical solver software.

The implementation of KPPA into GEOS-Chem has been named Flexchem, for "flexible chemistry". The advantage of using Flexchem over the existing SMVGEAR/KPP code is that you will be able to make changes to the chemistry mechanism by just changing an input file. The current SMVGEAR/KPP code requires many steps in order to change the mechanism.

The work is ongoing, but we envision that Flexchem could be a standard GEOS-Chem option within several months.

High-performance computing with GEOS-Chem

NASA/GMAO will use GEOS-Chem for a 7km resolution simulation

NASA/GMAO is planning on running a version of the GEOS-DAS system on the cubed-sphere grid at 7km horizontal resolution (aka the "Nature run") by June 2015. GEOS-Chem will be used as the chemical operator in this simulation.

Mike Long is currently adding Flexchem to the development version of GEOS-Chem that will be used in the "Nature run". The GEOS-Chem Support Team is assisting Mike in this effort.

At this time, the "Nature run" has taken precedence over other GEOS-DAS/GEOS-Chem activities.

The ESMF/MPI version of GEOS-Chem now compiles and runs!

We have succeeded in compiling and running GEOS-Chem in a high-performance computing (HPC) environment. GEOS-Chem can now utilize the Earth System Modeling Framework (ESMF) with Message-Passing Interface (MPI) parallelization to run on distributed computing architectures. It also uses the MPI-enabled NASA/GMAO finite-volume dynamics core (FVdycore) as the transport operator.

At present, we have gotten the HPC-enabled GEOS-Chem to run on both the Odyssey computer at Harvard, as well as the Discover supercomputer at NASA. Several beta testers have downloaded the code. Further testing is ongoing.

Still to do: bring the latest HEMCO emissions updates from v10-01h into the HPC-enabled GEOS-Chem.

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