GEOS-Chem Classic

Release 14.6.0

GEOS-Chem Support Team

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GETTING STARTED

This site provides instructions for **GEOS-Chem Classic**, the single-node mode of operation of the GEOS-Chem model. We provide instruction for downloading and compiling GEOS-Chem Classic, plus its required software libraries.

Note: If you would like to run GEOS-Chem on more than one node of a computing system, consider using GEOS-Chem High Performance (GCHP).

GEOS-Chem is a global 3-D model of atmospheric composition driven by assimilated meteorological observations from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office. It is applied by research groups around the world to a wide range of atmospheric composition problems.

- GEOS-Chem Overview
- Narrative description of GEOS-Chem

Cloning and building from source code ensures you will have direct access to the latest available versions of GEOS-Chem Classic, provides additional compile-time options, and allows you to make your own modifications to GEOS-Chem Classic source code.

CHAPTER

ONE

QUICKSTART GUIDE

This quickstart guide is for quick reference on how to download, build, and run **GEOS-Chem Classic**, which is the single-node instance of GEOS-Chem.

Tip: Please also see our GCHP Quickstart Guide if you would like to run GEOS-Chem across using more than one computational node.

This guide assumes that your environment satisfies GEOS-Chem Classic *hardware* and *software* requirements. This means you should load a *compute environment* such that programs like **cmake** are available before continuing. If you do not have some of the required software dependencies, you can find instructions for installing external dependencies in our Spack instructions.

For simplicity we will also refer to **GEOS-Chem Classic** as simply **GEOS-Chem** on this page. More detailed instructions on downloading, compiling, and running GEOS-Chem can be found in the User Guide elsewhere on this site.

1.1 1. Clone GEOS-Chem Classic

Download the source code:

```
$ git clone --recurse-submodules https://github.com/geoschem/GCClassic.git GCClassic
$ cd GCClassic
```

Tip: If you wish, you may choose a different name for the source code folder, e.g.

```
$ git clone --recurse-submodules https://github.com/geoschem/GCClassic.git my_code_dir
$ cd my_code_dir
```

Upon download you will have the most recently released version. You can check what this is by printing the last commit in the git log and scanning the output for tag.

```
$ git log -n 1
```

Tip: To use an older GEOS-Chem Classic version (e.g. 14.0.0), follow these additional steps:

```
$ git checkout tags/14.0.0                  # Points HEAD to the tag "14.0.0"
$ git branch version_14.0.0                 # Creates a new branch at tag "14.0.0"
```

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```
$ git checkout version_14.0.0              # Checks out the version_14.0.0 branch
$ git submodule update --init --recursive  # Reverts submodules to the "14.0.0" tag
```

You can do this for any tag in the version history. For a list of all tags, type:

```
$ git tag
```

If you have any unsaved changes, make sure you commit those to a branch prior to updating versions.

1.2 2. Create a run directory

Navigate to the `run/` subdirectory. To *create a run directory*, run the script `./createRunDir.sh`:

```
$ cd run/
$ ./createRunDir.sh
```

Creating a run directory is interactive, meaning you will be asked multiple questions to set up the simulation. For example, running `createRunDir.sh` will prompt questions about configurable settings such as simulation type, grid resolution, meteorology source, and number of vertical levels. It will also ask you where you want to store your run directory and what you wish to name it, including whether you want to use the default name, e.g. `gc_4x5_merra2_fullchem`. We recommend storing run directories in a place that has a large storage capacity. It does not need to be in the same location as your source code. When creating a run directory you can quit and start from scratch at any time.

For demonstration purposes, we will use a full chemistry simulation run directory with the default name (`gc_merra2_4x5_fullchem`). The steps to setup and run other types of GEOS-Chem Classic simulations follow the same pattern as the examples shown below.

Attention: The first time you create a run directory, you will be asked to provide *registration information*. Please answer all of the questions, as it will help us to keep track of GEOS-Chem usage worldwide. We will also add your information to the GEOS-Chem Users web page.

Important: The convection scheme used for GEOS-FP met generation changed from RAS to Grell-Freitas with impact on GEOS-FP meteorology files starting June 1, 2020, specifically enhanced vertical transport. In addition, there is a bug in convective precipitation flux following the switch where all values are zero. While this bug is automatically fixed by computing fluxes online for runs starting on or after June 1 2020, the fix assumes meteorology year corresponds to simulation year. Due to these issues we recommend splitting up GEOS-FP runs in time such that a single simulation does not run across June 1, 2020. Instead. set one run to stop on June 1 2020 and then restart a new run from there. If you wish to use a GEOS-FP meteorology year different from your simulation year please create a GEOS-Chem GitHub issue for assistance.

1.3 3. Load your environment

Always make sure that all libraries and environment variables are loaded prior to building GEOS-Chem Classic. An easy way to do this is to write an *environment file* and load that file every time you work with GEOS-Chem. To make this extra easy you can create a symbolic link to your environment file within your run directory or for reference. For example, do the following in your new run directory to have a handy link to the environment you plan on using.

```
$ cd /path/to/gc_4x5_merra2_fullchem   # Skip if you are already here
$ ln -s ~/envs/gcc.gfortran10.env gcc.env
```

Then every time you start up a session to work with GEOS-Chem in your run directory you can easily load your environment.

```
$ source gcc.env
```

1.4 4. Configure your build

You may build GEOS-Chem Classic from within the run directory or from anywhere else on your system. But we recommend that you always build GEOS-Chem Classic from within the run directory. This is convenient because it keeps all build files in close proximity to where you will run the model. For this purpose the GEOS-Chem run directory includes a build directory called `build/`.

First, navigate to the `build/` folder of your run directory:

```
$ cd /path/to/gc_4x5_merra2_fullchem  # Skip if you are already here
$ cd build
```

The next step is to *configure your build*. These are persistent settings that are saved to your build directory. A useful configuration option is `-DRUNDIR`. This option lets you specify one or more run directories that GEOS-Chem is "installed" to; that is, where where the executable is copied, when you do **`make install`**.

Configure your build so it installs GEOS-Chem to the run directory you created in Step 2. The run directory is one directory level higher than the `build` directory. Also located one level higher than the build directory is the `CodeDir` symbolic link to the top-level GEOS-Chem source code directory. Use the following command to configure your build:

```
$ cmake ../CodeDir -DRUNDIR=..
```

GEOS-Chem has a number of *additional configuration options* you can add here. For example, to compile with RRTMG after running the above command:

Note: The `.` in the **`cmake`** command above is important. It tells CMake that your current working directory (i.e., `.`) is your build directory.

```
$ cmake . -DRRTMG=y
```

A useful configuration option is to build in **debug mode**. Doing this is a good idea if you encountered an error (such as a segmentation fault) in a previous run and need more information about where the error happened and why.

```
$ cmake . -DCMAKE_BUILD_TYPE=Debug
```

Click here for more information on configuration options.

1.5 5. Compile and install

Compiling GEOS-Chem Classic should take about a minute, but it can vary depending on your system, your compiler, and your configuration options. To maximize build speed you should compile GEOS-Chem in parallel using as many cores as are available. Do this with the `-j` flag from the `build/` directory:

```
$ cd /path/to/gc_4x5_merra2_fullchem/build   # Skip if you are already here
$ make -j
```

Upon successful compilation, install the compiled executable to your run directory:

```
$ make install
```

This copies executable `build/bin/gcclassic` and supplemental files to your run directory.

Note: You can update build settings at any time:

1. Navigate to your build directory.
2. Update your build settings with **`cmake`** (only if they differ since your last execution of cmake)
3. Recompile with **`make -j`**. Note that the build system automatically figures out what (if any) files need to be recompiled.
4. Install the rebuilt executable with **`make install`**.

If you do not install the executable to your run directory you can always get the executable from the directory **`build/bin`**.

1.6 6. Configure your run directory

Now, navigate to your run directory:

```
$ cd /path/to/gcc_4x5_merra2_fullchem
```

You should review these files before starting a simulation:

- ***geoschem_config.yml***
  - Controls several frequently-updated simulation settings (e.g. start and end time, which operations to turn on/off, etc.)
- ***HISTORY.rc***
  - Controls GEOS-Chem diagnostic settings.
- ***HEMCO_Diagn.rc***
  - Controls emissions diagnostic settings via HEMCO.
- ***HEMCO_Config.rc***
  - Controls which emissions inventories and other non-emissions data will be read from disk (via HEMCO).

Attention: If you wish to spin up a GEOS-Chem simulation with a restart file that has (1) missing species or (2) a timestamp that does not match the start date in *geoschem_config.yml*, simply change the time cycle flag for the SPC_ entry in *HEMCO_Config.rc* from

```
* SPC_ ... $YYYY/$MM/$DD/$HH EFYO xyz 1 * - 1 1
```

to

```
* SPC_ ... $YYYY/$MM/$DD/$HH CYS xyz 1 * - 1 1
```

This will direct HEMCO to read the closest date available (C), to use the simulation year (Y), and to skip any species (S) not found in the restart file.

Skipped species will be assigned the initial concentration (units: $mol\ mol^{-1}$ w/r/t dry air) specified by its `BackgroundVV` entry in *species_database.yml*. If the species does not have a `BackgroundVV` value specified, then its initial concentration will be set to 1.0×10^{-20} instead.

Please see our *Customize simulations with research options* Supplemental Guide to learn how you can customize your simulation by activating alternate science options in your simulations.

1.7 7. Download input data

Before you can run your GEOS-Chem Classic simulation, you must first *download the required input data*. These data include:

- *Meteorological fields* (e.g. GEOS-FP, MERRA-2, GEOS-IT, or GCAP2)
- *Emissions inventories*
- *Inputs for GEOS-Chem modules (e.g. Cloud-J)*
- *Initial conditions for starting GEOS-Chem simulations*

Tip: If your institution has several GEOS-Chem users, then someone may have already downloaded these data for you. If this is the case, you may *start running your your GEOS-Chem Classic simulation* right away.

The easiest way to download data is to perform a *dry-run simulation*. This is a GEOS-Chem Classic simulation that steps through time, but does not perform computations or read data files from disk. Instead, the dry-run simulation prints a list of all data files that the simulation would have read.

To start a dry-run simulation, type this command:

```
$ ./gcclassic --dryrun | tee log.dryrun
```

This will generate the `log.dryrun` log file, which contains the list of data files to be downloaded.

Once the dry-run simulation has finished, use the `download_data.py` file (included in your run directory) to *download the required data*.

Note: Depending on your system, you might have to activate a Conda or Mamba environment containing a version of Python before running the `download.data.py` script. Ask your sysadmin.

To start the data download, type:

```
$ ./download_data.py log.dryrun geoschem+http
```

This will download data from the *GEOS-Chem Input Data* portal using the HTTP data transfer protocol.

Tip: If you have AWS CLI (command line interface) installed on your system, you can use this command instead:

```
$ ./download_data.py log.dryrun geoschem+aws
```

This will use the AWS CLI data download protocol instead, which should be faster than regular HTTP connections. This is the command you should use if you are running GEOS-Chem Classic in an AWS EC2 instance.

We also maintain *separate data portals* for special nested-grid domains as well as the GCAP 2.0 meteorology.

For more information about dry-run simulations, please see our *Download data with a dry-run simulation* chapter.

1.8 8. Run your simulation

If you used an *environment file* to load software libraries prior to building GEOS-Chem then you should load that file prior to running. To *run GEOS-Chem Classic*, type at the command line:

```
$ ./gcclassic
```

If you wish to send output to a log file, use:

```
$ ./gcclassic > GC.log 2>&1
```

We recommend *running GEOS-Chem Classic as a batch job*, although you can also do short runs interactively. Running GEOS-Chem as a batch job means that you *write a script (usually bash)* and then you submit that script to your local job scheduler (SLURM, LSF, etc.). If you write a batch script you can include sourcing your *environment file* within the script to ensure you always use the intended environment. Submitting GEOS-Chem as a batch job is slightly different depending on your scheduler. If you aren't familiar with scheduling jobs on your system, ask your system administrator for guidance.

Those are the basics of using GEOS-Chem Classic! See this user guide, step-by-step guides, and reference pages for more detailed instructions.

CHAPTER

TWO

MEET ALL HARDWARE REQUIREMENTS

If you are a first-time GEOS-Chem Classic user, please take a moment to make sure that your computer system meets certain hardware and software requirements. These are described in the following chapters.

2.1 Computer system

You will need to have access to one (or both) of these types of computational resources in order to use GEOS-Chem Classic:

2.1.1 A Unix-like computer system

GEOS-Chem Classic can only be used on computers with operating systems that are **Unix-like**. This includes all flavors of Linux (e.g. Ubuntu, Fedora, Red-Hat, Rocky Linux, Alma Linux, etc) and BSD Unix (including MacOS X, which is a BSD derivative).

Attention: While it is possible to run a Linux instance on a PC with the Windows Subsystem for Linux, we have found that PCs typically lack the memory and disk space to run most GEOS-Chem simulations. We therefore recommend using a computational cluster or the *Amazon cloud* instead.

If your institution has computational resources (e.g. a shared computer cluster with many cores, sufficient *disk storage* and *memory*), then you can run GEOS-Chem Classic there. Contact your sysadmin or IT support staff for assistance.

2.1.2 An account on the Amazon Web Services cloud

If your institution lacks computational resources (or if you need additional computational resources), then you should consider signing up for access to the Amazon Web Services cloud. Using the cloud has the following advantages:

- You can run GEOS-Chem without having to invest in local hardware and maintenance personnel.
- You won't have to download any meteorological fields or emissions data. All of the necessary data input for GEOS-Chem will be available on the cloud.
- You can initialize your computational environment with all of the required software (e.g. compilers, libraries, utilities) that you need for GEOS-Chem.
- Your GEOS-Chem runs will be 100% reproducible, because you will initialize your computational environment the same way every time.
- You will avoid GEOS-Chem compilation errors due to library incompatibilities.

- You will be charged for the computational time that you use, and if you download data off the cloud.

You can learn more about how to use GEOS-Chem on the cloud by visiting this tutorial (cloud.geos-chem.org).

2.2 Memory requirements

If you plan to run GEOS-Chem on a local computer system, please make sure that your system has sufficient memory to run your simulations.

2.2.1 Sufficient memory to run GEOS-Chem

For the $4^\circ \times 5^\circ$ "standard" simulation

- 8-15 GB RAM

For the $2^\circ \times 2.5^\circ$ "standard" simulation:

- 30-40 GB RAM
- 20 GB memory (MaxRSS)
- 26 GB virtual memory (MaxVMSize)

Our standard GEOS-Chem Classic 1-month full-chemistry benchmark simulations use a little under 12 GB of system memory. This is mostly due to the fact that the benchmark simulations archive the "kitchen sink"—that is, most diagnostic outputs are requested so that the benchmark simulation can be properly evaluated. But a typical GEOS-Chem Classic production simulation would not require all of these diagnostic outputs, and thus would use much less memory than the benchmark simulations.

2.2.2 Extra memory for special simulations

You may want to consider at least 30 GB RAM if you plan on doing any of the following:

- Running high-resolution (e.g. $1^\circ \times 1.25^\circ$ or higher resolution) global simulations
- Running high-resolution (e.g. $0.25^\circ \times 0.3125^\circ$ or $0.5^\circ \times 0.625^\circ$
- Running $2^\circ \times 2.5^\circ$ and generating a lot of diagnostic output. The more diagnostics you turn on, the more memory GEOS-Chem Classic will require).

2.3 Disk space requirements

The following sections will help you assess how much disk space you will need on your server to store GEOS-Chem Classic *input data* and *output data*.

2.3.1 Space for GEOS-Chem Classic input data

The data format used by GEOS-Chem Classic is *COARDS-compliant netCDF*. This is a standard file format used for Earth Science applications. See our *netCDF guide* for more information.

Emissions input fields

Please see our *Emissions input data* section for more information.

Meteorology fields

The amount of disk space that you will need depends on two things:

1. Which type of met data you will use, and
2. How many years of met data you will download

Table 1: Disk space needed for 1-year of MERRA-2 data

Resolution	Type	Size GB/yr
$1^\circ \times 1.25^\circ$	Global	~30
$2^\circ \times 2.5^\circ$	Global	~110
$0.5^\circ \times 0.625^\circ$	Nested Asia (aka AS)	~115
$0.5^\circ \times 0.625^\circ$	Nested Europe (aka EU)	~58
$0.5^\circ \times 0.625^\circ$	Nested North America (aka NA)	~110

Table 2: Disk space needed for 1-year of GEOS-FP data

Resolution	Type	Size GB/yr
$1^\circ \times 1.25^\circ$	Global	~30
$2^\circ \times 2.5^\circ$	Global	~120
$0.25^\circ \times 0.3125^\circ$	Nested Asia (aka AS)	~175
$0.25^\circ \times 0.3125^\circ$	Nested Europe (aka EU)	~175
$0.25^\circ \times 0.3125^\circ$	Nested North America (aka NA)	~175

GCAP 2.0: to be added

Obtaining emissions data and met fields

There are several ways to obtain the input data required for GEOS-Chem classic. These are described in more detail in the following sections.

1. Perform a *GEOS-Chem dry-run simulation*;
2. Download and manage data with the *bashdatacatalog tool*;
3. Transfer data with Globus **GEOS-Chem data (WashU)** endpoint;
4. Direct FTP access from the WashU data portal;
5. Direct access from the Amazon data portal using AWS S3 Explorer.

Also see our *Download input data* chapter for more data download options.

2.3.2 Space for data generated by GEOS-Chem Classic

Monthly-mean output

We can look to the **GEOS-Chem Classic** full-chemistry benchmark simulations for a rough upper limit of how much disk space is needed for diagnostic output. The GEOS-Chem 13.0.0 vs. 12.9.0 1-month benchmark simulation generated approximately 837 MB/month of output. Of this amount, diagnostic output files accounted for ~646 MB and restart files accounted for ~191 MB.

We say that this is an upper limit, because benchmark simulations archive the "kitchen sink"–all species concentrations, various aerosol diagnostics, convective fluxes, dry dep fluxes and velocities, J-values, various chemical and meteorological quantities, transport fluxes, wet deposition diagnostics, and emissions diagnostics. Most GEOS-Chem users would probably not need to archive this much output.

GEOS-Chem Classic specialty simulations–simulations for species with first-order loss by prescribed oxidant fields (i.e. Hg, CH4, CO2, CO)–will produce much less output than the benchmark simulations. This is because these simulations typically only have a few species.

Reducing output file sizes

You may subset the horizontal and vertical size of the diagnostic output files in order to save space. For more information, please see our section on *GEOS-Chem History diagnostics*.

Furthermore, since GEOS-Chem 13.0.0, we have modified the diagnostic code so that diagnostic arrays are only dimensioned with enough elements necessary to save out the required output. For example, if you only wish to output the SpeciesConc_O3 diagnostic, GEOS-Chem will dimension the relevant array with (NX,NY,NZ,1) elements (1 because we are only archiving 1 species). This can drastically reduce the amount of memory that your simulation will require.

Timeseries output

Archiving hourly or daily timeseries output would require much more disk space than the monthly-mean output. The disk space actually used will depend on how many quantities are archived and what the archival frequency is.

CHAPTER

THREE

MEET ALL SOFTWARE REQUIREMENTS

If you are a first-time GEOS-Chem Classic user, please take a moment to make sure that your computer system meets certain hardware and software requirements. These are described in the following chapters.

3.1 Supported compilers

GEOS-Chem is written in the Fortran programming language. However, you will also need C and C++ compilers to install certain libraries (like *netCDF*) on your system.

3.1.1 Intel

The **`Intel Compiler Suite`** is our recommended proprietary compiler suite.

Intel compilers produce well-optimized code that runs extremely efficiency on machines with Intel CPUs. Many universities and institutions will have an Intel site license that allows you to use these compilers.

The GCST has tested **`GEOS-Chem Classic`** with these versions (but others may work as well):

- 23.0.0
- 19.0.5.281
- 19.0.4

Older compiler versions than these may either be incompatible with GEOS-Chem, or may cause unexpected results. We hope to be able to port GEOS-Chem to the latest Intel 2024 compiler suite (`icx` for C, C++ and `ifx` for Fortran) in the near future.

Best way to install: Direct from Intel (Older versions may require purchase of a site license or a student license)

Tip: Intel 2021 and later may be obtained for free, or installed with a package manager such as Spack.

3.1.2 GNU

The **GNU Compiler Collection** (or **GCC** for short) is our recommended open-source compiler suite.

Because the GNU Compiler Collection is free and open source, this is a good choice if your institution lacks an Intel site license, or if you are running GEOS-Chem on the Amazon EC2 cloud environment.

The GCST has tested **GEOS-Chem Classic** with these versions (but others may work as well):

- 12.2.0
- 11.2.0
- 11.1.0
- 10.2.0
- 9.3.0
- 9.2.0
- 8.2.0
- 7.4.0
- 7.3.0
- 7.1.0
- 6.2.0

We recommend using GCC 10 or later if possible. We have not thoroughly tested GEOS-Chem with compiler versions more recent than GCC 12 as of January 2025.

Best way to install: *With Spack*.

3.1.3 Other compilers

We currently have no plans to port GEOS-Chem to compilers other than *Intel* and *GNU*. But when we interface GEOS-Chem into external models (such as CESM); all compilers used by the parent model can successfully parse GEOS-Chem source code.

3.2 Required software packages

3.2.1 Git

Git is the de-facto software industry standard package for source code management. A version of Git usually ships with most Linux OS builds.

The GEOS-Chem source code can be downloaded using the Git source code management system. GEOS-Chem software repositories are stored at the https://github.com/geoschem organization page.

Best way to install: git-scm.com/downloads. But first check if you have a version of Git pre-installed.

3.2.2 CMake

CMake is software that directs how the GEOS-Chem source code is compiled into an executable. You will need **CMake** version 3.13 or later to build GEOS-Chem Classic.

Best way to install: *With Spack*.

3.2.3 GNU Make

GNU Make is software that can build executables from Makefiles that are created by *CMake*.

While GNU Make is not required for GEOS-Chem 13.0.0 and later, some external libraries that you might need to build will require GNU Make. Therefore it is best to download GNU Make along with CMake.

Best way to install: *With Spack*.

3.2.4 netCDF

GEOS-Chem input and output data files use the netCDF file format (cf. *netCDF*). NetCDF is a self-describing file format that allows meadata (descriptive text) to be stored alongside data values.

Best way to install: *With Spack*.

3.3 Optional but recommended software packages

3.3.1 GCPy

GCPy is our recommended python companion software to GEOS-Chem.

While **GCPy** is not a general-purpose plotting package, it does contain many useful functions for creating zonal mean and horizontal plots from GEOS-Chem output. It also contains scripts to generate plots and tables from GEOS-Chem benchmark simulations.

Best way to install: From PyPi (see gcpy.readthedocs.io)

3.3.2 gdb and cgdb

The GNU debugger (gdb) and its graphical interface (cgdb) are very useful tools for tracking down the source of GEOS-Chem errors, such as segmentation faults, out-of-bounds errors, etc.

Best way to install: *With Spack*.

3.3.3 ncview

The ncview program is a netCDF file viewer. While it does not produce publication-quality output, ncview can let you easily examine the contents of a netCDF data file (such as those which are input and output by GEOS-Chem). Ncview is very useful for debugging and development.

3.3.4 nco

The netCDF operators (nco) are powerful command-line tools for editing and manipulating data in netCDF format.

Best way to install: *With Spack*.

3.3.5 cdo

The Climate Data Operators (cdo) are powerful command-line utilities for editing and manipulating data in netCDF format.

Best way to install: *With Spack*.

3.3.6 KPP

The Kinetic PreProcessor (KPP) translates a chemical mechanism specification from user-configurable input files to Fortran-90 source code. You will need to use **`KPP`** if you plan on updating any of the chemical mechanisms that ship with GEOS-Chem.

Best way to install: Clone from github.com/KineticPreProcessor/KPP and build the the KPP executable from source.

3.3.7 flex and bison

Flex is the Fast Lexical Analyzer, and bison is a general purpose parser-generator. *KPP* uses both **`flex`** and **`bison`** to parse chemical mechanism definition files. Depending on your setup, these packages might have already been installed for you.

Best way to install: *With Spack*.

CHAPTER

FOUR

CUSTOMIZE YOUR LOGIN ENVIRONMENT

Tip: You may *skip ahead* if you will be using **GEOS-Chem Classic** on an Amazon EC2 cloud instance. When you initialize the EC2 instance with one of the pre-configured Amazon Machine Images (AMIs) all of the required software libraries will be automatically loaded.

Tip: If your computer system lacks the required software packages for **GEOS-Chem Classic**, you can build them with the Spack package manager. For detailed instructions, please see our *Build required software with Spack* supplemental guide.

Each time you log in to your computer system, you'll need to load the *software libraries* needed by GEOS-Chem into your environment. You can do this with a script known as an **environment file**, as described in the following chapters:

4.1 Environment files

An environment file is a script that:

1. Loads software libraries into your login environment. This is often done with a module manager such as **lmod**, **spack**, or **environment-modules**.
2. Stores settings for GEOS-Chem and its dependent libraries in shell variables called environment variables.

You will **source** the environment file each time you log in with a command such as:

```
$ . ~/my-environment-file   # or whatever you name it
```

Tip: Keep a separate environment file for each combination of modules that you will use. Example environment files for *GNU* and *Intel* compilers and related software are provided in the following sections.

For general information about how libraries are loaded, see *Load software into your environment*.

4.2 Sample environment file for GNU 12.2.0 compilers

Below is a sample environment file (based on an enviroment file for the Harvard Cannon computer cluster). This file will load software libraries built with the GNU 12.2.0 compilers.

Note: This environment file shown below assumes that required software packages for **GEOS-Chem Classic** are available as pre-built modules. If your computer system does not have these packages pre-installed, you can build them with Spack. Please see our *Build required software with Spack* supplemental guide for detailed instructions.

Save the code below (with any appropriate modifications for your own computer system) to a file named `~/gcclassic.gnu12.env`.

```
############################################################################
#
# Environment file for GCClassic + GNU Compiler Collection 12.2.0
#
############################################################################

# Display message (if we are in a terminal window)
if [[ $- = *i* ]] ; then
  echo "Loading modules for GEOS-Chem Classic, please wait ..."
fi

#============================================================================
# Unload all previously-unloaded software
#============================================================================

# Unload packages loaded with "module load"
module purge

#============================================================================
# Load software packages for GNU 12.2.0
#============================================================================
if [[ $- = *i* ]] ; then
  echo "... Loading FASRC-built software, please wait ..."
fi

# Pre-built modules needed for GEOS-Chem
# (NOTE: These may be named differently on your system)
module load gcc/12.2.0-fasrc01              # gcc / g++ / gfortran
module load openmpi/4.1.4-fasrc01           # MPI
module load netcdf-c/4.9.2-fasrc01          # netcdf-c
module load netcdf-fortran/4.6.0-fasrc02    # netcdf-fortran
module load flex/2.6.4-fasrc01              # Flex lexer (needed for KPP)
module load cmake/3.25.2-fasrc01            # CMake (needed to compile)

#============================================================================
# Environment variables and related settings
# (NOTE: Lmod will define <module>_HOME variables for each loaded module)
#============================================================================

# Make all files world-readable by default
```

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```
umask 022

# Set number of threads for OpenMP.  If running in a SLURM environment,
# use the number of requested cores.  Otherwise use 8 cores for OpenMP.
if [[ "x${SLURM_CPUS_PER_TASK}" == "x" ]]; then
    export OMP_NUM_THREADS=8
else
    export OMP_NUM_THREADS="${SLURM_CPUS_PER_TASK}"
fi

# Max out the stacksize memory limit
export OMP_STACKSIZE="500m"

# Compilers
export CC="gcc"
export CXX="g++"
export FC="gfortran"
export F77="${FC}"

# netCDF
if [[ "x${NETCDF_HOME}" == "x" ]]; then
    export NETCDF_HOME="${NETCDF_C_HOME}"
fi
export NETCDF_C_ROOT="${NETCDF_HOME}"
export NETCDF_FORTRAN_ROOT=${NETCDF_FORTRAN_HOME}

# KPP 3.0.0+
export KPP_FLEX_LIB_DIR=${FLEX_HOME}/lib64

#=============================================================================
# Set limits
#=============================================================================

ulimit -c unlimited   # coredumpsize
ulimit -u 50000       # maxproc
ulimit -v unlimited   # vmemoryuse
ulimit -s unlimited   # stacksize

#=============================================================================
# Print information
#=============================================================================

module list

echo ""
echo "Environment:"
echo ""
echo "CC                  : ${CC}"
echo "CXX                 : ${CXX}"
echo "FC                  : ${FC}"
echo "KPP_FLEX_LIB_DIR    : ${KPP_FLEX_LIB_DIR}"
echo "MPI_HOME            : ${MPI_HOME}"
```

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```
echo "NETCDF_HOME          : ${NETCDF_HOME}"
echo "NETCDF_FORTRAN_HOME  : ${NETCDF_FORTRAN_HOME}"
echo "OMP_NUM_THREADS      : ${OMP_NUM_THREADS}"
echo ""
echo "Done sourcing ${BASH_SOURCE[0]}"
```

To activate the settings contained in the environment file, type:

```
$ . ~/gcclassic.gnu12.env
```

You may also place the above command within your *GEOS-Chem run script*, which will be discussed in a subsequent chapter.

4.3 Sample environment file for Intel 2023 compilers

Below is a sample environment file (based on an enviroment file for the Harvard Cannon computer cluster). This file will load software libraries built with the Intel 2023 compilers.

Note: This environment file shown below assumes that required software packages for **GEOS-Chem Classic** are available as pre-built modules. If your computer system does not have these packages pre-installed, you can build them with Spack. Please see our *Build required software with Spack* supplemental guide for detailed instructions.

Add the code below (with the appropriate modifications for your system) into a file named `~/gcclassic.intel23.env`.

```
###############################################################################
#
# Environment file for GCClassic + Intel 2023 compilers
#
###############################################################################

# Unload all modules first
module purge

# Load modules
module load intel/23.0.0-fasrc01           # icc / i++ / gfortran
module load intelmpi/2021.8.0-fasrc01      # MPI
module load netcdf-fortran/4.6.0-fasrc03   # netCDF-Fortran
module load flex/2.6.4-fasrc01             # Flex lexer (needed for KPP)
module load cmake/3.25.2-fasrc01           # CMake (needed to compile)

#==============================================================================
# Environment variables and related settings
# (NOTE: Lmod will define <module>_HOME variables for each loaded module
#==============================================================================

# Make all files world-readable by default
umask 022

# Set number of threads for OpenMP.  If running in a SLURM environment,
```

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```
# use the number of requested cores.  Otherwise use 8 cores for OpenMP.
if [[ "x${SLURM_CPUS_PER_TASK}" == "x" ]]; then
    export OMP_NUM_THREADS=8
else
    export OMP_NUM_THREADS="${SLURM_CPUS_PER_TASK}"
fi

# Max out the stacksize memory limit
export OMP_STACKSIZE="500m"

# Compilers
export CC="icx"
export CXX="icx"
export FC="ifort"
export F77="${FC}"

# netCDF
if [[ "x${NETCDF_HOME}" == "x" ]]; then
   export NETCDF_HOME="${NETCDF_C_HOME}"
fi
export NETCDF_C_ROOT="${NETCDF_HOME}"
export NETCDF_FORTRAN_ROOT="${NETCDF_FORTRAN_HOME}"

# KPP 3.0.0+
export KPP_FLEX_LIB_DIR="${FLEX_HOME}/lib64"

#=============================================================================
# Set limits
#=============================================================================

ulimit -c unlimited   # coredumpsize
ulimit -u 50000       # maxproc
ulimit -v unlimited   # vmemoryuse
ulimit -s unlimited   # stacksize

#=============================================================================
# Print information
#=============================================================================

module list

echo ""
echo "Environment:"
echo ""
echo "CC                  : ${CC}"
echo "CXX                 : ${CXX}"
echo "FC                  : ${FC}"
echo "KPP_FLEX_LIB_DIR    : ${KPP_FLEX_LIB_DIR}"
echo "MPI_HOME            : ${MPI_HOME}"
echo "NETCDF_HOME         : ${NETCDF_HOME}"
echo "NETCDF_FORTRAN_HOME : ${NETCDF_FORTRAN_HOME}"
echo "OMP_NUM_THREADS     : ${OMP_NUM_THREADS}"
```

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```
echo ""
echo "Done sourcing ${BASH_SOURCE[0]}"
```

To activate the settings contained in the environment file, type:

```
$ . ~/gcclassic.intel23.env
```

You may also place the above command within your *GEOS-Chem run script*, which will be discussed in a subsequent chapter.

4.4 Set environment variables for compilers

The sample *GNU* and *Intel* environment files set the **environment variables** listed below in order to select the desired C, C++, and Fortran compilers:

Table 1: Environment variables that specify compilers

Variable	Specifies the:	GNU name	Intel name
`CC`	C compiler	`gcc`	`icx`
`CXX`	C++ compiler	`g++`	`icx`
`FC`	Fortran compiler	`gfortran`	`ifort`

Note: GEOS-Chem Classic only requires the Fortran compiler. But you will also need the C and C++ compilers if you plan to build other software packages (*such as KPP*) or *install libraries manually*.

Also, older Intel compiler versions used `icc` as the name for the C compiler and `icpc` as the name of the C++ compiler. These names have been deprecated in Intel 2023 and will be removed from future Intel compiler releases.

The commands used to define `CC`, `CXX`, and `FC` are:

```
# for GNU
export CC=gcc
export CXX=g++
export FC=gfortran
```

or

```
# for Intel
export CC=icx
export CXX=icx
export FC=ifort
```

4.5 Set environment variables for parallelization

GEOS-Chem Classic uses OpenMP parallelization, which is an implementation of shared-memory (aka serial) parallelization.

Important: OpenMP-parallelized programs (such as GEOS-Chem Classic) cannot execute on more than 1 computational node. Most modern computational nodes typically contain between 16 and 64 cores. Therefore, **GEOS-Chem Classic** simulations will not be able to take advantage of more cores than these.

We recommend that you consider using GCHP for more computationally-intensive simulations.

In the the sample environment files for *GNU* and *Intel*, we define the following **environment varaiables** for OpenMP parallelization:

OMP_NUM_THREADS

The `OMP_NUM_THREADS` environment variable sets the number of computational cores (aka threads) that you would like GEOS-Chem Classic to use.

For example, the command below will tell **GEOS-Chem Classic** to use 8 cores within parallel sections of code:

```
$ export OMP_NUM_THREADS=8
```

We recommend that you define `OMP_NUM_THREADS` not only in your environment file, but also in your *GEOS-Chem run script*.

OMP_STACKSIZE

In order to use **GEOS-Chem Classic** with OpenMP parallelization, you must request the maximum amount of stack memory in your Unix environment. (The stack memory is where local automatic variables and temporary `$OMP PRIVATE` variables will be created.)

Add the following lines to your system startup file (e.g. `.bashrc`) and to your *GEOS-Chem run scripts*:

```
ulimit -s unlimited
export OMP_STACKSIZE=500m
```

The **ulimit -s unlimited** will tell the bash shell to use the maximum amount of stack memory that is available.

The environment variable `OMP_STACKSIZE` must also be set to a very large number. In this example, we are nominally requesting 500 MB of memory. But in practice, this will tell the GNU Fortran compiler to use the maximum amount of stack memory available on your system. The value **500m** is a good round number that is larger than the amount of stack memory on most computer clusters, but you can increase this if you wish.

4.5.1 Errors caused by incorrect environment variable settings

Be on the lookout for these errors:

1. If *OMP_NUM_THREADS* is set to 1, then your simulation will execute using only one computational core. This will make your simulation take much longer than necessary.
2. If *OMP_STACKSIZE* environment variable is not included in your environment file (or if it is set to a very low value), you might encounter a *Segmentation fault encountered after TPCORE initialization* error. In this case, GEOS-Chem Classic "thinks" that it does not have enough memory to perform the simulation, even though sufficient memory may be present.

CHAPTER

FIVE

KEY REFERENCES

Bey *et al.* [2001] is the first reference to GEOS-Chem that includes a detailed model description. It is suitable as an original reference for the model. It only describes a model for gas-phase tropospheric oxidant chemistry. Subsequent original references for major additional model features are:

1. Park *et al.* [2004] for aerosol chemistry;
2. Y.X. Wang *et al.* [2004] for the nested model;
3. Henze *et al.* [2007] for the model adjoint;
4. Selin *et al.* [2007] for the mercury simulation;
5. Trivitayanurak *et al.* [2008] for TOMAS aerosol microphysics;
6. Yu and Luo [2009] for APM aerosol microphysics;
7. Eastham *et al.* [2014] and for stratospheric chemistry;
8. Keller *et al.* [2014] and Lin *et al.* [2021] for HEMCO;
9. Long *et al.* [2015] for the grid-independent GEOS-Chem;
10. Prather [2015] for Cloud-J;
11. Eastham *et al.* [2018] for the high-performance GEOS-Chem (GCHP);
12. Hu *et al.* [2018] for GEOS-Chem within the GEOS ESM (GEOS-GC);
13. Lin *et al.* [2020] for GEOS-Chem within WRF (WRF-GC);
14. Zhuang *et al.* [2019] and Zhuang *et al.* [2020] for implementations of GEOS-Chem Classic and GCHP on the cloud;
15. Bindle *et al.* [2021] for the stretched-grid capability in GCHP;
16. Murray *et al.* [2021] for GEOS-Chem driven by GISS GCM fields (GCAP 2.0);
17. Bukosa *et al.* [2023] for the carbon simulation;
18. Lin *et al.* [2023] for KPP 3.0.0 with adaptive auto-reduction solver;
19. Miller *et al.* [2024] for HETerogeneous vectorized or Parallel (HETPv1.0).

References

CHAPTER

SIX

DOWNLOAD SOURCE CODE

In the following chapters, you will learn how to download the GEOS-Chem source code from Github.

6.1 Source code repositories

The **GEOS-Chem Classic** source code is distributed into several GitHub repositories (aka "repos"), as described below. This setup allows the GEOS-Chem core science routines to be easily integrated into several modeling contexts, such as:

- GEOS-Chem Classic
- GCHP
- GEOS-Chem within the NASA/GEOS ESM
- GEOS-Chem within CESM
- GEOS-Chem withn WRF (aka WRF-GC)

This repository setup also aligns with our GEOS-Chem Vision and Mission statements.

6.1.1 GEOS-Chem repositories

The bulk of the GEOS-Chem Classic code is contained in three repositories:

GEOS-Chem "Science Codebase"

The **GEOS-Chem "Science Codebase"** repository (https://github.com/geoschem/geos-chem) contains the GEOS-Chem science routines, plus:

- Scripts to create GEOS-Chem run directories, plus template configuration files for all simulations;
- Scripts to create GEOS-Chem integration tests;
- Interfaces (i.e. the driver programs) for GEOS-Chem Classic, GCHP, etc.

HEMCO

The **HEMCO** repository (https://github.com/geoschem/HEMCO) contains the source code for the Harmonized Emissions Component, which is used to read and regrid emissions, met fields, and other inputs to GEOS-Chem.

GCClassic

The **GCClassic** repository (https://github.com/geoschem/GCClassic) is a lightweight wrapper that encompasses GEOS-Chem and HEMCO. We say that GCClassic is the **superproject** (i.e. top-level source code folder), and that GEOS-Chem (science codebase) and HEMCO are **submodules**.

6.1.2 Other code packages used by GEOS-Chem

GEOS-Chem uses a few code packages that are maintained separately. These are inlined to GEOS-Chem as Git submodules.

Cloud-J

The **Cloud-J** repository (https://github.com/geoschem/Cloud-J) contains the source code for the Cloud-J photolysis package. This is used to compute reaction rates for photo-dissociation reactions in the GEOS-Chem fullchem and Hg chemistry mechanisms.

Reference: Prather [2015]

ISORROPIA/HETP

The **ISORROPIA/HETP** repository (https://github.com/geoschem/HETerogeneous-vectorized-or-Parallel) contains the source code for HETP, which is an implementation of the ISORROPIA II aerosol thermodynamics scheme written in modern Fortran.

Reference: Miller *et al.* [2024]

geos-chem-shared-docs

The **geos-chem-shared-docs** repository (https://github.com/geoschem/geos-chem-shared-docs) contains common documentation files that are shared by the GEOS-Chem, GCHP, and HEMCO ReadTheDocs pages. This repository is maintained by the GEOS-Chem Support Team.

6.2 Download instructions

Follow these directions to download the GEOS-Chem Classic source code.

6.2.1 Clone GCClassic and fetch submodules

To download the latest stable GEOS-Chem Classic version, type:

```
$ git clone --recurse-submodules https://github.com/geoschem/GCClassic.git
```

This command does the following:

1. Clones the *GCClassic* repo from GitHub to a local folder named `GCClassic`;
2. Clones the *GEOS-Chem "Science Codebase"* repo from GitHub to `GCClassic/src/GEOS-Chem`;
3. Clones the *HEMCO* repo from GitHub to `GCClassic/src/HEMCO`;
4. Clones the *Cloud-J* repo from GitHub to `GCClassic/src/Cloud-J`;
5. Clones the *ISORROPIA/HETP* repo from GitHub to `GCClassic/src/HETP`; and
6. Clones the *geos-chem-shared-docs* from GitHub to `GCClassic/docs/source/geos-chem-shared-docs`.

Tip: To download GEOS-Chem Classic source code into a folder named something other than `GCClassic`, supply the name of the folder at the end of the **`git clone`** command. For example:

```
git clone --recurse-submodules https://github.com/geoschem/GCClassic.git my-code-dir
```

will download the GEOS-Chem Classic source code into `my-code-dir` instead of `GCClassic`.

Once the **`git clone`** process starts, you should see output similar to this:

```
$ git clone https://github.com/geoschem/GCClassic.git
Cloning into 'GCClassic'...
remote: Enumerating objects: 4410, done.
remote: Counting objects: 100% (1309/1309), done.
remote: Compressing objects: 100% (629/629), done.
remote: Total 4410 (delta 714), reused 1257 (delta 676), pack-reused 3101
Receiving objects: 100% (4410/4410), 2.10 MiB | 8.12 MiB/s, done.
Resolving deltas: 100% (2377/2377), done.
Submodule 'geos-chem-shared-docs' (https://github.com/geoschem/geos-chem-shared-docs.
↪git) registered for path 'docs/source/geos-chem-shared-docs'
Submodule 'Cloud-J' (https://github.com/geoschem/Cloud-J.git) registered for path 'src/
↪Cloud-J'
Submodule 'GEOS-Chem' (https://github.com/geoschem/geos-chem.git) registered for path
↪'src/GEOS-Chem'
Submodule 'HEMCO' (https://github.com/geoschem/hemco.git) registered for path 'src/HEMCO'
Submodule 'src/HETerogeneous-vectorized-or-Parallel' (https://github.com/geoschem/
↪HETerogeneous-vectorized-or-Parallel) registered for path 'src/HETP'
Cloning into '/n/holyscratch01/jacob_lab/ryantosca/tests/14.4.0/release/example/docs/
↪source/geos-chem-shared-docs'...
remote: Enumerating objects: 356, done.
remote: Counting objects: 100% (110/110), done.
remote: Compressing objects: 100% (71/71), done.
remote: Total 356 (delta 66), reused 79 (delta 39), pack-reused 246
Receiving objects: 100% (356/356), 524.63 KiB | 8.46 MiB/s, done.
Resolving deltas: 100% (205/205), done.
Cloning into '/n/holyscratch01/jacob_lab/ryantosca/tests/14.4.0/release/example/src/
↪Cloud-J'...
```

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```
remote: Enumerating objects: 488, done.
remote: Counting objects: 100% (149/149), done.
remote: Compressing objects: 100% (56/56), done.
remote: Total 488 (delta 104), reused 102 (delta 93), pack-reused 339
Receiving objects: 100% (488/488), 715.91 KiB | 9.67 MiB/s, done.
Resolving deltas: 100% (241/241), done.
Cloning into '/n/holyscratch01/jacob_lab/ryantosca/tests/14.4.0/release/example/src/GEOS-
↪Chem'...
remote: Enumerating objects: 88738, done.
remote: Counting objects: 100% (8421/8421), done.
remote: Compressing objects: 100% (2309/2309), done.
remote: Total 88738 (delta 6574), reused 7742 (delta 6093), pack-reused 80317
Receiving objects: 100% (88738/88738), 98.58 MiB | 11.35 MiB/s, done.
Resolving deltas: 100% (72704/72704), done.
Cloning into '/n/holyscratch01/jacob_lab/ryantosca/tests/14.4.0/release/example/src/HEMCO
↪'...
remote: Enumerating objects: 4752, done.
remote: Counting objects: 100% (1546/1546), done.
remote: Compressing objects: 100% (423/423), done.
remote: Total 4752 (delta 1177), reused 1426 (delta 1117), pack-reused 3206
Receiving objects: 100% (4752/4752), 2.88 MiB | 21.06 MiB/s, done.
Resolving deltas: 100% (3458/3458), done.
Cloning into '/n/holyscratch01/jacob_lab/ryantosca/tests/14.4.0/release/example/src/HETP
↪'...
remote: Enumerating objects: 97, done.
remote: Counting objects: 100% (97/97), done.
remote: Compressing objects: 100% (69/69), done.
remote: Total 97 (delta 37), reused 68 (delta 21), pack-reused 0
Receiving objects: 100% (97/97), 81.51 KiB | 937.00 KiB/s, done.
Resolving deltas: 100% (37/37), done.
Submodule path 'docs/source/geos-chem-shared-docs': checked out
↪'285d5904561a34d7c7941681a4fed19a68e1201f'
Submodule path 'src/Cloud-J': checked out '3162ea8baa9ab69c3b8473270abc0188ad54501b'
Submodule path 'src/GEOS-Chem': checked out 'c4c4c146ed9cd6bb8af42f080b766a0a0119b4a5'
Submodule path 'src/HEMCO': checked out 'fddcae53f73327e0da7f0a505b4d07a53dd0930b'
Submodule 'geos-chem-shared-docs' (https://github.com/geoschem/geos-chem-shared-docs.
↪git) registered for path 'src/HEMCO/docs/source/geos-chem-shared-docs'
Cloning into '/n/holyscratch01/jacob_lab/ryantosca/tests/14.4.0/release/example/src/
↪HEMCO/docs/source/geos-chem-shared-docs'...
remote: Enumerating objects: 356, done.
remote: Counting objects: 100% (110/110), done.
remote: Compressing objects: 100% (71/71), done.
remote: Total 356 (delta 66), reused 79 (delta 39), pack-reused 246
Receiving objects: 100% (356/356), 524.63 KiB | 8.33 MiB/s, done.
Resolving deltas: 100% (205/205), done.
Submodule path 'src/HEMCO/docs/source/geos-chem-shared-docs': checked out
↪'4bb2b11e35953a8b0a8e1aec9161479bf0fc6bb6'
Submodule path 'src/HETP': checked out '2a99b24625ed26cf87ae88697ddd6cf8bbdec812'
```

When the **`git clone`** process has finished, navigate into the `GCClassic` folder and get a directory listing:

```
$ cd GCClassic
```

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```
$ ls -CF src/*
src/CMakeLists.txt

src/Cloud-J:
AUTHORS.txt   CMakeLists.txt  CONTRIBUTING.md  LICENSE    src/        tables/
CHANGELOG.md  CMakeScripts/   docs/            README.md  SUPPORT.md  tools/

src/GEOS-Chem:
APM/          CMakeLists.txt  GeosRad/   Headers/     KPP/         ObsPack/   run/
AUTHORS.txt   CMakeScripts/   GeosUtil/  History/     LICENSE.txt  PKUCPL/    test/
CHANGELOG.md  GeosCore/       GTMM/      Interfaces/  NcdfUtil/    README.md

src/HEMCO:
AUTHORS.txt   CMakeLists.txt  CONTRIBUTING.md  LICENSE.txt  run/    src/
CHANGELOG.md  CMakeScripts/   docs/            README.md    spack@  SUPPORT.md

src/HETP:
CHANGELOG.md  CMakeLists.txt  CMakeScripts/  LICENSE  README.md  src/
```

This confirms that the `GCClassic/src/GEOS-Chem` and `GCClassic/src/HEMCO` folders have been populated with source code from the GitHub repositories listed above.

Tip: To use an older GEOS-Chem Classic version (e.g. 14.0.0), follow these additional steps:

```
$ git checkout tags/14.0.0                  # Points HEAD to the tag "14.0.0"
$ git branch version_14.0.0                 # Creates a new branch at tag "14.0.0"
$ git checkout version_14.0.0               # Checks out the version_14.0.0 branch
$ git submodule update --init --recursive   # Reverts submodules to the "14.0.0" tag
```

You can do this for any tag in the version history. For a list of all tags, type:

```
$ git tag
```

If you have any unsaved changes, make sure you commit those to a branch prior to updating versions.

6.2.2 Create a branch in src/GEOS-Chem for your work

Whter the **`git clone`** command *described above* finishes, the *GEOS-Chem Science Codebase* submodule code (in folder `GCClassic/src/GEOS-Chem`) and the *HEMCO* submodule code (in folder `GCClassic/src/HEMCO`) will be in **detached HEAD state**. In other words, the code is checked out but a branch is not created. Adding new code to a detached HEAD state is very dangerous and should be avoided. You should instead make a branch it the same point as the detached HEAD, and then add your own modifications into that branch.

Navigate from `GCClassic` to `GCClassic/src/GEOS-Chem`:

```
$ cd src/GEOS-Chem
```

and then type:

```
$ git branch
```

You will see output similar to this:

```
*(HEAD detached at xxxxxxxx)
main
```

where `xxxxxxxx` denotes the hash of the commit at which the code has been checked out.

At ths point, you may now create a branch in which to store your own modifications to the GEOS-Chem science codebase. Type:

```
$ git branch feature/my-git-updates
$ git checkout feature/my-git-updates
```

Instead of `feature/my-git-updates`, you may choose a name that reflects the nature of your updates (e.g. `feature/new_reactions`, etc.).

Note: This naming convention adheres to the Github Flow conventions (i.e. new feature branches start with `feature/`, bug fix branches start with `bugfix/`, etc.

If you now type:

```
$ git branch
```

You will see that we are checked out onto the branch that you just created and are no longer in detached HEAD state.

```
* feature/my-git-updates
main
```

At this point, you may proceed to add your modifications into the GEOS-Chem Science Codebase.

Note: If you need to also modify *HEMCO* source code, repeat the process above to create your own working branch in `GCClassic/src/HEMCO`.

6.2.3 See additional resources

For more information about downloading the GEOS-Chem source code, please see the following Youtube video tutorials:

- Getting started with GEOS-Chem 13 (by Melissa Sulprizio)
- Managing branches between superproject and submodules (by Bob Yantosca)

CHAPTER

SEVEN

CREATE A RUN DIRECTORY

Please see the following sections for more information on how to create run directories for GEOS-Chem Classic simulations:

7.1 First-time user registration

We have introduced a online user registration system starting with GEOS-Chem Classic 14.0.0. The first time that you create a run directory, you will be prompted to provide contact information and a summary about how you plan to use GEOS-Chem. This information will be kept at a secure cloud-based server.

Even if you are a long-time GEOS-Chem user, we ask that you answer all of the questions. Your responses will help us to keep an accurate count of GEOS-Chem users and to keep the list of GEOS-Chem users current.

The user registration dialog (and where you will type in your repsonses) is shown below.

```
============================================================
GEOS-CHEM RUN DIRECTORY CREATION
============================================================

Initiating User Registration:
You will only need to fill this information out once.
Please respond to all questions.

------------------------------------------------------------
What is your name?
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
What is your email address?
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
What is the name of your research institution?
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
What is the name of your principal invesigator?
(Enter 'self' if you are the principal investigator.)
```

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```
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
Please provide the web site for your institution
(group website, company website, etc.)?
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
Please provide your github username (if any) so that we
can recognize you in submitted issues and pull requests.
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
Where do you plan to run GEOS-Chem?
(e.g. local compute cluster, AWS, other supercomputer)?
------------------------------------------------------------
>>> type your response and hit ENTER

------------------------------------------------------------
Please briefly describe how you plan on using GEOS-Chem
so that we can add you to 'GEOS-Chem People and Projects'
(https://geoschem.github.io/geos-chem-people-projects-map/)
------------------------------------------------------------
>>> type your response and hit ENTER
Successful Registration
```

If you do not see the `Successful Registration` message, check your internet connection and try again. If the problem persists, open a new Github issue.

7.2 Example: Create a full-chemistry simulation run directory

Let us walk through the process of creating a run directory for a global GEOS-Chem full-chemistry simulation.

1. Navigate to the GCClassic superproject folder and get a directory listing:

   ```
   $ cd /path/to/your/GCClassic
   $ ls -CF
   AUTHORS.txt     CMakeScripts/    LICENSE.txt  SUPPORT.md  run@  test@
   CMakeLists.txt  CONTRIBUTING.md  README.md    docs/       src/
   ```

   As mentioned previously, `run@` is a symbolic link. It actually points to the to the `src/GEOS-Chem/run/GCClassic` folder. This folder contains several scripts and template files for run directory creation.

2. Navigate to the run folder and get a directory listing:

   ```
   $ cd run
   $ ls -CF
   archiveRun.sh*                gitignore                   init_rd.sh*
   createRunDir.sh*              HEMCO_Config.rc.templates/  README.md
   ```

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```
geoschem_config.yml.templates/  HEMCO_Diagn.rc.templates/   runScriptSamples/
getRunInfo*                     HISTORY.rc.templates/       setupForRestarts.sh*
```

You can see several folders (highlighted in the directory display with /) and a few executable scripts (highlighted with *). The script we are interested in is `createRunDir.sh`.

3. Run the `createRunDir.sh` script. Type:

```
$ ./createRunDir.sh
```

4. You will then be prompted to supply information about the run directory that you wish to create:

```
=============================================================
GEOS-CHEM RUN DIRECTORY CREATION
=============================================================


-------------------------------------------------------------
Choose simulation type:
-------------------------------------------------------------
   1. Full chemistry
   2. Aerosols only
   3. Carbon
   4. Hg
   5. POPs
   6. Tagged O3
   7. Trace metals
   8. TransportTracers
   9. CH4
  10. CO2
  11. Tagged CO
>>>
```

To create a run directory for the full-chemistry simulation, type **1** followed by the **ENTER** key.

Tip: To exit, the run directory creation process, type `Ctrl-C` at any prompt.

5. You will then be asked to specify any additional options for the full-chemistry simulation (such as adding the RRTMG radiative transfer model, APM or TOMAS microphysics, etc.)

```
-------------------------------------------------------------
Choose additional simulation option:
-------------------------------------------------------------
  1. Standard
  2. Benchmark
  3. Complex SOA
  4. Marine POA
  5. Acid uptake on dust
  6. TOMAS
  7. APM
```

(continues on next page)

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```
  8. RRTMG
>>>
```

For the standard full-chemistry simulation, type **1** followed by **ENTER**.

To add an option to the full-chemistry simulation, type a number between **2** and **8** and press **ENTER**.

6. You will then be asked to specify the meteorology type for the simulation (GEOS-FP, MERRA-2), or GCAP 2.0).

> **Attention:** We are still evaluating GEOS-Chem with the new NASA GEOS-IT meterorology product. Please select one of the other meteorology options for the time being.

```
------------------------------------------------------------
Choose meteorology source:
------------------------------------------------------------
  1. MERRA-2 (Recommended)
  2. GEOS-FP
  3. GEOS-IT (Beta release)
  4. GISS ModelE2.1 (GCAP 2.0)
>>>
```

You should use the recommended option (MERRA-2) if possible. Type **1** followed by **ENTER**.

Important: The convection scheme used for GEOS-FP met generation changed from RAS to Grell-Freitas with impact on GEOS-FP meteorology files starting June 1, 2020. For this reason we recommend using MERRA-2 instead of GEOS-FP if running a simulation across June 1, 2020 to avoid unexpected discontinuities. Additional information about the impact of the convection change is at geoschem/geos-chem#1409.

---

7. The next menu will prompt you for the horizontal resolution that you wish to use:

```
------------------------------------------------------------
Choose horizontal resolution:
------------------------------------------------------------
  1. 4.0  x 5.0
  2. 2.0  x 2.5
  3. 0.5  x 0.625
>>>
```

If you wish to set up a global simulation, type either **1** or **2** followed by **ENTER**.

If you wish to set up a nested-grid simulation, type **3** and hit **ENTER**. Then you will be followed by a nested-grid menu:

```
------------------------------------------------------------
Choose horizontal grid domain:
------------------------------------------------------------
  1. Global
  2. Asia
  3. Europe
  4. North America
```

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```
  5. Custom
>>>
```

Select your preferred horizontal domain, followed by **ENTER**.

8. You will then be prompted for the vertical dimension of the grid.

```
------------------------------------------------------------
Choose number of levels:
------------------------------------------------------------
  1. 72 (native)
  2. 47 (reduced)
>>>
```

For most simulations, you will want to use **72** levels. Type **1** followed by **ENTER**.

For some memory-intensive simulations (such as nested-grid simulations), you can use 47 levels. Type **2** followed by **ENTER**.

9. You will then be prompted for the folder in which you wish to create the run directory.

```
------------------------------------------------------------
Enter path where the run directory will be created:
------------------------------------------------------------
>>>
```

You may enter an absolute path (e.g. `$HOME/myusername/my-run-dirs` followed by **ENTER)**.

You may also enter a relative path (e.g `~/my-run-dirs` followed by **ENTER**). In this case you will see that the `./createRunDir.sh` script will expand the path to an absolute path.

10. The next menu will prompt you for the run directory name.

```
------------------------------------------------------------
Enter run directory name, or press return to use default:

NOTE: This will be a subfolder of the path you entered above.
------------------------------------------------------------
>>>
```

You should use the default run directory name whenever possible. Type **ENTER** to select the default. You will then see output similar to this:

```
-- Using default directory name gc_4x5_merra2_fullchem
```

or if you are creating a nested grid simulation:

```
-- Using default directory name gc_05x0625_merra2_fullchem
```

and then:

```
-- See rundir_vars.txt for summary of default run directory settings
-- This run directory has been set up to start on 20190701
-- A restart file for this date has been copied to the Restarts subdirectory
-- You may add more restart files using format GEOSChem.Restart.YYYYMMDD_HHmmz.nc4
-- Change simulation start and end dates in configuration file geoschem_config.yml
```

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```
-- Default frequency and duration of diagnostics are set to monthly
-- Modify diagnostic settings in HISTORY.rc and HEMCO_Config.rc
```

11. The next menu will prompt you with:

    ```
    ------------------------------------------------------------
    Do you want to track run directory changes with git? (y/n)
    ------------------------------------------------------------
    ```

    Type **y** and then **ENTER**. Then you will be able to track changes that you make to GEOS-Chem configuration files with Git. This can be a lifesaver when debugging—you can revert to an earlier state and then start fresh.

    You will then see this output:

    ```
    Initialized empty Git repository in /path/to/gc_4x5_merra2_fullchem/.git/
    ```

12. The next (and final) menu will ask you:

    ```
    ------------------------------------------------------------
    Do you want to build the KPP-Standalone Box Model? (y/n)
    ------------------------------------------------------------
    >>>
    ```

    Type **y** and then **ENTER** you wish to build the **KPP-Standalone Box Model**, or **n** then **ENTER** to skip this step. If you choose to build KPP-Standalone, you will be given this reminder:

    ```
    >>>> REMINDER: You must compile with options: -DKPPSA=y <<<<
    ```

    Please see the Supplemental Guide entitled *Use the KPP-Standalone box model to test chemical mechanisms* for further usage instructions.

    Lastly, you will see a message to indicate that run directory creation has completed successfully.

    ```
    Created /path/to/gc_4x5_merra2_fullchem
    ```

    You may now navigate to this directory and start editing the *GEOS-Chem configuration files*.

7.3 Example: Create a carbon gases simulation run directory

The process of creating run directories for the GEOS-Chem specialty simulations is similar to that of the *previous example*. But the number of menus that you need to select from will likely be fewer than for the full-chemistry simulation. We'll use the carbon gases simulation as an example.

1. Navigate to the `GCClassic` superproject folder and get a directory listing:

    ```
    $ cd /path/to/your/GCClassic
    $ ls -CF
    AUTHORS.txt   CMakeLists.txt  CONTRIBUTING.md  LICENSE.txt  run@    src/       ␣
    ↪test@
    CHANGELOG.md  CMakeScripts/   docs/            README.md    spack@  SUPPORT.md
    ```

As mentioned previously, `run@` is a symbolic link. It actually points to the to the `src/GEOS-Chem/run/GCClassic` folder. This folder contains several scripts and template files for run directory creation.

2. Navigate to the run folder and get a directory listing:

```
$ cd run
$ ls -CF
archiveRun.sh*                  gitignore                   init_rd.sh*
createRunDir.sh*                HEMCO_Config.rc.templates/  README.md
geoschem_config.yml.templates/  HEMCO_Diagn.rc.templates/   runScriptSamples/
getRunInfo*                     HISTORY.rc.templates/       setupForRestarts.sh*
```

You can see several folders (highlighted in the directory display with `/`) and a few executable scripts (highlighted with `*`). The script we are interested in is `createRunDir.sh`.

3. Run the **`createRunDir.sh`** script.. Type:

```
$ ./createRunDir.sh
```

4. You will then be prompted to supply information about the run directory that you wish to create:

```
=============================================================
GEOS-CHEM RUN DIRECTORY CREATION
=============================================================

-------------------------------------------------------------
Choose simulation type:
-------------------------------------------------------------
   1. Full chemistry
   2. Aerosols only
   3. Carbon
   4. Hg
   5. POPs
   6. Tagged O3
   7. Trace metals
   8. TransportTracers
   9. CH4
  10. CO2
  11. Tagged CO
>>>
```

To select the GEOS-Chem carbon gases specialty simulation, type **`3`** followed by **`ENTER`**.

Tip: To exit, the run directory creation process, type `Ctrl-C` at any prompt.

---

5. You will be asked if you wish to set up a carbon simulation with all species (CH4, CO, CO2, OCS), or with just one of these species:

```
-------------------------------------------------------------
Do you wish to use a single advected species?
-------------------------------------------------------------
```

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```
  1. Use all species
  2. Use CH4 only
  3. Use CO2 only
  4. Use CO only
  5. Use OCS only
>>>
```

Let's pick the carbon simulation with all species. Type **1** followed by **ENTER**.

6. You will then be asked to specify the meteorology type for the simulation (GEOS-FP, MERRA-2), or GCAP 2.0):

> **Attention:** We are still evaluating GEOS-Chem with the new NASA GEOS-IT meterorology product. Please select one of the other meteorology options for the time being.

```
------------------------------------------------------------
Choose meteorology source:
------------------------------------------------------------
  1. MERRA-2 (Recommended)
  2. GEOS-FP
  3. GEOS-IT (Beta release)
  4. GISS ModelE2.1 (GCAP 2.0)
>>>
```

To accept the recommended meteorology (MERRA-2), type **1** followed by **ENTER**.

Important: The convection scheme used for GEOS-FP met generation changed from RAS to Grell-Freitas with impact on GEOS-FP meteorology files starting June 1, 2020. For this reason we recommend using MERRA-2 instead of GEOS-FP if running a simulation across June 1, 2020 to avoid unexpected discontinuities. Additional information about the impact of the convection change is at geoschem/geos-chem#1409.

---

7. The next menu will prompt you for the horizontal resolution that you wish to use:

```
------------------------------------------------------------
Choose horizontal resolution:
------------------------------------------------------------
  1. 4.0  x 5.0
  2. 2.0  x 2.5
  3. 0.5  x 0.625
>>>
```

If you wish to set up a global simulation, type either **1** or **2** followed by **ENTER**.

If you wish to set up a nested-grid simulation, type **3** and hit **ENTER**. Then you will be followed by a nested-grid menu:

```
------------------------------------------------------------
Choose horizontal grid domain:
------------------------------------------------------------
  1. Global
  2. Asia
```

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```
  3. Europe
  4. North America
  5. Custom
>>>
```

Type the number of your preferred option and then hit **ENTER**.

8. You will then be prompted for the vertical dimension of the grid.

```
------------------------------------------------------------
Choose number of levels:
------------------------------------------------------------
  1. 72 (native)
  2. 47 (reduced)
>>>
```

For most simulations, you will want to use 72 levels. Type **1** followed by **ENTER**.

For some memory-intensive simulations (such as nested-grid simulations), you can use 47 levels. Type **2** followed by **ENTER**.

9. You will then be prompted for the folder in which you wish to create the run directory.

```
------------------------------------------------------------
Enter path where the run directory will be created:
------------------------------------------------------------
>>>
```

You may enter an absolute path (e.g. `$HOME/myusername/my-run-directories`) followed by **ENTER**.

You may also enter a relative path (e.g. `~/my-run-directories`) followed by **ENTER**). In this case you will see that the `./createRunDir.sh` script will expand the path to an absolute path.

10. The next menu will prompt you for the run directory name.

```
------------------------------------------------------------
Enter run directory name, or press return to use default:

NOTE: This will be a subfolder of the path you entered above.
------------------------------------------------------------
>>>
```

You should use the default run directory name whenever possible. Type **ENTER**. The script will display the following output:

```
-- Using default directory name gc_4x5_merra2_carbon
```

or if you are creating a nested grid simulation:

```
-- Using default directory name gc_05x0625_merra2_carbon
```

and then

```
-- See rundir_vars.txt for summary of default run directory settings
-- This run directory has been set up to start on 20190101
-- A restart file for this date has been copied to the Restarts subdirectory
```

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```
-- You may add more restart files using format GEOSChem.Restart.YYYYMMDD_HHmmz.nc4
-- Change simulation start and end dates in configuration file geoschem_config.yml
-- Default frequency and duration of diagnostics are set to monthly
-- Modify diagnostic settings in HISTORY.rc and HEMCO_Config.rc
```

11. The last menu will prompt you with:

    ```
    ------------------------------------------------------------
    Do you want to track run directory changes with git? (y/n)
    ------------------------------------------------------------
    >>>
    ```

    Type **y** and then **ENTER**. Then you will be able to track changes that you make to GEOS-Chem configuration files with Git. This can be a lifesaver when debugging—you can revert to an earlier state and then start fresh.

    You will then see output similar to this:

    ```
    Initialized empty Git repository in /path/to/gc_4x5_merra2_carbon/.git/

    Created /path/to/gc_4x5_merra2_carbon

    >>>> REMINDER: You must compile with options: -DMECH=carbon <<<<
    ```

    You can navigate to this directory and then start editing the *GEOS-Chem configuration files*.

    Because the carbon simulation requires special compilation instructions, a reminder will be displayed with the proper command to use during the configuration step.

The procedure to set up run directories for other GEOS-Chem Classic simulations is similar to that shown above.

7.4 Run directory files and folders

Each GEOS-Chem Classic run directory that you create will contain the files and folders listed below. The *GEOS-Chem and HEMCO configuration files* in the run directory will be appropriate to the type of simulation that you have selected.

archiveRun.sh

This script can be used to create an archive of the run directory. Run this script with:

```
$ ./archiveRun.sh directory-name
```

Where `directory-name` is the name of the archive folder. This can be either a relative path or an absolute path.

build/

This is a blank directory where you can direct **CMake** to *configure and build* the GEOS-Chem source code.

build_info/

This folder is created when you *compile GEOS-Chem*. It contains information about the options that were passed to **CMake** during the configuration and build process.

cleanRunDir.sh

Typing

```
$ ./cleanRunDir.sh
```

will remove log files and diagnostic output files left over from a previous GEOS-Chem simulation.

CodeDir

Symbolic link to the top-level source code folder (i.e. the `GCClassic` superproject folder).

CreateRunDirLogs/rundir_vars.txt

Log file containing environment variable settings used in run directory creation. Running the `init_rd.sh` script on this file will create a duplicate run directory.

download_data.py

Use this Python script to download data from one of the GEOS-Chem data portals to your disk space. See our *Download data with a dry-run simulation* chapter for more information.

download_data.yml

Configuration file for `download_data.py`.

geoschem_config.yml

The main GEOS-Chem configuration file (see *Configure your simulation*).

getRunInfo

This file is now deprecated and will be removed in a future version.

HEMCO_Config.rc

The main HEMCO configuration file (see *Configure your simulation*).

HEMCO_Config.rc.gmao_metfields

HEMCO configuration file snippet containing entries for reading the GMAO meteorological fields. This file will only be present if you are using GEOS-FP or MERRA-2 meteorology to drive your GEOS-Chem simulation.

HEMCO_Config.rc.gcap2_metfields

HEMCO configuration file snippet containing entries for reading the GCAP2 meteorological fields. This file will only be present if you are using GCAP2 meteorology to drive your GEOS-Chem simulation.

HEMCO_Diagn.rc

Configuration file for HEMCO diagnostics (see *Configure your simulation*).

HISTORY.rc

Configuration file for GEOS-Chem History diagnostics (see *Configure your simulation*).

metrics.py

This Python script can be used to print the OH metrics for a full-chemistry simulation. Typing:

```
$ ./metrics.py
```

will generate output such as:

```
================================================================================
GEOS-Chem FULL-CHEMISTRY SIMULATION METRICS

Simulation start : 2019-07-01 00:00:00z
Simulation end   : 2019-07-01 01:00:00z
================================================================================

Mass-weighted mean OH concentration    = 10.04682154969 x 10^5 molec cm-3
```

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```
CH3CCl3 lifetime w/r/t tropospheric OH = 6.3189 years

CH4 lifetime w/r/t tropospheric OH     = 10.6590 years
```

OutputDir/

Blank directory where GEOS-Chem diagnostic output files will be created.

README.md

README file (in Markdown format) with containing links to information about GEOS-Chem.

Restarts/

Directory where GEOS-Chem *restart files* will be created.

Restarts/GEOSChem.Restart.YYYYMMDD_hhmmzz.nc4

Restart file containing initial conditions for the GEOS-Chem simulation.

> **Attention:** The restart file that is created when you generate a run directory should not be used to start a production simulation. We recommend that you "spin up" your simulation for at least 6 months to a year in order to remove the signature of the initial conditions.

runScriptSamples

Symbolic link to the folder in the GEOS-Chem "Science Codebase"" repository that contains sample scripts for running GEOS-Chem.

species_database.yml

YAML file containing metadata (e.g. molecular weight, Henry's law constants, wetdep and drydep parameters, etc.) for each species used in the various GEOS-Chem simulations. You should not have to edit this file unless you are adding new species to your GEOS-Chem simulation. The *species_database.yml* file will be discussed in more detail in a following section.

CHAPTER

EIGHT

COMPILE THE SOURCE CODE

In this chapter, we will describe how you can compile GEOS-Chem Classic. Compiling creates an **executable file** that you can run on your computer system.

The compilation process involves the following steps:

8.1 Configure with CMake

You should think of CMake as an interactive tool for configuring GEOS-Chem Classic's build. For example, compile-time options like disabling multithreading and turning on components (e.g. APM, RRTMG) are all configured with CMake commands.

Besides configuring GEOS-Chem's build, CMake also performs checks on your build environment to detect problems that would cause the build to fail. If it identifies a problem, like a missing dependency or mismatched run directory and source code version numbers, CMake will print an error message that describes the problem.

If you are new to CMake and would like a rundown of how to use the **`cmake`** command, check out Liam Bindle's Cmake Tutorial. This tutorial is not necessary, but it will make you more familiar with using CMake and help you better understand what is going on.

Below are the steps for building GEOS-Chem with CMake.

8.1.1 Navigate to your run directory

In this example, we will compile the GEOS-Chem code for the full-chemistry simulation. Navigate to your run directory and get a directory listing as shown below:

```
$ cd /path/to/gc_4x5_merra2_fullchem
$ ls
archiveRun.sh*     download_data.py*    HEMCO_Config.rc.gmao_metfields  README.md
build/             download_data.yml    HEMCO_Diagn.rc                  Restarts/
cleanRunDir.sh*    geoschem_config.yml  HISTORY.rc                      runScriptSamples@
CodeDir@           getRunInfo*          metrics.py*                     species_database.
↪yml
CreateRunDirLogs/  HEMCO_Config.rc      OutputDir/
```

Note that each GEOS-Chem run directory that you generate has a folder named `build/`. This is where we will run CMake.

8.1.2 Navigate to the build directory

The build directory is where CMake and your compilers are going to put the files they generate. For this example, we will use the `build/` folder that was automatically generated in the GEOS-Chem Classic run directory. For GCHP you will need to create one.

```
$ cd build
```

Tip: If you find yourself switching between different compilers, you can create multiple build directories with different names (e.g. `build_gfortran10`, `build_ifort19`, etc).

8.1.3 Initialize the build directory

Next, we need to initialize the build directory. Type:

```
$ cmake ../CodeDir -DRUNDIR=..
```

where `../CodeDir` is the symbolic link from our run directory to the GEOS-Chem source code directory. CMake will generate output similar to this:

```
=================================================================
GCClassic X.Y.Z (superproject wrapper)
Current status: X.Y.Z
=================================================================
-- Found NetCDF: /path/to/netcdf-fortran/lib/libnetcdff.so
-- Useful CMake variables:
  + CMAKE_PREFIX_PATH:    /path/to/netcdf-c/
  ...             /path/to/netcdf-fortran/
  + CMAKE_BUILD_TYPE:     Release
-- Run directory setup:
  + RUNDIR:       /path/to/run/directory
-- Threading:
  * OMP:          *ON*  OFF
-- Found OpenMP_Fortran: -fopenmp (found version "4.5")
-- Found OpenMP: TRUE (found version "4.5")
-- General settings:
  * MECH:         **fullchem**  carbon  Hg  custom
  * USE_REAL8:    *ON*  OFF
  * SANITIZE:      ON  *OFF*
-- Components:
  * TOMAS:         ON  *OFF*
  * TOMAS_BINS:   *NA*  15  40
  * APM:           ON  *OFF*
  * RRTMG:         ON  *OFF*
  * GTMM:          ON  *OFF*
  * HCOSA:         ON  *OFF*
  * LUO_WETDEP:    ON  *OFF*
  * FASTJX:        ON  *OFF*
=================================================================
HEMCO A.B.C
Current status: A.B.C
```

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```
=================================================================
=================================================================
HETP D.E.F
=================================================================
=================================================================
Cloud-J G
Current status: G
=================================================================
=================================================================
GEOS-Chem X.Y.Z (science codebase)
Current status: X.Y.Z
=================================================================
Creating /path/to/run/directory/CodeDir/src/GEOS-Chem/Interfaces/GCClassic/gc_classic_
↪version.H
-- Configuring done
-- Generating done
-- Build files have been written to: /path/to/run/directory
```

Your CMake command's output contains important information about your build's configuration.

Note: The text `X.Y.Z`, `A.B.C`, `D.E.F.`, and `G` refer to the version numbers (in semantic versioning style) of the *GCClassic*, *HEMCO*, *ISORROPIA/HETP*, and *Cloud-J* repositories, respectively.

The *GEOS-Chem "Science Codebase"* and GCClassic repositories share the same version number `X.Y.Z`.

8.1.4 Configure your build with extra options

Your build directory is now configured to compile GEOS-Chem using all default options. If you do not wish to change anything further, you may *skip ahead to the next section*.

However, if you wish to modify your build's configuration, simply invoke CMake once more with optional parameters. Use this format:

```
$ cmake . -DOPTION=value
```

Note that the `.` argument is necessary. It tells CMake that your current working directory (i.e. `.`) is your build directory. The output of **`cmake`** tells you about your build's configuration. Options are prefixed by a + or * in the output, and their values are displayed or highlighted.

Tip: If you are colorblind or if you are using a terminal that does not support colors, refer to the CMake FAQ for instructions on disabling colorized output. For a detailed explanation of CMake output, see the next section.

The table below contains the list of GEOS-Chem build options that you can pass to CMake. GEOS-Chem will be compiled with the default build options, unless you explicitly specify otherwise.

`RUNDIR`

Defines the path to the run directory.

In this example, our build directory is a subfolder of the run directory, so we can use `-DRUNDIR=..`. If your build directory is somewhere else, then specify the path to the run directory as an absolute path.

CMAKE_BUILD_TYPE

Specifies the type of build. Accepted values are:

Release

Tells CMake to configure GEOS-Chem in **Release** mode. This means that all optimizations will be applied and all debugging options will be disabled. **(Default option)**.

Debug

Turns on several runtime error checks. This will make it easier to find errors but will adversely impact performance. Only use this option if you are actively debugging.

MECH

Specifies the chemical mechanism that you wish to use:

fullchem

Activates the **fullchem** mechanism. The source code files that define this mechanism are stored in `KPP/fullchem`. **(Default option)**

Hg

Activates the **Hg** mechanism. The source code files that define this mechanism are stored in `KPP/Hg`.

carbon

Activates the **carbon** mechanism (CH4-CO-CO2-OCS). The source code files that define this mechanism are stored in `KPP/carbon`.

custom

Activates a **custom** mechanism defined by the user. The source code files that define this mechanism are stored in `KPP/custom`.

OMP

Determines if GEOS-Chem Classic will activate OpenMP parallelization. Accepted values are:

y

Activates OpenMP parallelization. **(Default option)**

GEOS-Chem Classic will execute on as many computational cores as is specified with *OMP_NUM_THREADS*.

n

Deactivates OpenMP parallelization. GEOS-Chem Classic will execute on a single computational core. Useful for debugging.

TOMAS

Configure GEOS-Chem with the TOMAS aerosol microphysics package. Accepted values are:

y

Activate TOMAS microphysics.

n

Deactivate TOMAS microphysics **(Default option)**

TOMAS_BINS

Specifies the number of size-resolved bins for TOMAS. Accepted values are:

15

Use 15 size-resolved bins with TOMAS simulations.

40

Use 40 size-resolved bins with TOMAS simulations.

APM

Configures GEOS-Chem to use the APM microphysics package. Accepted values are:

y

Activate APM microphysics.

n

Deactivate APM microphysics. **(Default option)**

RRTMG

Configures GEOS-Chem to use the RRTMG radiative transfer model. Accepted values are:

y

Activates the RRTMG radiative transfer model.

n

Deactivates the RRTMG radiative transfer model. **(Default option)**

HCOSA

Compiles the HEMCO standalone executable.

LUO_WETDEP

Configures GEOS-Chem to use the Luo et al., 2020 wet deposition scheme.

Note: The Luo et al 2020 wet deposition scheme will eventually become the default wet deposition schem in GEOS-Chem. We have made it an option for the time being while further evaluation is being done.

Accepted values are:

y

Activates the Luo et al., 2020 wet deposition scheme.

n

Deactivates the Luo et al., 2020 wet deposition scheme. **(Default option)**

FASTJX

Configures GEOS-Chem to use the legacy FAST-JX v7.0 photolysis mechanism instead of its successor *Cloud-J*.

Note: We recommend using FAST-JX for the mercury simulation instead of Cloud-J. Further work is needed to make the mercury simulation compatible with Cloud-J. Once that work is completed the legacy FAST-JX option will be deleted from the model.

Accepted values are:

y

Uses the legacy FAST-JX v7.0 photolysis scheme rather than Cloud-J.

n

Uses the Cloud-J photolyis scheme rather than legacy FAST-JX. **(Default option)**

SANITIZE

Activates the AddressSanitizer/LeakSanitizer functionality in GNU Fortran to identify memory leaks. Accepted values are:

y

Activates AddressSanitizer/LeakSanitizer

n

Deactivates AddressSanitizer/LeakSanitizer **(Default option)**.

If you plan to use the **`make -j install`** option (recommended) to copy your executable to your run directory, you must reconfigure CMake with the **`RUNDIR=/path/to/run/dir`** option. Multiple run directories can be specified by a semicolon separated list. A warning is issues if one of these directories does not look like a run directory. These paths can be relative paths or absolute paths. Relative paths are interpreted as relative to your build directory. For example:

```
$ cmake . -DRUNDIR=/path/to/run/dir
```

For example if you wanted to build GEOS-Chem with all debugging flags on, you would type:

```
$ cmake . -DCMAKE_BUILD_TYPE=Debug
```

or if you wanted to turn off OpenMP parallelization (so that GEOS-Chem executes only on one computational core), you would type:

```
$ cmake . -DOMP=n
```

etc.

8.1.5 Understand CMake output

As you can see from the example CMake output listed above, GEOS-Chem Classic contains code from the various repositories:

1. GCClassic wrapper (aka "the superproject"):

   ```
   ================================================================
   GCClassic X.Y.Z (superproject wrapper)
   Current status: X.Y.Z
   ================================================================
   ```

   where `X.Y.Z` specifies the GEOS-Chem Classic "major", "minor", and "patch" version numbers.

   Note: If you are cloning GEOS-Chem Classic between official releases, you may the see `Current status` reported like this:

   ```
   X.Y.Z-alpha.n-C-gabcd1234.dirty  or

   X.Y.Z.rc.n-C.gabcd1234.dirty
   ```

   We will explain these formats below.

   ---

2. HEMCO (Harmonized Emissions Component) submodule:

   ```
   ================================================================
   HEMCO A.B.C
   Current status: A.B.C
   ================================================================
   ```

where `A.B.C` specifies the HEMCO "major", "minor", and "patch" version numbers. The HEMCO version number differs from GEOS-Chem because it is kept in a separate repository, and is considered a separate package.

3. GEOS-Chem submodule:

```
==================================================================
GEOS-Chem X.Y.Z (science codebase)
Current status: X.Y.Z
==================================================================
```

The GEOS-Chem science codebase and GEOS-Chem Classic wrapper will always share the same version number.

During the build configuration stage, CMake will display the **version number** (e.g. `X.Y.Z`) as well as the **current status of the Git repository** (e.g. `TAG-C-gabcd1234.dirty`) for GCClassic, GEOS-Chem, and HEMCO.

4. Similar messages will be displayed for the *Cloud-J* and *ISORROPIA/HETP* repositories.

Let's take the Git repository status of GCClassic as our example. The status string uses the same format as the **`git describe --tags`** command, namely:

```
TAG-C-gabcd1234.dirty
```

where

`TAG`

Indicates the most recent tag in the GCClassic superproject repository.

Tags may use the following notations:

- `X.Y.Z`: Denotes an official release
- `X.Y.Z-rc.n`: Denotes a release candidate
- `X.Y.Z-alpha.n`: Denotes an internal "alpha" benchmark

where `n` is the number of the release candidate or alpha benchmark (starting from 0).

`C`

Indicates the number of commits that were made on top of the commit that is referred to by *`TAG`*.

`g`

Indicates that the version control system is Git.

`abcd1234`

Indicates the Git commit hash. This is an alphanumeric string that denotes the commit at the `HEAD` of the GCClassic repository.

`.dirty`

If present, indicates that there are uncommitted updates atop the *`abcd1234`* commit in the GCClassic repository.

Under each header are printed the various *options that have been selected*.

8.2 Compile with Make

Now that CMake has created the Makefiles that are needed to compile GEOS-Chem, you may proceed as follows:

8.2.1 Build the GEOS-Chem Classic executable

Use the **make** command to build the GEOS-Chem executable. Type:

```
$ make -j
[  1%] Built target KPP_FirstPass
[  1%] Building Fortran object src/Cloud-J/src/Core/CMakeFiles/CloudJ_Core.dir/cldj_fjx_
↪sub_mod.F90.o
[  1%] Building Fortran object src/Cloud-J/src/Core/CMakeFiles/CloudJ_Core.dir/cldj_init_
↪mod.F90.o
[  1%] Building Fortran object src/Cloud-J/src/Core/CMakeFiles/CloudJ_Core.dir/cldj_osa_
↪sub_mod.F90.o
[  3%] Building Fortran object src/Cloud-J/src/Core/CMakeFiles/CloudJ_Core.dir/cldj_sub_
↪mod.F90.o
[  4%] Linking Fortran static library libCloudJ_Core.a
[  4%] Built target CloudJ_Core
[  6%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/charpak_mod.
↪F90.o
[  6%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/errcode_mod.
↪F90.o
[  7%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/precision_
↪mod.F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/input_opt_
↪mod.F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/state_grid_
↪mod.F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/CMN_FJX_MOD.
↪F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/CMN_SIZE_mod.
↪F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/aermass_
↪container_mod.F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/inquireMod.
↪F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/qfyaml_mod.
↪F90.o
[  9%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/diaglist_mod.
↪F90.o

... etc ...

[ 93%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/sulfate_
↪mod.F90.o
[ 93%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/fullchem_
↪mod.F90.o
[ 93%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/mixing_mod.
↪F90.o
[ 93%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/carbon_mod.
```

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```
↪F90.o
[ 95%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/chemistry_
↪mod.F90.o
[ 95%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/gc_
↪environment_mod.F90.o
[ 96%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/emissions_
↪mod.F90.o
[ 96%] Building Fortran object src/GEOS-Chem/GeosCore/CMakeFiles/GeosCore.dir/cleanup.
↪F90.o
[ 98%] Linking Fortran static library libGeosCore.a
[ 98%] Built target GeosCore
Scanning dependencies of target gcclassic
[ 98%] Building Fortran object src/CMakeFiles/gcclassic.dir/GEOS-Chem/Interfaces/
↪GCClassic/main.F90.o
[100%] Linking Fortran executable ../bin/gcclassic
[100%] Built target gcclassic
```

Tip: The `-j` argument tells **`make`** that it can execute as many jobs as it wants simultaneously. For example, if you have 8 cores, then the build process may attempt to compile 8 files at a time.

If you want to restrict the number of simultaneous jobs (e.g. you are compiling on a machine with limited memory), you can can use e.g. **`make -j4`**, which should only try to compile 4 files at a time.

8.2.2 Install the executable in your run directory

Now that the `gcclassic` executable is built, install it to your run directory with **`make install`**. For this to work properly, you must tell CMake where to find your run directory by configuring CMake with `-DRUNDIR=/path/to/run/directory` *as described above*. Type:

```
$ make install
[  1%] Built target KPP_FirstPass
[  4%] Built target CloudJ_Core
[ 13%] Built target Headers
[ 13%] Built target JulDay
[ 18%] Built target NcdfUtil
[ 24%] Built target GeosUtil
[ 26%] Built target ObsPack
[ 27%] Built target HeadersHco
[ 29%] Built target JulDayHco
[ 33%] Built target NcdfUtilHco
[ 33%] Built target GeosUtilHco
[ 47%] Built target HCO
[ 56%] Built target HCOX
[ 58%] Built target HCOI_Shared
[ 60%] Built target HETP_core
[ 69%] Built target KPP
[ 72%] Built target History
[ 98%] Built target GeosCore
[100%] Built target gcclassic
Install the project...
```

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```
-- Install configuration: "Release"
-- Installing: /path/to/run/directory/build_info/CMakeCache.txt
-- Installing: /path/to/run/directory/build_info/summarize_build
-- Installing: /path/to/run/directory/gcclassic
-- Set runtime path of "/path/to/run/directory/gcclassic" to ""
```

Let's now navigate back to the run directory and get a directory listing:

```
$ cd ..
$ ls -CF
archiveRun.sh*     download_data.py*    HEMCO_Config.rc.gmao_metfields  Restarts/
build/             download_data.yml    HEMCO_Diagn.rc                  runScriptSamples@
build_info/        gcclassic*           HISTORY.rc                      species_database.
↪yml
cleanRunDir.sh*    geoschem_config.yml  metrics.py*
CodeDir@           getRunInfo*          OutputDir/
CreateRunDirLogs/  HEMCO_Config.rc      README.md
```

You should now see the **gcclassic** executable and a `build_info` directory there. GEOS-Chem has now been configured, compiled, and installed in your run directory.

Please see the *Run directory files and folders* section for more information about the contents of the run directory.

You are now ready to run a GEOS-Chem simulation!

8.2.3 Remove compiler-generated files when no longer needed

In older versions of GEOS-Chem, you could use a GNU Make command such as **make clean** or **make realclean** to remove all object (`.o`), library (`.a`), module (`.mod`) files, as well as the previously-built executable file from the GEOS-Chem source code folder.

All of the files created by Cmake during the configuration and compilation stages are placed in the `build/` folder in your run directory (or in the location that you have specified with the `-DRUNDIR=/path/to/run/dir` option.). Therefore, if you wish to build the **GEOS-Chem Classic** executable from scratch, all you have to do is to remove all of the files from the build folder. It's as simple as that!

You can also create a new build folder with this command:

```
$ mv build was.build
$ mkdir build
```

and then later on, you can remove the old build folder:

```
$ rm -rf was.build
```

This avoids the temptation to use **rm -rf ***, which can potentially wipe out all of your files if used incorrectly.

8.3 Get a summary of compilation options

The compilation process will create a folder in your run directory named `build_info`. Navigate into this folder and get a directory listing:

```
$ cd build_info
$ ls -CF
CMakeCache.txt  summarize_build*
```

`CMakeCache.txt` contains the **CMake cache**, which is a complete listing of all compilation settings. `summarize_build` is a script that will print the most important of these CMake cache settings.

If you run `summarize_build`:

```
$ ./summarize_build
```

You will get output similar to this:

```
$ ./summarize_build
## Compiler Info
#  Family:   GNU
#  Version:  10.2.0
#  Which:    /n/sw/helmod-rocky8/apps/Core/gcc/10.2.0-fasrc01/bin/gfortran

## Compiler Options (global)
-DCMAKE_Fortran_FLAGS=""
-DCMAKE_Fortran_FLAGS_RELEASE="-O3"

## Compiler Options (GEOS-Chem)
-DGEOSChem_Fortran_FLAGS_GNU="-cpp;-w;-std=legacy;-fautomatic;-fno-align-commons;-
↪fconvert=big-endian;-fno-range-check;-mcmodel=medium;-fbacktrace;-g;-DLINUX_GFORTRAN;-
↪ffree-line-length-none"
-DGEOSChem_Fortran_FLAGS_RELEASE_GNU="-O3;-funroll-loops"

## Compiler Options (HEMCO)
-DHEMCO_Fortran_FLAGS_GNU="-cpp;-w;-std=legacy;-fautomatic;-fno-align-commons;-
↪fconvert=big-endian;-fno-range-check;-mcmodel=medium;-fbacktrace;-g;-DLINUX_GFORTRAN;-
↪ffree-line-length-none"
-DHEMCO_Fortran_FLAGS_RELEASE_GNU="-O3;-funroll-loops"

## GEOS-Chem Components Settings
-DTOMAS="OFF"
-DTOMAS_BINS="NA"
-DAPM="OFF"
-DRRTMG="OFF"
-DGTMM="OFF"
-DHCOSA="OFF"
-DLUO_WETDEP="OFF"
-DFASTJX="OFF"
```

Here you can see the compiler flags that were used as well as the options that were selected.

CHAPTER

NINE

CONFIGURE YOUR SIMULATION

Note: We recommend that you configure your simulation before downloading data files. You can use the configuration settings with a *dry-run simulation* to download only the data that you will need.

You will need to edit various **configuration files** in order to specify options for your GEOS-Chem Classic simulation. These are described below.

9.1 Commonly-updated configuration files

When starting a new GEOS-Chem Classic simulation, you will usually edit most (if not all) of these configuration files:

9.1.1 geoschem_config.yml

Starting with GEOS-Chem 14.0.0, the `input.geos` configuration file (plain text) has been replaced with by the `geoschem_config.yml` file. This file is in YAML format, which is a text-based markup syntax used for representing dictionary-like data structures.

The `geoschem_config.yml` file contains several sections. Only The sections relevant to a given type of simulation are present. For example, *`fullchem`* simulation options (such as aerosol settings and photolysis settings) are omitted from the `geoschem_config.yml` file for the *`CH4`* simulation.

Note: Settings that are not relevant to GCHP will be excluded from the `geoschem_config.yml` file that ships with the GCHP run directory. We will note these excluded settings below. All other settings in `geoschem_config.yml` will be treated in in the same way as in GEOS-Chem Classic.

Simulation settings

```
#============================================================================
# Simulation settings
#============================================================================
simulation:
  name: fullchem
  start_date: [20190701, 000000]
  end_date: [20190801, 000000]
  root_data_dir: /path/to/ExtData
```

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```
met_field: MERRA2
species_database_file: ./species_database.yml
species_metadata_output_file: OutputDir/geoschem_species_metadata.yml
verbose:
  activate: false
  on_cores: root       # Allowed values: root all
use_gcclassic_timers: false
```

The `simulation` section contains general simulation options:

name

Specifies the type of GEOS-Chem simulation. Accepted values are

fullchem

Full-chemistry simulation.

aerosol

Aerosol-only simulation.

carbon

Coupled carbon gases simulation (CH4-CO-CO2-OCS), implemented as a KPP mechanism (cf Bukosa *et al.* [2023]).

You must configure your build with with `-DMECH=carbon` in order to use this simulation. For more information, please see:

- GEOS-Chem Classic configuration instructions or
- GCHP configuration instructions

CH4

Methane simulation.

This simulation will eventually be superseded by the *carbon* simulation.

CO2

Carbon dioxide simulation.

This simulation will eventually be superseded by the *carbon* simulation.

Hg

Mercury simulation.

You must configure your build with with `-DMECH=Hg` in order to use this simulation. For more information, please see:

- GEOS-Chem Classic configuration instructions or
- GCHP configuration instructions

POPs

Persistent organic pollutants (aka POPs) simulation.

> **Attention:** The POPs simulation is currently stale. We look to members of the GEOS-Chem user community take the lead on updating this simulation.

tagCH4

Methane simulation with species tagged by geographic region or other criteria.

This simulation will eventually be superseded by the *carbon* simulation.

tagCO

Carbon dioxide simulation, with species tagged by geographic region and other criteria.

This simulation will eventually be superseded by the *carbon* simulation.

tagO3

Ozone simulation (using specified production and loss rates), with species tagged by geographical region.

TransportTracers

Transport Tracers simulation, with both radionuclide and passive_species. Useful for evaluating model transport.

metals

Trace metals simulation

start_date

Note: This option is omitted for GCHP. The simulation start date is specified in the `CAP.rc` and `cap_restart` files.

Specifies the starting date and time of the simulation in list notation `[YYYYMMDD, hhmmss]`.

end_date

Note: This option is omitted for GCHP. Duration is specified in the `cap_restart` file.

Specifies the ending date and time of the simulation in list notation `[YYYYMMDD, hhmmss]`.

root_data_dir

Note: This option is omitted for GCHP. All data paths (with the exception of the aerosol optics and photolysis paths) are specified in the `ExtData.rc` file.

Path to the root data directory. All of the data that GEOS-Chem Classic reads must be located in subfolders of this directory.

met_field

Note: This option is omitted for GCHP. Met field source is described in file paths of the in the `ExtData.rc` file.

Name of the meteorology product that will be used to drive GEOS-Chem. Accepted values are:

MERRA2

The MERRA-2 meteorology product from NASA/GMAO. MERRA-2 is a stable reanalysis product, and extends from approximately 1980 to present. **(Recommended option)**

GEOS-FP

The GEOS-FP meteorology product from NASA/GMAO. GEOS-FP is an operational data product and, unlike MERRA-2, periodically receives science updates.

GCAP2

The GCAP-2 meteorology product, archived from the GISS-2 GCM. GCAP-2 has hundreds of years of data available, making it useful for simulations of historical climate.

species_database_file

Path to the *GEOS-Chem Species Database* file. This is stored in the run directory file `./species_database.yml`. You should not have to edit this setting.

species_metadata_output_file

Path to the `geoschem-species-metadata.yml` file. This file contains echoback of information from *species_database.yml*, but only for species that are defined in this simulation (instead of all possible species). This facilitates interfacing GEOS-Chem with external models such as CESM.

verbose:

Menu controlling verbose printout. Starting with GEOS-Chem 14.2.0 and HEMCO 3.7.0, most informational printouts are now deactivated by default. You may choose to activate them (e.g. for debugging and/or testing) with the options below:

activate

Activates (`true`) or deactivates (`false`) printing extra informational printout to the screen and/or log file.

on_cores:

Specify on which computational cores informational printout should be done.

root

Print extra informational output only on the root core. Use this setting for GEOS-Chem Classic.

all

Print extra informational output on all cores. Consider using this when using GEOS-Chem as GCHP, or in MPI-based external models (NASA GEOS, CESM, etc.).

use_gcclassic_timers

Note: This setting is omitted for GCHP, as the MAPL library provides all timer functionality.

Activates (`true`) or deactivates (`false`) the GEOS-Chem Classic timers. If activated, information about how long each component of GEOS-Chem Classic took to execute will be printed to the screen and/or the log file The same information will also be written in JSON format to a file named gcclassic_timers.json.

You can set this option to `false` unless you are running benchmark or timing simulations.

Grid settings

Note: Grid settings are omitted for GCHP. Grid specifications are contained in the `GCHP.rc` file instead.

```
#============================================================================
# Grid settings
#============================================================================
```

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```
grid:
  resolution: 4.0x5.0
  number_of_levels: 72
  longitude:
    range: [-180.0, 180.0]
    center_at_180: true
  latitude:
    range: [-90.0, 90.0]
    half_size_polar_boxes: true
  nested_grid_simulation:
    activate: true
    buffer_zone_NSEW: [0, 0, 0, 0]
```

The `grid` section contains settings that define the grid used by GEOS-Chem Classic:

resolution

Specifies the horizontal resolution of the grid. Accepted values are:

4.0x5.0

The global $4^\circ \times 5^\circ$ GEOS-Chem Classic grid.

2.0x2.5

The global $2.0^\circ \times 2.5^\circ$ GEOS-Chem Classic grid.

0.5x0.625

The global $0.5^\circ \times 0.625^\circ$ GEOS-Chem Classic grid (*MERRA2* only). Can be used for global or nested simulations.

0.5x0.625

The global $0.25^\circ \times 0.3125^\circ$ GEOS-Chem Classic grid (*GEOS-FP* and *MERRA2*). Can be used for global or nested simulations.

number_of_levels

Number of vertical levels to use in the simulation. Accepted values are:

72

Use 72 vertical levels. This is the native vertical resolution of *MERRA2* and *GEOS-FP*.

47

Use 47 vertical levels (for *MERRA2* and *GEOS-FP*).

40

Use 40 vertical levels (for *GCAP2*).

longitude

Settings that define the longitude dimension of the grid. There are two sub-options:

range

The minimum and maximum longitude values (grid box edges), specified in list format.

center_at_180

If `true`, then westernmost grid boxes are centered at -180° longitude (the International Date Line). This is true for both *MERRA2* and *GEOS-FP*.

If `false`, then the westernmost grid boxes have their westernmost edges at -180° longitude. This is true for the *GCAP2* grid.

latitude

Settings to define the latitude dimension of the grid. There are two sub-options:

range

The minimum and maximum latitude values (grid box edges), specified in list format.

use_halfpolar_boxes

If `true`, then the northernmost and southernmost grid boxes will be $\frac{1}{2}$ the extent of other grid boxes. This is true for both *MERRA2* and *GEOS-FP*.

If `false`, then all grid boxes will have the same extent in latitude. This is true for the *GCAP2* grid.

nested_grid_simulation

Settings for nested-grid simulations. There are two sub-options:

activate

If `true`, this indicates that the simulation will use a sub-window of the horizontal grid.

If `false`, this indicates that the simulation will use the entire global grid extent.

buffer_zone_NSEW

Specifies the nested grid latitude offsets (# of grid boxes) in list format `[N-offset, S-offset, E-offset, W-offset]`. These offsets are used to define an inner window region in which transport is actually done (aka the "transport window"). This "transport window" is always smaller than the actual size of the nested grid region in order to properly account for the boundary conditions.

- For global simulations, use: `[0, 0, 0, 0]`.
- For nested-grid simulations, we recommend using: `[3, 3, 3, 3]`.

Timesteps settings

Note: Timesteps settings are omitted for GCHP. Timesteps are specified in the `CAP.rc` file.

```
#============================================================================
# Timesteps settings
#============================================================================
timesteps:
  transport_timestep_in_s: 600
  chemistry_timestep_in_s: 1200
  radiation_timestep_in_s: 10800
```

The `timesteps` section specifies the frequency at which various GEOS-Chem operations occur.

The table below contains our recommended GEOS-Chem Classic timestep settings.

GEOS-Chem Classic Resolution	Transport	Chemistry
$4° \times 5°$	600s (10m)	1200s (20m)
$2° \times 2.5°$	600s (10m)	1200s (20m)
$0.5° \times 0.625°$	300s (5m)	600s (10m)
$0.25° \times 0.3125°$	300s (5m)	600s (10m)
$0.125° \times 0.15625°$	150s (2.5m)	300s (5m)

The Courant limit on the latitude-longitude grid constrains the choice of transport timestep for a given horizontal resolution. We choose a chemistry timestep that is double the transport timestep (i.e. Strang operator splitting).

Note: GCHP, which uses the FVdycore advection scheme on the cubed-sphere grid, does not have similar restrictions for timesteps.

See Philip *et al.* [2016] for a comprehensive study on GEOS-Chem timesteps. For some practical tips on speeding up your simulations, see:

- Speeding up GEOS-Chem Classic simulations
-

transport_timestep_in_s

Specifies the "heartbeat" timestep of GEOS-Chem.. This is the frequency at which transport, cloud convection, PBL mixing, and wet deposition will be done.

chemistry_timestep_in_s

Specifies the frequency at which chemistry and emissions will be done.

radiation_timestep_in_s

Specifies the frequency at which the RRTMG radiative transfer model will be called (valid for *fullchem* simulations only). We recommend using a timestep of 10800s (3h), as the RRTMG calculations are computationally intensive.

Operations settings

This section of `geoschem_config.yml` is included for all simulations. However, some of the options listed below will be omitted for simulations that do not require them.

There are several sub-sections under `operations`:

Chemistry

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  chemistry:
    activate: true
    linear_chemistry_aloft:
      activate: true
      use_linoz_for_O3: true
    active_strat_H2O:
      activate: true
      use_static_bnd_cond: true
    gamma_HO2: 0.2
    autoreduce_solver:
      activate: false
      use_target_threshold:
        activate: true
```

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```
    oh_tuning_factor: 0.00005
    no2_tuning_factor: 0.0001
  use_absolute_threshold:
    scale_by_pressure: true
    absolute_threshold: 100.0
  keep_halogens_active: false
  append_in_internal_timestep: false

  # ... following sub-sections omitted ...
```

The `operations:chemistry` section contains settings for chemistry:

activate

Activates (`true`) or deactivates (`false`) chemistry in GEOS-Chem.

linear_chemistry_aloft

Determines how linearized chemistry will be applied in the stratosphere and/or mesosphere. (Only valid for *fullchem* simulations).

There are two sub-options:

activate

Activates (`true`) or deactivates (`false`) linearized stratospheric chemistry in the stratosphere and/or mesosphere.

use_linoz_for_O3

If `true`, Linoz stratospheric ozone chemistry will be used.

If `false`, Synoz (i.e. a synthetic flux of ozone across the tropopause) will be used instead of Linoz.

active_strat_H2O

Determines if water vapor as modeled by GEOS-Chem will be allowed to influence humidity fields. (Only valid for *fullchem* simulations)

There are two sub-options:

activate

Allows (`true`) or disallows (`false` the H2O species in GEOS-Chem to influence specific humidity and relative humidity.

use_static_bnd_cond

Allows (`true`) or diasallows (`false`) a static boundary condition.

TODO Clarify this

gamma_HO2

Specifies γ, the uptake coefficient for HO_2 heterogeneous chemistry.

Recommended value: `0.2`.

autoreduce_solver

Menu for controlling the adaptive mechanism auto-reduction feature, which is available in KPP 3.0.0. and later versions. See Lin *et al.* [2023] for details.

activate

If `true`, the mechanism will be integrated using the Rosenbrock method with the adaptive auto-reduction feature.

If `false`, the mechanism will be integrated using the traditional Rosenbrock method.

Default value: `false`.

use_target_threshold

Contains options for defining ∂ (the partitioning threshold between "fast" and "slow" species") by considering the production and loss of key species (OH for daytime, NO2 for nighttime).

activate

Activates (`true`) or deactivates (`false`) using OH and NO2 to determine ∂.

Default value: `true`.

oh_tuning_factor

Specifies α_{OH}, which is used to compute ∂.

no2 tuning factor

Specifies α_{NO2}, which is used to compute ∂.

use_pressure_threshold

Contains options for setting an absolute threshold ∂ that may be weighted by pressure.

scale_by_pressure

Activates (`true`) or deactivates (`false`) using a pressure-dependent method to determine ∂.

absolute_threshold

The absolute partitioning threshold ∂.

If *scale_by_pressure* is `true`, and `use_target_threshold:activate` is `false` , the value for ∂ specified here will be scaled by the ratio P/P_{sfc}. where P is the grid box pressure and P_{sfc} is the surface pressure for the column.

keep_halogens_active

If `true`, then all halogen species will be considered "fast". This may be necessary in order to obtain realistic results for ozone and other important species.

If `false`, then halogen species will be determined as "slow" or "fast" depending on the partitioning threshold ∂.

Default value: `true`

append_in_internal_timestep

If `true`, any "slow" species that later become "fast" will be appended to the list of "fast" species.

If `false`, any "slow" species that later become "fast" will NOT be appended to the list of "fast" species.

Default value: `false`

Convection

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  convection:
```

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```
    activate: true

  # ... following sub-sections omitted ...
```

The **operations:convection** section contains settings for cloud convection:

activate
: Activates (`true`) or deactivates (`false`) cloud convection in GEOS-Chem.

Dry deposition

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  dry_deposition:
    activate: true
    CO2_effect:
      activate: false
      CO2_level: 600.0
      reference_CO2_level: 380.0
    diag_alt_above_sfc_in_m: 10

  # ... following sub-sections omitted ...
```

The `operations:dry_deposition` section contains settings that for dry deposition:

activate
: Activates (`true`) or deactivates (`false`) dry deposition.

CO2_effect
: This sub-section contains options for applying the simple parameterization for the CO2 effect on stomatal resistance.

  activate
  : Activates (`true`) or deactivates (`false`) the CO2 effect on stomatal resistance in dry deposition.

    Default value: `false`.

  CO2_level
  : Specifies the CO2 level (in ppb).

  reference_CO2_level
  : Specifies the reference CO2 level (in ppb).

diag_alt_above_sfc_in_m:
: Specifies the altitude above the surface (in m) to used with the ConcAboveSfc diagnostic collection.

PBL mixing

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  pbl_mixing:
    activate: true
    use_non_local_pbl: true

  # ... following sub-sections omitted ...
```

The `operations:pbl_mixing` section contains settings that for planetary boundary layer (PBL) mixing:

activate

Activates (`true`) or deactivates (`false`) planetary boundary layer mixing in GEOS-Chem Classic.

use_non_local_pbl

If `true`, then the non-local PBL mixing scheme (VDIFF) will be used. (Default option)

If `false`, then the full PBL mixing scheme (TURBDAY) will be used.

Photolysis

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  photolysis:
    activate: true
    cloud-j:
      cloudj_input_dir: ${RUNDIR_DATA_ROOT}/CHEM_INPUTS/CLOUD_J/v2025-01/
      num_levs_with_cloud: 34
      cloud_scheme_flag: 3
      opt_depth_increase_factor: 1.050
      min_top_inserted_cloud_OD: 0.005
      cloud_overlap_correlation: 0.33
      num_cloud_overlap_blocks: 6
      sphere_correction: 1
      num_wavelength_bins: 18
      use_H2O_UV_absorption: true
    fast-jx:
      fastjx_input_dir: /path/to/ExtData/CHEM_INPUTS/FAST_JX/v2024-05/
    overhead_O3:
      use_online_O3_from_model: true
      use_column_O3_from_met: true
```

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```
    use_TOMS_SBUV_O3: false
  photolyze_nitrate_aerosol:
    activate: true
    NITs_Jscale: 100.0
    NIT_Jscale: 100.0
    percent_channel_A_HONO: 66.667
    percent_channel_B_NO2: 33.333

# ... following sub-sections omitted ...
```

The `operation:photolysis` section contains settings for photolysis. This section only applies to fullchem, Hg, and aerosol-only simulations.

activate

Activates (`true`) or deactivates (`false`) photolysis.

> **Attention:** You should always keep photolysis turned on in your simulations. Disabling photolysis should only be done when debugging.

cloud-j:

Specifies various options for the Cloud-J photolysis package.

> **Note:** The Cloud-J settings have been preset to the recommended values. You should not need to modify these settings (unless you are investigating how aerosol and cloud interactions impact photolysis).

cloudj_input_dir

Specifies the path to the Cloud-J configuration files containing information about species cross sections and quantum yields.

num_levs_with_cloud

Specifies the number of levels that can contain clouds, which is a required input for the Cloud-J photolysis module. This value is pre-set to the proper value for the vertical grid that your simulation will use.

GEOS-Chem variable:	`Input_Opt%NLevs_Phot_Cloud`
Cloud-J variable	`LWEPAR`

cloud_scheme_flag

Specifies the cloud option used in the computation of photolyis rates.

GEOS-Chem variable:	`Input_Opt%CLDFLAG`
Cloud-J variable	`LWEPAR`

opt_depth_increase_factor

Specifies the factor increase in cloud optical depth from a given layer to the layer below.

GEOS-Chem variable:	`Input_Opt%OD_Increase_Factor`
Cloud-J variable	`ATAU`

`min_top_inserted_cloud_OD`

Specifies the minimum cloud OD in the uppermost inserted layer.

GEOS-Chem variable:	`Input_Opt%Min_Cloud_OD`
Cloud-J variable	`ATAU0`

`cloud_overlap_correlation`

Specifies the cloud de-corellation between max-overlap blocks, where 0.00 is random overlap. This option is only used when *`cloud_scheme_flag`* is set to 5 or higher.

GEOS-Chem variable:	`Input_Opt%Cloud_Corr`
Cloud-J variable	`CLDCOR`

`num_cloud_overlap_blocks`

Specifies the number of maximum-overlap blocks.

GEOS-Chem variable:	`Input_Opt%Num_Max_Overlap`
Cloud-J variable	`LNRG`

`sphere_correction`

Specifies the type of spherical correction to be applied.

GEOS-Chem variable:	`Input_Opt%OD_Increase_Factor`
Cloud-J variable	`ATM0`

`num_wavelength_bins`

Specifies the number of wavelength bins to use in the computation of photolysis reaction rates.

GEOS-Chem variable:	`Input_Opt%Num_WV_Bins`
Cloud-J variable	`ATM0`

`use_H2O_UV_absorption`

Specifies whether to enable (`true`) or disable (`false`) UV absorption of water vapor in the computations for photolysis rates. Default value: `true`.

GEOS-Chem variable:	`Input_Opt%Use_H2O_UV_Abs`
Cloud-J variable	`USEH2OUV`

`fast-jx`

Specifies various options for the FAST-JX photolysis package.

> **Attention:** FAST-JX is currently used only by the Hg (mercury) simulation, In the near future, the Hg simulation will be updated to use Cloud-J, and FAST_JX will be retired from GEOS-Chem.

fastjx_input_dir

Specifies the path to the legacy FAST_JX configuration files containing information about species cross sections and quantum yields. These are used to define several aerosol optical properties even when FAST-JX is not used.

Note that FAST-JX is off by default and Cloud-J is used instead. You can use legacy FAST-JX instead of Cloud-J by configuring with `-DFASTJX=y` during build.

overhead_O3

This section contains settings that control which overhead ozone sources are used for photolysis

use_online_O3_from_model

Activates (`true`) or deactivates (`false`) using online O3 from GEOS-Chem in the extinction calculations for photolysis.

Recommended value: `true`

use_column_O3_from_met

Activates (`true`) or deactivates (`false`) using ozone columns (e.g. TO3) from the meteorology fields.

Recommended value: `true`.

use_TOMS_SBUV_O3

Activates (`true`) or deactivates (`false`) using ozone columns from the TOMS-SBUV archive will be used.

Recommended value: `false`.

photolyze_nitrate_aerosol

This section contains settings that control options for nitrate aerosol photolysis.

activate

Activates (`true`) or deactivates (`false`) nitrate aerosol photolysis.

Recommended value: `true`.

NITs_Jscale

Scale factor (percent) for JNO3 that photolyzes NITs aerosol.

NIT_Jscale

Scale factor (percent) for JHNO2 that photolyzes NIT aerosol.

percent_channel_A_HONO

Fraction of JNITs/JNIT in channel A (HNO2) for NITs photolysis.

percent_channel_B_HO2

Fraction of JNITs/JNIT in channel B (NO2) for NITs photolysis.

RRTMG radiative transfer model

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  rrtmg_rad_transfer_model:
```

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```
    activate: false
    aod_wavelengths_in_nm:
      - 550
    longwave_fluxes: false
    shortwave_fluxes: false
    clear_sky_flux: false
    all_sky_flux: false
    fixed_dyn_heating: false
    seasonal_fdh: false
    read_dyn_heating: false
    co2_ppmv: 390.0

  # .. following sub-sections omitted ...
```

The `operations:rrtmg_rad_transfer_model` section contains settings for the RRTMG radiative transfer model:

This section only applies to *fullchem* simultions.

activate

Activates (`true`) or deactivates (`false`) the RRTMG radiative transfer model.

Default value: `false`.

aod_wavelengths_in_nm

Specify wavelength(s) for the aerosol optical properties in nm (in YAML sequence format) Up to three wavelengths can be selected. The specified wavelengths are used for the photolysis mechanism (either legacy FAST-JX or Cloud-J) regardless of whether the RRTMG radiative transfer model is used.

longwave_fluxes

Activates (`true`) or deactivates (`false`) RRTMG longwave flux calculations.

Default value: `false`.

shortwave_fluxes

Activates (`true`) or deactivates (`false`) RRTMG shortwave calculations.

Default value: `false`.

clear_sky_flux

Activates (`true`) or deactivates (`false`) RRTMG clear-sky flux calculations.

Default value: `false`.

all_sky_flux

Activates (`true`) or deactivates (`false`) RRTMG all-sky flux calculations.

Default value: `false`.

fixed_dyn_heating

Activates (`true`) or deactivates (`false`) fixed dynamic heating (FDH) approximation as described by Forster *et al.* [1997].

Default value: `false`.

seasonal_fdh

Activates (`true`) or deactivates (`false`) seasonally-evolving fixed dynamic heating (SEFDH) approzimation as described by Kiehl *et al.* [1999].

> **Attention:** This option has not been extensively tested, and is considered experimental.

Default value: `false`.

read_dyn_heating

Activates (`true`) or deactivates (`false`) reading previously-archived dynamical heating outputs from disk.

Default value: `false`.

co2_ppmv

Specify the value of CO2 [in parts per million by volume] to be used in radiative forcing calculations.

Default value: `390.0`.

Transport

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  transport:
    gcclassic_tpcore:                # GEOS-Chem Classic only
      activate: true                 # GEOS-Chem Classic only
      fill_negative_values: true     # GEOS-Chem Classic only
      iord_jord_kord: [3, 3, 7]      # GEOS-Chem Classic only
    transported_species:
      - ACET
      - ACTA
      - AERI
      # ... etc more transported species ...

# .. following sub-sections omitted ...
```

The `operations:transport` section contains settings for species transport:

gcclassic_tpcore

> **Note:** These settings are omitted for GCHP, which uses the FVdycore advection package instead.

Contains options that control species transport in GEOS-Chem Classic with the TPCORE advection scheme:

activate

Activates (`true`) or deactivates (`false`) species transport in GEOS-Chem Classic.

Default value: `true`.

fill_negative_values

If `true`, negative species concentrations will be replaced with zeros.

If `false`, no change will be made to species concentrations.

Default value: `true`.

iord_jord_kord

Specifies advection options (in list format) for TPCORE in the longitude, latitude, and vertical dimensions. The options are listed below:

1. 1st order upstream scheme (use for debugging only)
2. 2nd order van Leer (full monotonicity constraint)
3. Monotonic PPM
4. Semi-monotonic PPM (same as 3, but overshoots are allowed)
5. Positive-definite PPM
6. Un-constrained PPM (use when fields & winds are very smooth) this option only when the fields and winds are very smooth.
7. Huynh/Van Leer/Lin full monotonicity constraint (KORD only)

Default (and recommended) value: `[3, 3, 7]`

transported_species

A list of species names (in YAML sequence format) that will be transported by the TPCORE advection scheme.

Wet deposition

```
#============================================================================
# Settings for GEOS-Chem operations
#============================================================================
operations:

  # .. preceding sub-sections omitted ...

  wet_deposition:
    activate: true
```

The `operations:wet_deposition` section contains settings for wet deposition.

activate

Activates (`true`) or deactivates (`false`) wet deposition in GEOS-Chem Classic.

Aerosols settings

This section of `geoschem_config.yml` is included for *`fullchem`* and *`aerosol`* simulations.

There are several sub-sections under `aerosols`:

Optics

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  optics:
    input_dir: /path/to/ExtData/CHEM_INPUTS/Aerosol_Optics/v2025-03/

  # .. following sub-sections omitted ...
```

optics

input_dir
Specifies the path to files used containing aerosol optical properties for computing aerosol optical depth.

Carbon aerosols

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  # ... preceding sub-sections omitted ...

  carbon:
    activate: true
    brown_carbon: false
    enhance_black_carbon_absorption:
      activate: true
      hydrophilic: 1.5
      hydrophobic: 1.0

  # .. following sub-sections omitted ...
```

The `aerosols:carbon` section contains settings for carbon aerosols:

activate
Activates (`true`) or deactivates (`false`) carbon aerosols in GEOS-Chem.

Default value: `true`.

brown_carbon
Activates (`true`) or deactivates (`false`) brown carbon aerosols in GEOS-Chem.

Default value: `false`.

enhance_black_carbon_absorption
Options for enhancing the absorption of black carbon aerosols due to external coating.

activate
Activates (`true`) or deactivates (`false`) black carbon absorption enhancement.

Default value: `true`.

hydrophilic

Absorption enhancement factor for hydrophilic black carbon aerosol (species name **BCPI**).

Default value: `1.5`

hydrophobic

Absorption enhancement factor for hydrophilic black carbon aerosol (species name **BCPO**).

Default value: `1.0`

Complex SOA

The `aerosols:complex_SOA` section contains settings for the complex SOA scheme used in GEOS-Chem.

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  # ... preceding sub-sections omitted ...

  complex_SOA:
    activate:  true
    semivolatile_POA: false

  # ... following sub-sections omitted ...
```

activate

Activates (`true`) or deactivates (`false`) the complex SOA scheme.

Default value:

- `true` for the *fullchem* benchmark simulation
- `false` for all other *fullchem* simulations

semivolatile_POA

Activates (`true`) or deactivates (`false`) the semi-volatile primary organic aerosol (POA) option.

Default value: `false`

Mineral dust aerosols

The `aerosols:dust` section contains settings for mineral dust aerosols.

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  # ... preceding sub-sections omitted ...

  dust:
    activate: true
    acid_uptake_on_dust: false
```

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```
  # ... following sub-sections omitted ...
```

activate

Activates (`true`) or deactivates (`false`) mineral dust aerosols in GEOS-Chem.

Default value: `true`

acid_uptake_on_dust

Activates (`true`) or deactivates (`false`) the acid uptake on dust option, which includes 12 additional species.

Default value: `false`

Sea salt aerosols

The `aerosols:sea_salt` section contains settings for sea salt aerosols:

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  # ... preceding sub-sections omitted ...

  sea_salt:
    activate: true
    SALA_radius_bin_in_um: [0.01, 0.5]
    SALC_radius_bin_in_um: [0.5,  8.0]
    marine_organic_aerosols: false

  # ... following sub-sections omitted ...
```

activate

Activates (`true`) or deactivates (`false`) sea salt aerosols.

Default value: `true`

SALA_radius_bin_in_um

Specifies the upper and lower boundaries (in nm) for accumulation-mode sea salt aerosol (aka **SALA**).

Default value: `0.01 nm - 0.5 nm`

SALC_radius_bin_in_um

Specifies the upper and lower boundaries (in nm) for coarse-mode sea salt aerosol (aka **SALC**).

Default value: `0.5 nm - 8.0 nm`

marine_organic_aerosols

Activates (`true`) or deactivates (`false`) emission of marine primary organic aerosols. This option includes two extra species (**MOPO** and **MOPI**).

Default value: `false`

Stratospheric aerosols

The `aerosols:sulfate` section contains settings for stratopsheric aerosols.

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  # ... preceding sub-sections omitted ...

  stratosphere:
    settle_strat_aerosol: true
    polar_strat_clouds:
      activate: true
      het_chem: true
    allow_homogeneous_NAT: false
    NAT_supercooling_req_in_K: 3.0
    supersat_factor_req_for_ice_nucl: 1.2
    calc_strat_aod: true

  # ... following sub-sections omitted ...
```

settle_strat_aerosol

Activates (`true`) or deactivates (`false`) gravitational settling of stratospheric solid particulate aerosols (SPA, trapezoidal scheme) and stratospheric liquid aerosols (SLA, corrected Stokes' Law).

Default value: `true`

polar_strat_clouds

Contains settings for how aerosols are handled in polar stratospheric clouds (PSC):

activate

Activates (`true`) or deactivates (`false`) formation of polar stratospheric clouds.

Default value: `true`

het_chem

Activates (`true`) or deactivates (`false`) heterogeneous chemistry within polar stratospheric clouds.

Default value: `true`

allow_homogeneous_NAT

Activates (`true`) or deactivates (`false`) heterogeneous formation of NAT from freezing of HNO3.

Default value: `false`

NAT_supercooling_req_in_K

Specifies the cooling (in K) required for homogeneous NAT nucleation.

Default value: `3.0`

supersat_factor_req_for_ice_nucl

Specifies the supersaturation factor required for ice nucleation.

Recommended values: `1.2` for coarse grids; `1.5` for fine grids.

calc_strat_aod

Includes (`true`) or excludes (`false`) online stratospheric aerosols in extinction calculations for photolysis.

Default value: `true`

Sulfate aerosols

The `aerosols:sulfate` section contains settings for sulfate aerosols:

```
#============================================================================
# Settings for GEOS-Chem aerosols
#============================================================================
aerosols:

  # ... preceding sub-sections omitted ...

  sulfate:
    activate: true
    metal_cat_SO2_oxidation: true
```

activate

Activates (`true`) or deactivates (`false`) sulfate aerosols.

Default value: `true`

metal_cat_SO2_oxidation

Activates (`true`) or deactivates (`false`) the metal catalyzed oxidation of SO2.

Default value: `true`

Extra diagnostics

The `extra_diagnostics` section contains settings for GEOS-Chem Classic diagnostics that are not archived by History diagnostics or HEMCO.

Obspack diagnostic

Note: These settings are omitted for GCHP, as ObsPack diagnostics can only be used with GEOS-Chem Classic.

The `extra_diagnostics:obspack` section contains settings for the Obspack diagnostic:

```
#============================================================================
# Settings for diagnostics (other than HISTORY and HEMCO)
#============================================================================
extra_diagnostics:

  obspack:
    activate: false
    quiet_logfile_output: false
    input_file: ./obspack_co2_1_OCO2MIP_2018-11-28.YYYYMMDD.nc
    output_file: ./OutputDir/GEOSChem.ObsPack.YYYYMMDD_hhmmz.nc4
```

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```
    output_species:
      - CO
      - 'NO'
      - O3

  # ... following sub-sections omitted ...
```

activate

Activates (`true`) or deactivates (`false`) ObsPack diagnostic output.

Default value: `true`

quiet_logfile_output

Deactivates (`true`) or activates (`false`) printing informational output to `stdout` (i.e. the screen or log file).

Default value: `false`

input_file

Specifies the path to an ObsPack data file (in netCDF format).

output_file

Specifies the path to the ObsPack diagnostic output file. This will be a file that contains data at the same locations as specified in *input_file*.

output_species

A list of GEOS-Chem species (as a YAML sequence) to archive to the output file.

Planeflight diagnostic

Note: These settings are omitted for GCHP, as the Planeflight diagnostics can only be used with GEOS-Chem Classic.

The `extra_diagnostics:planeflight` section contains settings for the GEOS-Chem planeflight diagnostic:

```
#============================================================================
# Settings for diagnostics (other than HISTORY and HEMCO)
#============================================================================
extra_diagnostics:

  # ... preceding sub-sections omitted ...

  planeflight:
    activate: false
    flight_track_file: Planeflight.dat.YYYYMMDD
    output_file: plane.log.YYYYMMDD

  # ... following sub-sections omitted ...
```

activate

Activates (`true`) or deactivates (`false`) the Planeflight diagnostic output.

Default value: `false`

flight_track_file

Specifies the path to a flight track file. This file contains the coordinates of the plane as a function of time, as well as the requested quantities to archive.

output_file

Specifies the path to the Planeflight output file. Requested quantities will be archived from GEOS-Chem along the flight track specified in *flight_track_file*.

Hg simulation options

This section of `geoschem_config.yml` is included for the mercury (Hg) simulation:

Hg sources

The `Hg_simulation_options:sources` section contains settings for various mercury sources.

```
#============================================================================
# Settings specific to the Hg simulation
#============================================================================
Hg_simulation_options:

  sources:
    use_dynamic_ocean_Hg: false
    use_preindustrial_Hg: false
    use_arctic_river_Hg: true

  # ... following sub-sections omitted ...
```

use_dynamic_ocean_Hg

Activates (`true`) or deactivates (`false`) the online slab ocean mercury model.

Default value: `false`

use_preindustrial_Hg

Activates (`true`) or deactivates (`false`) the preindustrial mercury simulation. This will turn off all anthropogenic emissions.

Default value: `false`

use_arctic_river_Hg

Activates (`true`) or deactivates (`false`) the source of mercury from arctic rivers.

Default value: `true`

Hg chemistry

The `Hg_simulation_options:chemistry` section contains settings for mercury chemistry:

```
#============================================================================
# Settings specific to the Hg simulation
#============================================================================
Hg_simulation_options:
```

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```
  # ... preceding sub-sections omitted ...

  chemistry:
    tie_HgIIaq_reduction_to_UVB: true

  # ... following sub-sections omitted ...
```

tie_HgIIaq_reduction_to_UVB

Activates (`true`) or deactivates (`false`) linking the reduction of aqueous oxidized mercury to UVB radiation. A lifetime of -1 seconds indicates the species has an infinite lifetime.

Default value: `true`

Options for simulations with carbon gases

These sections of `geoschem_config.yml` are included for simulations with carbon gases (*carbon*, *CH4*, *CO2*, *tagCO*, *tagCH4*).

CH4 observational operators

The `CH4_simulation_options:use_observational_operators` section contains options for using satellite observational operators for CH4:

```
#============================================================================
# Settings specific to the CH4 simulation / Integrated Methane Inversion
#============================================================================
CH4_simulation_options:

  use_observational_operators:
    AIRS: false
    GOSAT: false
    TCCON: false

  # ... following sub-sections omitted ...
```

AIRS

Activates (`true`) or deactivates (`false`) the AIRS observational operator.

Default value: `false`

GOSAT

Activates (`true`) or deactivates (`false`) the GOSAT observational operator.

Default value: `false`

TCCON

Activates (`true`) or deactivates (`false`) the GOSAT observational operator.

Default value: `false`

CH4 analytical inversion options

The `ch4_simulation_options:analytical_inversion` section contains options for analytical inversions with the Integrated Methane Inversion workflow (aka IMI). The IMI will automatically modify several of these options based on the inversion parameters that you specify.

```
#============================================================================
# Settings specific to the CH4 simulation / Integrated Methane Inversion
#============================================================================
CH4_simulation_options:

  # ... preceding sub-sections omitted ...

  analytical_inversion:
    perturb_OH_boundary_conditions: false
    CH4_boundary_condition_ppb_increase_NSEW: [0.0, 0.0, 0.0, 0.0]
```

perturb_CH4_boundary_conditions

Activates (`true`) or deactivatees (`false`) perturbation of CH4 nested-grid boundary conditions in analytical inversions.

Default value: `false`

CH4_boundary_condition_ppb_increase_NSEW

Specifies the perturbation amount (in ppbv) to apply to the north, south, east and west CH4 nested-grid boundary conditions. Used in conjunction with the *perturb_CH4_boundary_conditions* option.

Default value: `[0.0, 0.0, 0.0, 0.0]` (no perturbation)

CO2 Sources

The `CO2_simulation_options:sources` section contains toggles for activating sources of CO_2:

```
#============================================================================
# Settings specific to the CO2 simulation
#============================================================================
CO2_simulation_options:

  sources:
    3D_chemical_oxidation_source: true

  # ... following sub-sections omitted ...
```

3D_chemical_oxidation_source

Activates (`true`) or deactivates (`false`) CO_2 production by archived chemical oxidation, as read by HEMCO.

Default value: `true`

CO2 tagged species

The `CO2_simulation_options:tagged_species` section contains toggles for activating tagged CO_2 species:

Attention: Tagged CO_2 tracers should be customized by each user and the present configuration will not work for resolutions other than $2.0^\circ \times 2.5^\circ$.

```
#============================================================================
# Settings specific to the CO2 simulation
#============================================================================
CO2_simulation_options:

  # ... preceding sub-sections omitted ...

  tagged_species:
    tag_bio_and_ocean_CO2: false
    tag_land_fossil_fuel_CO2: false

  # .. following sub-sections omitted ...
```

tag_bio_and_ocean_CO2

Activates (`true`) or deactivates (`false`) tagging of biosphere regions (28), ocean regions (11), and the rest of the world (ROW) as specified in `Regions_land.dat` and `Regions_ocean.dat` files.

tag_land_fossil_fuel_CO2:

Activates (`true`) or deactivates (`false`) tagging of land and ocean fossil fuel regions.

CO chemical sources

The `tagged_CO_simulation_options` section contains settings for the *carbon* simulation and tagged CO simulation.

```
#============================================================================
# Settings specific to the tagged CO simulation
#============================================================================

tagged_CO_simulation_options:
  use_fullchem_PCO_from_CH4: true
  use_fullchem_PCO_from_NMVOC: true
```

use_fullchem_PCO_from_CH4

Activates (`true`) or deactivates (`false`) applying the production of CO from CH_4. This field is archived from a 1-year or 10-year *fullchem* benchmark simulation and is read from disk via HEMCO.

Default value: `true`

use_fullchem_PCO_from_NMVOC

Activates (`true`) or deactivates (`false`) applying the production of CO from non-methane volatile organic compounds (VOCs). This field is archived from a 1-year or 10-year *fullchem* benchmark simulation and is read from disk via HEMCO.

Default value: `true`

9.1.2 HEMCO_Config.rc

GEOS-Chem Classic relies on the Harmonized Emissions Component (aka HEMCO) for file I/O, regridding, and computing emissions fluxes. Settings for HEMCO can be updated in the HEMCO configuration file, which is named `HEMCO_Config.rc`.

The HEMCO online manual at hemco.readthedocs.io contains detailed instructions about the structure and contents of `HEMCO_Config.rc`, so we will not replicate that content in this Guide. Instead, we will provide a short summary with links to the relevant documentation.

General HEMCO settings

Define general simulation parameters in the Settings section of `HEMCO_Config.rc`. This includes data paths, global diagnostic options, and verbose output options.

```
###############################################################################
### BEGIN SECTION SETTINGS
###############################################################################

ROOT:                         /path/to/hemco/data/dir
METDIR:                       /path/to/hemco/met/dir
GCAPSCENARIO:                 not_used
GCAPVERTRES:                  47
Logfile:                      *
DiagnFile:                    HEMCO_Diagn.rc
DiagnPrefix:                  ./OutputDir/HEMCO_diagnostics
DiagnFreq:                    00000000 010000
Wildcard:                     *
Separator:                    /
Unit tolerance:               1
Negative values:              0
Only unitless scale factors: false
Verbose:                      false
VerboseOnCores:               root       # Accepted values: root all

### END SECTION SETTINGS ###
```

Extension switches

Turn individual emissions inventories on/off in the Extension Switches section of `HEMCO_Config.rc`. Emission inventories are specified as either Base Emissions (i.e. read from files on disk) or Extensions (i.e. computed using meteorological inputs).

```
###############################################################################
### BEGIN SECTION EXTENSION SWITCHES
###############################################################################
# ExtNr ExtName                 on/off  Species  Years avail.
0       Base                    : on    *
# ----- MAIN SWITCHES ------------------------------------------------------
    --> EMISSIONS               :       true
    --> METEOROLOGY             :       true
    --> CHEMISTRY_INPUT         :       true
```

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```
# ----- RESTART FIELDS ------------------------------------------------------
    --> GC_RESTART             :       true
    --> HEMCO_RESTART          :       true
# ----- NESTED GRID FIELDS --------------------------------------------------
    --> GC_BCs                 :       false
# ----- REGIONAL INVENTORIES ------------------------------------------------
    --> APEI                   :       false    # 1989-2014
    --> NEI2016_MONMEAN        :       false    # 2002-2020
    --> DICE_Africa            :       false    # 2013
# ----- GLOBAL INVENTORIES --------------------------------------------------
    --> CEDSv2                 :       true     # 1750-2019
    --> CEDS_GBDMAPS           :       false    # 1970-2017
    --> CEDS_GBDMAPS_byFuelType:       false    # 1970-2017

... etc ...

# ------------------------------------------------------------------------------
100     Custom                 : off   -
101     SeaFlux                : on    DMS/ACET/ALD2/MENO3/ETNO3/MOH
102     ParaNOx                : on    NO/NO2/O3/HNO3
    --> LUT data format        :       nc
    --> LUT source dir         :       $ROOT/PARANOX/v2015-02
103     LightNOx               : on    NO
    --> CDF table              :       $ROOT/LIGHTNOX/v2014-07/light_dist.ott2010.dat
104     SoilNOx                : on    NO
    --> Use fertilizer NOx     :       true

... etc ...

### END SECTION EXTENSION SWITCHES ###
```

Base emissions

Note: You do not have to edit this section if you just wish to run GEOS-Chem Classic with its default emissions configuration.

Specify how emissions and other data sets will be read from disk in the Base Emissions section of `HEMCO_Config.rc`.

```
##############################################################################
### BEGIN SECTION BASE EMISSIONS
##############################################################################

# ExtNrName sourceFile sourceVar sourceTime C/R/E SrcDim SrcUnit Species ScalIDs Cat Hier

(((EMISSIONS

#==============================================================================
# --- APEI (Canada) ---
#==============================================================================
```

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```
(((APEI
0 APEI_NO   $ROOT/APEI/v2016-11/APEI.0.1x0.1.nc NOx 1989-2014/1/1/0 RF xy kg/m2/s NO  ␣
↪25/1002/115    1 30
0 APEI_CO   $ROOT/APEI/v2016-11/APEI.0.1x0.1.nc CO  1989-2014/1/1/0 RF xy kg/m2/s CO  ␣
↪26/52/1002     1 30
0 APEI_SOAP -                                   -   -               -  -  -       SOAP␣
↪26/52/1002/280 1 30
0 APEI_SO2  $ROOT/APEI/v2016-11/APEI.0.1x0.1.nc SOx 1989-2014/1/1/0 RF xy kg/m2/s SO2 ␣
↪60/1002        1 30
0 APEI_SO4  -                                   -   -               -  -  -       SO4 ␣
↪60/65/1002     1 30
0 APEI_pFe  -

... etc ...

### END SECTION BASE EMISSIONS ###
```

Scale factors

Define scale factors for emissions inventories and other data sets in the Scale Factors section of `HEMCO_Config.rc`.

```
#==============================================================================
# --- Scale factors used for species conversions ---
#==============================================================================

# Units carbon to species conversions
# Factor = # carbon atoms * MW carbon) / MW species
40 CtoACET MATH:58.09/(3.0*12.0)   - - - xy unitless 1
41 CtoALD2 MATH:44.06/(2.0*12.0)   - - - xy unitless 1
42 CtoALK4 MATH:58.12/(4.3*12.0)   - - - xy unitless 1

... etc ...
# VOC speciations
(((RCP_3PD.or.RCP_45.or.RCP_60.or.RCP_85
50 KET2MEK    0.25  - - - xy unitless 1
51 KET2ACET   0.75  - - - xy unitless 1
)))RCP_3PD.or.RCP_45.or.RCP_60.or.RCP_85

... etc ...

### END SECTION SCALE FACTORS ###
```

Masks

Define masks for emissions and other data sets in the Masks section of `HEMCO_Config.rc`

```
  ###############################################################################
  ### BEGIN SECTION MASKS
  ###############################################################################

  # ScalID Name sourceFile sourceVar sourceTime C/R/E SrcDim SrcUnit Oper Lon1/Lat1/Lon2/
↪Lat2

  (((EMISSIONS

  #==============================================================================
  # Country/region masks
  #==============================================================================
  (((APEI
  1002 CANADA_MASK $ROOT/MASKS/v2018-09/Canada_mask.geos.1x1.nc                  MASK    ␣
↪ 2000/1/1/0 C xy 1 1 -141/40/-52/85
  )))APEI

  (((NEI2016_MONMEAN
  1007 CONUS_MASK  $ROOT/MASKS/v2018-09/CONUS_Mask.01x01.nc                      MASK    ␣
↪ 2000/1/1/0 C xy 1 1 -140/20/-50/60
  )))NEI2016_MONMEAN

  ... etc ...

  )))EMISSIONS

  ### END SECTION MASKS ###

  ### END OF HEMCO INPUT FILE ###

.. _cfg-hco-gchp-gcc:
```

Usage differences between GCHP and GEOS-Chem Classic

`HEMCO_Config.rc` is used in GCHP for masking and scaling within HEMCO. The input file and read frequency information is not used because MAPL ExtData handles file input rather than HEMCO in GCHP. Items at the top of the file that are ignored include:

- `ROOT` data directory path
- `METDIR` path
- `DiagnPrefix`
- `DiagnFreq`
- `Wildcard`

The `ROOT` data directory and `METDIR` paths are instead specified by the symbolic links in the run directory. Diagnostic filename and frequency information are specified in `HISTORY.rc`. Emissions diagnostics in GCHP are output in the same way and with the same file format as other diagnostic collections in GCHP. Please note, however, that all emissions diagnostics are vertically flipped relative to other diagnostics, with level 1 corresponding to top-of-atmosphere.

In the *Base emissions* section and beyond, columns that are ignored include:

- `sourceFile`
- `sourceVar`
- `sourceTime`
- `C/R/E`
- `SrcDim`
- `SrcUnit`

Because GCHP uses NASA MAPL code to read and regrid input files the file path, variable name, and data frequency are specified in GCHP config file `ExtData.rc`. Input data dimensions and units are not needed since they are taken directly from the file during read.

Note that some GEOS-Chem simulations require that all species be present in the restart file. For GEOS-Chem Classic you can get around this by updating the `C/R/E` flags in `HEMCO_Config.rc`. In GCHP that part of `HEMCO_Config.rc` is not used. To configure your run to allow missing species in the restart file you instead need to flip a switch in config file `setCommonRunSettings.sh`. Search for string `Require_Species_in_Restart` in the file. If set to 1 it will require species, and if set to 0 it will not.

Also beware that one entry in `HEMCO_Config.rc` is changed when script `setCommonRunSettings.sh` is executed in the run script prior to running GCHP. The online dust mass tuning factor gets replaced by a value specific to your configured grid resolution.

One entry also gets propagated to another configuration file by `setCommonRunSettings.sh`. Lightning entries in `ExtData.rc` get commented or uncommented depending on whether lightning climatology is turned on in `HEMCO_Config.rc`.

9.1.3 HEMCO_Diagn.rc

In your run directory, you will find a copy of the HEMCO diagnostic configuration file (named `HEMCO_Diagn.rc`) corresponding to the *HEMCO_Config.rc* file. You will only need to edit this file if you wish to change the default diagnostic output configuration.

Format

A snippet of the `HEMCO_Diagn.rc` for the *fullchem* simulation is shown below:

```
###############################################################################
#####  ALD2 emissions                                                     #####
###############################################################################
EmisALD2_Total      ALD2   -1     -1  -1   3   kg/m2/s  ALD2_emission_flux_from_all_
↪sectors
EmisALD2_Anthro     ALD2   0      1   -1   3   kg/m2/s  ALD2_emission_flux_from_
↪anthropogenic
EmisALD2_BioBurn    ALD2   111    -1  -1   2   kg/m2/s  ALD2_emission_flux_from_biomass_
↪burning
EmisALD2_Biogenic   ALD2   0      4   -1   2   kg/m2/s  ALD2_emission_flux_from_biogenic_
↪sources
EmisALD2_Ocean      ALD2   101    -1  -1   2   kg/m2/s  ALD2_emission_flux_from_ocean
EmisALD2_PlantDecay ALD2   0      3   -1   2   kg/m2/s  ALD2_emission_flux_from_decaying_
↪plants
EmisALD2_Ship       ALD2   0      10  -1   2   kg/m2/s  ALD2_emission_flux_from_ships
```

Columns:

1. netCDF variable name for the requested diagnostic quantity
2. Species name
3. Extension number (`-1` means sum over all extensions)
4. Category (`-1` means sum over all categories)
5. Hierarchy (`-1` means sum over all hierarchies)
6. Dimension of data (`1`: scalar, `2`: lon-lat, `3`: lon-lat-lev)
7. Units
8. Value for the `long_name` netCDF variable attribute

The prefix (e.g. `OutputDir/HEMCO_diagnostics`) for HEMCO diagnostics output files are specified in the Settings section of the HEMCO_Config.rc file.

Usage differences between GCHP and GEOS-Chem Classic

Emissions diagnostics (beginning with `Emis` or `Inv`) listed in `HEMCO_Diagn.rc` will not be archived to disk unless they are also included in the `Emissions` collection of the GCHP HISTORY.rc file. This is because GCHP relies on the MAPL **`HISTORY`** component for diagnostic archival, and thus all diagnostic ouptuts must be listed in the GCHP `HISTORY.rc` file.

Also note that the GCHP `Emissions` collection is archived such that level 1 corresponds to the top-of-atmosphere and level 72 corresponds to the surface (aka `lev:positive = 'down'`). This is in contrast to all other GCHP diagnostic collections, where level 1 is the surface and level 72 is top-of-atmopshere (aka `lev:positive = 'up'`).

9.1.4 HISTORY.rc

This content has been migrated to our *Archive output with the History diagnostics* supplemental guide.

All of the above-mentioned files are included in your *GEOS-Chem Classic run directory*.

Please see our *Customize simulations with research options* Supplemental Guide to learn how you can customize your simulation by activating alternate science options in your simulations.

9.2 Less-commonly updated configuration files

If you need to add or delete species, or to change the default photolysis and/or chemistry mechanism settings in your simulation, you'll need to edit these configuration files:

9.2.1 species_database.yml

Note: You will only need to edit `species_database.yml` if you are adding new species to a GEOS-Chem simulation.

The *GEOS-Chem Species Database* is a YAML file that contains a listing of metadata for each species used by GEOS-Chem. The Species Database is included in your run directory as file `species_database.yml`, a snippet of which is shown below.

```yaml
# GEOS-Chem Species Database
# Core species only (neglecting microphysics)
# NOTE: Anchors must be defined before any variables that reference them.
A3O2:
  Formula: CH3CH2CH2OO
  FullName: Primary peroxy radical from C3H8
  Is_Gas: true
  MW_g: 75.10
ACET:
  DD_F0: 1.0
  DD_Hstar: 1.0e+5
  Formula: CH3C(O)CH3
  FullName: Acetone
  Henry_CR: 5500.0
  Henry_K0: 2.74e+1
  Is_Advected: true
  Is_DryDep: true
  Is_Gas: true
  Is_Photolysis: true
  MW_g: 58.09

... etc ...

AERI:
  DD_DvzAerSnow: 0.03
  DD_DvzMinVal: [0.01, 0.01]
  DD_F0: 0.0
  DD_Hstar: 0.0
  Formula: I
  FullName: Iodine on aerosol
  Is_Advected: true
  Is_Aerosol: true
  Is_DryDep: true
  Is_WetDep: true
  MW_g: 126.90
  WD_AerScavEff: 1.0
  WD_KcScaleFac: [1.0, 0.5, 1.0]
  WD_RainoutEff: [1.0, 0.0, 1.0]
  WD_RainoutEff_Luo: [0.4, 0.0, 1.0]

... etc ...
```

Important: Species NO (nitrogen oxide) must be listed in `species_database.yml` as `'NO':`. This will avoid YAML readers mis-intepreting this as `no` (meaning `false`).

Each species name begins in the first column of the file, followed by a `:`. Underneath the species name follows an indented block of *species properties* in `Property: Value` format.

Some properties listed above are only applicable to gas-phase species, and others to aerosol species. But at the very least, each species should have the following properties defined:

- `Formula`

- `FullName`
- `MW_g`
- Either `Is_Gas` or `Is_Aerosol`

For more information about species properties, please see *View GEOS-Chem species properties* in the Supplemental Guides section.

9.2.2 Aerosol, chemistry, and photolysis configuration files

Note: You should not modify these files unless:

1. You need to update aerosol optical properties (such as cross-sections) that are used to compute aerosol optical depth.
2. You need to add or remove species for which photolysis rates will be computed.
3. You need to modify the GEOS-Chem chemical mechanism.

Aerosol optics configuration files

The following files (stored in the `ExtData/CHEM_INPUTS/AEROSOL_OPTICS/Aerosol_Optics` directory tree) contain optical properties for several aerosol species. See the *geoschem_config.yml* file for the current file path specification.

File	Contains optical properties for ...
`brc.dat`	Brown carbon optical properties
`dust.dat`	Mineral dust optical properties
`org.dat`	Organic carbon optical properties
`so4.dat`	Sulfate optical properties
`soot.dat`	Black carbon optical properties
`ssa.dat`	Accumulation-mode sea salt aerosol
`ssc.dat`	Coarse-mode sea salt aerosol
`h2so4.dat`	Sulfuric acid

The properties are provided at multiple wavelengths to be used in the online calculation of the aerosol optical depth diagnostics. Up to three wavelentghs can be selected in the Radiation Menu of input.geos. These properties are also used for in the RRTMG radiative transfer model (if enabled).

Chemical mechanism configuration files

GEOS-Chem Classic and GCHP simulations use source code generated by The Kinetic PreProcessor. If you need to update the default chemistry mechanism, you will need to do the following steps:

1. Modify the relevant KPP configuration files (described below);
2. Run KPP to generate updated solver source code;
3. Recompile the GEOS-Chem source code to create a new executable;
4. Run your simulation.

Chemical mechanism configuration files are located in these folders:

KPP/fullchem

Contains configuration files for the default "full-chemistry" mechanism (NOx + Ox + aerosols + Br + Cl + I).

- `fullchem.kpp`: Main configuration file for the **fullchem** mechanism.
- `fullchem.eqn`: List of species and reactions for the **fullchem** mechanism.

KPP/carbon

Contains configuration files for the carbon gases mechanism (CH4-CO2-CO-OCS):

- `carbon.kpp`: Main configuration file for the **carbon** mechanism.
- `carbon.eqn`: List of species and reactions for the **carbon** mechanism.

KPP/custom

Contains configuration files that you can edit if you need to create a custom mechanism. We recommend that you create the custom in this folder and leave `KPP/fullchem` and `KPP/Hg` untouched.

- `custom.kpp`: Copy of `fullchem.kpp`
- `custom.eqn`: Copy of `fullchem.eqn`.

KPP/Hg

Contains configuration files for the mercury chemistry mechanism:

- `Hg.kpp`: Main configuration file for the **Hg** mechanism.
- `Hg.eqn`: List of species and reactions for the **Hg** mechanism.

Please see the following references for more information about KPP:

1. The KPP user manual (kpp.readthedocs.io)
2. Supplemental Guide: *Update chemical mechanisms with KPP*

Photolysis configuration files

Configuration files containing photolysis parameters (such as quantum yields, cross sections, branching ratios, etc.) may be found in subdirectories of `ExtData/CHEM_INPUTS/CLOUD-J/`. See the *geoschem_config.yml* file for the current file path specifications.

At present, the mercury (Hg) simulation still uses the legacy **FAST-JX** photolysis scheme. Configuration files for **FAST-JX** may be found in the `ExtData/CHEM_INPUTS/FAST-JX/` directory tree.

CHAPTER

TEN

DOWNLOAD INPUT DATA

In the following chapters, you will learn how to download input data for your GEOS-Chem simulation.

Note: If you are located at an institution with several GEOS-Chem users, the input data for GEOS-Chem Classic may have already been downloaded to a shared data directory on your system. If this is the case for you, feel fee to skip ahead to the *Run your simulation* chapter.

10.1 GEOS-Chem Input Data on AWS cloud

The GEOS-Chem Input Data portal provides essential datasets for GEOS-Chem Classic, GCHP, and HEMCO. This includes NASA/GMAO MERRA-2 and GEOS-FP *meteorological products*, *chemistry input data*, *emissions input data*, and other smaller datasets such as model *initial conditions*. We will continuously upload and maintain the data in an S3 Bucket (s3://geos-chem) for convenient access.

Note: We are pleased to announce that the GEOS-Chem Input Data portal is part of the AWS Open Data Sponsorship Program. As a result, **the data is completely free to use**. You will NOT incur any data egress fees when downloading data from the s3://geos-chem bucket. This is now the recommended repository for GEOS-Chem data download.

In the following chapters, we will describe how the GEOS-Chem Input Data portal is organized and how to access the data stored there.

10.1.1 Why do we store GEOS-Chem data on the cloud?

Storing the GEOS-Chem Input Data portal on the AWS cloud offers several advantages:

Scalability

Cloud storage scales seamlessly to accommodate growing datasets without the need for physical infrastructure upgrades.

Accessibility

Data hosted on the cloud can be *accessed from anywhere in the world*, facilitating collaboration among teams. Data stored at the GEOS-Chem Input Data portal is covered by the AWS Open Data Sponsorship Program. and may be downloaded without incurring any data egress fees.

Performance

Setting up a high-resolution nested simulation often requires significant time to retrieve the necessary meteorological fields. The new paradigm to solve this big data challenge is to "move compute to data", meaning that computations are performed directly in the cloud environment where the data is already available. This approach leverages Amazon's considerable infrastructure, providing users with a more customized computing environment (For more information, see Running GCHP on AWS).

10.1.2 The GEOS-Chem Input Data portal

The main GEOS-Chem Input Data portal is hosted at the AWS S3 bucket s3://geos-chem. From here you may download the data required to run **GEOS-Chem Classic**, **GCHP**, or **HEMCO standalone** simulations.

Note: We are pleased to announce that the GEOS-Chem Input Data portal is part of the AWS Open Data Sponsorship Program. As a result, **the data is completely free to use**. You will NOT incur any data egress fees when downloading data from the s3://geos-chem bucket. This is now the recommended repository for GEOS-Chem data download.

We also maintain *additional portals for special meteorology products*.

Data organization

The GEOS-Chem Input Data portal is structured into the following categories:

1. *Initial conditions input data* (aka Restart files)
2. *Chemistry input data*
3. *Emissions input data*
4. *Meteorology input data*

Initial conditions input data

Initial conditions include initial species concentrations (aka Restart files) used to start a GEOS-Chem simulation.

Chemistry input data

Chemistry input data includes:

- Tables of aerosol optical properties
- Quantum yields and cross sections for photolysis using either **Cloud-J** or legacy **FAST-JX**
- Climatology data for **Linoz** stratospheric ozone chemistry
- Boundary conditions for **UCX** stratospheric chemistry routines

Emissions input data

Emissions input data includes the following data:

- Emissions inventories
- Input data for **HEMCO** Extensions
- Input data for **GEOS-Chem** specialty simulations
- Scale factors
- Mask definitions
- Surface boundary conditions
- Leaf area indices
- Land cover map

Meteorology input data

GEOS-Chem Classic be driven by the following meteorology products:

1. MERRA-2
2. GEOS-FP
3. GEOS-IT
4. GCAP 2.0 (available at the atmos.earth.rochester.edu data portal)

> **Attention:** We are still evaluating GEOS-Chem with the new NASA GEOS-IT meterorology product. For the time being, you should use one of the other meteorology options.

Data access

You may access the GEOS-Chem Input Data portal in several ways, as described below.

AWS S3 Explorer

You can browse the contents of the GEOS-Chem Input Data portal with the **AWS S3 Explorer** interface. Simply point your web browser to the following link:

- https://geos-chem.s3.amazonaws.com/index.html.

This is an easy way for you to familiarize yourself with the directory structure. Before downloading large amounts of data, we recommend that you use the AWS S3 Explorer to find the path to the relevant data directories.

AWS CLI (command-line interface)

You can also use the AWS command-line interface (aka **AWS CLI**) to browse and download data from the GEOS-Chem Input Data portal.

For example, if you have an AWS account and have installed AWS CLI on your system, you may use this command to get a data listing:

```
$ aws s3 ls s3://geos-chem/   # Get a directory listing
```

If you do not have an AWS account (or do not wish to open one), you may still use AWS CLI to access or download data via anonymous login, which is completely free. Simply add the `--no-sign-request` flag after each AWS CLI command, such as:

```
$ aws s3 ls --no-sign-request s3://geos-chem/   # Get a directory listing via anonymous␣
↪login
```

For detailed instructions about using AWS CLI, please see: *Tutorial: Accessing GEOS-Chem Input Data using AWS CLI*.

HTTP or wget download

You can also access the GEOS-Chem Input Data portal via the alternate web link http://geoschemdata.wustl.edu.

As with the AWS S3 Explorer, you can navigate through the web interface to find the data sets that you wish to download. You can then use the **wget** command to download the data.

Dry-run simulation (GEOS-Chem Classic and HEMCO standalone only)

If you plan to run a GEOS-Chem Classic or HEMCO standalone simulation, we recommend first performing a **dry-run simulation**. The dry-run simulation workflow is as follows:

1. Configure your GEOS-Chem Classic or HEMCO standalone simulation.
2. Run GEOS-Chem Classic or HEMCO standalone with the `--dryrun` flag. This will generate a list of required data files.
3. Pass this list to a Python script, which will download the data to your computer system or AWS EC2 instance.

For more information, please see the following links:

- GEOS-Chem Classic dry-run instructions
- HEMCO standalone dry-run instructions

Globus

Many institutions use the **Globus** file transfer utility, which has much higher data download speeds than normal SSH or HTTP connections.

If your institution uses Globus, you can download data from the **GEOS-Chem Data (WashU)** endpoint to your computer system.

Bashdatacatalog

We have created the **bashdatacatalog** tool to facilitate downloading large amounts of data from the GEOS-Chem Input Data portal. Please see our *Manage a data archive with bashdatacatalog* guide for usage instructions.

Example directory structure

The directory structure of the GEOS-Chem Input Data portal adheres to the format listed below. You can see easily browse through the portal using one of the following web links:

- https://geos-chem.s3.amazonaws.com/index.html (Recommended)
- http://geoschemdata.wustl.edu

```
ExtData/
│
├── GEOSCHEM-RESTARTS/
│   ├── GC_14.2.0/
│   ├── GC_14.3.0/
│   └── ...
│
├── CHEM_INPUTS/
│   ├── CLOUD-J/
│   ├── FAST-JX/
│   └── ...
│
├── HEMCO/
│   ├── UVALBEDO/
│   └── ...
│
├── GEOS_0.5x0.625/
│   ├── MERRA2/
│   │   ├── 2023/
│   │   ├── 2024/
│   │   └── ...
│   └── ...
│
├── GEOS_0.25x0.3125/
│   ├── GEOS_FP/
│   │   ├── 2023/
│   │   ├── 2024/
│   │   └── ...
│   ├── GEOS_FP_Raw/
│   └── ...
│
└── ...
```

10.1.3 Tutorial: Accessing GEOS-Chem Input Data using AWS CLI

This tutorial will guide you through the process of accessing and using the *GEOS-Chem Input Data* with AWS CLI. Alternatively, you can access the data via AWS S3 Explorer.

Note: When you open an AWS account you will be asked for credit card information. But even if you don't have (or don't wish to open) an AWS account, you may still access and download the GEOS-Chem Input Data using AWS CLI with anonymous login, which is completely free.

The workflow is:

1. *Install AWS CLI*
   - This step only has to be done once.
2. *Configure AWS CLI*
   - You may skip this step if you do not have (or do not wish to open) an AWS account.
3. *Download data from the GEOS-Chem Input Data portal*.
4. *Run a GEOS-Chem Classic, GCHP, or HEMCO standalone simulation*.

Install AWS CLI

Follow the installation instructions from the AWS CLI User Guide.

Configure AWS CLI (if you already have an AWS account)

Note: You may *skip ahead to the next section* if you do not have (or do not wish to open) an AWS account but wish to access the data via anonymous login.

Configure AWS CLI with this command:

```
$ aws configure
```

and supply your credentials when prompted.

For instructions on `aws configure`, refer to the Configure the AWS CLI .

Access and download data

Step 1: List available data

To view the available data in the GEOS-Chem Input Data S3 bucket, use one of the following commands:

If you have an AWS account:

```
$ aws s3 ls s3://geos-chem/
```

If you do not have an AWS account:

```
$ aws s3 ls --no-sign-request s3://geos-chem/
```

Tip: Adding the `--no-sign-request` flag to any AWS CLI command will access or download data via anonymous login.

Step 2: Navigate through the directories

You can navigate through the directories to find the specific data you need. For example,

If you have an AWS account:

```
$ aws s3 ls s3://geos-chem/GEOS_0.5x0.625/MERRA2/2024/05
```

If you do not have an AWS account:

```
$ aws s3 ls --no-sign-request s3://geos-chem/GEOS_0.5x0.625/MERRA2/2024/05
```

Step 3: Download the data

Tip: If you are using **`GEOS-Chem Classic`** or the **`HEMCO standalone model`**, you can download data with a dry-run simulation, while still using the AWS CLI data transfer protocol.

Once you have located the data you need, you can download it to your local cluster or an EC2 instance. For example,

If you have an AWS account:

```
$ aws s3 cp s3://geos-chem/GEOS_0.5x0.625/MERRA2/2024/05 ./ --recursive
```

If you do not have an AWS account:

```
$ aws s3 cp --no-sign-request s3://geos-chem/GEOS_0.5x0.625/MERRA2/2024/05 ./ --recursive
```

This command will copy the data to your current path.

Run simulations using downloaded data

Once you have *downloaded the data* from the GEOS-Chem Input Data portal to your computer system or EC2 instance, you may run a **`GEOS-Chem Classic`**, **`GCHP`**, or **`HEMCO standalone`** simulation. Please refer to the relevant user guide listed below.

- GEOS-Chem Classic Quickstart Guide
- GCHP Quickstart Guide
- HEMCO Standalone Guide

Running GCHP on AWS

If you wish to use the computing resources on AWS to run GCHP and are seeking for an AMI, feel free to check our Set up AWS ParallelCluster guide.

10.2 Additional portals for meteorology data

As discussed in the previous chapter, the *GEOS-Chem Input Data* portal is the main source of input data for **GEOS-Chem Classic**, **GCHP**, and the **HEMCO standalone model**. This portal contains the entire catalog of emissions inventories, chemical inputs, initial conditions, and most years of GEOS-FP, MERRA-2, and GEOS-IT meteorology.

We also maintain two additional data portals for special data sets.

10.2.1 GEOS-Chem Nested Input Data

Note: Data stored at the GEOS-Chem Nested Input Data portal is covered by the AWS Open Data Sponsorship Program. and may be downloaded without incurring any data egress fees.

We are still adding data to the GEOS-Chem Nested Input Data portal. As of this writing (January 2025), not all data may have been uploaded yet. We thank you for your patience.

The GEOS-Chem Nested Input data portal stores GEOS-FP and MERRA-2 meteorology fields that have been cropped to specific nested-grid domains. These data can be used to perform high-resolution inversions with the Integrated Methane Inversion (IMI) workflow.

Table 1: Available nested-grid meteorology (2018 to present day)

Product	Horizontal resolution	Nested-grid domains
GEOS-FP	$0.125° \times 0.15625$	AF (Africa) AS (Asia) EU (Europe) ME (Middle East) NA (North America) OC (Oceania) RU (Russia) SA (South America)
MERRA 2	$0.5° \times 0.625°$	AS (Asia) EU (Europe) NA (North America)

The data can be accessed by:

- AWS S3 Explorer (https://gcgrid.s3.amazonaws.com/index.html)
- Direct HTTP or wget download
- *Dry-run simulation*

The GEOS-Chem Nested Input Data portal is also part of the AWS Open Data Sponsorship Program.

10.2.2 GCAP 2.0 meteorology hosted at U. Rochester

The atmos.earth.rochester.edu portal (curated by Lee Murray at the University of Rochester) contains the GCAP 2.0 meteorological data inputs for use with GEOS-Chem simulations.

The data can be accessed by:

- Direct HTTP or wget download (http://atmos.earth.rochester.edu/input/gc/ExtData/)
- *Dry run simulation*

10.3 Restart files

In the following chapers, you will learn about **restart files** and how they are used.

10.3.1 What is a restart file?

Restart files contain species concentrations, as well as other quantities that are needed to initialize GEOS-Chem simulations. GEOS-Chem simulations use two separate restart files.

`GEOSChem.Restart.YYYYMMDD_hhmmz.nc4`

Format: netCDF

Description: The *GEOS-Chem Classic restart file*. Contains species concentrations that are read at simulation startup.

GEOS-Chem writes a restart file at the end of each simulation. This allows a long simulation to be split into several individual run stages. For example, the restart file that was created at 00:00 UTC on August 1, 2019 is named: `GEOSChem.Restart.20190801_0000z.nc4`. The `z` character indicates "Zulu" time (aka UTC).

GEOS-Chem restart files are created in the `Restarts/` folder of your *GEOS-Chem run directory* directory.

`HEMCO_restart.YYYYMMDDhhmm.nc`

Format: netCDF

Description: The *HEMCO restart file*. HEMCO archives certain quantities (mostly pertaining to soil NOx and biogenic emissions in order to facilitate long GEOS-Chem simulations with several run stages.

HEMCO restart files are created in the `Restarts/` folder of your *GEOS-Chem run directory* directory.

When you run a GEOS-Chem simulation, it will write new GEOS-Chem restart files at the intervals you specify in *HISTORY.rc*. New HEMCO restart files are written with frequency configured in *HEMCO_Config.rc*.

Viewing and manipulating restart files

Please see the following sections of our Supplemental Guide: *Work with netCDF files* for more information on how you can view and manipulate data in restart files:

1. *Useful tools*
2. *Regrid netCDF files*
3. *Add a new variable to a netCDF file*
4. *Crop netCDF files*
5. *Chunk and deflate a netCDF file to improve I/O*

10.3.2 GEOS-Chem restart files

How are restart files read into GEOS-Chem?

GEOS-Chem restart files are read via HEMCO. The entries listed below have been added to `HEMCO_Config.rc` (and may vary slightly for different simulation types). These fields are obtained from HEMCO and copied to the appropriate `State_Chm` and `State_Met` fields in routine `Get_GC_Restart` (located in `GeosCore/hcoi_gc_main_mod.F90`).

```
#==============================================================================
# --- GEOS-Chem restart file ---
#==============================================================================
(((GC_RESTART
* SPC_            ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 SpeciesRst_?ALL?
 ↪$YYYY/$MM/$DD/$HH EFYO xyz 1 * - 1 1
* DELPDRY         ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Met_DELPDRY
 ↪$YYYY/$MM/$DD/$HH EY   xyz 1 * - 1 1
* KPP_HVALUE      ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_KPPHvalue
 ↪$YYYY/$MM/$DD/$HH EY   xyz 1 * - 1 1
* WETDEP_N        ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_WetDepNitrogen
 ↪$YYYY/$MM/$DD/$HH EY   xy  1 * - 1 1
* DRYDEP_N        ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_DryDepNitrogen
 ↪$YYYY/$MM/$DD/$HH EY   xy  1 * - 1 1
* SO2_AFTERCHEM   ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_SO2AfterChem
 ↪$YYYY/$MM/$DD/$HH EY   xyz 1 * - 1 1
* H2O2_AFTERCHEM ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_H2O2AfterChem
 ↪$YYYY/$MM/$DD/$HH EY   xyz 1 * - 1 1
* AEROH2O_SNA     ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_AeroH2OSNA
 ↪$YYYY/$MM/$DD/$HH EY   xyz 1 * - 1 1
* ORVCSESQ        ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_ORVCSESQ
 ↪$YYYY/$MM/$DD/$HH EY   xyz 1 * - 1 1
* JOH             ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_JOH
 ↪$YYYY/$MM/$DD/$HH EY   xy  1 * - 1 1
* JNO2            ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_JNO2
 ↪$YYYY/$MM/$DD/$HH EY   xy  1 * - 1 1
* STATE_PSC       ./Restarts/GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_StatePSC
 ↪$YYYY/$MM/$DD/$HH EY   xyz count * - 1 1
)))GC_RESTART
```

GEOS-Chem species (the `SPC_` entry) use HEMCO time cycle flag `EFYO` by default. Other restart file fields use the time cycle flag `EY`. These are explained below.

E

: **`Exact`**: Stops with an error if the date of the simulation is different than the file timestamp.

F

: **`Forced`**: Stops with an error if the file isn't found.

Y

: **`Simulation Year`**: Only reads the data for the simulation year but not for other years.

O

: **`Once`**: Does not keep cycling in time but only reads the file once.

When reading the **species concentrations** (time cycle flag: `EFYO`) from the restart file, HEMCO will cause your simulation to stop with an error if:

1. The restart file is missing, or;
2. Any species is not found in the restart file, or;
3. The date in the restart file (which is usually 20190101 or 20190701, depending on your simulation) differs from the start date listed in *geoschem_config.yml*.

When reading **other restart file fields** (time cycle flag: `EY`). HEMCO will stop with an error if:

1. The restart file is missing, or
2. The date in the restart file (which is usually 20190101 or 20190701, depending on your simulation) differs from the start date listed in *geoschem_config.yml*.

Attention: If you wish to spin up a GEOS-Chem simulation with a restart file that has (1) missing species or (2) a timestamp that does not match the start date in *geoschem_config.yml*, simply change the time cycle flag from

```
* SPC_ ... $YYYY/$MM/$DD/$HH EFYO xyz 1 * - 1 1
```

to

```
* SPC_ ... $YYYY/$MM/$DD/$HH CYS xyz 1 * - 1 1
```

This will direct HEMCO to read the closest date available (`C`), to use the simulation year (`Y`), and to skip any species (`S`) not found in the restart file.

Skipped species will be assigned the initial concentration (units: $mol\ mol^{-1}$ w/r/t dry air) specified by its `BackgroundVV` entry in *species_database.yml*. If the species does not have a `BackgroundVV` value specified, then its initial concentration will be set to 1.0×10^{-20} instead.

How can I determine the date of a restart file?

To determine the date of a netCDF restart file, you may use **`ncdump`**. For example:

```
ncdump -v time -t GEOSChem.Restart.YYYYMMDD_hhmmz.nc4
```

The **`-t`** option will return the time value in human-readable date-time strings rather than numerical values in unit such as `"hours since 1985-1-1 00:00:0.0.`

Where can I get a restart file for my simulation?

GEOS-Chem Classic *run directories* are configured to use sample GEOS-Chem restart files in **`netCDF`** format. These files are available for download at the *The GEOS-Chem Input Data portal* portal.

Tip: We recommend that you download restart files to your disk space with either a dry-run simulation or with the bashdatacatalog. This will ensure that the proper files will be downloaded.

If you have the `ExtData/GEOSCHEM_RESTARTS` folder in your GEOS-Chem data paths, then a sample restart file will be copied to your run directory when you *generate a new GEOS-Chem classic run directory*.

Monthly GEOS-Chem restart files from the GEOS-Chem 14.0.0 10-year benchmark may be found here.

Attention: The sample restart files do not reflect the actual atmospheric state and should only be used to "spin up" the model. In other words, they should be used as initial values in an initialization simulation to generate more accurate initial conditions for your production runs.

For how long should I spin up before starting a production simulation?

Doing a 6-month year spin up is usually sufficient for full-chemistry simulations. We recommend ten years for ozone, carbon dioxide, and methane simulations, and four years for radon-lead-beryllium simulations. If you are in doubt about how long your spin up should be for your simulation, we recommend contacting the GEOS-Chem Working Group that specializes in your area of research.

You may spin up the model starting at any year for which there is met data, but you should always start your simulations at the month and day corresponding to the restart file to more accurately capture seasonal variation. If you want to start your production run at a specific date, we recommend doing a spin up for the appropriate number of years plus the number of days needed to reach your ultimate start date. For example, if you want to do a production simulation starting on 2019/12/01, you could spin up the model for one year using the initial GEOS-FP restart file dated 2019/07/01 and then use the new restart file to spin up the model for five additional months, from 2019/07/01 to 2019/12/01.

How do I check my initial conditions?

To ensure you are using the expected initial conditions for your simulation, please check the GEOS-Chem log file. You should see something like:

```
HEMCO: Opening ./Restarts/GEOSChem.Restart.20190701_0000z.nc4
     - Found all CN     met fields for 2011/01/01 00:00
     - Found all A1     met fields for 2019/07/01 00:30
     - Found all A3cld  met fields for 2019/07/01 01:30
     - Found all A3dyn  met fields for 2019/07/01 01:30
     - Found all A3mstC met fields for 2019/07/01 01:30
     - Found all A3mstE met fields for 2019/07/01 01:30
     - Found all I3     met fields for 2019/07/01 00:00
 Initialize DELP_DRY from restart file
     - Found all I3     met fields for 2019/07/01 03:00
================================================================================
R E S T A R T   F I L E   I N P U T
Min and Max of each species in restart file [mol/mol]:
Species   1,     ACET: Min = 1.000458833E-22  Max = 6.680149323E-09
Species   2,     ACTA: Min = 6.574137699E-23  Max = 6.108235029E-10
Species   3,     AERI: Min = 4.122849756E-16  Max = 1.213838925E-11
Species   4,     ALD2: Min = 4.186668786E-23  Max = 4.571487633E-09
...
```

If a species is not found in the restart file, you may see something like:

```
Species 178,       pFe: Use background = 9.999999683E-21
```

How are GEOS-Chem restart files written?

GEOS-Chem restart files are now saved via the History component. A *Restart collection* has been defined in *HISTORY.rc* and fields saved out to the restart file can be modified in that file.

10.3.3 HEMCO restart files

In this chapter, you will learn more about HEMCO restart files.

Do I need a HEMCO restart file for my initial spin-up run?

Using a HEMCO restart file for your initial spin up run is optional.

The HEMCO restart file contains fields for initializing variables required for Soil NOx emissions, MEGAN biogenic emissions, and the UCX chemistry quantities. The HEMCO restart file that comes with a run directory may only be used for the date and time indicated in the filename. HEMCO will automatically recognize when a restart file is not available for the date and time required, and in that case HEMCO will use default values to initialize those fields. You can also force HEMCO to use the default initialization values by setting `HEMCO_RESTART` to false in `HEMCO_Config.rc`.

For more information

Please see HEMCO diagnostics (at hemco.readthedocs.io) for more information about restart files and other diagnostic outputs from HEMCO.

10.4 Download data with a dry-run simulation

Tip: If you are located at an institution with many other GEOS-Chem users, then the necessary input data might have already been downloaded and stored in a commmon directory on your system. Ask your sysadmin or IT support staff.

Please see our *Download input data* chapter for other ways in which you can download the necessary input data for GEOS-Chem.

A **`dry-run`** is a is a **`GEOS-Chem Classic`** simulation that steps through time, but does not perform computations or read data files from disk. Instead, a dry-run simulation prints a list of all data files that a regular GEOS-Chem simulation would have read. The dry-run output also denotes whether each data file was found on disk, or if it is missing. This output can be fed to a script which will download the missing data files to your computer system.

You may generate dry-run output for any of the GEOS-Chem Classic simulation types (*`fullchem`*, *`carbon`*, *`TransportTracers`*, etc.)

In the following chapters, you will learn how to you can download data using the output from a dry-run simulation:

10.4.1 Execute a dry-run simulation

Follow the steps below to perform a GEOS-Chem Classic dry-run simulation:

Complete preliminary setup

Make sure that you have done the following steps;

1. *Downloaded GEOS-Chem Classic source code*
2. *Compiled the source code*
3. *Configured your simulation*

Then doublecheck these settings in the following *configuration files*:

geoschem_config.yml

1. *start_date*: Set the start date and time for your simulation.
2. *end_date*: Set the end date and time for your simulation.
3. *met_field*: Check if the meteorology setting (*GEOS-FP*, *MERRA2*, *GCAP2*) is correct for your simulation.

   Important: The convection scheme used for GEOS-FP met generation changed from RAS to Grell-Freitas with impact on GEOS-FP meteorology files starting June 1, 2020. For this reason we recommend using MERRA-2 instead of GEOS-FP if running a simulation across June 1, 2020 to avoid unexpected discontinuities. Additional information about the impact of the convection change is at geoschem/geos-chem#1409.

4. *root_data_dir*: Make sure that the path to `ExtData` is correct.

HISTORY.rc

1. Set the frequency and duration for each *diagnostic collection* to be consistent with the settings in *geoschem_config.yml*.

HEMCO_Config.rc

1. Check the Settings section to make sure that diagnostic frequency `DiagnFreq`: is set to the interval that you wish (e.g. `Monthly`, `Daily`, `YYYYMMDD hhmmss`, etc).
2. Check the Extension Settings section, to make sure all of the required emissions inventories and data sets for your simulation have been switched on.

Tip: You can reduce the amount of data that needs to be downloaded for your simulation by turning off inventories that you don't need.

Run the executable with the `--dryrun` flag

Run the GEOS-Chem Classic executable file at the command line with the **`--dryrun`** command-line argument as shown below:

```
$ ./gcclassic --dryrun | tee log.dryrun
```

The **`tee`** command will send the output of the dryrun to the screen as well as to a file named `log.dryrun`.

The `log.dryrun` file will look somewhat like a regular GEOS-Chem log file but will also contain a list of data files and whether each file was found on disk or not. This information will be used by the `download_data.py` script in the next step.

You may use whatever name you like for the dry-run output log file (but we prefer `log.dryrun`). You will need this file to download data (*see the next chapter*).

10.4.2 Download data from dry-run output

Once you have successfully executed a GEOS-Chem dry-run, you can use the output from the dry-run (contained in the `log.dryrun` file) to download the data files that GEOS-Chem will need to perform the corresponding "production" simulation. You may download from different *data repositories*.

Important: Before you use the `download_data.py` script, make sure to initialize a Mamba or Conda environment with the relevant command shown below:

```
$ mamba activate ENV-NAME   # If using Mamba

$ conda activate ENV-NAME   # If using Conda
```

Here `ENV-NAME` is the name of your environment.

Also make sure that you have installed the PyYAML module to your conda environment. PyYAML will allow the `download_data.py` script to read certain configurable settings from a YAML file in your run directory.

The Python environment for GCPy has all of the proper packages that you need to download data from a dry-run simulation. For more information, please see gcpy.readthedocs.io.

Choose a data portal

You can *download input data* from any of the portals listed below.

Table 2: GEOS-Chem data portals and access methods

Portal	S3 Explorer	AWS CLI	HTTP	Bashdata-catalog	Globus
GEOS-Chem Input Data (The main source of GEOS-Chem input data)	Yes	Yes	Yes	Yes	Yes
GEOS-Chem Nested Input Data	Yes	Yes	Yes	No	No
GCAP 2.0 meteorology hosted at U. Rochester	No	No	Yes	No	No

Run the `download_data.py` script on the dryrun log file

Navigate to your GEOS-Chem run directory where you executed the dry-run and type.

```
$ ./download_data.py log.dryrun PORTAL-NAME
```

where:

- `download_data.py` is the dry-run data download program (written in Python). It is included in each *GEOS-Chem Classic run directory* that you create.
- `log.dryrun` is the log file from your GEOS-Chem dry-run simulation.
- `PORTAL-NAME` specifies the data portal that you wish to download from. Allowed values are:

Table 3: Allowed values for the `PORTAL-NAME` argument to `download_data.py`

Value	Downloads from portal	With this command	Via this method
geoschem+aws	*GEOS-Chem Input Data*	**`aws s3 cp`**	AWS CLI
geoschem+http	*GEOS-Chem Input Data*	**`wget`**	HTTP
nested+aws	*GEOS-Chem Nested Input Data*	**`aws s3 cp`**	AWS CLI
nested+http	*GEOS-Chem Nested Input Data*	**`wget`**	HTTP
rochester	*GCAP 2.0 met data @ Rochester*	**`wget`**	HTTP

For example, to download data from the *GEOS-Chem Input Data* portal using the AWS CLI download (which is faster than HTTP download), use this command:

```
$ ./download_data.py log.dryrun geoschem+s3
```

Note: You must have the AWS CLI (command-line interface) software installed on your system before in order to use the `geoschem+aws` or `nested+aws` options in the table listed above.

The `download_data.py` program will generate a **log of unique data files** (i.e. with all duplicate listings removed), which looks similar to this:

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!! LIST OF (UNIQUE) FILES REQUIRED FOR THE SIMULATION
!!! Start Date       : 20190701 000000
!!! End Date         : 20190701 010000
!!! Simulation       : fullchem
!!! Meteorology      : MERRA2
!!! Grid Resolution  : 4.0x5.0
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
./HEMCO_Config.rc
./HEMCO_Config.rc.gmao_metfields
./HEMCO_Diagn.rc
./HISTORY.rc
./Restarts/GEOSChem.Restart.20190701_0000z.nc4 --> /home/ubuntu/ExtData/GEOSCHEM_
↪RESTARTS/GC_14.5.0/GEOSChem.Restart.fullchem.20190701_0000z.nc4
./Restarts/HEMCO_restart.201907010000.nc
./geoschem_config.yml
/path/to/ExtData/CHEM_INPUTS/CLOUD_J/v2024-09/FJX_j2j.dat
```

(continues on next page)

(continued from previous page)

```
/path/to/ExtData/CHEM_INPUTS/CLOUD_J/v2024-09/FJX_scat-aer.dat
/path/to/ExtData/CHEM_INPUTS/CLOUD_J/v2024-09/FJX_scat-cld.dat
/path/to/ExtData/CHEM_INPUTS/CLOUD_J/v2024-09/FJX_scat-ssa.dat
/path/to/ExtData/CHEM_INPUTS/CLOUD_J/v2024-09/FJX_spec.dat
/path/to/ExtData/CHEM_INPUTS/FastJ_201204/fastj.jv_atms_dat.nc
/path/to/ExtData/CHEM_INPUTS/Linoz_200910/Linoz_March2007.dat
/path/to/ExtData/CHEM_INPUTS/Olson_Land_Map_201203/Olson_2001_Drydep_Inputs.nc
/path/to/ExtData/CHEM_INPUTS/UCX_201403/NoonTime/Grid4x5/InitCFC_JN2O_01.dat

 ... etc ...
```

This name of this "unique" log file will be the same as the log file with dryrun ouptut, with `.unique` appended. In our above example, we passed `log.dryrun` to `download_data.py`, so the "unique" log file will be named `log.dryrun.unique`. This "unique" log file can be very useful for documentation purposes.

Skip download, but create log of unique files

If you wish to only produce the *log of unique data files without downloading any data, then type the following command from within your GEOS-Chem run directory:

```
$ ./download_data.py log.dryrun skip-download
```

or for short:

```
$ ./download_data.py log.dryrun skip
```

This can be useful if you already have the necessary data downloaded to your system but wish to create the log of unique files for documentation purposes (such as for benchmark simulations, etc.)

CHAPTER

ELEVEN

RUN YOUR SIMULATION

In the following chapters, you will learn how to run your GEOS-Chem Classic simulation on your computer system.

11.1 Create a run script

We recommend that you create a **run script** for your GEOS-Chem simulation. This is a bash script containing the commands to run GEOS-Chem.

A sample run script for the Simple Linux Utility for Resource Management (SLURM) is shown below. SLURM is a "scheduler"—a root-level program that decides if there are sufficient resources (cores, memory, available time) for a job to run. If not, SLURM will delay starting the job until resources free up.

Note: If your computer system uses a different scheduler (e.g. LSF, PBS), simply replace the SLURM-specific commands with the equivalent commands for your scheduler. Ask your sysadmin or IT staff for more information.

```
#!/bin/bash

#SBATCH -c 8
#SBATCH -N 1
#SBATCH -t 0-12:00
#SBATCH -p PARTITION
#SBATCH --mem=15000
#SBATCH --mail-type=END

################################################################################
### Sample GEOS-Chem Classic run script (using SLURM).
###
### If you are running a nested-grid simulation at fine resolution, you
### will likely need to request additional memory, cores, and time.
###
### -c           : Requests this many cores
### -N           : Requests a single node
### --mem        : Requests this amount of memory in GB
### -p           : Requests these partitions where the job can run
### -t           : Requests time for the job (days-hours:minutes)
###  --exclusive : Reserves entire nodes (i.e. to prevent backfilling jobs)
################################################################################

# Source the environment file you have created for your system
```

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```
source /path/to/gcclassic.gnu10.env

# Set the proper # of threads for OpenMP
# SLURM_CPUS_PER_TASK ensures this matches the number you set with -c above
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# Run GEOS_Chem.  The "time" command will return CPU and wall times.
# Stdout and stderr will be directed to the "GC.log" log file
# (you can change the log file name below if you wish)
srun -c $OMP_NUM_THREADS time -p ./gcclassic >> GC.log

# Exit normally
exit 0
```

Important commands in the run script are listed below:

#SBATCH `-c 8`

Tells SLURM to request 8 computational cores. You may choose a different number of cores depending on the type of node you are using. Most modern computer clusters have nodes with up to 64 (or more) cores.

#SBATCH `-N 1`

Tells SLURM to request 1 computational node.

Important: GEOS-Chem Classic uses OpenMP, which is a shared-memory parallelization model. Using OpenMP limits GEOS-Chem Classic to one computational node.

#SBATCH `-t 0-12:00`

Tells SLURM to request 12 hours of computational time. The format is `D-hh:mm` or (`days-hours:minutes`).

#SBATCH `-p PARTITION`

Tells SLURM to run GEOS-Chem Classic in the computational partition (aka "queue") named `PARTITION`. Ask your IT staff for a list of the available partitions (queues) on your system.

Note: With SLURM, you may specify more than one partition with:

```
#SBATCH -p PARTITION1,PARTITION2,PARTITION3,...
```

Your job will run on whichever partition first has sufficient resources.

If you have different scheduler on your system, ask your sysadmin or IT staff if your scheduler allows you to specify multiple partitions when submitting jobs.

#SBATCH `--mem=15000`

Tells SLURM to reserve 15000 MB (15 GB) of memory for the simulation.

#SBATCH `--mail-type=END`

Tells SLURM to send an email upon completion (successful or unsuccesful) of the simulation.

export `OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK`

Specifies how many computational cores that GEOS-Chem Classic should use. The environment variable `SLURM_CPUS_PER_TASK` will fill in the number of cores requested (in this example, we used `#SBATCH -c 8`, which requests 8 cores).

time -p ./gcclassic > GC.log 2>&1

Executes the GEOS-Chem Classic executable and pipes the output (both stdout and stderr streams) to a file named GC.log.

The time -p command will print the amount of time (both CPU time and wall time) that the simulation took to complete to the end of GC.log.

The following commands should already be present in your environment file. Otherwise, add these to the run script before the command to the gcclassic executable.

ulimit -s unlimited

Tells the bash shell to remove any restrictions on stack memory. This is the place in GEOS-Chem's memory where temporary variables (including *PRIVATE variables for OpenMP parallel loops*) get created.

export OMP_STACKSIZE=500m

Tells the GEOS_Chem executable to use as much memory as it needs for allocating *PRIVATE variables in OpenMP parallel loops*.

srun -c $OMP_NUM_THREADS

Tells SLURM to run the GEOS-Chem Classic executable using the number of cores specified in *OMP_NUM_THREADS*.

11.2 Complete this pre-run checklist

Now that you have created a *run script* for GEOS-Chem Classic, take a moment to make sure that you have completed all required setup steps before running your simulation.

11.2.1 First-time setup

1. If this is your first-time using GEOS-Chem, make sure that you *registered as a new user* when you created the run directory.
2. Make sure that your computational environment meets all of the *hardware* and *software* requirements for GEOS-Chem Classic.

11.2.2 Each-time setup

1. Make sure that you have *properly configured your login environment* (i.e. load necessary software modules after login, etc.)
2. Create a *GEOS-Chem Classic run directory*, and make sure that it is correct for the simulation you wish to perform.

   Attention: The initial *restart file that is included with your run directory* does not reflect the actual atmospheric state and should only be used to "spin-up" the model. We recommend a spin-up period of 6 months to 1 year (depending on the type of simulation you are using).

3. *Edit configuration files* to specify the runtime behavior of GEOS-Chem Classic..

> **Attention:** Be aware that GEOS-FP meteorology is an operational (i.e. evolving) product that is subject to assimilation system updates.
>
> On the other hand, the MERRA-2 meteorology is a 40+ year reanalysis product performed with a "frozen" version of the NASA GEOS assimilation system. Thus, MERRA-2 is preferable for studies ranging over multiple years or decades.

Important: The convection scheme used for GEOS-FP met generation changed from RAS to Grell-Freitas with impact on GEOS-FP meteorology files starting June 1, 2020, specifically enhanced vertical transport. In addition, there is a bug in convective precipitation flux following the switch where all values are zero. While this bug is automatically fixed by computing fluxes online for runs starting on or after June 1 2020, the fix assumes meteorology year corresponds to simulation year. Due to these issues we recommend splitting up GEOS-FP runs in time such that a single simulation does not run across June 1, 2020. Instead. set one run to stop on June 1 2020 and then restart a new run from there. If you wish to use a GEOS-FP meteorology year different from your simulation year please create a GEOS-Chem GitHub issue for assistance.

---

4. *Configure and build* the source code into an executable file.
5. Create a *GEOS-Chem Classic run script* to your run directory and edit it for the particulars of your simulation and computer system.
6. Make sure that your run script contains the proper settings for *OpenMP parallelization*, either by sourcing an environment file, or by manually adding the settings to the run script.
7. Be aware of *ways in which you can speed up your GEOS-Chem Classic simulations*.

11.3 Submit your run script to a scheduler

Many shared computer systems use a **scheduler** to determine in which order submitted jobs will run.

If your computer system uses the SLURM scheduler, then you can use the following command to submit your GEOS-Chem Classic *run script* to a computational queue:

```
sbatch geoschem.run
```

The SLURM scheduler will then decide when your job starts based on paramaters such as current load on the system and past cluster usage (sometimes known as **fairshare**). If there is high demand on the cluster, your job may remain in **pending state** for a few hours (or sometimes days!) before it starts.

If your computer system uses a different scheduler (e.g. LSF, PBS, etc.) then ask your sysadmin or IT staff about the commands that are needed to submit jobs.

11.4 Or run the script from the command line

If your computer system does not use a scheduler, or if you are logged into an Amazon Web Services (AWS) cloud instance, then you can run GEOS-Chem Classic directly from the terminal command line.

Here is a sample run script for interactive use. It is similar to the *run script shown previously*, with a few edits:

```
#!/bin/bash

################################################################################
### Sample GEOS-Chem run script for interactive use
################################################################################

# Set the proper # of threads for OpenMP
export OMP_NUM_THREADS=8

# Max out stack memory available to GEOS-Chem
ulimit -s unlimited
export OMP_STACKSIZE=500m

# Run GEOS-Chem.  The "time" command will return CPU and wall times.
# Stdout and stderr will be directed to the "GC.log" log file
# (you can change the log file name below if you wish)
time -p ./gcclassic > GC.log 2>&1

# Exit normally
exit 0
```

The modifications entail:

1. Removing the SLURM-specific commands (i.e. `#SBATCH`, `$SLURM_CPUS__PER_TASK`, and `srun`).
2. Manually specifying the number of cores that you wish GEOS-Chem to use (`export $OMP_NUM_THREADS=8`).

Note: If you are logged into an AWS cloud instance, you can add

```
export OMP_NUM_THREADS=`ncpus`
```

to the run script. This will automatically set *OMP_NUM_THREADS* to the available number of cores.

To run GEOS-Chem interactively, type:

```
$ ./geoschem.run > GC.log 2>&1 &
```

This will run the job in the background. To monitor the progress of the job you can type:

```
$ tail -f GC.log
```

which will show the contents of the log file as they are being written.

Another way to view output from GEOS-Chem in real time is to use the **tee** command . This will print output to the screen and also send the same output to a log file. Type:

```
$ ./geoschem.run | tee GC.log
```

11.5 Verify a successful simulation

There are several ways to verify that your GEOS-Chem Classic run was successful:

1. The following output can be found at the end of the log file:

```
**************  E N D  O F  G E O S -- C H E M  **************
```

2. NetCDF files (e.g. `OutputDir/GEOSChem*.nc4` and `OutputDir/HEMCO*.nc`) are present.
3. *Restart files* (e.g. `GEOSChem.Restart.YYYYMMDD_hhmmz.nc4` and `HEMCO_restart.YYYYMMDDhh.nc`) for ending date `YYYYMMDD hhmm` are present.
4. Your scheduler log file (e.g. `slurm-xxxxx.out`, where `xxxxx` is the job id) is free of errors.

If your run stopped with an error, please see the following resources:

- *Understand what error messages mean*
- *Debug GEOS-Chem and HEMCO errors*
- Submitting GEOS-Chem support requests

11.6 Minimize differences in multi-stage runs

If you need to split up a very long simulation (e.g. 1 model year or more) into multiple stages, keep these guidelines in mind:

1. Make sure `GC_RESTART` and `HEMCO_RESTART` options are set to `true:` in *HEMCO_Config.rc*.
2. To ensure your *restart_files* are read and species concentrations are properly initialized, check your GEOS-Chem log file for the following output:

```
================================================================================
R E S T A R T  F I L E  I N P U T
Min and Max of each species in restart file [mol/mol]:``
Species   1,       NO: Min = 1.000000003E-30  Max = 1.560991691E-08
Species   2,       O3: Min = 3.135925075E-09  Max = 9.816152669E-06
Species   3,      PAN: Min = 3.435056848E-25  Max = 1.222619450E-09
...
```

   Actual values may differ. If you see `Use background = ...` for most or all species, that suggests your restart file was not found. To avoid using the wrong restart file make sure to use time cycle flag `EY` in HEMCO_Config.rc (cf. *How are restart files read into GEOS-Chem?*).

11.7 Speed up a slow simulation

GEOS-Chem Classic performance is continuously monitored by the GEOS-Chem Support Team by means of benchmark simulations and ad-hoc timing tests. In this chapter, we provide some practical tips that you can use to speed up your simulations.

11.7.1 Use a coarser chemistry timestep

The table below contains our recommended GEOS-Chem Classic timestep settings.

GEOS-Chem Classic Resolution	Transport	Chemistry
$4° \times 5°$	600s (10m)	1200s (20m)
$2° \times 2.5°$	600s (10m)	1200s (20m)
$0.5° \times 0.625°$	300s (5m)	600s (10m)
$0.25° \times 0.3125°$	300s (5m)	600s (10m)
$0.125° \times 0.15625°$	150s (2.5m)	300s (5m)

The Courant limit on the latitude-longitude grid constrains the choice of transport timestep for a given horizontal resolution. We choose a chemistry timestep that is double the transport timestep (i.e. Strang operator splitting).

If you wish to speed up your simulation, try increasing the chemistry timestep. Chemistry is the GEOS-Chem operation that takes the longest to execute, so increasing the interval between calls to the chemistry solver will reduce the run time accordingly. But you should also verify that the increased chemistry timestep allows your simulation to faithfully capture diurnal variations, etc.

See Philip *et al.* [2016] for a comprehensive study on GEOS-Chem timesteps.

11.7.2 Use the Rosenbrock solver with auto-reduction

The GEOS-Chem full-chemistry mechanism uses the KPP Rosenbrock solver, which has an automatic mechanism reduction option as described in Lin *et al.* [2023]. This automatic mechanism reduction feature separates species into "fast" and "slow" categories based on their chemical production or loss rates. "Fast" species are integrated with the full Rosenbrock algorithm, while "slow" species will have a simple 1st-order loss applied to them. This approach has been shown to reduce the time spent in chemistry by 20 to 30 percent.

The automatic mechanism reduction option is disabled by default, but can be enabled by toggiing this switch in *geoschem_config.yml*:

```
autoreduce_solver:
  activate: false  # <=== set to true to activate auto-reduction
```

11.7.3 Turn off unwanted diagnostics

Several diagnostics are turned on by default in *the HISTORY.rc* configuration file. The more diagnostics that are turned on, the more I/O operations need to be done, resulting in longer simulation execution times. Disabling diagnostics that you do not wish to archive can result in a faster simulation.

11.7.4 Disable debugging options

If you previously configured GEOS-Chem with the : *CMAKE_BUILD_TYPE* option set to `Debug`, then several run-time debugging checks will be activated. These include:

- Checking for array-out-of-bounds errors
- Checking for floating-point math exceptions (e.g. div-by-zero)
- Disabling compiler optimizations

These options can be useful in detecting errors in your GEOS-Chem Classic simulation, but result in a much slower simulation. If you plan on running a long Classic simulation, make sure that you *configure and build GEOS-Chem Classic* so that *CMAKE_BUILD_TYPE* is set to `Release`.

11.7.5 Reduce the amount of files that need to be read

If you are developing a new data set (such as an emissions inventory) for GEOS-Chem, we recommend that you prepare data files with multiple timestamps rather than one file per timestamp. For example, if your data set has hourly time resolution, consider creating one file for each day, with each file containing 24 hours of data, etc.

The greatest amount of overhead in I/O occurs when new data files (in netCDF format) are opened. This also usually involves decompression of the file contents, which is computationally intensive. Reducing the number of times that GEOS-Chem has to open and close netCDF files can substantially improve performance.

11.7.6 Speeding up GEOS-Chem Classic nested-grid simulations

Use these tips to speed up your GEOS-Chem nested-grid simulations:

Crop nested-grid meteorology inputs

Your simulation should not read global high-resolution ($0.5^\circ \times 0.625^\circ$ or finer) meteorology fields. The overhead in reading and regridding these global fields can significantly impact your simulation. Instead, consider cropping high-resolution meteorology fields to the extent of your nested domain. This can easily be done with the netCDF operators or the Climate Data Operators; see our *Work with netCDF files* supplemental guide for more information.

Increase the size of the transport buffer zone

By default, nested *buffer_zone_NSEW* option is set to 3 boxes in each cardinal direction. Increasing this number will reduce the amount of grid boxes in which transport will be performed, which should also reduce the overall run time.

CHAPTER

TWELVE

VIEW OUTPUT FILES

In this chapter, you will learn more about the **output files** that are generated by GEOS-Chem Classic simulations.

12.1 Log files

Log files redirect the output of Fortran `PRINT*` or `WRITE` statements to a file. You can check the log files for an "echo-back" of simulation options, as well as error messages.

12.1.1 GEOS-Chem and HEMCO log file

File name: `GC.log` (or similar)

Contains an "echo-back" of input options that were specified in *geoschem_config.yml* and *HISTORY.rc*, as well as information about what is happening at each GEOS-Chem timestep. If your GEOS-Chem Classic simulation dies with an error, a detailed error message will be printed in this log file.

In GEOS-Chem 14.1.0 and later versions, information about emissions, met fields, and other relevant data that are read from disk and processed by HEMCO is now sent to this log file (instead of to `HEMCO.log`).

12.1.2 GEOS-Chem log file with dry-run output

File name: `log.dryrun` (or similar)

Contains the full path names of all input files (configuration files, meteorology files, emissions files) that are read by GEOS-Chem. This will allow users to download only those files that their GEOS-Chem simulation requires, thus speeding up the data downloading process.

For more information, please see the *dry run* chapter.

12.1.3 GEOS-Chem species metadata log

File name: `OutputDir/geoschem_species_metadata.yml`

Contains metadata (taken from the *GEOS-Chem species database*) in YAML format for only those species that are used in the simulation. This facilitates coupling GEOS-Chem to other Earth System Models.

12.1.4 Timers log file

File name: `gcclassic_timers.json` (in JSON format).

The timers log file is created when you set `use_gcclassic_timers: true` in *the Simulation Settings section of geoschem_config.yml*. It contains "wall-clock" times that measure how long each component of GEOS-Chem took to execute. This information is used by the GEOS-Chem benchmarking scripts that execute on the Amazon cloud computing platform.

12.1.5 Scheduler log file

File name: Specific to each scheduler.

If you used a batch scheduler such as SLURM, PBS, LSF, etc. to submit your GEOS-Chem Classic simulation, then output from the Unix stdout and/or stderr streams may be printed to this file. This file may contain important error messages.

12.2 History diagnostics output

GEOS-Chem History diagnostics are comprised of several **diagnostic collections**. Each diagnostic collection contains a series of **diagnostic fields** that may be archived from a GEOS-Chem Classic simulation.

In the *HISTORY.rc configuration file* (which is located in your *GEOS-Chem Classic run directory*, you will find a list of **default diagnostic collections**. These are collections that have been predefined for you. You may edit the this configuration file to select which diagnostic collections you wish to archive from your GEOS-Chem Classic simulation. You may also define your own custom diagnostic collectinons.

The filenames listed below correspond to the default diagnostic collections in the *HISTORY.rc configuration file*.

Table 1: GEOS-Chem History diagnostics output files

History output file	Diagnostic collection	Used in simulations
`GEOSChem.AdvFluxVert.YYYYMMDD_hhhmmz.nc4`	*AdvFluxVert*	`fullchem`
`GEOSChem.AerosolMass.YYYYMMDD_hhhmmz.nc4`	*AerosolMass*	`fullchem aerosol`
`GEOSChem.Aerosols.YYYYMMDD_hhhmmz.nc4`	*Aerosols*	`fullchem aerosol`
`GEOSChem.BoundaryConditions.YYYYMMDD_hhhmmz.nc4`	*BoundaryConditions*	Nested-grid simulations
`GEOSChem.Carbon.YYYYMMDD_hhhmmz.nc4`	*Carbon*	`carbon`
`GEOSChem.CH4.YYYYMMDD_hhhmmz.nc4`	*CH4*	`CH4`
`GEOSChem.CloudConvFlux.YYYYMMDD_hhhmmz.nc4`	*CloudConvFlux*	All simulations
`GEOSChem.CO.YYYYMMDD_hhhmmz.nc4`	*CO*	`CH4`
`GEOSChem.CO2.YYYYMMDD_hhhmmz.nc4`	*CO2*	`CH4`
`GEOSChem.ConcAboveSfc.YYYYMMDD_hhhmmz.nc4`	*ConcAboveSfc*	`fullchem`
`GEOSChem.ConcAfterChem.YYYYMMDD_hhhmmz.nc4`	*ConcAfterChem*	`fullchem`
`GEOSChem.DryDep.YYYYMMDD_hhhmmz.nc4`	*DryDep*	All simulations with dry-
`GEOSChem.JValues.YYYYMMDD_hhhmmz.nc4`	*JValues*	`fullchem`
`GEOSChem.KppARDiags.YYYYMMDD_hhhmmz.nc4`	*KppARDiags*	`fullchem`
`GEOSChem.KppDiags.YYYYMMDD_hhhmmz.nc4`	*KppDiags*	`fullchem`
`GEOSChem.LevelEdgeDiags.YYYYMMDD_hhhmmz.nc4`	*LevelEdgeDiags*	All simulations
`GEOSChem.MercuryChem.YYYYMMDD_hhhmmz.nc4`	*MercuryChem*	`Hg`
`GEOSChem.MercuryEmis.YYYYMMDD_hhhmmz.nc4`	*MercuryEmis*	`Hg`
`GEOSChem.MercuryOcean.YYYYMMDD_hhhmmz.nc4`	*MercuryOcean*	`Hg`
`GEOSChem.Metrics.YYYYMMDD_hhhmmz.nc4`	*Metrics*	`fullchem`

continues on next page

Table 1 – continued from previous page

History output file	Diagnostic collection	Used in simulations
GEOSChem.ProdLoss.YYYYMMDD_hhhmmz.nc4	*ProdLoss*	*fullchem aerosol tagCO tagO3*
GEOSChem.RadioNuclide.YYYYMMDD_hhhmmz.nc4	*RadioNuclide*	*TransportTracers*
GEOSChem.Restart.YYYYMMDD_hhhmmz.nc4	*Restart*	All simulations
GEOSChem.RRTMG.YYYYMMDD_hhhmmz.nc4	*RRTMG*	All simulations
GEOSChem.RxnConst.YYYYMMDD_hhhmmz.nc4	*RxnConst*	*fullchem CH4 Hg*
GEOSChem.RxnRates.YYYYMMDD_hhhmmz.nc4	*RxnRates*	*fullchem CH4 Hg*
GEOSChem.SatDiagn.YYYYMMDD_hhhmmz.nc4	*SatDiagn*	All simulations
GEOSChem.SatDiagnEdge.YYYYMMDD_hhhmmz.nc4	*SatDiagnEdge*	All simulations
GEOSChem.SpeciesConc.YYYYMMDD_hhhmmz.nc4	*SpeciesConc*	All simulations
GEOSChem.StateChm.YYYYMMDD_hhhmmz.nc4	*StateChm*	All simulations
GEOSChem.StateMet.YYYYMMDD_hhhmmz.nc4	*StateMet*	All simulations
GEOSChem.StratBM.YYYYMMDD_hhhmmz.nc4	*StratBM*	All simulations
GEOSChem.Tomas.YYYYMMDD_hhhmmz.nc4	*Tomas*	All simulations
GEOSChem.UVFlux.YYYYMMDD_hhhmmz.nc4	*UVFlux*	All simulations
GEOSChem.WetLossConv.YYYYMMDD_hhhmmz.nc4	*WetLossConv*	All simulations with wet-deposited species
GEOSChem.WetLossLS.YYYYMMDD_hhhmmz.nc4	*WetLossLS*	All simulations with wet-deposited species

12.3 Other diagnostic output files

12.3.1 HEMCO diagnostic output

HEMCO diagnostics generate *netCDF-format* files in the `OutputDir/` subdirectory of your *GEOS-Chem run directory*. You may change this filepath by editing the *HEMCO_Config.rc* configuration file.

HEMCO diagnostic files use the naming convention `HEMCO_diagnostics.YYYYMMDDhhmm.nc`, where `YYYYMMDD` and `hhmm` refer to the model date and time at which each file was created.

For more information, please see our HEMCO user manual at hemco.readthedocs.io.

12.3.2 Planeflight diagnostic output

The *GEOS-Chem plane-following diagnostic* generates text files in the top-level of your *GEOS-Chem Classic run directory*. You may change this filepath by editing the *planeflight section of geoschem_config.yml*.

Planeflight diagnostic files use the naming convention `plane.log.YYYYMMDDhhmm`, where `YYYYMMDD` refers to the model date at which each diagnostic file is created.

12.3.3 ObsPack diagnostic output

The *GEOS-Chem ObsPack diagnostic* generates *netCDF-format* files in the top-level of your *GEOS-Chem Classic run directory*. You may change this filepath by editing the *ObsPack section of geoschem_config.yml*.

ObsPack diagnostic files use the naming convention `GEOS-Chem.ObsPack.YYYYMMDD_hhmmz.nc4`, where `YYYYMMDD` and `hhmm` refers to the model date a which each diagnostic file is created, and `z` refers to UTC (aka Zulu time).

GEOS-Chem Classic and HEMCO also create *restart files*, which have been discussed previously.

CHAPTER

THIRTEEN

DIAGNOSTICS REFERENCE

In the following chapters, you will learn about the types of diagnostic outputs you can generate with GEOS-Chem Classic.

13.1 GEOS-Chem History diagnostics

Please see our *Archive output with the History diagnostics* supplemental guide for detailed instructions about archiving GEOS-Chem diagnostic quantities.

13.2 HEMCO diagnostics

Information about diagnostic output from HEMCO (the Harmonized Emissions Component) may be found on our HEMCO ReadTheDocs site.

13.3 Planeflight diagnostic

On this page we provide information about the GEOS-Chem planeflight diagnostic, which allows you to save certain diagnostic quantities along flight tracks or at the position of ground observations. This can be more efficient in terms of storage than saving out 3-D data files via the *GEOS-Chem History diagnostics*.

Important: Several diagnostic quantities were disabled when the SMVGEAR chemistry solver was replaced with the FlexChem implementation of **KPP** (cf: *Update chemical mechanisms with KPP*). Therefore, you may find that functionality is not currently working. We look to GEOS-Chem community members to help us maintain the planeflight diagnostic.

13.3.1 The Planeflight.dat.YYYYMMDD configuration file

The `Planeflight.dat.YYYYMMDD` files allow you to specify the diagnostic quantities (species, reaction rates, met fields) that you want to print out for a specific longitude, latitude, altitude, and time. A sample `Planeflight.dat.YYYYMMDD` file is given below. Of course if you have lots of flight track data points, your file will be much longer.

If the plane flight following diagnostic is switched on, then it will look for a new `Planeflight.dat.YYYYMMDD` file each day. If a `Planeflight.dat.YYYYMMDD` file is found for a given day, then GEOS-Chem will save out diagnostic quantities along the flight track(s) to the `plane.log.YYYYMMDD` file.

Format

```
Planeflight.dat -- Input file for planeflight diagnostic
GCST
July 2018
------------------------------------------------------------
9     <-- # of variables to be output (listed below)
------------------------------------------------------------
TRA_001
TRA_002
TRA_003
GMAO_TEMP
GMAO_ABSH
GMAO_RELH
GMAO_IIEV
GMAO_JJEV
GMAO_LLEV
------------------------------------------------------------
  Now give the times and locations of the flight
------------------------------------------------------------
Point   Type DD-MM-YYYY HH:MM     LAT      LON ALT/PRE        OBS
    1   Scrz 30-06-2012 13:53  -46.43    51.85  202.00   1765.030
    2   Scrz 30-06-2012 13:53  -46.43    51.85  202.00   1765.060
    3   Sush 30-06-2012 16:25  -54.85   -68.31   32.00   1764.750
    4   Sush 30-06-2012 16:25  -54.85   -68.31   32.00   1765.610
    5   Sllb 30-06-2012 17:13   54.95  -112.45  588.00   1891.200
    6   Sllb 30-06-2012 17:13   54.95  -112.45  588.00   1891.310
99999   END  00-00-0000 00:00    0.00     0.00    0.00      0.000
```

The data in this text file can be read and plotted using GAMAP routines CTM_READPLANEFLIGHT and PLANE_PLOT.

Requesting diagnostic quantities

The first part of the `Planeflight.dat.YYYYMMDD` file allows you to request several diagnostic quantities that you would like to be archived along the plane's flight track. These are listed in the table below.

You must make sure that you have specified the number of requested quantities properly, or you will get an input error.

Important: Several planeflight diagnostic quantities had to be disabled when the SMVGEAR chemical solver was replaced by the FlexChem implementation of the KPP chemical solver. Therefore, you may find that not all of the planeflight diagnostic quantities listed below are still functional. Please report any issues to the GEOS-Chem Support Team by opening a new Github issue.

Table 1: Planeflight diagnostic archivable quantities

Quantity	Description	Units
`TRA_nnn`	Species concentration (nnn = species index)	v/v dry
`OH`, `HO2`, etc.	Species concentration	molec/cm3
`RO2`	Concentration of RO2 family	v/v dry
`AN`	Concentration of AN family	v/v dry

continues on next page

Table 1 – continued from previous page

Quantity	Description	Units
NOy	Concentration of NOy family	v/v dry
GMAO_TEMP	Temperature	K
GMAO_ABSH	Absolute humidity	unitless
GMAO_SURF	Aerosol surface area	cm2/cm3
GMAO_PSFC	Surface pressure	hPa
GMAO_UWND	Zonal winds	m/s
GMAO_VWND	Meridional winds	m/s
GMAO_IIEV	Longitude index	unitless
GMAO_JJEV	Latitude index	unitless
GMAO_LLEV	Level index	unitless
GMAO_RELH	Relative humidity	%
GMAO_PSLV	Sea level pressure	hPa
GMAO_AVGW	Water vapor mixing ratio	v/v
GMAO_THTA	Potential temperature	K
GMAO_PRES	Pressure at center of grid box	hPa
GMAO_ICEnn	SEAICEnn fields	unitless
AODC_SULF	Column AOD, sulfate	unitless
AODC_BLKC	Column AOD, black carbon	unitless
AODC_ORGC	Column AOD, organic carbon	unitless
AODC_SALA	Column AOD, fine sea salt	unitless
AODC_SALC	Column AOD, coarse sea salt	unitless
AODC_DUST	Column AOD, dust	unitless
AODB_SULF	Column AOD, sulfate (below aircraft)	unitless
AODB_BLKC	Column AOD, black carbon (below aircraft)	unitless
AODB_ORGC	Column AOD, organic carbon (below aircraft)	unitless
AODB_SALA	Column AOD, fine sea salt (below aircraft)	unitless
AODB_SALC	Column AOD, coarse sea salt (below aircraft)	unitless
AODB_DUST	Column AOD, dust (below the aircraft)	unitless
TMS_nnn	Nucleation rates (TOMAS)	
HG2_FRACG	Frac of Hg(II) in gas phase	unitless
HG2_FRACP	Frac Hg(II) in particle phase	unitless
ISOR_HPLUS	ISORROPIA H+	M
ISOR_PH	ISORROPIA pH	unitless
ISOR_AH2O	ISORROPIA aerosol water	ug/m3 air
ISOR_HSO4	ISORROPIA bifulfate	M
TIME_LT	Local time	hours
AQAER_RAD	Aqueous aerosol radius	cm
AQAER_SURF	Aqueous aerosol surface area	cm2/cm3
PROD_xxxx	Production rates (needs updating)	molec/cm3/s
REA_nnn	Reaction rates (Needs updating)	molec/cm3/s

Specifying the flight track

The next section of the `Planeflight.dat.YYYYMMDD` file is where you will specify the points that make up the flight track.

Quantity	Description
`POINT`	A sequential index of flight track points.
`TYPE`	Identifier for the plane (or station)
`DD`	Day of the observation
`MM`	Month of the observation
`YYYY`	Year of the observation
`HH`	Hour of the observation (UTC)
`MM`	Minute of the observation (UTC)
`LAT`	Latitude (deg), range -90 to +90
`LON`	Longitude (deg), range -180 to +180
`ALT/PRE`	Altitude [m] or Pressure [hPa] of the observation[1]
`OBS`	Value of the observation (if known), used to compare to model output

Notes

Important: The `TYPE` column can be used to specify the aircraft type and flight number to distinguish between multiple plane flight tracks.

The planeflight diagnostic will automatically set `L=1` if it does not recognize `TYPE`. When using a new flight track, make sure to add your `TYPE` to this IF statement if you do not wish to use L=1 for that type value.

The plane.log.YYYYMMDD output file

The `plane.log.YYYYMMDD` file contains output from the planeflight diagnostic.

Format

```
POINT    TYPE YYYYMMDD HHMM     LAT     LON   PRESS        OBS     T-IND P-I I-IND J-IND␣
↪ TRA_001     GMAO_TEMP   ...
    1    Scrz 20120630 1353  -46.43   51.85  981.74   1765.030 000061277 002 00047 00012␣
↪ 1.785E-006  2.780E+002  ...
    2    Scrz 20120630 1353  -46.43   51.85  981.74   1765.060 000061277 002 00047 00012␣
↪ 1.785E-006  2.780E+002  ...
    3    Sush 20120630 1625  -54.85  -68.31  949.77   1764.750 000061281 002 00023 00010␣
↪ 1.784E-006  2.746E+002  ...
    4    Sush 20120630 1625  -54.85  -68.31  949.77   1765.610 000061281 002 00023 00010␣
↪ 1.784E-006  2.746E+002  ...
    5    Sllb 20120630 1713   54.95 -112.45  876.13   1891.200 000061283 005 00015 00037␣
↪ 1.906E-006  2.942E+002  ...
```

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[1] Altitude is only supported for CCGG or tower data. All other observations must specify pressure in hPa. This can be obtained from the "static pressure" field as measured by the aircraft. See this code block in planeflight_mod.F90 for details.

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```
    6    Sllb 20120630 1713   54.95 -112.45  876.13   1891.310 000061283 005 00015 00037␣
↪ 1.906E-006  2.942E+002  ...
```

Columns

Table 2: Cp;

Column	Description
`POINT`	Flight track data point number (for reference)
`TYPE`	Aircraft/flight number ID or ground station ID
`YYYYMMDD`	Year, month, and day (UTC or each flight track point
`HHMM`	Hour and minute (UTC) for each flight track point
`LAT`	Latitude (-90 to 90 degrees) for each flight track point
`LON`	Longitude (-180 to 180 degrees) for each flight track point
`PRESS`	Pressure in hPa for each flight track point
`OBS`	Observation value from the flight campaign
`T-IND`	Time index
`P-IND`	GEOS-Chem level index
`I-IND`	GEOS-Chem longitude index
`J-IND`	GEOS-Chem latitude index
`TRA_001` etc.	Diagnostic quantities requested in `Planeflight.dat.YYMMDD`

13.4 ObsPack diagnostic

On this page we provide information about the ObsPack diagnostic in GEOS-Chem, which is intended to sample GEOS-Chem data at specified coordinates and times (e.g. corresponding to surface or flight track measurements). This feature was written by Andy Jacobson of NOAA and Andrew Schuh of Colorado State University and implemented in GEOS-Chem 12.2.0.

Attention: The GEOS-Chem ObsPack diagnostic was originally developed for use with the ObsPack GLOBALVIEWplus CO2 product. The data files in this product contain a particular netCDF variable named `CT_sampling_strategy` that GEOS-Chem uses to quickly determine the time-averaging window for aggregating observations.

We have recently learned that the ObsPack GLOBALVIEWplus CH4 data product currently lacks the `CT_sampling_strategy` variable, and thus is incompatible with GEOS-Chem.

The best workaround for now is to preprocess ObsPack GLOBALVIEWplus CH4 data files with one of the following Python tools before attempting to read them into GEOS-Chem:

- process_obspack by James East
- gcpy_campaigns by Jessica Haskins

13.4.1 Specifying ObsPack diagnostic options

The ObsPack Menu section of input.geos is where you define the following settings:

1. Turning ObsPack or off
2. Specifying which GEOS-Chem species you would like to archive.
   - At present, you can archive individual species, or all advected species.
3. Specifying the names of input files
   - These are the files from which coordinate data will be read)
4. Specifying the names of output files
   - These are the files that will contain GEOS-Chem data sampled by the ObsPack diagnostic.

13.4.2 Input file format

The ObsPack diagnostic reads input information (such as coordinates, sampling method, and observation ID's) from netCDF files having the format shown below. You will need to prepare an input file for each YYYY/MM/DD date on which you would like to obtain ObsPack diagnostic output from GEOS-Chem. (The ObsPack diagnostic will skip over days on which it cannot find an input file.)

ObsPack input files can be downloaded the NOAA website: https://gml.noaa.gov/ccgg/obspack/.

Attention: Starting in ObsPack v6, `time_components` indicates the start-time of the sampling interval, not the center time. For the center time, we need to read the `time` variable. The `time` variable represents the center of the averaging window in all ObsPack data versions.

Obspack file metadata

Here is the metadata from an ObsPack data file. We have only displayed the variables that the ObsPack module needs to read.

```
netcdf obspack_co2_1_GLOBALVIEWplus_v6.0_2020-09-11.20190408 {
dimensions:
        obs = UNLIMITED ; // (3111 currently)
        calendar_components = 6 ;
        string_of_200chars = 200 ;
        string_of_500chars = 500 ;
variables:
        int obs(obs) ;
                obs:long_name = "obs" ;
                obs:_Storage = "chunked" ;
                obs:_ChunkSizes = 1024 ;
                obs:_Endianness = "little" ;
        int time(obs) ;
                time:units = "Seconds since 1970-01-01 00:00:00 UTC" ;
                time:_FillValue = -999999999 ;
                time:long_name = "Seconds since 1970-01-01 00:00:00 UTC" ;
                time:_Storage = "chunked" ;
                time:_ChunkSizes = 778 ;
```

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```
                time:_DeflateLevel = 5 ;
                time:_Endianness = "little" ;
        ...
        float latitude(obs) ;
                latitude:units = "degrees_north" ;
                latitude:_FillValue = -1.e+34f ;
                latitude:long_name = "Sample latitude" ;
                latitude:_Storage = "chunked" ;
                latitude:_ChunkSizes = 778 ;
                latitude:_DeflateLevel = 5 ;
                latitude:_Endianness = "little" ;
        float longitude(obs) ;
                longitude:units = "degrees_east" ;
                longitude:_FillValue = -1.e+34f ;
                longitude:long_name = "Sample longitude" ;
                longitude:_Storage = "chunked" ;
                longitude:_ChunkSizes = 778 ;
                longitude:_DeflateLevel = 5 ;
                longitude:_Endianness = "little" ;
        float altitude(obs) ;
                altitude:units = "meters" ;
                altitude:_FillValue = -1.e+34f ;
                altitude:long_name = "sample altitude in meters above sea level" ;
                altitude:comment = "Altitude is surface elevation plus sample intake␣
↪height in meters above sea level." ;
                altitude:_Storage = "chunked" ;
                altitude:_ChunkSizes = 778 ;
                altitude:_DeflateLevel = 5 ;
        ...
        char obspack_id(obs, string_of_200chars) ;
                obspack_id:long_name = "Unique ObsPack observation id" ;
                obspack_id:comment = "Unique observation id string that includes obs_id,␣
↪dataset_id and obspack_num." ;
                obspack_id:_Storage = "chunked" ;
                obspack_id:_ChunkSizes = 1, 200 ;
                obspack_id:_DeflateLevel = 5 ;
        ...
        int CT_sampling_strategy(obs) ;
                CT_sampling_strategy:_FillValue = -9 ;
                CT_sampling_strategy:long_name = "model sampling strategy" ;
                CT_sampling_strategy:values = "How to sample model. 1=4-hour avg; 2=1-
↪hour avg; 3=90-min avg; 4=instantaneous" ;
                CT_sampling_strategy:_Storage = "chunked" ;
                CT_sampling_strategy:_ChunkSizes = 778 ;
                CT_sampling_strategy:_DeflateLevel = 5 ;
                CT_sampling_strategy:_Endianness = "little"

... omitting global attributes etc. ...
```

Notes

1. The ObsPack ID string should be 200 characters long.
2. If you have coordinate data in another format (e.g. a text-based *Planeflight.dat* file) then you'll need to create a netCDF file using the format shown above, or else ObsPack will not be able to read it.

13.4.3 Output file format

The ObsPack diagnostic will produce a file called `GEOSChem.ObsPack.YYYYMMDD_hhmmz.nc4` for each day where an *input file* has been specified. (You can change the output file name in the ObsPack Menu in `input.geos`.

Below is shown an ObsPack output file for the GEOS-Chem methane simulation. If you are using the ObsPack diagnostic with other GEOS-Chem simulations, your output files will look similar to this, except for the species names.

```
netcdf GEOSChem.ObsPack.20180926_0000z.nc4 {
dimensions:
        obs = UNLIMITED ; // (662 currently)
        species = 1 ;
        char_len_obs = 200 ;
variables:
        char obspack_id(obs, char_len_obs) ;
                obspack_id:long_name = "obspack_id" ;
                obspack_id:units = "1" ;
        int nsamples(obs) ;
                nsamples:long_name = "no. of model samples" ;
                nsamples:units = "1" ;
                nsamples:comment = "Number of discrete model samples in average" ;
        int averaging_interval(obs) ;
                averaging_interval:long_name = "Amount of model time over which this␣
↪observation is averaged" ;
                averaging_interval:units = "seconds" ;
        int averaging_interval_start(obs) ;
                averaging_interval_start:long_name = "Start of averaging interval" ;
                averaging_interval_start:units = "seconds since 1970-01-01 00:00:00 UTC"␣
↪;
                averaging_interval_start:calendar = "standard" ;
        int averaging_interval_end(obs) ;
                averaging_interval_end:long_name = "End of averaging interval" ;
                averaging_interval_end:units = "seconds since 1970-01-01 00:00:00 UTC" ;
                averaging_interval_end:calendar = "standard" ;
        float lon(obs) ;
                lon:long_name = "longitude" ;
                lon:units = "degrees_east" ;
        float lat(obs) ;
                lat:long_name = "latitude" ;
                lat:units = "degrees_north" ;
        float u(obs) ;
                u:long_name = "Zonal component of wind" ;
                u:units = "m s^-1" ;
        float v(obs) ;
                v:long_name = "Meridional component of wind" ;
                v:units = "m s^-1" ;
```

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```
        float blh(obs) ;
                blh:long_name = "Boundary layer height" ;
                blh:units = "m" ;
        float q(obs) ;
                q:long_name = "mass_fraction_of_water_inair" ;
                q:units = "kg water (kg air)^-1" ;
        float pressure(obs) ;
                pressure:long_name = "pressure" ;
                pressure:units = "Pa" ;
        float temperature(obs) ;
                temperature:long_name = "temperature" ;
                temperature:units = "K" ;
        float CH4(obs) ;
                CH4:long_name = "Methane" ;
                CH4:units = "mol mol-1" ;
                CH4:_FillValue = -1.e+34f ;

// global attributes:
                :history = "GEOS-Chem simulation at 2019/01/11 14:54" ;
                :conventions = "CF-1.4" ;
                :references = "www.geos-chem.org; wiki.geos-chem.org" ;
                :model_start_date = "2018/09/26 00:00:00 UTC" ;
                :model_end_date = "2018/09/27 00:00:00 UTC" ;
}
```

You can several different types of netCDF-reading software to read and plot data from Obspack diagnostic output files. We recommend using either Python scripts or Jupyter notebooks.

13.4.4 Known issues

Unit conversions are currently done for all species

In routine `ObsPack_Sample` (located in module `ObsPack/obspack_mod.F90`), the following algorithm is used:

```
! Ensure that units of species are "v/v dry", which is dry=
! air mole fraction.  Capture the InUnit value, this is=
! what the units are prior to this call.  After we sample=
! the species, we'll call this again requesting that the=
! species are converted back to the InUnit values.=

... THEN DO THE DATA SAMPLING ..............................................
... i.e. determine which GEOS-Chem grid boxes to include in the averaging ...

! Return State_Chm%SPECIES to whatever units they had
! coming into this routine
call Convert_Spc_Units( am_I_root, Input_Opt, State_Met,                &
```

The routine `Convert_Spc_Units` performs unit conversions for all of the species in the `State_Chm%Species` array, regardless of whether they are being archived with ObsPack or not. This can lead to a bottleneck in performance, as `ObsPack_Sample` is called on every GEOS-Chem "heartbeat" timestep.

What would be more efficient would be to do the unit conversion only for hose species that are being archived by

ObsPack. A typical full-chemistry simulation includes about 200 species. But if we are only using ObsPack to archive 10 of these species, GEOS-Chem would execute much faster if we were doing unit conversions for only the 10 archived species instead of all 200 species.

This issue is currently unresolved.

CHAPTER

FOURTEEN

AEROSOL-ONLY SIMULATION

14.1 Overview

The **GEOS-Chem aerosol-only simulation** is an offline simulation for aerosol tracers only. It uses archived monthly mean OH, NO3, O3 and total nitrate concentrations archived from a previous full-chemistry simulation (more on that below), as well as production and loss rates for H2O2. This simulation does not provide "tagged" capabilities, but reduces the suite of tracers from full chemistry.

NOTES:

1. The aerosol-only simuation is currently functional in GEOS-Chem Classic.
2. There is currently no aerosol-only run directory for GCHP. Interested users are encouraged to make this modification on their own.
3. OH concentrations are archived from the most recent 10-year benchmark simulation.
4. O3, NO3 and total nitrate (HNO3+NIT) concentrations, as well as production rates and photolysis rates for H2O2 are archived from the most recent 10-year benchmark simulation.

14.2 List of species

Table 1: Transported species

Species	Description	Formula	MW (g)
BCPI	Hydrophilic black carbon aerosol	C	12.01
BCPO	Hydrophobic black carbon aerosol	C	12.01
DMS	Dimethyl sulfide	(CH3)2S	62.13
DST1	Dust aerosol, Reff = 0.7 microns	Dust	29.0
DST2	Dust aerosol, Reff = 1.4 microns	Dust	29.0
DST3	Dust aerosol, Reff = 2.4 microns	Dust	29.0
DST4	Dust aerosol, Reff = 4.5 microns	Dust	29.0
H2O2	Hydrogen peroxide	H2O2	34.02
MSA	Methyl sulfonic acid	CH4SO3	96.1
NH3	Ammonia	NH3	17.04
NH4	Ammonium	NH4	18.05
NIT	Inorganic nitrates	not listed	62.01
NITs	Inorganic nitrates on surface of seasalt aerosol	not listed	31.4
OCPI	Hydrophilic organic carbon aerosol	not listed	12.01
OCPO	Hydrophobic organic carbon aerosol	not listed	12.01
pFe	Anthropogenic iron	Fe	55.85
SALA	Fine (0.01-0.05 microns) sea salt aerosol	not listed	31.4
SALAAL	Accumulation mode sea salt alkalinity	not listed	31.4
SALACL	Chloride in Accumulation mode sea salt aerosol	not listed	35.45
SALC	Coarse (0.5-8 microns) sea salt aerosol	not listed	31.4
SALCAL	Coarse mode sea salt alkalinity	not listed	31.4
SALCCL	Chloride in Coarse mode sea salt aerosol	not listed	35.45
SO2	Sulfur dioxide	SO2	64.04
SO4	Sulfate	SO4	96.06
SO4s	Sulfate on surface of seasalt aerosol	not listed	31.4
SOAP	SOA Precursor - lumped species for simplified SOA parameterization	not listed	150.0
SOAS	SOA Simple - simplified non-volatile SOA parameterization	not listed	150.0

CHAPTER

FIFTEEN

CARBON GASES SIMULATION

15.1 Overview

The **GEOS-Chem carbon gases simulation** carbon simulation combines the chemistry reactions of the individual CH4, CO2, and tagged CO simulations. Users may configure the GEOS-Chem carbon gases simulation to use all of the advected species, or any one of the advected species.

Attention: The carbon gases simulation is slated to replace the individual CH4, CO2, and tagged CO simulations, likely in GEOS-Chem version 14.7.0.

Reference: Bukosa, B., Fisher, J., Deutscher, N., and Jones, D. A Coupled CH4, CO and CO2 Simulation for Improved Chemical Source Modelling. Atmosphere, 14:764, 2023, DOI: 10.3390/atmos14050764.

15.2 List of species

Table 1: Transported species

Species	Description	Formula	MW (g)
CH4	Methane	CH4	16.04
CO	Carbon monoxide	CO	28.01
CO2	Carbon dioxide	CO2	44.01
OCS (aka COS)	Carbonyl sulfate	OCS	60.07

Table 2: Non-transported species

Species	Description	Formula	MW (g)
COfromCH4	CO produced from methane oxidation (carbon mechanism)	CO	28.01
COfromNMVOC	CO produced from non-methane VOCs oxidation (carbon mechanism)	CO	28.01
CO2fromOH	Carbon dioxide loss by OH (carbon mechanism)	CO2	44.01
Dummy	Dummy species (carbon mechanism)	not listed	1.0
FixedOH	Hydroxyl radical (external input for carbon mechanism)	OH	17.01
FixedCl	Atomic chlorine (external input for carbon mechanism)	Cl	35.45
DummyCH4	Methane (external input for carbon mechanism)	CH4	16.04
DummyNMVOC	CO produced from NMVOC oxidation (external input for carbon mechanism)	CO	28.01

CHAPTER

SIXTEEN

FULLCHEM SIMULATION

16.1 Overview

The GEOS-Chem **fullchem** (aka "full-chemistry") simulation uses a detailed NOx-Ox-hydrocarbons-aerosols-halogens mechanism.

You may choose one of several fullchem simulation options at *run directory creation time*.

Option	Description
Standard	The default full chemistry simulation. Uses a simple SOA species and precursor.
Benchmark	The configuration used for performing GEOS-Chem benchmark simulations. Uses all of the species in the standard simulation, but also carries complex SOA species for diagnostic purposes.
Complex SOA	Replaces the simple SOA species and precursor with the Pye et al. [2010] complex SOA scheme.
Complex SOA plus semi-volatile POA	Replaces the simple SOA species and precursor with the Pye et al. 2010 complex SOA scheme, plus semi-volatile POA species.
Marine POA	Adds species MOPI (hydrophilic marine POA) and MOPO (hydrophobic marine POA).
Acid uptake on dust	Adds several species to track how acids are taken up by dust and other aerosols.
TOMAS	Replaces the default bulk aerosol scheme with TOMAS Aerosol Microphysics.
APM	Replaces the default bulk aerosol scheme with the APM Aerosol Microphysics.
RRTMG	Enables the RRTMG radiative transfer model, which can be used to compute radiative forcings for certain species.

Most GEOS-Chem users typically run the **Standard** simulation.

16.2 List of species, by option

16.2.1 Standard

The **Standard** fullchem option uses the following species:

Table 1: Transported species (Standard option)

Species	Description	Formula	MW (g)
ACET	Acetone	CH3C(O)CH3	58.09

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Table 1 – continued from previous page

Species	Description	Formula	MW (g)
ACTA	Acetic acid	CH3C(O)OH	60.06
ACR	Acrolein	C3H4O	56.06
AERI	Iodine on aerosol	I	126.9
ALD2	Acetaldehyde	CH3CHO	44.06
ALK4	Lumped C4+C5 Alkanes	not listed	58.12
ALK4N2	Lumped alkyl nitrate from ALK4	RO2NO	119.1
ALK4P	Peroxide from ALK4O2	CH3CH2CH2CH2OOH	90.14
ALK6	Lumped >= C6 Alkanes	C7H16	100.2
AONITA	Aerosol-phase organonitrates from aromatics	C6H6O6N	189.12
APAN	Peroxyacryloyl nitrate	C3H3NO5	133.06
APINP	Hydroperoxide from APIN	C10H18O3	186.28
APINN	1st gen organic nitrate from APIN	C10H17NO4	215.28
AROMCHO	ACCOMECHO from MCM	C5H6O4	130.1
AROMP4	Generic C4 product of aromatics	C4H4O2	68.08
AROMP5	C5 unsaturated dicarbonyl	C5H6O2	98.1
AROMPN	Lumped PN from aromatics	C5H5NO8	207.1
ATOOH	ATO2 peroxide	CH3C(O)CH2OOH	90.09
BALD	Benzaldehyde	C7H6O	106.12
BCPI	Hydrophilic black carbon aerosol	C	12.01
BCPO	Hydrophobic black carbon aerosol	C	12.01
BENZ	Benzene	C6H6	78.12
BENZP	Phenyl hydroperoxide	C6H6O2	110.11
BPINO	Ketone from BPIN	C9H14O	186.28
BPINN	Saturated 1st gen BPIN organic nitrate	C10H17NO4	215.28
BPINP	Peroxide from BPIN	C10H18O3	186.28
BPINOOH	2nd-gen peroxide from BPIN	C9H14O3	186.28
BPINON	Saturated 2nd gen BPIN organic nitrate	C9H13NO4	215.28
Br	Atomic bromine	Br	79.9
Br2	Molecular Bromine	Br2	159.8
BrCl	Bromine chloride	BrCl	115.45
BrNO2	Nitryl bromide	BrNO2	125.91
BrNO3	Bromine nitrate	BrNO3	141.91
BrO	Bromine monoxide	BrO	95.9
BrSALA	Fine sea salt bromine	Br	79.9
BrSALC	Coarse sea salt bromine	Br	79.9
BUTDI	Butenedial	C4H4O2	84.07
BUTN	C4H6 alkyl nitrate	C4H7NO4	133.1
BZCO3H	Perbenzoic acid	C6H5CO3H	138.12
BZPAN	Peroxybenzoylnitrate	C7H5O5N	183.12
C96O2H	Peroxide from APIN 2nd gen	C9H16O3	186.28
C96N	Saturated 2nd gen monoterpene organic nitrate	C9H15NO4	215.28
C2H2	Acetylene (aka Ethyne)	C2H2	26.05
C2H4	Ethylene	C2H4	28.05
C2H6	Ethane	C2H6	30.08
C3H8	Propane	C3H8	44.11
C4H6	1,3-butadiene	C4H6	54.09
CCl4	Carbon tetrachloride	CCl4	153.82
CFC11	CFC-11	CCl3F	137.37
CFC113	CFC-113	C2Cl3F3	187.38
CFC114	CFC-114	C2Cl2F4	170.92

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Table 1 – continued from previous page

Species	Description	Formula	MW (g)
CFC115	CFC-115	C2ClF5	154.47
CFC12	CFC-12	CCl2F2	120.91
CH2Br2	Dibromomethane	CH2Br2	173.83
CH2Cl2	Dichloromethane	CH2Cl2	84.93
CH2I2	Diiodomethane	CH2I2	267.84
CH2IBr	Bromoiodomethane	CH2IBr	220.84
CH2ICl	Chloroiodomethane	CH2ICl	176.38
CH2O	Formaldehyde	CH2O	30.03
CH3Br	Methyl bromide	CH3Br	94.94
CH3CCl3	Methyl chloroform	CH3CCl3	133.35
CH3Cl	Chloromethane	CH3Cl	50.45
CH3I	Methyl iodide	CH3I	141.94
CH4	not listed	CH4	16.04
CHBr3	Bromoform	CHBr3	252.73
CHCl3	Chloroform	CHCl3	119.35
Cl	Atomic chlorine	Cl	35.45
Cl2	Molecular chlorine	Cl2	70.9
Cl2O2	Dichlorine dioxide	Cl2O2	102.91
ClNO2	Nitryl chloride	ClNO2	81.45
ClNO3	Chlorine nitrate	ClNO3	97.45
ClO	Chlorine monoxide	ClO	51.45
ClOO	Chlorine dioxide	ClOO	67.45
CLOCK	Clock tracer for diagnosing age of air	not listed	1.0
CO	not listed	CO	28.01
CSL	Cresols	C7H8O	108.14
DMS	Dimethyl sulfide	(CH3)2S	62.13
DST1	Dust aerosol, Reff = 0.7 microns	not listed	29.0
DST2	Dust aerosol, Reff = 1.4 microns	not listed	29.0
DST3	Dust aerosol, Reff = 2.4 microns	not listed	29.0
DST4	Dust aerosol, Reff = 4.5 microns	not listed	29.0
EBZ	Ethylbenzene	C8H10	106.167
EOH	Ethanol	C2H5OH	46.07
ETHLN	Ethanol nitrate	CHOCH2ONO2	105.06
ETHN	hydroxy-nitrooxy-ethane	HOCH2CH2ONO2	107.07
ETHP	hydroxy-hydroperoxy-ethane	HOCH2CH2OOH	78.07
ETNO3	Ethyl nitrate	C2H5ONO2	91.08
ETP	Ethylhydroperoxide	CH3CH2OOH	62.08
FURA	Furan	C4H4O	68.07
GLYC	Glycoaldehyde	HOCH2CHO	60.06
GLYX	Glyoxal	CHOCHO	58.04
HACTA	Hydroxyacetic/glycolic acid	HOCH2CO2H	76.0514
H1211	Halon 1211, Freon 12B1	CBrClF2	165.36
H1301	Halon 1301, Freon 13B1	CBrF3	148.91
H2402	Halon 2402	C2Br2F4	259.82
H2O	Water vapor	H2O	18.02
H2O2	Hydrogen peroxide	H2O2	34.02
HAC	Hydroxyacetone	HOCH2C(O)CH3	74.08
HBr	Hypobromic acid	HBr	80.91
HC5A	isoprene-4,1-hydroxyaldehyde	C5H8O2	100.13
HCFC123	HCFC-123, Freon 123	C2HCl2F3	152.93

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Table 1 – continued from previous page

Species	Description	Formula	MW (g)
HCFC141b	HCFC-141b, Freon 141b	C(CH3)Cl2F	116.94
HCFC142b	HCFC-142b, Freon 142b	C(CH3)ClF2	100.5
HCFC22	HCFC-22, Freon 22	CHClF2	86.47
HCl	Hydrochloric acid	HCl	36.45
HCOOH	Formic acid	HCOOH	46.03
HI	Hydrogen iodide	HI	127.91
HMHP	Hydroxymethyl hydroperoxide	HOCH2OOH	64.05
HMML	hydroxymethyl-methyl-a-lactone	C4H6O3	102.1
HMS	Hydroxymethanesulfonate	HOCH2SO3	111.1
HNO2	Nitrous acid	HNO2	47.01
HNO3	Nitric acid	HNO3	63.01
HNO4	Peroxynitric acid	HNO4	79.01
HOBr	Hypobromous acid	HOBr	96.91
HOCl	Hypochlorous acid	HOCl	52.45
HOI	Hypoiodous acid	HOI	143.89
HONIT	2nd gen monoterpene organic nitrate	not listed	215.0
HPALD1	d-4,1-C5-hydroperoxyaldehyde	C5H8O3	116.13
HPALD2	d-1,4-C5-hydroperoxyaldehyde	C5H8O3	116.13
HPALD3	b-2,1-C5-hydroperoxyaldehyde	C5H8O3	116.13
HPALD4	b-3,4-C5-hydroperoxyaldehyde	C5H8O3	116.13
HPETHNL	Hydroperoxy ethanal	HOOCH2CHO	76.06
I	Atomic iodine	I	126.9
I2	Molecular iodine	I2	253.8
I2O2	Diiodine dioxide	I2O2	285.8
I2O3	Diiodine trioxide	I2O3	301.8
I2O4	Diiodine tetraoxide	I2O4	317.8
IBr	Iodine monobromide	IBr	206.9
ICHE	Isoprene hydroxy-carbonyl-epoxides	C5H8O3	116.13
ICl	Iodine monochloride	ICl	162.45
ICN	Lumped isoprene carbonyl-nitrates	C5H7NO4	145.13
ICPDH	Isoprene dihydroxy hydroperoxycarbonyl	C5H10O5	150.15
IDC	Lumped isoprene dicarbonyls	C5H6O2	98.11
IDCHP	Isoprene dicarbonyl hydroxy dihydroperoxide	C5H8O5	148.13
IDHDP	Isoprene dihydroxy dihydroperoxide	C5H12O6	168.17
IDHPE	Isoprene dihydroxy hydroperoxy epoxide	C5H10O5	150.15
IDN	Lumped isoprene dinitrates	C5H8N2O6	192.15
IEPOXA	trans-Beta isoprene epoxydiol	C4H10O3	106.14
IEPOXB	cis-Beta isoprene epoxydiol	C4H10O3	106.14
IEPOXD	Delta isoprene epoxydiol	C4H10O3	106.14
IHN1	Isoprene-d-4,1-hydroxynitrate	C5H9NO4	147.15
IHN2	Isoprene-b-1,2-hydroxynitrate	C5H9NO4	147.15
IHN3	Isoprene-b-4,3-hydroxynitrate	C5H9NO4	147.15
IHN4	Isoprene-d-4,1-hydroxynitrate	C5H9NO4	147.15
INDIOL	Generic aerosol-phase organonitrate hydrolysis product	not listed	102.0
INO	Nitrosyl iodide	INO	156.91
INPB	Lumped b-hydroperoxy isoprene nitrates	C5H9NO5	163.15
INPD	Lumped d-hydroperoxy isoprene nitrates	C5H9NO5	163.15
IO	Iodine monoxide	IO	142.9
IONITA	Aer-phase organic nitrate from isoprene precursors	not listed	14.01
IONO	Nitryl iodide	IONO	172.91

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Table 1 – continued from previous page

Species	Description	Formula	MW (g)
IONO2	Iodine nitrate	IONO2	188.91
IPRNO3	Isopropyl nitrate	C3H7ONO2	105.11
ISALA	Fine sea salt iodine	I	126.9
ISALC	Coarse sea salt iodine	I	126.9
ISOP	Isoprene	CH2=C(CH3)CH=CH2	68.13
ITCN	lumped isoprene tetrafunctional carbonylnitrates	C5H9NO7	195.15
ITHN	Lumped isoprene tetrafunctional hydroxynitrates	C5H11NO7	197.17
LIMAL	Aldehyde from limonene	C10H16O2	186.28
LIMKB	2nd gen ketone from limonene	C10H16O3	186.28
LIMKET	Ketone from limonene	C10H16O2	186.28
LIMN	Saturated 1st gen limonene organic nitrate	C10H17NO4	215.28
LIMNB	Saturated 1st gen LIMO organic nitrate	C10H15NO4	215.28
LIMO	Limonene	C10H16	136.26
LIMO2H	Acid from LIMO	C10H18O3	186.28
LIMO3H	Peracid from LIMO	C10H18O4	186.28
LIMPAN	PAN from LIMO	C10H17NO4	215.28
LVOC	Gas-phase low-volatility non-IEPOX product of RIP ox	C5H14O5	154.19
LVOCOA	Aer-phase low-volatility non-IEPOX product of RIP ox	C5H14O5	154.19
MACR	Methacrolein	CH2=C(CH3)CHO	70.1
MACR1OOH	Peracid from MACR	CH2=C(CH3)C(O)OOH	102.1
MAP	Peroxyacetic acid	CH3C(O)OOH	76.06
MCRDH	Dihydroxy-methacrolein	C4H8O3	104.12
MCRENOL	Lumped enols from MVK/MACR	C4H6O2	86.1
MCRHN	Nitrate from MACR	HOCH2C(ONO2)(CH3)CHO	149.11
MCRHNB	Nitrate from MACR	O2NOCH2C(OH)(CH3)CHO	149.11
MCRHP	Hydroxy-hydroperoxy-methacrolein	HOCH2C(OOH)(CH3)CHO	120.12
MCT	Catechols and methyl catechols	C7H8O2	124.0
MEK	Methyl Ethyl Ketone	RC(O)R	72.11
MEKPN	MEK peroxyacetyl nitrate	C3H5NO6	151.07
MENO3	Methyl nitrate	CH3ONO2	77.05
MGLY	Methylglyoxal	CH3COCHO	72.07
MOH	Methanol	CH3OH	32.05
MONITA	Aer-phase organic nitrate from monoterpene precursors	not listed	14.01
MONITS	Saturated 1st gen monoterpene organic nitrate	C10H17NO4	215.28
MONITU	Unsaturated 1st gen monoterpene organic nitrate	C10H17NO4	215.28
MP	Methyl hydro peroxide	CH3OOH	48.05
MPAN	Peroxymethacroyl nitrate (PMN)	CH2=C(CH3)C(O)OONO2	147.1
MPN	Methyl peroxy nitrate	CH3O2NO2	93.05
MSA	Methyl sulfonic acid	CH4SO3	96.1
MTPA	a-pinene, b-pinene, sabinene, carene	not listed	136.26
MTPO	Terpinene, terpinolene, myrcene, ocimene, other monoterpenes	not listed	136.26
MVK	Methyl vinyl ketone	CH2=CHC(=O)CH3	70.09
MVKDH	dihydroxy-MVK	HOCH2CH2OHC(O)CH3	105.13
MVKHC	MVK hydroxy-carbonyl	C4H6O3	102.1
MVKHCB	MVK hydroxy-carbonyl	C4H6O3	102.1
MVKHP	MVK hydroxy-hydroperoxide	C4H8O4	120.12
MVKN	Nitrate from MVK	HOCH2CH(ONO2)C(=O)CH3	149.12
MVKPC	MVK hydroperoxy-carbonyl	OCHCH(OOH)C(O)CH3	118.1
MYRCO	Aldehyde or ketone from myrcene	C10H18O3	186.28
N2O	Nitrous oxide	N2O	44.02

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Table 1 – continued from previous page

Species	Description	Formula	MW (g)
N2O5	Dinitrogen pentoxide	N2O5	108.02
NH3	Ammonia	NH3	17.04
NH4	Ammonium	NH4	18.05
NIT	Inorganic nitrates	not listed	62.01
NITs	Inorganic nitrates on surface of seasalt aerosol	not listed	31.4
NO	Nitrogen oxide	NO	30.01
NO2	Nitrogen dioxide	NO2	46.01
NO3	Nitrate radical	NO3	62.01
NPHEN	Nitrophenols	C6H5NO3	139.11
NPRNO3	n-propyl nitrate	C3H7ONO2	105.11
O3	Ozone	O3	48.0
OClO	Chlorine dioxide	OClO	67.45
OCPI	Hydrophilic organic carbon aerosol	not listed	12.01
OCPO	Hydrophobic organic carbon aerosol	not listed	12.01
OCS	Carbonyl sulfide	COS	60.07
OIO	Iodine dioxide	OIO	158.9
PAN	Peroxyacetyl nitrate	CH3C(O)OONO2	121.06
pFe	Anthropogenic iron	Fe	55.85
PHAN	Peroxyhydroxyacetic nitric anhydride	C2H3NO6	137.0483
PHEN	Phenol	C6H6O	94.11
PIN	Saturated 1st gen monoterpene organic nitrate	C10H17NO4	215.28
PINAL	Pinonaldehyde	C10H16O2	186.28
PINONIC	Pinonic acid	C10H18O3	186.28
PINO3H	Pinonic peracid	C10H18O4	186.28
PINPAN	PAN from pinonaldehyde	C10H17NO4	215.28
PIP	Peroxide from MTPA	C10H18O3	186.28
PP	Peroxide from PO2	HOCH2CH(OOH)CH3	92.11
PPN	Lumped peroxypropionyl nitrate	CH3CH2C(O)OONO2	135.08
PROPNN	Propanone nitrate	CH3C(=O)CH2ONO2	119.08
PRPE	Lumped >= C3 alkenes	C3H6	42.09
PRPN	Peroxide from PRN1	O2NOCH2CH(OOH)CH3	137.11
PYAC	Pyruvic acid	C3H4O3	88.07
R4N2	Lumped alkyl nitrate	RO2NO	119.1
R4P	Peroxide from R4O2	CH3CH2CH2CH2OOH	90.14
R7N2	C7 Lumped alkyl nitrate	RO2NO	161.2
R7P	Peroxide from R7O2	C7H16O2	132.2
RA3P	Peroxide from A3O2	CH3CH2CH2OOH	76.11
RB3P	Peroxide from B3O2	CH3CH(OOH)CH3	76.11
RCHO	Lumped aldehyde >= C3	CH3CH2CHO	58.09
RCOOH	> C2 organic acids	C2H5C(O)OH	74.09
RIPA	1,2-ISOPOOH	C5H10O3	118.15
RIPB	4,3-ISOPOOH	C5H10O3	118.15
RIPC	d-1,4-ISOPOOH	C5H10O3	118.15
RIPD	d-4,1-ISOPOOH	C5H10O3	118.15
RNO3	Lumped aromatic nitrate	RO2NO	203.15
RP	Peroxide from RCO3	CH3CH2C(O)OOH	90.09
SALA	Fine (0.01-0.05 microns) sea salt aerosol	not listed	31.4
SALAAL	Accumulation mode sea salt alkalinity	not listed	31.4
SALACL	Chloride in Accumulation mode sea salt aerosol	not listed	35.45
SALC	Coarse (0.5-8 microns) sea salt aerosol	not listed	31.4

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Table 1 – continued from previous page

Species	Description	Formula	MW (g)
SALCAL	Coarse mode sea salt alkalinity	not listed	31.4
SALCCL	Chloride in Coarse mode sea salt aerosol	not listed	35.45
SO2	Sulfur dioxide	SO2	64.04
SO4	Sulfate	SO4	96.06
SO4s	Sulfate on surface of seasalt aerosol	not listed	31.4
SOAGX	Aerosol-phase glyoxal	C2H2O2	58.04
SOAIE	Aerosol-phase IEPOX	C5H10O3	118.15
SOAP	SOA Precursor - lumped species for simplified SOA parameterization	not listed	150.0
SOAS	SOA Simple - simplified non-volatile SOA parameterization	not listed	150.0
STYR	Styrene	C8H8	104.1491
TLFUONE	Aromatic furanones	C5H6O2	98.1
TMB	Trimethylbenzenes	C8H10	106.167
TOLU	Toluene	C7H8	92.15
XYLE	Xylene	C8H10	106.18

Table 2: Non-transported species (Standard option)

Species	Description	Formula	MW (g)
A3O2	Primary peroxy radical from C3H8	CH3CH2CH2OO	75.1
ACRO2	Peroxy radical from ACR	C3H5O4	105.07
ACO3	Peroxyacetyl radical for APAN	C3H3O3	87.054
ALK4N1	Peroxy radical from ALK4N2	C4H8NO5	150.13
ALK4O2	Peroxy radical from ALK4	C4H9O2	89.13
AROMRO2	hydroxy-peroxy radical from aromatics	C6H7O3	127.0
AROMCO3	Lumped aromatic peroxyacetyl radical	C5H5O6	161.09
ATO2	Peroxy radical from acetone	CH3C(O)CH2O2	89.08
B3O2	B3O2	CH3CH(OO)CH3	75.1
BENZO	alkoxy radical from aromatics	C6H5O	93.0
BENZO2	peroxy radical from aromatics	C6H5O2	109.0
BRO2	Peroxy radical from BENZ oxidation	C6H7O5	159.13
BUTO2	peroxy radical from C4H6	C4H7O3	103.097
BZCO3	Acyl peroxy radical from benzaldehyde	C7H5O3	137.0
C4HVP1	C4 hydroxy-vinyl peroxy radicals from HPALDS	C4H7O3	103.11
C4HVP2	C4 hydroxy-vinyl peroxy radicals from HPALDS	C4H7O3	103.11
CH2OO	Criegee intermediate	CH2OO	46.03
CH3CHOO	Criegee intermediate	CH3CHOO	60.06
CO2	Carbon dioxide	CO2	44.01
ETO	alkoxy radical from ETOO	HOCH2CH2O	61.06
ETOO	peroxy radical from ethene	HOCH2CH2OO	77.06
ETO2	ETO2	CH3CH2OO	61.07
GCO3	Peroxyacetyl radical for PHAN	HOCH2CO3	91.0428
H	Atomic hydrogen	H	1.01
HO2	Hydroperoxyl radical	HO2	33.01
HPALD1OO	HPALD1OO	C5H7O5	147.12
HPALD2OO	HPALD2OO	C5H7O5	147.12
ICHOO	Peroxy radical from IEPOXD	C5H9O5	149.14
ICNOO	Peroxy radicals from ICN	C5H8NO7	194.14
IDHNBOO	Peroxy radicals from INPB	C5H10NO7	196.16
IDHNDOO1	Peroxy radicals from INPD	C5H10NO7	196.16

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Table 2 – continued from previous page

Species	Description	Formula	MW (g)
IDHNDOO2	Peroxy radicals from INPD	C5H10NO7	196.16
IDNOO	IDNOO	C5H9N2O6	241.14
IEPOXAOO	Peroxy radical from trans-Beta isoprene epoxydiol	C5H8O5	149.14
IEPOXBOO	peroxy radical from cis-Beta isoprene epoxydiol	C5H9O5	149.14
IHOO1	Peroxy radical from OH addition to isoprene at C1	C5H9O3	117.14
IHOO4	Peroxy radical from OH addition to isoprene at C4	C5H9O3	117.14
IHPNBOO	Peroxy radicals from INPB	C5H10NO8	212.16
IHPNDOO	Peroxy radicals from INPD	C5H10NO8	212.16
IHPOO1	Peroxy radical from ISOPOOH	C5H11O6	167.16
IHPOO2	Peroxy radical from ISOPOOH	C5H11O6	167.16
IHPOO3	Peroxy radical from ISOPOOH	C5H11O6	167.16
INA	Alkoxy radical from INO2D	C5H8NO4	146.14
INO2B	beta-peroxy radicals from isoprene + NO3	C5H8NO5	162.14
INO2D	delta-peroxy radicals from isoprene + NO3	C5H8NO5	162.14
ISOPNOO1	Peroxy radicals from IHN2	C5H10NO7	196.16
ISOPNOO2	Peroxy radicals from IHN3	C5H10NO7	196.16
KO2	Peroxy radical from >3 ketones	C4H5O3	101.09
LBRO2H	Dummy species to track oxidation of BRO2 by HO2	not listed	159.13
LBRO2N	Dummy species to track oxidation of BRO2 by NO	not listed	159.13
LIMO2	Peroxy radical from LIMO	C10H17O3	185.27
APINO2	Peroxy radical from APIN	C10H17O3	185.27
PINO3	Acylperoxy radical from APIN	C10H17O3	185.27
C96O2	2nd-gen peroxy radical from APIN	C10H17O3	185.27
BPINO2	Peroxy radical from BPIN	C10H17O3	185.27
BPINOO2	2nd-gen peroxy radical from BPIN	C10H17O3	185.27
LIMKO2	2nd-gen peroxy radical from LIMO	C10H17O3	185.27
LIMO3	Acylperoxy radical from LIMO	C10H17O3	185.27
LISOPOH	Dummy species to track oxidation of ISOP by OH	not listed	68.13
LISOPNO3	Dummy species to track oxidation of ISOP by NO3	not listed	68.13
LNRO2H	Dummy species to track oxidation of NRO2 by HO2	not listed	159.17
LNRO2N	Dummy species to track oxidation of NRO2 by NO	not listed	159.17
LTRO2H	Dummy species to track oxidation of TRO2 by HO2	not listed	173.16
LTRO2N	Dummy species to track oxidation of TRO2 by NO	not listed	173.16
LXRO2H	Dummy species to track oxidation of XRO2 by HO2	not listed	187.19
LXRO2N	Dummy species to track oxidation of XRO2 by NO	not listed	187.19
MACR1OO	Peroxyacyl radical from MACR + OH	CH2=C(CH3)C(O)OO	101.09
MACRNO2	Product of MCRHN + OH	C4H6NO7	180.1
MCO3	Peroxyacetyl radical	CH3C(O)OO	75.05
MCROHOO	Peroxy radical from MACR + OH	C4H7O4	119.11
MEKCO3	not listed	C3H5O4	105.07
MO2	Methylperoxy radical	CH3O2	47.04
MVKOHOO	Peroxy radical from MVK + OH	C4H7O4	119.11
N	Atomic nitrogen	N	14.01
NAP	Naphtalene/IVOC surrogate	C10H8	128.18
NRO2	Peroxy radical from NAP oxidation	C10H7O2	159.17
O	Ground state atomic oxygen	O(3P)	16.0
O1D	Excited atomic oxygen (1D)	O(1D)	16.0
OH	Hydroxyl radical	OH	17.01
OLND	Monoterpene-derived NO3-alkene adduct	C10H16NO5	230.27
OLNN	Monoterpene-derived NO3 adduct	C10H16NO5	230.27

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Table 2 – continued from previous page

Species	Description	Formula	MW (g)
OTHRO2	Other C2 RO2 not from C2H6 oxidation	CH3CH2OO	61.07
PIO2	Peroxy radical from MTPA	C10H17O3	185.27
PO2	Peroxy radical from propene	HOCH2CH(OO)CH3	91.1
PRN1	Peroxy radical from propene + NO3	O2NOCH2CH(OO)CH3	136.09
R4N1	Peroxy radical from R4N2	C4H8NO5	150.13
R4O2	Peroxy radical from isoprene and MTPA alkyl generation	C4H9O2	89.13
R7O2	Peroxy radical from ALK6	C7H15O2	131.19
R7N1	Peroxy radical from R7N2	C7H15NO5	161.2
RCO3	Peroxypropionyl radical	CH3CH2C(O)OO	89.08
ROH	> C2 alcohols	C3H7OH	60.11
TLFUO2	not listed	C5H7O5	147.1
TRO2	Peroxy radical from TOLU oxidation	C7H9O5	173.16
XRO2	Peroxy radical from TOLU oxidation	C8H11O5	187.19
PH2SO4	SO4 from gas-phase chemistry	not listed	96.06
PSO4AQ	SO4 from cloud chemistry	not listed	96.06
ZRO2	RO2 for making lumped aromatic nitrate	C7H9O5	173.16
H2	Molecular hydrogen	H2	2.02
N2	Molecular nitrogen	N2	28.02
O2	Molecular oxygen	O2	32.0

16.2.2 Benchmark

Fullchem simulations with the **Benchmark** option allow the **`GEOS-Chem Support Team <https://geoschem.github.io/support-team.html`_** `to perform simulations that document the performance and evolution of GEOS-Chem over time.

Benchmark simulations use all of the *Standard species*, as well as the *Complex SOA species* listed below. However, the complex SOA species are carried solely for diagnostic purposes.

16.2.3 Complex SOA

Fullchem simulations with **Complex SOA** option use all of the *Standard species*, plus 15 additional transported species.

Table 3: Additional transported species (Complex SOA)

Species	Description	MW (g)
ASOA1	Lumped non-volatile aerosol products of light aromatics + IVOCs	150.0
ASOA2	Lumped non-volatile aerosol products of light aromatics + IVOCs	150.0
ASOA3	Lumped non-volatile aerosol products of light aromatics + IVOCs	150.0
ASOAN	Lumped non-volatile aerosol products of light aromatics + IVOCs	150.0
ASOG1	Lumped non-volatile gas products of light aromatics + IVOCs	150.0
ASOG2	Lumped non-volatile gas products of light aromatics + IVOCs	150.0
ASOG3	Lumped non-volatile gas products of light aromatics + IVOCs	150.0
TSOA0	Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation	150.0
TSOA1	Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation	150.0
TSOA2	Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation	150.0
TSOA3	Lumped semivolatile aerosol products of monoterpene + sesquiterpene oxidation	150.0
TSOG0	Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation	150.0
TSOG1	Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation	150.0
TSOG2	Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation	150.0
TSOG3	Lumped semivolatile gas products of monoterpene + sesquiterpene oxidation	150.0

You may archive several complex SOA diagnostic quantities to the *AerosolMass History collection*.

16.2.4 Complex SOA plus semi-volatile POA

Fullchem simulations with **`Complex SOA plus semi-volatile POA`** use all of the *Standard species* and *Complex SOA species*, plus several additional transported primary organic aerosol species.

Table 4: Additional transported species (Complex SOA with SVPOA)

Species	Description	MW (g)
OPOA1	Lumped aerosol product of SVOC oxidation	12.01
OPOA2	Lumped aerosol product of SVOC oxidation	12.01
OPOG1	Lumped gas product of SVOC oxidation	12.01
OPOG2	Lumped gas product of SVOC oxidation	12.01
POA1	Lumped aerosol primary SVOCs	12.01
POA2	Lumped aerosol primary SVOCs	12.01
POG1	Lumped gas primary SVOCs	12.01
POG2	Lumped gas primary SVOCs	12.01

16.2.5 Marine POA

Fullchem simulations with **`Marine POA`** use all of the *Standard species*, plus two additional transported aerosol species.

Table 5: Additional transported species (Marine POA)

Species	Description	Formula	MW (g)
MOPI	Hydrophilic marine organic carbon aerosol	C	12.01
MOPO	Hydrophobic marine organic carbon aerosol	C	12.01

16.2.6 Acid uptake on dust

Fullchem simulations with **`Acid uptake on dust`** use all of the *Standard species*, plus 12 additional transported species.

Table 6: Additional transported species (Acid uptake on dust)

Species	Description	MW (g)
DSTAL1	Dust alkalinity, Reff = 0.7 μm	29.0
DSTAL2	Dust alkalinity, Reff = 1.4 μm	29.0
DSTAL3	Dust alkalinity, Reff = 2.4 μm	29.0
DSTAL4	Dust alkalinity, Reff = 4.5 μm	29.0
NITD1	Nitrate on dust, Reff = 0.7 μm	29.0
NITD2	Nitrate on dust, Reff = 1.4 μm	29.0
NITD3	Nitrate on dust, Reff = 2.4 μm	29.0
NITD4	Nitrate on dust, Reff = 4.5 μm	29.0
SO4D1	Sulfate on dust, Reff = 0.7 μm	29.0
SO4D2	Sulfate on dust, Reff = 1.4 μm	29.0
SO4D3	Sulfate on dust, Reff = 2.4 μm	29.0
SO4D4	Sulfate on dust, Reff = 4.5 μm	29.0

16.2.7 TOMAS aerosol microphysics

Fullchem simulations with **`TOMAS aerosol microphysics`** use all of the *Standard species*, plus several additional size-resolved aerosol species. Note that the bulk dust species (DST1, DST2, DST3, DST4) species are replaced with size-resolved dust species (DUST1 .. DUST40).

Table 7: Additional transported species (TOMAS)

Species	Description	MW (g)
AW01 .. AW40	Aerosol water, size bins 1 .. 40	18.0
DUST01 .. DUST40	Mineral dust, size bins 1 .. 40	100.0
ECIL01 .. ECIL40	Hydrophilic elemental carbon, size bins 1 .. 40	12.01
ECOB01 .. ECOB40	Hydrophobic elemental carbon, size bins 1 .. 40	12.01
H2SO4:	Sulfuric acid	98.0
NK01 .. NK40	Aerosol number, size bins 1..40	1.0
OCIL01 .. OCIL40	Hydrophilic organic carbon, size bins 1 .. 40	12.01
OCOB01 .. OCOB40	Hydrophilic organic carbon, size bins 1 .. 40	12.01
SF01 .. SF40	Sulfate aerosol, size bins 1 .. 40	96.0
SS01 .. SS40	Sea salt aerosol, size bins 1 .. 40	58.5

You must request TOMAS aerosol microphysics at configuration time. You may select either TOMAS with 15 size-resolved bins or with 40 size-resolved bins. Please see *this section* for configuration and compilation instructions.

You may archive several TOMAS diagnostic quantities to the *TOMAS History collection*.

16.2.8 APM aerosol microphysics

Fullchem simulations with **`APM aerosol microphysics`** use all species listed in the *Standard*, as well as the following species:

Table 8: Additional transported species (APM)

Species	Description	MW (g)
APMAMINE1	APM amines 1	31.0
APMAMINE2	APM amines 2	45.0
APMAMINE3	APM amines 3	59.0
APMBCBIN01 .. APMBCBIN15	APM black carbon, size bins 01 .. 15	12.01
APMCTBC1	APM CTSO4	96.0
APMCTBC2	APM CTSLVSOA	181.0
APMCTDST1	APM CTSO4	96.0
APMCTDST2	APM CTLVSOA	181.0
APMCTOC1	APM CTSO4	96.0
APMCTOC2	APM CTLVSOA	181.0
APMCTSEA1	APM CTSO4	96.0
APMCTSEA2	APM CTLVSOA	181.0
APMDSTBIN01 .. APMDSTBIN15	APM Dust	29.0
APMH2SO4	APM sulfuric acid	98.0
APMLVSOA	APM LVSOA	181.0
APMLVSOG	APM LV secondary organic gas	181.0
APMOCBIN01 .. APMOCBIN15	APM organic carbon, size bins 01 .. 15	12.01
APMSEABIN01 .. APMSEABIN20	APM sea salt, size bins 01 .. 20	12.01
APMSPBIN01 .. APMSPBIN40	APM sulfate, size bins 01 .. 40	96.0

You must request APM aerosol microphysics at configuration time. Please see *this section* for configuration and compilation instructions.

16.2.9 RRTMG radiative transfer model

Fullchem simulations with the **`RRTMG radiative transfer model`** use the *Standard species*. No additional species are included. Radiative forcing diagnostics can be archived to the *RRTMG History collection*.

CHAPTER

SEVENTEEN

HG (MERCURY) SIMULATION

17.1 Overview

From the abstract to Shah et al. 2021:

> We present a new chemical mechanism for HgO, HgI/HgII atmospheric cycling, including recent laboratory and computational data, and implement it in the GEOS-Chem global atmospheric chemistry model for comparison to observations. Our mechanism includes the oxidation of Hg0 by Br and OH, subsequent oxidation of HgI by ozone and radicals, respeciation of HgII in aerosols and cloud droplets, and speciated HgII photolysis in the gas and aqueous phases. The tropospheric Hg lifetime against deposition in the model is 5.5 months, consistent with observational constraints. The model reproduces the observed global surface Hg0 concentrations and HgII wet deposition fluxes. Br and OH make comparable contributions to global net oxidation of Hg0 to HgII. Ozone is the principal HgI oxidant, enabling the efficient oxidation of Hg0 to HgII by OH. BrHgIIOH and HgII(OH)2, the initial HgII products of Hg0 oxidation, respeciate in aerosols and clouds to organic and inorganic complexes, and volatilize to photostable forms. Reduction of HgII to Hg0 takes place largely through photolysis of aqueous HgII–organic complexes. 71% of model HgII deposition is to the oceans. Major uncertainties for atmospheric Hg chemistry modeling include Br concentrations, stability and reactions of HgI, and speciation and photoreduction of HgII in aerosols and clouds.

Reference: Shah, V., D.J. Jacob, C.P. Thackray, X. Wang, E.M. Sunderland, T.S. Dibble, A. Saiz-Lopez, I. Cernusak, V. Kello, P.J. Castro, R. Wu, and C. Wang, *Improved mechanistic model of the atmospheric redox chemistry of mercury*, Environ. Sci. Technol., 55, 14445-14456, 2021, DOI: 10.1021/acs.est.1c03160

17.2 List of species

Table 1: Transported species

Species	Description	Formula	MW (g)
Hg0	Elemental mercury	Hg	200.59
HgBr	not listed	HgBr	200.59
HgBrNO2	not listed	BrHgONO	200.59
HgBrHO2	not listed	BrHgOOH	200.59
HgBrClO	not listed	BrHgOCl	200.59
HgBrBrO	not listed	BrHgOBr	200.59
HgBr2	not listed	HgBr2	200.59
HgBrOH	not listed	BrHgOH	None
HgBrO	HgBrO	HgBrO	200.59
HgClNO2	not listed	ClHgONO	200.59

continues on next page

Table 1 – continued from previous page

Species	Description	Formula	MW (g)
HgClHO2	not listed	ClHgOOH	200.59
HgClClO	not listed	ClHgOCl	200.59
HgClBrO	not listed	ClHgOBr	200.59
HgClBr	not listed	HgBrCl	200.59
HgClOH	not listed	ClHgOH	None
HgCl	not listed	HgCl	200.59
HgClO	not listed	ClHgO	200.59
HgOHNO2	not listed	HOHgONO	200.59
HgOHHO2	not listed	HOHgOOH	200.59
HgOHClO	not listed	HOHgOCl	None
HgOHBrO	not listed	HOHgOBr	200.59
HgOHOH	not listed	HOHgOH	200.59
HgOH	not listed	HgOH	200.59
HgOHO	not listed	HgOHO	200.59
HgCl2	not listed	HgCl2	200.59
Hg2ClP	not listed	HgCln	200.59
Hg2ORGP	not listed	R-Hg	200.59
Br	Atomic bromine	Br	79.9
Cl	Atomic chlorine	Cl	35.45
OH	Hydroxyl radical	OH	17.01
NO2	Nitrogen dioxide	NO2	46.01
NO	Nitrogen oxide	NO	30.01
O3	Ozone	O3	48.0
HO2	Hydroperoxyl radical	HO2	33.01
BrO	Bromine monoxide	BrO	95.9
ClO	Chlorine monoxide	ClO	51.45
CO	not listed	CO	28.01
CH4	not listed	CH4	16.04

CHAPTER

EIGHTEEN

METALS SIMULATION

18.1 Overview

From the abstract of Xu et al. [2019]:

> Trace metal distributions are of relevance to understand sources of fine particulate matter (PM2.5), PM2.5-related health effects, and atmospheric chemistry. However, knowledge of trace metal distributions is lacking due to limited ground-based measurements and model simulations. This study develops a simulation of 12 trace metal concentrations (Si, Ca, Al, Fe, Ti, Mn, K, Mg, As, Cd, Ni and Pb) over continental North America for 2013 using the GEOS-Chem chemical transport model. Evaluation of modeled trace metal concentrations with observations indicates a spatial consistency within a factor of 2. The spatial distribution of trace metal concentrations reflects their primary emission sources. Crustal element (Si, Ca, Al, Fe, Ti, Mn, K) concentrations are enhanced over the central US from anthropogenic fugitive dust and over the southwestern U.S. due to natural mineral dust. Heavy metal (As, Cd, Ni and Pb) concentrations are high over the eastern U.S. from industry. K is abundant in the southeast from biomass burning. High concentrations of Mg are observed along the coast from sea spray. The spatial pattern of PM2.5 mass is most strongly correlated with Pb, Ni, As and K due to their signature emission sources. Challenges remain in accurately simulating observed trace metal concentrations. Halving anthropogenic fugitive dust emissions in the 2011 National Air Toxic Assessment (NATA) inventory and doubling natural dust emissions in the default GEOS-Chem simulation was necessary to reduce biases in crustal element concentrations. A fivefold increase of anthropogenic emissions of As and Pb was necessary in the NATA inventory to reduce the national-scale bias versus observations by more than 80%, potentially reflecting missing sources.

Reference Xu, J.-W., R.V. Martin, B.H. Henderson, J. Meng, Y.B. Oztaner, J.L. Hand, A. Hakami, M. Strum, and S.B. Phillips, *Simulation of airborne trace metals in fine particulate matter over North America*, Atmos. Environ., 214, 116883, 2019, DOI: 10.1016/j.atmosenv.2019.116883

18.2 List of species

Table 1: Transported species

Species	Description	Formula	MW (g)
AlF1	not listed	Al	26.98
AlF2	not listed	Al	26.98
AsF1	not listed	As	74.92
AsF2	not listed	As	74.92
CaF1	not listed	Ca	40.08
CaF2	not listed	Ca	40.08
CaC3	not listed	Ca	40.08

continues on next page

Table 1 – continued from previous page

Species	Description	Formula	MW (g)
CaC4	not listed	Ca	40.08
CdF1	not listed	Cd	112.41
CdF2	not listed	Cd	112.41
FeF1	not listed	Fe	55.84
FeF2	not listed	Fe	55.84
KF1	not listed	K	39.1
KF2	not listed	K	39.1
KC3	not listed	K	39.1
KC4	not listed	K	39.1
MgF1	not listed	Mg	24.31
MgF2	not listed	Mg	24.31
MgC3	not listed	Mg	24.31
MgC4	not listed	Mg	24.31
MnF1	not listed	Mn	54.94
MnF2	not listed	Mn	54.94
NiF1	not listed	Ni	58.69
NiF2	not listed	Ni	58.69
PbF1	not listed	Pb	210.0
PbF2	not listed	Pb	210.0
SiF1	not listed	not listed	28.09
SiF2	not listed	not listed	28.09
TiF1	not listed	Ti	47.87
TiF2	not listed	Ti	47.87

CHAPTER

NINETEEN

TAGGED O3 SIMULATION

19.1 Overview

The **GEOS-Chem tagged ozone simulation** allows you to use archived ozone production and loss rates to perform a simulation for geographically tagged ozone tracers without having to run the full-chemistry simulation. The tagged O3 simulation is also used to spin up the ozone into steady-state when validating a new meterorolgical field product.

19.2 List of species

Table 1: Transported species

Species	Description	Formula	MW (g)
O3	Ozone	O3	48.0
O3Strat	Ozone produced in the stratosphere	O3	48.0
O3ut	Ozone produced in the upper troposphere	O3	48.0
O3mt	Ozone produced in the middle troposphere	O3	48.0
O3row	Ozone produced in the rest of the world	O3	48.0
O3pcbl	Ozone produced in the Pacific Ocean boundary layer	O3	48.0
O3nabl	Ozone produced in the North America boundary layer	O3	48.0
O3atbl	Ozone produced in the Atlantic Ocean boundary layer	O3	48.0
O3eubl	Ozone produced in the European boundary layer	O3	48.0
O3afbl	Ozone produced in the African boundary layer	O3	48.0
O3asbl	Ozone produced in the Asian boundary layer	O3	48.0
O3init	Ozone from the initial condition	O3	48.0
O3usa	Ozone produced over the United States in PBL	O3	48.0

CHAPTER

TWENTY

TRANSPORTTRACERS SIMULATION

20.1 Overview

The **GEOS-Chem Rn-Pb-Be simulation** was based on that of the old Harvard/GISS CTM model. In version 12.2.0, this simulation was extended to include additional passive species for benchmarking purposes and for diagnosing transport in GEOS-Chem. At this time the simulation was renamed to the **TransportTracers** simulation.

In GEOS-Chem 14.2.0, the TransportTracers simulation was further modified so that species names and definitions are now consistent with GMAO's tracer gridded component (aka TR_GridComp). This will facilitate comparison of transport within GEOS-Chem, GCHP, and GEOS.

Reference Liu, H., D. Jacob, I. Bey, and R.M. Yantosca, *Constraints from 210Pb and 7Be on wet deposition and transport in a global three-dimensional chemical tracer model driven by assimilated meteorological fields*, J. Geophys. Res, 106, D11, 12109-12128, 2001.

20.2 List of species

Table 1: Transported species

Species	Description	Formula	MW (g)
Rn222	Radon-222 isotope	Rn222	222.0
Pb210	Lead-210 isotope	Pb210	210.0
Pb210s	Lead-210 isotope stratospheric-source tracer	Pb210	210.0
Be7	Beryllium-7 isotope	Be7	7.0
Be7s	Beryllium-7 isotope stratospheric-source tracer	Be7	7.0
Be10	Beryllium-10 isotope	Be10	10.0
Be10s	Beryllium-10 isotope stratospheric-source tracer	Be10	10.0
aoa	Age of air uniform source tracer	not listed	1.0
aoa_bl	Age of air uniform source tracer with sink restricted to the boundary layer	not listed	1.0
aoa_nh	Age of air uniform source tracer with surface sink restricted to a zone in the northern hemisphere	not listed	1.0
CH3I	Methyl iodide	CH3I	141.94
CO_25	Anthropogenic CO 25 day tracer	CO	28.01
CO_50	Anthropogenic CO 50 day tracer	CO	28.01
e90	Constant burden 90 day tracer	not listed	1.0
e90_n	Constant burden Northern Hemisphere 90 day tracer	not listed	1.0
e90_s	Constant burden Southern Hemisphere 90 day tracer	not listed	1.0
nh_5	Northern Hemisphere 5 day tracer	not listed	1.0
nh_50	Northern Hemisphere 50 day tracer	not listed	1.0
Passive-Tracer	Passive tracer for mass conservation evaluation	not listed	1.0
SF6	Sulfur hexafluoride	SF6	146.06
st80_25	Stratosphere source 25 day tracer	not listed	1.0

CHAPTER

TWENTYONE

GEOS-CHEM CLASSIC FOLDER TREE

The tables below list the folders in which various components of GEOS-Chem Classic reside.

```
GCClassic
|
+---CMakeScripts                          # Utility functions for CMake
|
+---docs                                  # Root directory for ReadTheDocs documentation
|   |
|   +---source                            # Subdivides documentation into subdirectories
|       |
|       +---gcclassic-user-guide          # Markup files (ReST format) for ReadTheDocs
|       |
|       +---geos-chem-shared-docs         # Submodule containing shared documentation␣
↪files
|       |                                 # (such as common supplemental guides)
|       |
|       +---getting-started               # Markup files (ReST format) for ReadTheDocs
|       |
|       +---help-and-reference            # Markup files (ReST format) for ReadTheDocs
|       |
|       +---_static                       # Static content (e.g. images) for ReadTheDocs
|       |
|       +---supplemental-guides           # Markup files (ReST format) for ReadTheDocs
|                                         # (Content specific to GEOS-Chem Classic)
|
+---run                                   # Link to src/GEOS-Chem/run/GCClassic
|
+---src                                   # Contains submodules used by GEOS-Chem␣
↪Classic
|   |
|   +---Cloud-J                           # Cloud-J submodule source code
|   |   |
|   |   +---CMakeScripts                  # Utility functions for CMake
|   |   |
|   |   +---docs                          # Cloud-J documentation files
|   |   |
|   |   +---src                           # Cloud-J source code
|   |   |
|   |   +---tables                        # Input lookup tables for Cloud-J
|   |   |
```

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```
|   |   +---tools                          # Tools for Cloud-J
|   |       |
|   |       +---AddXs                      # Source code to add new cross-sections
|   |
|   +---GEOS_Chem                          # GEOS-Chem submodule, contains
|   |   |
|   |   +---APM                            # Source code for APM microphysics module
|   |   |
|   |   +---CMakeScripts                   # Utility functions for CMake
|   |   |
|   |   +---GeosCore                       # Source code for most GEOS-Chem science␣
↪routines
|   |   |
|   |   +---GeosRad                        # RRTMG radiative transfer model source code
|   |   |
|   |   +---GeosUtil                       # Source code for various utility routines
|   |   |
|   |   +---GTMM                           # Global Terrestrial Mercury Model source code
|   |   |                                  # (NOTE: This feature has fallen into disuse)
|   |   |
|   |   +---Headers                        # Source code for defining the GEOS-Chem␣
↪state objects
|   |   |
|   |   +---History                        # Source code for History diagnostics
|   |   |
|   |   +---Interfaces                     # Driver code for various implementations of␣
↪GEOS-Chem
|   |   |   |
|   |   |   +---CESM                       # Source code to connect GEOS-Chem to CESM
|   |   |   |
|   |   |   +---GCClassic                  # "Main program" source code for GEOS-Chem␣
↪Classic
|   |   |   |
|   |   |   +---GCHP                       # "Main program" source code for GCHP
|   |   |   |
|   |   |   +---GEOS                       # Source code to connect GEOS-Chem in the␣
↪NASA GEOS ESM
|   |   |
|   |   +---KPP                            # Root folder KPP-generated solver code
|   |   |   |
|   |   |   +---carbon                     # KPP-generated code for the carbon mechanism
|   |   |   |
|   |   |   +---custom                     # "Sandbox" for generating custom mechanisms
|   |   |   |
|   |   |   +---fullchem                   # KPP-generated code for the full-chemistry␣
↪mechanism
|   |   |   |
|   |   |   +---Hg                         # KPP-generated code for the mercury (Hg)␣
↪mechanism
|   |   |
|   |   +---NcdfUtil                       # Source code for netCDF file I/O
|   |   |
```

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```
|   |   +---ObsPack                         # Source code for the ObsPack diagnostic
|   |   |
|   |   +---PKUCPL                          # Source code for PKU two way coupler
|   |   |                                   # (NOTE: This feature has fallen into disuse)
|   |   |
|   |   +---run                             # Root folder for run directory creation␣
↪scripts
|   |   |   |
|   |   |   +---CESM                        # Rundir creation scripts/files for CESM
|   |   |   |
|   |   |   +---GCClassic                   # Rundir creation scripts/files for GEOS-CHem␣
↪Classic
|   |   |   |
|   |   |   +---GCHP                        # Rundir creation scripts/files for GCHP
|   |   |   |
|   |   |   +---GEOS                        # Rundir creation scripts/files for NASA GEOS␣
↪ESM
|   |   |   |
|   |   |   +---shared                      # Common scripts and configuration file␣
↪snippets
|   |   |   |
|   |   |   +---WRF                         # Rundir creation scripts/files for WRF-GC
|   |   |
|   |   +---test                            # Root folder for integration test scripts
|   |       |
|   |       +---difference                  # Scripts to compare the results of two␣
↪integrationtests
|   |       |
|   |       +---integration                 # Top-level integration test folder
|   |       |   |
|   |       |   +---GCClassic               # Scripts to run integration tests for GEOS-
↪Chem Classic
|   |       |   |
|   |       |   +---GCHP                    # Scripts to run integration tests for GCHP
|   |       |
|   |       +---parallel                    # Top-level parallelization test folder
|   |       |   |
|   |       |   +---GCClassic               # Scripts to run parallel tests for GEOS-Chem␣
↪Classic
|   |       |
|   |       +---shared                      # Common scripts for integration & parallel␣
↪tests
|   |
|   +---HEMCO                               # Harmonized Emissions Component (HEMCO)␣
↪submodule
|   |   |
|   |   +---CMakeScripts                    # Utility functions for CMake
|   |   |
|   |   +---docs                            # Root directory for ReadTheDocs documentation
|   |   |   |
|   |   |   +---source                      # Subdivides documentation into subdirectories
|   |   |       |
```

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```
|   |   |       +---coupling                # Markup files (ReST format) for ReadTheDocs
|   |   |       |
|   |   |       +---geos-chem-shared-docs   # Submodule containing shared documentation␣
↪files
|   |   |       |                           # (such as common supplemental guides)
|   |   |       |
|   |   |       +---hco-ref-guide           # Markup files (ReST format) for ReadTheDocs
|   |   |       |
|   |   |       +---hco-sa-guide            # Markup files (ReST format) for ReadTheDocs
|   |   |       |
|   |   |       +---reference               # Markup files (ReST format) for ReadTheDocs
|   |   |       |
|   |   |       +---_static                 # Static content (e.g. images) for ReadTheDocs
|   |   |
|   |   +---run                             # Rundir creation scripts/files for HEMCO␣
↪standalone
|   |   |
|   |   +---src                             # Top-level source code folder
|   |       |
|   |       +---Core                        # Source code for core HEMCO routines
|   |       |
|   |       +---Extensions                  # Source code for HEMCO extensions
|   |       |   |
|   |       |   +---PreProcess              # Scripts for creating the FINN or GFED␣
↪include file
|   |       |
|   |       +---Interfaces                  # Driver programs for the various HEMCO␣
↪implementations
|   |       |   |
|   |       |   +--GEOS                     # Source code to connect HEMCO to the NASA␣
↪GEOS ESM
|   |       |   |
|   |       |   +--MAPL_ESMF                # Source code to run HEMCO in the ESMF/MAPL␣
↪environment
|   |       |   |
|   |       |   +--Shared                   # Common files for run directory creation
|   |       |   |
|   |       |   +--Standalone               # "Main Program" for the HEMCO standalone␣
↪model
|   |       |
|   |       +---Shared                      # Top-level folder for shared code
|   |           |
|   |           +---GeosUtil                # Local copies of source code in GEOS-Chem/
↪GeosUtil
|   |           |
|   |           +---Headers                 # Local copies of source code in GEOS-Chem/
↪Headers
|   |           |
|   |           +---NcdfUtil                # Local copies of source code in GEOS-Chem/
↪NcdfUtil
|   |
|   +---HETP                                # ISORROPIA/HETP submodule source code
```

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```
|       |
|       +---CMakeScripts                    # Utility functions for CMake
|       |
|       +---Core                            # Source code for HETP
|       |
|       +---Test                            # "Main program" for testing HETP in␣
↪standalone mode
|
|
+---spack                                   # Link to docs/source/geos-chem-shared-docs/
↪spack
|
+---test                                    # Link to src/GEOS-Chem/test
```

CHAPTER

TWENTYTWO

SAMPLE GEOS-CHEM RUN SCRIPTS

Here are some sample run scripts that you can adapt for your own purposes.

22.1 For clusters using the Slurm scheduler

Here is a sample GEOS-Chem run script for computational clusters that use the SLURM scheduler to control jobs:

22.1.1 Run script for Slurm

Save this code to a file named `geoschem.run.slurm`:

```
#!/bin/bash

#SBATCH -c 24
#SBATCH -N 1
#SBATCH -t 0-12:00
#SBATCH -p MYPARTITION
#SBATCH --mem=30000
#SBATCH --mail-type=END

############################################################################
### Sample GEOS-Chem run script for SLURM
### You can increase the number of cores with -c and memory with --mem,
### particularly if you are running at very fine resolution (e.g. nested-grid)
############################################################################
# Source the environment file that you created
source /path/to/gcclassic.gnu10.env

# Set the proper # of threads for OpenMP
# SLURM_CPUS_PER_TASK ensures this matches the number you set with -c above
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# NOTE: If the environment file does not max out the available
# stack memory for GEOS-Chem, you may uncomment these lines here:
#ulimit -s unlimited
#export OMP_STACKSIZE=500m

# Run GEOS_Chem.  The "time" command will return CPU and wall times.
# Stdout and stderr will be directed to the "GC.log" log file
```

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```
# (you can change the log file name below if you wish)
srun -c $OMP_NUM_THREADS time -p ./gcclassic >> GC.log
```

Important: If you forget to define `OMP_NUM_THREADS` in your run script, then **GEOS-Chem Classic** will execute using one core. This can cause your simulations to take much longer than is necessary!

Then make `geoschem.run.slurm` executable:

```
$ chmod 755 geoschem.run.slurm
```

For more information about how Slurm is set up on your particular cluster, ask your sysadmin.

22.1.2 Submitting jobs with Slurm

To schedule a **GEOS-Chem Classic** job with Slurm, use this command:

```
$ sbatch geoschem.run.slurm
```

22.2 For Amazon Web Services EC2 cloud instances

When you log into an Amazon Web Services EC2 instance, you will receive an entire node with as many **vCPUs** as you have requested. A vCPU is equivalent to the number of computational cores. Most cloud instances have twice as many vCPUs as physical CPUs (i.e. each CPU chip has 2 cores).

Tip: To find out how many vCPUs are available in your instance, you can use then **nproc** command.

22.2.1 Run script for Amazon EC2

Save the code below to a file named `geoschem.run.aws`:

```
#!/bin/bash

################################################################################
### Sample GEOS-Chem run script for Amazon Web Services EC2 instances
################################################################################

# Load your bash-shell customizations
source ~/.bashrc

### NOTE: We do not have to load an environment file
### because all libraries are contained in the Amazon
### Machine Image (AMI) used to initialize the instance.

# In an AWS cloud instance, you own the entire node, so there is no need
# to use a scheduler like SLURM.  You can just use the `nproc` command
# to specify the number of cores that GEOS-Chem should use.
```

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```
export OMP_NUM_THREADS=$(nproc)

# NOTE: If your `/.bashrc file does not max out the available
# stack memory for GEOS-Chem, you may uncomment these lines here:
#ulimit -s unlimited
#export OMP_STACKSIZE=500m

# Run GEOS_Chem.  The "time" command will return CPU and wall times.
# Stdout and stderr will be directed to the "GC.log" log file
# (you can change the log file name below if you wish)
time -p ./gcclassic >> GC.log 2>&1
```

And then make the `geoschem.run.aws` file executable:

```
$ chmod 755 geoschem.run.aws
```

22.2.2 Running jobs on AWS

When you are on an AWS EC2 instance, you own the entire node, so it is not necessary to use a scheduler. You can run your GEOS-Chem job in with this command:

```
$ ./geoschem.run.aws &
```

This will run your job in the background and send all output (i.e. program output and error output) to `log`.

CHAPTER

TWENTYTHREE

LOAD SOFTWARE INTO YOUR ENVIRONMENT

This supplemental guide describes the how to load the required software dependencies for **GEOS-Chem** and **HEMCO** into your computational environment.

23.1 On the Amazon Web Services Cloud

All of the required software dependencies for **GEOS-Chem** and **HEMCO** will be included in the Amazon Machine Image (AMI) that you use to initialize your Amazon Elastic Cloud Compute (EC2) instance. For more information, please see our our GEOS-Chem cloud computing tutorial.

23.2 On a shared computer cluster

If you plan to use **GEOS-Chem** or **HEMCO** on a shared computational cluster (e.g. at a university or research institution), then there is a good chance that your IT staff will have already installed several of the required software dependencis.

Depending on your system's setup, there are a few different ways in which you can activate these software pacakges in your computational environment, as shown below.

23.2.1 1. Check if libraries are available as modules

Many high-performance computing (HPC) clusters use a module manager such as Lmod or environment-modules to load software packages and libraries. A module manager allows you to load different compilers and libraries with simple commands.

One downside of using a module manager is that you are locked into using only those compiler and software versions that have already been installed on your system by your sysadmin or IT support staff. But in general, module managers succeed in ensuring that only well-tested compiler/software combinations are made available to users.

Tip: Ask your sysadmin or IT support staff for the software loading instructions specific to your system.

1a. Module load example

The commands shown below are specific to the Harvard Cannon cluster, but serve to demonstrate the process. Note that the names of software packages being loaded may contain version numbers and/or ID strings that serve to differentiate one build from another.

```
module load gcc/12.2.0-fasrc01              # gcc / g++ / gfortran
module load openmpi/4.1.4-fasrc01           # MPI
module load netcdf-c/4.9.2-fasrc01          # netcdf-c
module load netcdf-fortran/4.6.0-fasrc02    # netcdf-fortran
module load flex/2.6.4-fasrc01              # Flex lexer (needed for KPP)
module load cmake/3.25.2-fasrc01            # CMake (needed to
compile)
```

Note that it is often not necessary to load all modules. For example, loading **netcdf-fortran** will also cause its dependencies (such as **netcdf-c**, **hdf5**, etc.) to also be loaded into your environment.

Here is a summary of what the above commands do:

module purge
: Removes all previously loaded modules

module load git/...
: Loads Git (version control system)

module load gcc/...
: Loads the GNU Compiler Collection (suite of C, C++, and Fortran compilers)

module load openmpi/...
: Loads the OpenMPI library (a dependency of netCDF)

module load netcdf/..
: Loads the netCDF library

Important: Depending on how the netCDF libraries have been installed on your system, you might also need to load the netCDF-Fortran library separately, e.g.:

```
module load netcdf-fortran/...
```

---

module load perl/...
: Loads Perl (scripting language)

module load cmake/...
: Loads Cmake (needed to compile GEOS-Chem)

module load flex/...
: Loads the Flex lexer (needed for The Kinetic PreProcessor).

23.2.2 2. Check if Spack-built libraries are available

If your system doesn't have a module manager installed, check to see if the required libraries for **GEOS-Chem** and **HEMCO** were *built with the Spack package manager*. Type

```
$ spack find
```

to locate any Spack-built software libraries on your system. If there Spack-built libraries are found, you may present, you may load them into your computational environment with **spack load** commands such as:

```
$ spack load gcc@12.2.0
$ spack load netcdf-c%gcc@12.2.0
$ spack load netcdf-fortran%gcc@12.2.0
... etc ...
```

When loading a Spack-built library, you can specify its version number. For example, **spack load gcc@12.2.0** tells Spack to load the GNU Compiler Collection version 12.2.0.

You may also specify a library by the compiler it was built with. For example, **spack load netcdf-fortran%gcc@12.2.0** tells Spack to load the version of netCDF-Fortran that was built with GNU Compiler Collection version 12.2.0.

These specification methods are often necessary to select a given library in case there are several available builds to choose from.

We recommend that you place **spack load** commands into an environment file.

If a Spack environment has been installed on your system, type:

```
spack env activate -p ENVIRONMENT-NAME
```

to load all of the libraries in the environment together.

To deactivate the environment, type:

```
spack deactivate
```

23.2.3 3. Check if libaries have been manually installed

If your computer system does not use a module manager and does not use Spack, check for a manual library installation. Very often, common software libraries are installed into standard locations (such as the `/usr/lib` or `/usr/local/lib` system folders). Ask your sysadmin for more information.

Once you know the location of the compiler and netCDF libraries, you can set the proper environment variables for GEOS-Chem and HEMCO.

23.2.4 4. If there are none of these, install them with Spack

If your system has none of the required software packages that **GEOS-Chem** and **HEMCO** need, then we recommend that you *use Spack to build the libraries yourself*. Spack makes the process easy and will make sure that all software dependences are resolved.

Once you have installed the libraries with Spack, you can load the libraries into your computational environment *as described above*.

CHAPTER

TWENTYFOUR

BUILD REQUIRED SOFTWARE WITH SPACK

This page has instructions for building **dependencies** for GEOS-Chem Classic, GCHP, and HEMCO These are the **software libraries** that are needed to compile and execute these programs.

Before proceeding, please also check if the dependencies for GEOS-Chem, GCHP, and HEMCO are already found on your computational cluster or cloud environment. If this is the case, you may use the pre-installed versions of these software libraries and won't have to install your own versions.

For more information about software dependencies, see:

- GEOS-Chem Classic software requirements
- GCHP software requirements
- HEMCO software requirements

24.1 Introduction

In the sections below, we will show you how to **build a single software environment containing all software dependencies for GEOS-Chem Classic, GCHP, and HEMCO**. This will be especially of use for those users working on a computational cluster where these dependencies have not yet been installed.

We will be using the Spack package manager to download and build all required software dependencies for GEOS-Chem Classic, GCHP and HEMCO.

Note: Spack is not the only way to build the dependencies. It is possible to download and compile the source code for each library manually. Spack automates this process, thus it is the recommended method.

You will be using this workflow:

1. *Install Spack and do first-time setup*
2. *Clone a copy of GCClassic, GCHP, or HEMCO*
3. *Install the recommended compiler*
4. *Build GEOS-Chem dependencies and useful tools*
5. *Add spack load commands to your environment file*
6. *Clean up*

24.2 Install Spack and do first-time setup

Decide where you want to install Spack (aka the **Spack root directory**). A few details you should consider are:

- The Spack root directory will be ~5-10 GB. Keep in mind that some computational clusters restrict the size of your home directory (aka `${HOME}`) to a few GB).
- This Spack root directory cannot be moved. Instead, you will have to reinstall Spack to a different directory location (and rebuild all software packages).
- The Spack root directory should be placed in a shared drive if several users need to access it.

Once you have chosen an location for the Spack root directory, you may continue with the Spack download and setup process.

Important: Execute all commands in this tutorial from the same directory. This is typically one directory level higher than the Spack root directory.

For example, if you install Spack as a subdirectory of `${HOME}`, then you will issue all commands from `${HOME}`.

Use the commands listed below to install Spack and perform first-time setup. You can copy-paste these commands, but lookout for lines marked with a `# (modifiable) ...` comment as they might require modification.

```
$ cd ${HOME}                              # (modifiable) cd to the install location you␣
↪chose

$ git clone -c feature.manyFiles=true https://github.com/spack/spack.git  # download␣
↪Spack

$ source spack/share/spack/setup-env.sh  # Load Spack

$ spack external find                     # Tell Spack to look for existing software

$ spack compiler find                     # Tell Spack to look for existing complilers
```

Note: If you should encounter this error:

```
$ spack external find
==> Error: 'name'
```

then Spack could not find any external software on your system.

Spack searches for executables that are located within your search path (i.e. the list of directories contained in your `$PATH` environment variable), but not within software modules. Because of this, you might have to *load a software package into your environment* before Spack can detect it. Ask your sysadmin or IT staff for more information about your system's specific setup.

After the first-time setup has been completed, an environment variable named `SPACK_ROOT`, will be created in your Unix/Linux environment. This contains to the absolute path of the Spack root directory. Use this command to view the value of `SPACK_ROOT`:

```
$ echo ${SPACK_ROOT}
/path/to/home/spack    # Path to Spack root, assumes installation to a subdir of ${HOME}
```

24.3 Clone a copy of GCClassic, GCHP, or HEMCO

The GCClassic, GCHP , and HEMCO repositories each contain a `spack/` subdirectory with customized Spack configuration files `modules.yaml` and `packages.yaml`. We have updated these YAML files with the proper settings in order to ensure a smooth software build process with Spack.

First, define the `model`, `scope_dir`, and `scope_args` environment variables as shown below.

```
$ model=GCClassic               # Use this if you will be working with GEOS-Chem Classic
$ model=GCHP                    # Use this if you will be working with GCHP
$ model=HEMCO                   # Use this if you will be working with HEMCO standalone

$ scope_dir="${model}/spack"    # Folder where customized YAML files are stored

$ scope_args="-C ${scope_dir}"  # Tell spack to for custom YAML files in scope_dir
```

You will use these environment variables in the steps below.

When you have completed this step, download the source code for your preferred model (e.g. GEOS-Chem Classic, GCHP, or HEMCO standalone):

```
$ git clone --recurse-submodules https://github.com/geoschem/${model}.git
```

24.4 Install the recommended compiler

Next, install the recommended compiler, **gcc** (aka the GNU Compiler Collection). Use the `scope_args` environment variable that you defined in the *previous step*.

```
$ spack ${scope_args} install gcc     # Install GNU Compiler Collection
```

Note: Requested version numbers for software packages (including the compiler) are listed in the `${scope_dir}/packages.yaml` file. We have selected software package versions that have been proven to work together. You should not have to change any of the settings in `${scope_dir}/packages.yaml`.

As of this writing, the default compiler is gcc 12.2.0 (includes C, C++, and Fortran compilers). We will upgrade to newer compiler and software package versions as necessary.

The compiler installation should take several minutes (or longer if you have a slow internet connection).

Register the compiler with Spack after it has been installed. This will allow Spack to use this compiler to build other software packages. Use this command:

```
$ spack compiler add $(spack location -i gcc)     # Register GNU Compiler Collection
```

You will then see output similar to this:

```
==> Added 1 new compiler to /path/to/home/.spack/linux/compilers.yaml
    gcc@X.Y.Z
==> Compilers are defined in the following files:
    /path/to/home/.spack/linux/compilers.yaml
```

where

- `/path/to/home` indicates the absolute path of your home directory (aka `${HOME}`)
- `X.Y.Z` indicates the version of the GCC compiler that you just built with Spack.

Tip: Use this command to view the list of compilers that have been registered with Spack:

```
$ spack compiler list
```

Use this command to view the installation location for a Spackguide-built software package:

```
$ spack location -i <package-name>
```

24.5 Build GEOS-Chem dependencies and useful tools

Once the compiiler has been built and registered, you may proceed to building the software dependencies for GEOS-Chem Classic, GCHP, and HEMCO.

The Spack installation commands that you will use take the form:

```
$ spack ${scope_args} install <package-name>%gcc^openmpi
```

where

- `${scope_args}` is the environment variable that *you defined above*;
- `<package-name>` is a placeholder for the name of the software package that you wish to install;
- `%gcc` tells Spack that it should use the GNU Compiler Collection version that you just built;
- `^openmpi` tells Spack to use OpenMPI when building software packages. You may omit this setting for packages that do not require it.

Spack will download and build `<package-name>` plus all of its dependencies that have not already been installed.

Note: Use this command to find out what other packages will be built along with `<package-name>`:

```
$ spack spec <package-name>
```

This step is not required, but may be useful for informational purposes.

Use the following commands to build dependencies for GEOS-Chem Classic, GCHP, and HEMCO, as well as some useful tools for working with GEOS-Chem data:

1. Build the **esmf** (Earth System Model Framework), **hdf5**, **netcdf-c**, **netcdf-fortran**, and **openmpi** packages:

   ```
   $ spack ${scope_args} install esmf%gcc^openmpi
   ```

   The above command will build all of the above-mentioned packages in a single step.

   Note: GEOS-Chem Classic does not require **esmf**. However, we recommend that you build ESMF anyway so that it will already be installed in case you decide to use GCHP in the future.

   ---

2. Build the **cdo** (Climate Data Operators) and **nco** (netCDF operators) packages. These are command-line tools for editing and manipulating data contained in netCDF files.

```
$ spack ${scope_args} install cdo%gcc^openmpi

$ spack ${scope_args} install nco%gcc^openmpi
```

3. Build the **ncview** package, which is a quick-and-dirty netCDF file viewer.

```
$ spack ${scope_args} install ncview%gcc^openmpi
```

4. Build the **flex** (Fast Lexical Analyzer) package. This is a dependency of the Kinetic PreProcessor (KPP), with which you can update GEOS-Chem chemical mechanisms.

```
$ spack ${scope_args} install flex%gcc
```

> **Note:** The **flex** package does not use OpenMPI. Therefore, we can omit `^openmpi` from the above command.

At any time, you may see a list of installed packages by using this command:

```
$ spack find
```

24.6 Add `spack load` commands to your environment file

We recommend "sourcing" the load_script that you created in the *previous section* from within an **environment file**. This is a file that not only loads the required modules but also defines settings that you need to run GEOS-Chem Classic, GCHP, or the HEMCO standalone.

Please see the following links for sample environment files.

- Sample GEOS-Chem Classic environment file
- Sample GCHP environment file
- Sample HEMCO environment file

Copy and paste the code below into a file named `${model}.env` (using the `${model}` environment variable that *you defined above*). Then replace any existing `module load` commands with the following code:

```
#==============================================================================
# Load Spackguide-built modules
#==============================================================================

# Setup Spack if it hasn't already been done
# ${SPACK_ROOT} will be blank if the setup-env.sh script hasn't been called.
# (modifiable) Replace "/path/to/spack" with the path to your Spack root directory
if [[ "x${SPACK_ROOT}" == "x" ]]; fi
   source /path/to/spack/source/spack/setup-env.sh
fi
```

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```
# Load esmf, hdf5, netcdf-c, netcdf-fortran, openmpi
spack load esmf%gcc^openmpi

# Load netCDF packages (cdo, nco, ncview)
spack load cdo%gcc^openmpi
spack load nco%gcc^openmpi
spack load ncview

# Load flex
spack load flex

#==============================================================================
# Set environment variables for compilers
#==============================================================================
export CC=gcc
export CXX=g++
export FC=gfortran
export F77=gfortran

#==============================================================================
# Set environment variables for Spack-built modules
#==============================================================================

# openmpi (needed for GCHP)
export MPI_ROOT=$(spack-location -i openmpi%gcc)

# esmf (needed for GCHP)
export ESMF_DIR=$(spack location -i esmf%gcc^openmpi)
export ESMF_LIB=${ESMF_DIR}/lib
export ESMF_COMPILER=gfortran
export ESMF_COMM=openmpi
export ESMF_INSTALL_PREFIX=${ESMF_DIR}/INSTALL_gfortran10_openmpi4

# netcdf-c
export NETCDF_HOME=$(spack location -i netcdf-c%gcc^openmpi)
export NETCDF_LIB=$NETCDF_HOME/lib

# netcdf-fortran
export NETCDF_FORTRAN_HOME=$(spack location -i netcdf-fortran%gcc^openmpi)
export NETCDF_FORTRAN_LIB=$NETCDF_FORTRAN_HOME/lib

# flex
export FLEX_HOME=$(spack location -i flex%gcc^openmpi)
export FLEX_LIB=$NETCDF_FORTRAN_HOME/lib
export KPP_FLEX_LIB_DIR=${FLEX_LIB}       # OPTIONAL: Needed for KPP
```

To apply these settings into your login environment, type

```
source ${model}.env  # One of GCClassic.env, GCHP.env, HEMCO.env
```

To test if the modules have been loaded properly, type:

```
$ nf-config --help   # netcdf-fortran configuration utility
```

If you see a screen similar to this, you know that the modules have been installed properly.

```
Usage: nf-config [OPTION]

Available values for OPTION include:

  --help        display this help message and exit
  --all         display all options
  --cc          C compiler
  --fc          Fortran compiler
  --cflags      pre-processor and compiler flags
  --fflags      flags needed to compile a Fortran program
  --has-dap     whether OPeNDAP is enabled in this build
  --has-nc2     whether NetCDF-2 API is enabled
  --has-nc4     whether NetCDF-4/HDF-5 is enabled in this build
  --has-f90     whether Fortran 90 API is enabled in this build
  --has-f03     whether Fortran 2003 API is enabled in this build
  --flibs       libraries needed to link a Fortran program
  --prefix      Install prefix
  --includedir  Include directory
  --version     Library version
```

24.7 Clean up

At this point, you can remove the `${model}` directory as it is not needed. (Unless you would like to keep it to build the executable for your research with GEOS-Chem Classic, GCHP, or HEMCO.)

The `spack` directory needs to remain. *As mentioned above*, this directory cannot be moved.

You can clean up any Spack temporary build stage information with:

```
$ spack clean -m
==> Removing cached information on repositories
```

That's it!

CHAPTER

TWENTYFIVE

CUSTOMIZE SIMULATIONS WITH RESEARCH OPTIONS

Most of the time you will want to use the "out-of-the-box" settings in your GEOS-Chem simulations, as these are the recommended settings that have been evaluated with benchmark simulations. But depending on your research needs, you may wish to use alternate simulation options. In this Guide we will show you how you can select these **research options** by editing the various GEOS-Chem and HEMCO configuration files.

25.1 Aerosols

25.1.1 Aerosol microphysics

GEOS-Chem incorporates two different aerosol microphysics schemes: APM (Yu and Luo [2009]) and TOMAS (Trivitayanurak *et al.* [2008]) as compile-time options for the full-chemistry simulation. Both APM and TOMAS are deactivated by default due to the extra computational overhead that these microphysics schemes require.

Follow the steps below to activate either APM or TOMAS microphysics in your full-chemistry simulation.

APM

1. Create a run directory for the Full Chemistry simulation with APM as the extra simulation option.
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DAPM=y
$ make -j
$ make install
```

TOMAS

1. Create a run directory for the Full Chemistry simulation with TOMAS as the extra simulation option.
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DTOMAS=y -DTOMAS_BINS=15
$ make -j
$ make install
```

This will create a GEOS-Chem executable for the TOMAS15 (15 size bins) simulation. To generate an executable for the TOMAS40 (40 size-bins) simulation, replace `-DTOMAS_BINS=15` with `-DTOMAS_BINS=40` in the `cmake` step above.

25.2 Chemistry

25.2.1 Adaptive Rosenbrock solver with mechanism auto-reduction

In Lin *et al.* [2023], the authors introduce an adaptive Rosenbrock solver with on-the-fly mechanism reduction in The Kinetic PreProcessor (KPP) version 3.0.0 and later. While this adaptive solver is available for all GEOS-Chem simulations that use the `fullchem` simulation, it is disabled by default.

To activate the adaptive Rosenbrock solver with mechanism auto-reduction, edit the line of `geoschem_config.yml` indicated below:

```
chemistry:
  activate: true
  # ... Previous sub-sections omitted
  autoreduce_solver:
    activate: false   # <== true activates the adaptive Rosenbrock solver
    use_target_threshold:
      activate: true
      oh_tuning_factor: 0.00005
      no2_tuning_factor: 0.0001
    use_absolute_threshold:
      scale_by_pressure: true
      absolute_threshold: 100.0
    keep_halogens_active: false
    append_in_internal_timestep: false
```

Please see the Lin *et al.* [2023] reference for a detailed explanation of the other adaptive Rosenbrock solver options.

25.2.2 Alternate chemistry mechanisms

GEOS-Chem is compiled "out-of-the-box" with KPP-generated solver code for the `fullchem` mechanism. But you must manually specify the mechanism name at configuration time for the following instances:

Carbon mechanism

Follow these steps to build an executable with the `carbon` mechanism:

1. Create a run directory for the Carbon simulation
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DMECH=carbon
$ make -j
$ make install
```

Custom full-chemistry mechanism

We recommend that you use the `custom` mechanism instead of directly modifying the `fullchem` mechanism. The `custom` mechanism is a copy of `fullchem`, but the KPP solver code will be generated in the `KPP/custom` folder instead of in `KPP/fullchem`. This lets you keep the `fullchem` folder untouched.

Follow these steps:

1. Create a run directory for the full-chemistry simulation (whichever configuration you need).
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DMECH=custom
$ make -j
$ make install
```

Hg mechanism

Follow these steps to build an executable with the `Hg` (mercury) mechanism:

1. Create a run directory for the Hg simulation.
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DMECH=Hg
$ make -j
$ make install
```

25.2.3 HO2 heterogeneous chemistry reaction probability

You may update the value of γ_{HO2} (reaction probability for uptake of HO2 in heterogeneous chemistry) used in your simulations. Edit the line of `geoschem_config.yml` indicated below:

```
chemistry:
  activate: true
  # ... Preceding sections omitted ...
  gamma_HO2: 0.2   # <=== add new value here
```

25.2.4 TransportTracers

In GEOS-Chem 14.2.0 and later versions, species belonging to the TransportTracers simulation (radionuclides and passive species) now have their properties defined in the `species_database.yml` file. For example:

```
CH3I:
  Background_VV: 1.0e-20
  Formula: CH3I
  FullName: Methyl iodide
  Henry_CR: 3.6e+3
  Henry_K0: 0.20265
```

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```
  Is_Advected: true
  Is_Gas: true
  Is_Photolysis: true
  Is_Tracer: true
  Snk_Horiz: all
  Snk_Mode: efolding
  Snk_Period: 5
  Snk_Vert: all
  Src_Add: true
  Src_Mode: HEMCO
  MW_g: 141.94
```

where:

- `Is_Tracer: true` indicates a TransportTracer species
- `Snk_*` define species sink properties
- `Src_*` define species source properties
- `Units`: specifies the default units for species (added mainly for age of air species at this time which are in `days`)

For TransportTracers species that have a source term in HEMCO, there will be corresponding entries in `HEMCO_Config.rc`:

```
--> OCEAN_CH3I             :       true

# ... etc ...

#============================================================================
# CH3I emitted over the oceans at rate of 1 molec/cm2/s
#============================================================================
(((OCEAN_CH3I
0 SRC_2D_CH3I 1.0 - - - xy molec/cm2/s CH3I 1000 1 1
)))OCEAN_CH3I
```

Sources and sinks for TransportTracers are now applied in the new source code module `GeosCore/tracer_mod.F90`.

Note: Sources and sinks for radionuclide species (Rn, Pb, Be isotopes) are currently not applied in `GeosCore/tracer_mod.F90` (but may be in the future). Emissions for radionuclide species are computed by the HEMCO `GC-Rn-Pb-Be` extension and chemistry is done in `GeosCore/RnPbBe_mod.F90`.

TransportTracer properties for radionuclide species have been added to `species_database.yml` but are currently commented out.

25.3 Diagnostics

25.3.1 GEOS-Chem and HEMCO diagnostics

Please see our Diagnostics reference chapter for an overview of how to archive diagnostics from GEOS-Chem and HEMCO.

25.3.2 RRTMG radiative transfer diagnostics

You can use the RRTMG radiative transfer model to archive radiative forcing fluxes to the `GeosRad` History diagnostic collection. RRTMG is implemented as a compile-time option due to the extra computational overhead that it incurs.

To activate RRTMG, follow these steps:

1. Create a run directory for the Full Chemistry simulation, with extra option RRTMG.
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DRRTMG=y
$ make -j
$ make install
```

Then also make sure to request the radiative forcing flux diagnostics that you wish to archive in the `HISTORY.rc` file.

25.4 Emissions

25.4.1 Offline vs. online emissions

Emission inventories sometimes include dynamic source types and nonlinear scale factors that have functional dependencies on local environmental variables such as wind speed or temperature, which are best calculated online during execution of the model. HEMCO includes a suite of additional modules (aka HEMCO extensions) that perform **online emissions** ccalculations for a variety of sources.

Some types of emissions are highly sensitive to meteorological variables such as wind speed and temperature. Because the meteorological inputs are regridded from their native resolution to the GEOS-Chem or HEMCO simulation grid, emissions computed with fine-resolution meteorology can significantly differ from emissions computed with coarse-resolution meteorology. This can make it difficult to compare the output of GEOS-Chem and HEMCO simulations that use different horizontal resolutions.

In order to provide more consistency in the computed emissions, we now make available for download **offline emissions**. These offline emissions are pre-computed with HEMCO standalone simulations using meteorological inputs at native horizontal resolutions possible. When these emissions are regridded within GEOS-Chem and HEMCO, the total mass emitted will be conserved regardless of the horizontal resolution of the simulation grid.

You should use offline emissions:

- For all GCHP simulations
- For full-chemistry simulations (except benchmark)

You should use online emissions:

- For benchmark simulations

- If you wish to assess the impact of changing/updating the meteorlogical inputs on emissions.

You may toggle offline emissions on (`true`) or off (`false`) in this section of `HEMCO_Config.rc`:

```
# ----- OFFLINE EMISSIONS -------------------------------------------------------
# To use online emissions instead set the offline emissions to 'false' and the
# corresponding HEMCO extension to 'on':
#   OFFLINE_DUST        - DustDead or DustGinoux
#   OFFLINE_BIOGENICVOC - MEGAN
#   OFFLINE_SEASALT     - SeaSalt
#   OFFLINE_SOILNOX     - SoilNOx
#
# NOTE: When switching between offline and online emissions, make sure to also
# update ExtNr and Cat in HEMCO_Diagn.rc to properly save out emissions for
# any affected species.
#-------------------------------------------------------------------------------
    --> OFFLINE_DUST           :       true     # 1980-2019
    --> OFFLINE_BIOGENICVOC    :       true     # 1980-2020
    --> OFFLINE_SEASALT        :       true     # 1980-2019
    -->  CalcBrSeasalt         :       true
    --> OFFLINE_SOILNOX        :       true     # 1980-2020
```

As stated in the comments, if you switch between offline and online emissions, you will need to activate the corresponding HEMCO extension:

Table 1: Offline emissions and corresponding HEMCO extensions

Offline base emission	Extension #	Corresponding HEMCO extension	Extension #
OFFLINE_DUST	0	DustDead	105
OFFLINE_BIOGENICVOC	0	MEGAN	108
OFFLINE_SEASALT	0	SeaSalt	107
OFFLINE_SOILNOX	0	SoilNOx	104

Example: Disabling offline dust emissions

1. Change the `OFFLINE_DUST` setting from `true` to `false` in `HEMCO_Config.rc`:

```
--> OFFLINE_DUST           :       false    # 1980-2019
```

2. Change the `DustDead` extension setting from `off` to `on` in `HEMCO_Config.rc`:

```
105     DustDead              : on    DST1/DST2/DST3/DST4
```

3. Change the extension number for all dust emission diagnostics from `0` (the extension number for base emissions) to `105` (the extension number for `DustDead`) in `HEMCO_Diagn.rc`.

```
###############################################################################
#####  Dust emissions                                                     #####
###############################################################################
EmisDST1_Total     DST1   -1    -1   -1   2   kg/m2/s  DST1_emission_flux_from_all_
↪sectors
EmisDST1_Anthro    DST1  105     1   -1   2   kg/m2/s  DST1_emission_flux_from_
↪anthropogenic
```

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```
EmisDST1_Natural   DST1  105     3   -1   2   kg/m2/s  DST1_emission_flux_from_
↪natural_sources
EmisDST2_Natural   DST2  105     3   -1   2   kg/m2/s  DST2_emission_flux_from_
↪natural_sources
EmisDST3_Natural   DST3  105     3   -1   2   kg/m2/s  DST3_emission_flux_from_
↪natural_sources
EmisDST4_Natural   DST4  105     3   -1   2   kg/m2/s  DST4_emission_flux_from_
↪natural_sources
```

To enable online emissions again, do the inverse of the steps listed above.

25.4.2 Sea salt debromination

In Zhu *et al.* [2018], the authors present a mechanistic description of sea salt aerosol debromination. This option was originally enabled by in GEOS-Chem 13.4.0, but was then changed to be an option (disabled by default) due to the impact it had on ozone concentrations.

Further chemistry updates to GEOS-Chem have allowed us to re-activate sea-salt debromination as the default option in GEOS-Chem 14.2.0 and later versions. If you wish to disable sea salt debromination in your simulations, edit the line in `HEMCO_Config.rc` indicated below.

```
107     SeaSalt               : on  SALA/SALC/SALACL/SALCCL/SALAAL/SALCAL/BrSALA/BrSALC/
↪MOPO/MOPI
    # ... Preceding options omitted ...
    --> Model sea salt Br-     :       true    # <== false deactivates sea salt␣
↪debromination
    --> Br- mass ratio         :       2.11e-3
```

25.5 Photolysis

25.5.1 Particulate nitrate photolysis

A study by Shah *et al.* [2023] showed that particulate nitrate photolysis increases GEOS-Chem modeled ozone concentrations by up to 5 ppbv in the free troposphere in northern extratropical regions. This helps to correct a low bias with respect to observations.

Particulate nitrate photolysis is turned on by default in GEOS-Chem 14.2.0 and later versions. You may disable this option by editing the line in `geoschem_config.yml` indicated below:

```
photolysis:
  activate: true
  # .. preceding sub-sections omitted ...
  photolyze_nitrate_aerosol:
    activate: true   # <=== false deactivates nitrate photolysis
    NITs_Jscale_JHNO3: 100.0
    NIT_Jscale_JHNO2: 100.0
    percent_channel_A_HONO: 66.667
    percent_channel_B_NO2: 33.333
```

You can also edit the other nitrate photolysis parameters by changing the appropriate lines above. See the Shah et al [2023] reference for more information.

25.6 Wet deposition

25.6.1 Luo et al 2020 wetdep parameterization

In Luo *et al.* [2020], the authors introduced an updated wet deposition parameterization, which is now incorporated into GEOS-Chem as a compile-time option. Follow these steps to activate the Luo et al 2020 wetdep scheme in your GEOS-Chem simulations.

1. Create a run directory for the type of simulation that you wish to use.
    - CAVEAT: Make sure your simulation uses at least one species that can be wet-scavenged.
2. Navigate to the `build` folder within the run directory.
3. Then type the following:

```
$ cmake .. -DLUO_WETDEP=y
$ make -j
$ make install
```

CHAPTER

TWENTYSIX

UNDERSTAND WHAT ERROR MESSAGES MEAN

In this Guide we provide information about the different types of errors that your GEOS-Chem simulation might encounter.

Important: Know the difference between warnings and errors.

Warnings are non-fatal informational messages. Usually you do not have to take any action when encountering a warning. Nevertheless, you should always try to investigate why the warning was generated in the first place.

Errors are fatal and will halt GEOS-Chem compilation or execution. Looking at the error message will give you some clues as to why the error occurred.

We strongly encourage that you try to debug the issue using the info both in this Guide and in our *Debug GEOS-Chem and HEMCO errors* Guide. Please see our Support Guidelines for more information.

26.1 Where does error output get printed?

GEOS-Chem Classic, GCHP, and HEMCO, like all Linux-based programs, send output to two streams: **stdout** and **stderr**.

Most output will go to the **stdout** stream, which takes I/O from the Fortran `WRITE` and `PRINT` commands. If you run e.g. GEOS-Chem Classic by just typing the executable name at the Unix prompt:

```
$ ./gcclassic
```

then the stdout stream will be printed to the terminal window. You can also redirect the stdout stream to a log file with the redirect command:

```
$ ./gcclassic > GC.log 2>&1
```

The **2>&1** tells the bash script to append the stderr stream (noted by `2`) to the stdout stream (noted by `1`). This will make sure that any error output also shows up in the log file.

You can also use the Linux **`tee`** command, which will send output both to a log file as well as to the terminal window:

```
$ ./gcclassic | tee GC.log 2>&1
```

Note: Please be aware of the following:

1. We have combined HEMCO and GEOS-Chem informational printouts as of GEOS-Chem 14.2.0 and HEMCO 3.7.0. In previous versions, HEMCO informational printouts would have been sent to a separate `HEMCO.log` file.

2. We have disabled most GEOS-Chem and HEMCO informational printouts by default, starting in GEOS-Chem 14.2.0 and HEMCO 3.7.0. These printouts may be restored (e.g. for debugging) by enabling verbose output in both `geoschem_config.yml` and `HEMCO_Config.rc`.
3. GCHP sends output to several log files as well as to the stdout and stderr streams. Please see gchp.readthedocs.io for more information.
4. When using GEOS-Chem 14.5.1 or later within CESM, HEMCO error messages will be sent to `atm.log` rather than `cesm.log`.

26.2 Compile-time errors

In this section we discuss some compilation warnings that you may encounter when building GEOS-Chem.

26.2.1 Cannot open include file netcdf.inc

```
error #5102: Cannot open include file 'netcdf.inc'
```

Problem: The **`netcdf-fortran`** library cannot be found.

Solution: Make sure that *all software dependencies have been installed* and *loaded into your Linux environment*.

26.2.2 KPP error: Cannot find -lfl

```
/usr/bin/ld: cannot find -lfl
error: ld returned exit 1 status
```

Problem:: The Kinetic PreProcessor (KPP) cannot find the **`flex`** library, which is one of its dependencies.

Solution: Make sure that *all software dependencies have been installed* and *loaded into your Linux environment*.

26.2.3 GNU Fortran internal compiler error

```
f951: internal compiler error: in ___ at ___
```

Problem: Compilation halted due to a compiler issue. These types of errors can indicate:

1. An undiagnosed bug in the compiler itself.
2. The inability of the compiler to parse source code adhering to the most recent Fortran language standard.
3. The inability of the compiler to parse legacy source code that is now deprecated.

Solution: Try switching to a newer compiler version. We recommend using GNU Compiler Collection (GCC) 10.0.0 or later.

26.2.4 This module file was not generated by any release of this compiler

```
error #7013: This module file was not generated by any release of this compiler.
[NETCDF] use netCDF --------^
```

Problem: The netCDF library was built with a different compiler than the compiler being used to build the GEOS-Chem or HEMCO standalone executable.

Solution: Build the GEOS-Chem or HEMCO standalone executable with the same compiler that was used to build netCDF and netCDF-Fortran.

26.3 Run-time errors

26.3.1 Excessive fall velocity error

```
GEOS-CHEM ERROR:  Excessive fall velocity?
STOP at  CALC_FALLVEL, UCX_mod
```

Problem: The fall velocity (in stratopsheric chemistry routine `Calc_FallVel` in module `GeosCore/ucx_mod.F90`) exceeds 10 m/s. This error will most often occur in GEOS-Chem Classic nested-grid simulations, and is usually caused when the initial conditions (from the restart file) are out of sync with the stratospheric dynamical conditions.

Solution:

1. Reduce the default timestep settings in `geoschem_config.yml`. You may need to use 300 seconds (transport) and 600 seconds (chemistry) or even smaller depending on the horizontal resolution of your simulation, or
2. Use a well-spun-up restart file.

26.3.2 Floating invalid or floating-point exception error

```
forrtl: error (65): floating invalid    # Error message from Intel Fortran Compiler

Floating point exception (core dumped)  # Error message from GNU Fortran compiler
```

Problem: An illegal floating-point math operation has occurred. This error can be generated if one of the following conditions has been encountered:

1. Division by zero
2. Underflow or overflow
3. Square root of a negative number
4. Logarithm of a negative number
5. Negative or Positive Infinity
6. Undefined value(s) used in an equation

Solution: Re-configure GEOS-Chem (or the HEMCO standalone) with the `-DCMAKE_RELEASE_TYPE=Debug` Cmake option. This will build in additional error checking that should alert you to where the error is occurring. Once you find the location of the error, you can take the appropriate steps, such as making sure that the denominator of an expression never goes to zero, etc.

26.3.3 Forced exit from Rosenbrock

```
Forced exit from Rosenbrock due to the following error:
--> Step size too small: T + 10*H = T or H < Roundoff
T=   3044.21151383269      and H=  1.281206877135470E-012
### INTEGRATE RETURNED ERROR AT:          40          68           1

Forced exit from Rosenbrock due to the following error:
--> Step size too small: T + 10*H = T or H < Roundoff
T=   3044.21151383269      and H=  1.281206877135470E-012
### INTEGRATE FAILED TWICE ###

################################################################################
### KPP DEBUG OUTPUT
### Species concentrations at problem box           40          68          1
################################################################################
... printout of species concentrations ...

################################################################################
### KPP DEBUG OUTPUT
### Species concentrations at problem box           40          68          1
################################################################################
... printout of reaction rates ...
```

Problem: The KPP Rosenbrock integrator could not converge to a solution at a particular grid box. This can happen when:

1. The absolute (`ATOL`) and/or relative (`RTOL`) *error tolerances* need to be refined.
2. A particular species has numerically underflowed or overflowed.
3. A division by zero occurred in the reaction rate computations.
4. A species has been set to a very low value in another operation (e.g. wet scavenging), thus causing the non-convergence.
5. The initial conditions of the simulation may be non-physical.
6. A data file (meteorology or emissions) may be corrupted.

If the non-convergence only happens once, then GEOS-Chem will revert to prior concentrations and reset the saved KPP internal timestep (`Hnew`) to zero before calling the Rosenbrock integrator again. In many instances, this is sufficient for the chemistry to converge to a soluiton.

In the case that the Rosenbrock integrator fails to converge to a solution twice in a row, all of the concentrations and reaction rates at the grid box will be printed to *stdout* and the simulation will terminate.

Solution: Look at the error printout. You will likely notice species concentrations or reaction rates that are extremely high or low compared to the others. This will give you a clue as to where in GEOS-Chem the error may have occurred.

Try performing some short test simulations, turning each operation (e.g. transport, PBL mixing, convection, etc). off one at a time. This should isolate the location of the error. Make sure to turn on verbose output in both `geoschem_config.yml` and `HEMCO_Config.rc`; this will send additional printout to the *stdout* stream. The clue to finding the error may become obvious by looking at this output.

Check your restart file to make sure that the initial concentrations make sense. For certain simulations, using initial conditions from a simulation that has been sufficiently spun-up makes a difference.

Use a netCDF file viewer like **`ncview`** to open the meteorology files on the day that the error occurred. If a file does not open properly, it is probably corrupted. If you suspect that the file may have been corrupted during download, then

download the file again from its original source. If this still does not fix the error, then the file may have been corrupted at its source. Please open a new Github issue to alert the GEOS-Chem Support Team.

More about KPP error tolerances

The error tolerances are set in the following locations:

1. **fullchem** mechanism: In routine `Do_FlexChem` (located in in `GeosCore/fullchem_mod.F90`).
2. **Hg** mechanism: In routine `ChemMercury` (located in `GeosCore/mercury_mod.F90`).

For example, in the fullchem mechanism, `ATOL` and `RTOL` are defined as:

```
!%%%%% CONVERGENCE CRITERIA %%%%%

! Absolute tolerance
ATOL      = 1e-2_dp

! Relative tolerance
! Changed to 0.5e-3 to avoid integrate errors by halogen chemistry
!  -- Becky Alexander & Bob Yantosca (24 Jan 2023)
RTOL      = 0.5e-3_dp
```

Convergence errors can occur because the system arrives to a state too far from the truth to be able to converge. By tightening (i.e. decreasing) the tolerances, you ensure that the system stays closer to the truth at every time step. Then, the problematic time steps will start the chemistry with a system closer to the true state, enabling the chemistry to converge.

CAVEAT: If the first time step of chemistry cannot converge, tightening the tolerances wouldn't work but loosening the tolerance would. So you might have to experiment a little bit in order to find the proper settings for `ATOL` and `RTOL` for your specific mechanism.

26.3.4 GEOS-Chem Classic simulation failed after TPCORE initialization

See this section: *Segmentation fault encountered after TPCORE initialization*

26.3.5 HEMCO Error: Cannot find field

```
HEMCO Error: Cannot find field ___.  Please check the name in the config file.
```

Problem: A GEOS-Chem Classic or HEMCO standalone simulation halts because HEMCO cannot find a certain input field.

Solution: Most of the time, this error indicates that a species is missing from the GEOS-Chem restart file. By default, the GEOS-Chem restart file (entry `SPC_` in HEMCO_Config.rc) uses time cycle flag `EFYO`. This setting tells HEMCO to halt if a species does not have an initial condition field contained in the GEOS-Chem restart file. Changing this time cycle flag to `CYS` will allow the simulation to proceed. In this case, species will be given a default background initial concentration, and the simulation will be allowed to proceed.

26.3.6 HEMCO Error: Cannot find file for current simulation time

```
HEMCO ERROR: Cannot find file for current simulation time:
./Restarts/GEOSChem.Restart.20190101_0000z.nc4 - Cannot get field SPC_ACET.
Please check file name and time (incl. time range flag) in the config. file
```

Problem: A GEOS-Chem Classic simulation failed because the timestamp of the restart file did not match the starting date/time of the simulation (as specified in `geoschem_config.yml`). This is the default behavior.

Solution: Change the time cycle flag for the SPC_ container in `HEMCO_Config.rc`.

```
HEMCO ERROR: Cannot find file for current simulation time:
./Restarts/GEOSChem.Restart.17120701_0000z.nc4 - Cannot get field SPC_NO.
Please check file name and time (incl. time range flag) in the config. file
```

Problem: A GEOS-Chem Classic simulation failed because HEMCO kept searching back in time to 1712 for a valid restart file timestamp.

Solution: Make sure that the file is at the path specified in `HEMCO_Config.rc`. HEMCO will try to look back in time starting with the current year and going all the way back to the year 1712 or 1713. So if you see 1712 or 1713 in the error message, that is a tip-off that the file is missing.

26.3.7 HEMCO Error: Cannot get field PS_NEXTDAY

```
HEMCO ERROR: Cannot find field with valid time stamp in
/path/to/ExtData/GEOS_4x5/MERRA2/YYYY/MM/MERRA2.YYYYMMDD.I3.4x5.nc4 - Cannot get field␣
↪PS_NEXTDAY.
Please check file name and time (incl. time range flag) in the config. file
```

Problem: A GEOS-Chem Classic or HEMCO standalone simulation failed because HEMCO could not find a valid timestamp for the `PS_NEXTDAY` entry in `HEMCO_Config.rc`. This usually indicates that the next day's met field data is missing.

Solution: Download met field data for the missing date from one of the the *GEOS-Chem data portals*.

26.3.8 HEMCO ERROR: Not enough time slices: BC_<species-name>

```
HEMCO ERROR: not enough time slices: BC_<species-name>
 --> LOCATION: HCO_GetPtr_3D (hco _emislist_mod.F90)
```

Problem: An error occurred because fewer time slices than expected were encountered when reading nested-grid transport boundary conditions from disk. GEOS-Chem Classic nested-grid simulations expect to find boundary condition at 3 hour temporal frequency (e.g. 00z, 03z, .. 21z).

Solution: Set the frequency of the GEOS-Chem *BoundaryConditions* collection to `030000` (i.e. every 3 hours) in `HISTORY.rc` file as shown below.

```
#============================================================================
# GEOS-Chem boundary conditions for use in nested grid simulations
# Available for all simulations
#============================================================================
  BoundaryConditions.template:   '%y4%m2%d2_%h2%n2z.nc4',
  BoundaryConditions.frequency:  00000000 030000
```

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```
 BoundaryConditions.duration:   00000100 000000
 ... etc ...
```

26.3.9 HEMCO Error: Time stamps may be wrong

```
HEMCO WARNING: ncdf reference year is prior to 1901 - time stamps may be wrong!
--> LOCATION: GET_TIMEIDX (hco_read_std_mod.F90)
```

Problem: HEMCO reads the files but gives zero emissions and shows the error listed above.

Solution: Do the following:

1. Reset the reference datetime in the netCDF file so that it is after 1901.
2. Make sure that the `time:calendar` string is either `standard` or `gregorian`. GEOS-Chem Classic, GCHP, and HEMCO can only read data placed on calendars with leap years.

GCST member Lizzie Lundgren writes:

> This HEMCO error occurs if the reference time for the netCDF file time dimension is prior to 1901. If you do **`ncdump -c filename`** you will be able to see the metadata for the time dimension as well as the time variable values. The time units should include the reference date.
>
> You can get around this issue by changing the reference time within the file. You can do this with **`cdo`** (Climate Data Operators) using the **`setreftime`** command.
>
> Here is a bash script example by GCST member Melissa Sulprizio that updates the calendar and reference time for all files ending in `*.nc` within a directory. This script was made for a user who ran into this issue. into the same issue. In that case the first file was for Jan 1, 1950, so that was made the new reference time. I would recommend doing the same for your dataset so that the first time variable value would be `0`. This script also compresses the file which we recommend doing.

```
#!/bin/bash

for file in *nc; do
    echo "Processing $file"

    # Make sure te calendar is "standard" and not e.g. 360 days
    cdo setcalendar,standard $file tmp.nc
    mv tmp.nc $file

    # Set file reference time to 1950-01-01 at 0z
    cdo setreftime,1950-01-01,0 $file tmp.nc
    mv tmp.nc $file

    # Compress the file
    nccopy -d1 -c "time/1" $file tmp.nc
    mv tmp.nc $file
done
```

> After you update the file you can then again do **`ncdump -c filename`** to check the time dimension. For the case above it looks like this after processing.

```
    double time(time) ;
           time:standard_name = "time" ;
           time:long_name = "time" ;
           time:bounds = "time_bnds" ;
           time:units = "days since 1950-01-01 00:00:00" ;
           time:calendar = "standard" ;
           . . .

time = 0, 31, 59, 90, 120, 151, 181, 212, 243, 273, 304, 334, 365, 396, 424,
     455, 485, 516, 546, 577, 608, 638, 669, 699, 730, 761, 790, 821, 851,``
     882, 912, 943, 974, 1004, 1035, 1065, 1096, 1127, 1155,  1186, 1216, 1247␣
↪. . .
```

26.3.10 HEMCO Run Error

```
================================================================================
GEOS-CHEM ERROR: HCO_RUN

HEMCO ERROR: Please check the log file for error messages!

STOP at HCOI_GC_RUN (hcoi_gc_main_mod.F90)
================================================================================
```

Problem: A GEOS-Chem simulation stopped in the `HCOI_GC_RUN` routine with an error message similar to that shown above.

Solution: Look at the output that was written to the *stdout and stderr* streams. Error messages containing `HCO` originate in HEMCO.

26.3.11 Integrator error code: -5, STOP at INTEGRATE_KPP

```
INTEGRATE RETURNED ERROR AT: I J L
GEOS-CHEM ERROR: Integrator error code : -5
STOP at INTEGRATE_KPP
```

Problem: A GEOS-Chem simulation halted because the KPP integrator could not solve the chemical mechanism at grid box `(I,J,L)`. This type of error most often occurs in GEOS-Chem nested-grid fullchem simulations when the boundary conditions contain nonrealistic concentrations.

Solution: Try changing the buffer values in the nested grid menu of `geoschem_config.yml` as shown below:

```
#============================================================================
# Grid settings
#============================================================================
grid:
  ... etc not shown ...
  nested_grid_simulation:
    activate: true
    buffer_zone_NSEW: [3,3,3,3]  # <==== Try changing to [6,6,6,6]
```

This will reduce the size of the window in which chemistry will be performed, and thus hopefully prevent unphysical concentrations from the boundary conditions from affecting the chemistry.

26.3.12 libnetcdff.so.7: cannot open shared object file: No such file or directory

```
$ ./gcclassic
./gcclassic: error while loading shared libraries:
libnetcdff.so.7: cannot open shared object file: No such file or directory
```

Problem: This error can be caused by the following issues:

1. You have attempted to compile GEOS-Chem or the HEMCO standalone model with a different compiler than what was used to build the netCDF-Fortran library.
2. The GEOS-Chem or HEMCO standalone executable cannot find the netCDF-Fortran library.

Solution:

1. Recompile GEOS-Chem or the HEMCO standalone model with the same compiler that was used to build the netCDF-Fortran library, or
2. Make sure that *all software dependencies have been installed* and *loaded into your Linux environment*.

26.3.13 Negative tracer found in WETDEP

```
WETDEP: ERROR at   40  67   1 for species    2 in area WASHOUT: at surface
 LS          :  T
 PDOWN       :    0.0000000000000000
 QQ          :    0.0000000000000000
 ALPHA       :    0.0000000000000000
 ALPHA2      :    0.0000000000000000
 RAINFRAC    :    0.0000000000000000
 WASHFRAC    :    0.0000000000000000
 MASS_WASH   :    0.0000000000000000
 MASS_NOWASH :    0.0000000000000000
 WETLOSS     :                        NaN
 GAINED      :    0.0000000000000000
 LOST        :    0.0000000000000000
 DSpc(NW,:)  :                        NaN   6.0358243778561746E-013   6.
↪5871997362336500E-013   7.2710915872550685E-013   8.0185772698102585E-013   8.
↪7883682997147595E-013   9.6396466805517407E-013   1.0574719517340253E-012   1.
↪1617302070198606E-012   1.2976219851862141E-012   1.4347568254382824E-012   1.
↪5772212240871896E-012   1.7071657565802178E-012   1.8443377617027378E-012   1.
↪9982208320328261E-012   2.1567932874822908E-012   2.2591568422224307E-012   2.
↪2208301198704935E-012   1.8475974519883714E-012   1.7716069173018996E-013   1.
↪7714395985520433E-013   1.7633649101242403E-013   1.6668529114369137E-013   1.
↪3548045738669223E-013   5.1061710020314286E-014   0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000        0.
↪0000000000000000        0.0000000000000000        0.0000000000000000
 Spc(I,J,:N) :                        NaN   3.5108056785061143E-009   3.
↪8363969256742307E-009   3.6615166033026556E-009   3.6780394914242783E-009   4.
↪1462343168230006E-009   4.7319942271993657E-009   5.1961472823088513E-009   5.
```

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```
↪4030830279477525E-009   5.5736845790195336E-009   5.7139596145766606E-009   5.
↪8629212873139874E-009   7.9742789235773213E-009   1.0334311421916619E-008   1.
↪0816150360971255E-008   1.1168715310744298E-008   1.1534959217017146E-008   1.
↪1809950282570185E-008   1.7969626885629474E-008   1.7430760762446019E-008   1.
↪7477810715818748E-008   1.7967321756900857E-008   1.8683742574601477E-008   1.
↪9309929368816065E-008   2.0262386892450682E-008   2.0489969814921647E-008   1.
↪9961590106306151E-008   2.2859284477873924E-008   1.3161046290246557E-008   6.
↪5857053651000387E-009   2.7535806161296159E-009   1.2708780077337107E-009   3.
↪6557775667039418E-010   6.1984105316417057E-011   2.6665694620973736E-011   8.
↪7599157145440813E-012   4.8009375158768866E-012   1.0086435318729046E-012   1.
↪3493529625353547E-013   1.6403790023674963E-014   2.7417226109948757E-015   4.
↪2031825835582592E-014   2.3778709382809943E-013   8.3223532851684382E-013   4.
↪5695049346098890E-012   6.9911523125704209E-012   2.5076669266356582E-012
================================================================================
================================================================================
GEOS-Chem ERROR: Error encountered in wet deposition!
 -> at SAFETY (in module GeosCore/wetscav_mod.F90)
================================================================================

================================================================================
GEOS-Chem ERROR: Error encountered in "Safety"!
 -> at Do_Washout_at_Sfc (in module GeosCore/wetscav_mod.F90)
================================================================================

================================================================================
GEOS-Chem ERROR:
 -> at WetDep (in module GeosCore/wetscav_mod.F90)
================================================================================

================================================================================
GEOS-Chem ERROR: Error encountered in "Wetdep"!
 -> at Do_WetDep (in module GeosCore/wetscav_mod.F90)
================================================================================

================================================================================
GEOS-CHEM ERROR: Error encountered in "Do_WetDep"!
STOP at  -> at GEOS-Chem (in GeosCore/main.F90)
================================================================================
     - CLEANUP: deallocating arrays now...
```

Problem: A GEOS-Chem simulation has encountered either negative or `NaN` (not-a-number) concentrations in the wet deposition module. This can indicate the following:

1. The wet deposition routines have removed too much soluble species from within a grid box.
2. Another operation (e.g. transport, convection, etc.) has removed too much soluble species from within a grid box.
3. A corrupted or incorrect meteorological input has caused too much rainout or washout to occur within a grid box (which leads to conditions 1 and/or 2 above).
4. An *array-out-of-bounds error* has corrupted a variable that is used in wet depoosition.
5. For nested-grid simulations, the transport timestep may be too large, thus resulting in grid boxes with zero or negative concentrations.

Solution: Re-configure GEOS-Chem and/or HEMCO with the `-DCMAKE_RELEASE_TYPE=Debug` CMake option. This adds in additional error checks that may help you find where the error occurs.

Also try adding some `PRINT*` statements before and after the call to `DO_WETDEP` to check the concentrations entering and leaving the wetdep module. That might give you an idea of where the concetnrations are going negative.

26.3.14 Permission denied error

```
geoschem.run: Permission denied
```

Problem: The script `geoschem.run` is not executable.

Solution: Change the permission of the script with:

```
$ chmod 755 geoschem.run
```

26.4 File I/O errors

26.4.1 List-directed I/O syntax error

```
# Error message from GNU Fortran
At line NNNN of file filename.F90
Fortran runtime error: Bad real number|integer number|character in item X of list input

# Error message from Intel Fortran
forrtl: severe (59): list-directed I/O syntax error, unit -5, file Internal List-
↪Directed Read
```

Problem: This error indicates that the wrong type of data was read from a text file. This can happen when:

1. Numeric input is expected but character input was read from disk (or vice-versa);
2. A **READ** statement in your code has been omitted or deleted.

Solution: Check configuration files (`geoschem_config.yml`, `HEMCO_Config.rc`, `HEMCO_Diagn.rc`, etc.) for syntax errors and omissions that could be causing this error.

26.4.2 NF90_Def_Var: Can not create compressed variable

```
NF90_Def_Var: can not create compressed variable : time
```

Problem: This error may be caused by the following issues:

1. You are attempting to build GEOS-Chem or the HEMCO standalone with a different compiler than what was used to build the netCDF libraries.
2. You are trying to write to a file that is write-protected.
3. You have exceeded your alloted disk quota.

Solution:

1. Build the GEOS-Chem or HEMCO standalone executable with the same compiler that was used to build netCDF and netCDF-Fortran, or

2. Change the permission of the output file so that it can be overwritten (`chmod 644 myfile.nc`), or
3. Remove unnecessary files so that you no longer exceed your alloted disk quota.

26.4.3 NF90_Def_Var: Can not define variable

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NF90_Def_var: can not define variable: ____

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

Code stopped from DO_ERR_OUT (in module NcdfUtil/m_do_err_out.F90)

This is an error that was encountered in one of the netCDF I/O modules,
which indicates an error in writing to or reading from a netCDF file!

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Problem: GEOS-Chem or HEMCO could not write a variable to a netCDF file. This error may be caused by:

1. The netCDF file is write-protected and cannot be overwritten.
2. The path to the netCDF file is incorrect (e.g. directory does not exist).
3. The netCDF file already contains a variable with the same name.

Solution: Try the following:

1. If GEOS-Chem or HEMCO will be overwriting any existing netCDF files (which can often happen during testing & development), make sure that the file and containing directory are not write-protected.
2. Make sure that the path where you intend to write the netCDF file exists.
3. Check your `HISTORY.rc` and `HEMCO_Diagn.rc` diagnostic configuration files to make sure that you are not writing more than one diagnostic variable with the same name.

26.4.4 NetCDF: HDF Error

```
NetCDF: HDF error
```

Problem: The netCDF library routines in GEOS-Chem or HEMCO cannot read a netCDF file. The error is occurring in the HDF5 library (upon which netCDF depends). This may indicate a corrupted or incomplete netCDF file.

Solution: Try re-downloading the file from the relevant *GEOS-Chem data portal*. Downloading a fresh copy of the file is often sufficient to fix this type of issue. If the error persists, please open a new GitHub issue to alert the GEOS-Chem Support team, as the corruption may have occured at the original source of the data.

26.4.5 NetCDF: Variable not found

```
In NcGet_Var_Attr_C: ____, NetCDF: Variable not found
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
Code stopped from DO_ERR_OUT (in module NcdfUtil/m_do_err_out.F90)
This is an error that was encountered in one of the netCDF I/O modules,
which indicates an error in writing to or reading from a netCDF file!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Problem: A GEOS-Chem Classic or HEMCO standalone simulation failed because an expected variable was not found in a netCDF file. This can occur especially if the netCDF file does not contain one of the COARDS-standard index variables (`time`, `lev`, `lat`, `lon`).

Solution: Use the isCoards script to check if your netCDF file is COARDS-compliant. You can then use the netCDF Operators (NCO) and/or Climate Data Operators (CDO) to edit your netCDF file accordingly. For more information, please see our supplemental guides:

- *Prepare COARDS-compliant netCDF files*
- *Work with netCDF files*

26.5 Segmentation faults and similar errors

```
SIGSEGV, segmentation fault occurred
```

Problem: GEOS-Chem or HEMCO tried to access an invalid memory location.

Solution: See the sections below for ways to debug segmentation fault errors.

26.5.1 Array-out-of-bounds error

```
Subscript #N of the array THISARRAY has value X which is less than the lower bound of Y

or

Subscript #N of the array THISARRAY has value A which is greater than the upper bound of␣
↪B
```

Problem: An array index variable refers to an element that lies outside of the array boundaries.

Solution: Reconfigure GEOS-Chem with the following options:

```
$ cd /path/to/build                 # Your GEOS-Chem or HEMCO build directory
$ cmake . -DCMAKE_BUILD_TYPE=Debug
```

This will enable several debugging options, including checking for array operations indices that going out of bounds. You wil get an error message similar to those shown above.

Use the **grep** command to search for all instances of the array (in this example, `THISARRAY`) in each source code folder:

```
grep -i THISARRAY *.F90    # -i means ignore uppercase/lowercase distinction
```

This should let you quickly locate the issue. Depending on the compiler that is used, you might also get a routine name and line number from the error output.

26.5.2 Segmentation fault encountered after TPCORE initialization

```
NASA-GSFC Tracer Transport Module successfully initialized
```

Problem: A GEOS-Chem simulation dies immediately after this text is printed to stdout.

Note: Starting in GEOS-Chem Classic 14.1.0, the text above will only be printed if you have activated verbose output in the `geoschem_config.yml` configuration file.

Solution: Increase the amount of stack memory available to GEOS-Chem and HEMCO. Please follow this link for detailed instructions.

26.5.3 Invalid memory access

```
severe (174): SIGSEGV, segmentation fault occurred
This message indicates that the program attempted an invalid memory reference.
Check the program for possible errors.
```

Problem: GEOS-Chem or HEMCO code tried to read data from an invalid memory location. This can happen when data is being read from a file into an array, but the array is too small to hold all the data.

Solution: Use a debugger (like **gdb**) to try to diagnose the situation. Also try increasing the dimensions of the array that you suspect might be too small.

26.5.4 Stack overflow

```
severe (174): SIGSEGV, possible program stack overflow occurred
Program requirements exceed current stacksize resource limit.
```

Problem: GEOS-Chem and/or HEMCO is using more **stack memory** than is currently available to the system. Stack memory is a reserved portion of the memory structure where short-lived variables are stored, such as:

1. Variables that are local to a given subroutine
2. Variables that are NOT globally saved
3. Variables that are NOT declared as an `ALLOCATABLE` array
4. Variables that are NOT declared as a `POINTER` variable or array
5. Variables that are included in an `!$OMP PRIVATE` or `!$OMP THREADPRIVATE`

Solution: Max out the amount of stack memory that is available to GEOS-Chem and HEMCO. See this section for instructions.

26.6 Less commmon errors

The errors listed below, which occur infrequently, are related to invalid memory operations. These can especially occur with `POINTER`-based variables.

26.6.1 Bus Error

Problem: GEOS-Chem or HEMCO is trying to reference memory that cannot possibly be there. The website StackOverflow.com has a definition of bus error and how it differs from a segmentation fault.

Solution: A bus error may occur when you call a subroutine with too many arguments. Check subroutine definitions and subroutine calls to make sure the correct number of arguments are passed.

26.6.2 Double free or corruption

```
*** glibc detected *** PROGRAM_NAME: double free or corruption (out): ____ ***
```

Problem: The following error is not common, but can occur under some circumstances. Usually this means one of the following has occurred:

1. You are deallocating the same variable more than once.
2. You are deallocating a variable that wasn't allocated, or that has already been deallocated.

Please see this link for more details.

Solution: Try setting all deleted pointers to `NULL()`.

You can also use a debugger like **gdb**, which will show you a backtrace from your crash. This will contain information about in which routine and line number the code crashed, and what other routines were called before the crash happened.

Remember these three basic rules when working with `POINTER`-based variables:

1. Set pointer to NULL after free.
2. Check for NULL before freeing.
3. Initialize pointer to NULL in the start.

Using these rules helps to prevent this type of error.

Also note, you may see this error when a software library required by GEOS-Chem and/or HEMCO is not (e.g. **netcdf** or **netcdf-fortran** has not been installed. GEOS-Chem and/or HEMCO may be making calls to the missing library, which results in the error. If this is the case, the solution would be to *install all required libraries*.

26.6.3 Dwarf subprogram entry error

```
Dwarf subprogram entry L_ROUTINE-NAME__LINE-NUMBER__par_loop2_2_576 has high_pc < low_pc.
This warning will not be repeated for other occurrences.
```

Problem: GEOS-Chem or HEMCO code tried to use a `POINTER`-based variable that is **unassociated** (i.e. not pointing to any other variable or memory) from within an OpenMP parallel loop.

This error can happen when a `POINTER`-based variable is set to `NULL()` where it is declared:

```
TYPE(Species), POINTER :: ThisSpc => NULL()
```

The above declaration causes use pointer variable `ThisSpc` to be implicitly declared with the `SAVE` attribute. This causes a segmentation fault, because all pointers used within an OpenMP parallel region must be associated and nullified on the same thread.

Solution: Make sure that any `POINTER`-based variables (such as `ThisSpc` in this example) point to their target and are nullified within the same OpenMP parallel loop.

```
TYPE(Species), POINTER :: ThisSpc   ! Do not set to NULL() here!!!

 ... etc ...

!$OMP PARALLEL DO(
!$OMP DEFAULT( SHARED ) &
!$OMP PRIVATE( I, J, L, N, ThisSpc, ... )
DO N = 1, nSpecies
DO L = 1, NZ
DO J = 1, NY
DO I = 1, NX

   ... etc ...

   ! Point to species database entry
   ThisSpc => State_Chm%Species(N)%Info

   ... etc ...

   ! Free pointer at end of loop
   ThisSpc => NULL()

ENDDO
ENDDO
ENDDO
ENDDO
```

Note that you must also add `POINTER`-based variables (such as `ThisSpc`) to the `!$OMP PRIVATE` clause for the parallel loop.

For more information about this type of error, please see this article.

26.6.4 Free: invalid size

```
Error in PROGRAM_NAME free(): invalid size: 0x00000000 0662e090
```

Problem: This error is not common. It can happen when:

1. You are trying to free a pointer that wasn't allocated.
2. You are trying to delete an object that wasn't created.
3. You may be trying to nullify or deallocate an object more than once.
4. You may be overflowing a buffer.
5. You may be writing to memory that you shouldn't be writing to.

Solution: Any number of programming errors can cause this problem. You need to use a debugger (such as **gdb**), get a backtrace, and see what your program is doing when the error occurs. If that fails and you determine you have

corrupted the memory at some previous point in time, you may be in for some painful debugging (it may not be too painful if the project is small enough that you can tackle it piece by piece).

See this post on StackOverFlow for more information.

26.6.5 Munmap_chunk: invalid pointer

```
** glibc detected *** PROGRAM_NAME: munmap_chunk(): invalid pointer: 0x00000000059aac30␣
↪***
```

Problem: This is not a common error, but can happen if you deallocate or nullify a `POINTER`-based variable that has already been deallocated or modified.

Solution: Use a debugger (like **gdb**) to see where in GEOS-Chem or HEMCO the error occurs. You will likely have to remove a duplicate `DEALLOCATE` or `=> NULL()` statement. See this link for more information.

26.6.6 Out of memory asking for NNNNN

```
Fatal compilation error: Out of memory asking for 36864.
```

Problem: This error may be caused by the `datasize` limit not being maxed out in your Linux login environment. For more informatin, see this link for more information.

Solution: Use this command to check the status of the `datasize` limit:

```
$ ulimit -d
unlimited
```

If the result of this command is not `unlimited`, then set it to unlimited with this command:

```
$ ulimit -d unlimited
```

Note: The two most important limits for GEOS-Chem and HEMCO are `datasize` and `stacksize` These should both be set to `unlimited`.

CHAPTER

TWENTYSEVEN

DEBUG GEOS-CHEM AND HEMCO ERRORS

If your **GEOS-Chem** or **HEMCO** simulation dies unexpectedly with an error or takes much longer to execute than it should, the most important thing is to try to isolate the source of the error or bottleneck right away. Below are some debugging tips that you can use.

27.1 Check if a solution has been posted to Github

We have migrated support requests from the GEOS-Chem wiki to **Github issues**. A quick search of Github issues (both open and closed) might reveal the answer to your question or provide a solution to your problem.

You should also feel free to open a new issue at one of these Github links:

- GEOS-Chem Classic new issues page
- GCHP new issues page
- HEMCO new issues page

If you are new to Github, we recommend viewing our Github tutorial videos at our GEOS-Chem Youtube site.

27.2 Check if your computational environment is configured properly

Many **GEOS-Chem** and **HEMCO** errors occur due to improper configuration settings (i.e. missing libraries, incorrectly-specified environment variables, etc.) in your computational environment. Take a moment and refer back to these manual pages (on ReadTheDocs) for information on configuring your environment:

- GEOS-Chem Classic manual
- GCHP manual
- HEMCO manual

27.3 Check any code modifications that you have added

If you have made modifications to a "fresh out-of-the-box" **GEOS-Chem** or **HEMCO** version, look over your code edits to search for sources of potential error.

You can also use Git to revert to the last stable version, which is always in the **main** branch.

27.4 Check if your runs exceeded time or memory limits

If you are running **GEOS-Chem** or **HEMCO** on a shared computer system, you will probably have to use a **job scheduler** (such as **SLURM**) to submit your jobs to a computational queue. You should be aware of the run time and memory limits for each of the queues on your system.

If your job uses more memory or run time than the computational queue allows, it can be cancelled by the scheduler. You will usually get an error message printed out to the stderr stream, and maybe also an email stating that the run was terminated. Be sure to check all of the log files created by your jobs for such error messages.

To solve this issue, try submitting your **GEOS-Chem** or **HEMCO** simulations to a queue with larger run-time and memory limits. You can also try splitting up your long simulations into several smaller stages (e.g. monthly) that take less time to run to completion.

27.5 Send debug printout to the log files

If your **GEOS-Chem** simulation stopped with an error, but you cannot tell where, turn on the the `debug_printout` option. This is found in the **Simulation Settings** section of `geoschem_config.yml`:

```
#============================================================================
# Simulation settings
#============================================================================
simulation:
  name: fullchem
  start_date: [20190701, 000000]
  end_date: [20190801, 000000]
  root_data_dir: /path/to/ExtData
  met_field: MERRA2
  species_database_file: ./species_database.yml
  debug_printout: false  # <---- set this to true
  use_gcclassic_timers: false
```

This will send additional output to the **GEOS-Chem** log file, which may help you to determine where the simulation stopped.

If your **HEMCO** simulation stopped with an error, turn on debug printout by editing the `Verbose` and `Warnings` settings at the top of the `HEMCO_Config.rc` configuration file:

```
###############################################################################
### BEGIN SECTION SETTINGS
###############################################################################

ROOT:                       /path/to/ExtData/HEMCO
METDIR:                     MERRA2
GCAP2SCENARIO:              none
GCAP2VERTRES:               none
Logfile:                    HEMCO.log
DiagnFile:                  HEMCO_Diagn.rc
DiagnPrefix:                ./OutputDir/HEMCO_diagnostics
DiagnFreq:                  Monthly
Wildcard:                   *
Separator:                  /
Unit tolerance:             1
```

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```
Negative values:             0
Only unitless scale factors: false
Verbose:                     0      # <---- set this to 3
Warnings:                    1      # <---- set this to 3
```

Both `Verbose` and `Warnings` settings can have values from 0 to 3. The higher the number, the more information will be printed out to the `HEMCO.log` file. A value of 0 disables debug printout.

Having this extra debug printout in your log file output may provide insight as to where your simulation is halting.

27.6 Look at the traceback output

An **error traceback** will be printed out whenever a **GEOS-Chem** or **HEMCO** simulation halts with an error. This is a list of routines that were called when the error occurred.

An sample error traceback is shown here:

```
forrtl: severe (174): SIGSEGV, segmentation fault occurred

Image              PC                Routine            Line        Source
gcclassic          0000000000C82023  Unknown               Unknown  Unknown
libpthread-2.17.s  00002AACE8015630  Unknown               Unknown  Unknown
gcclassic          000000000095935E  error_mod_mp_erro         437  error_mod.F90
gcclassic          000000000040ABB7  MAIN__                    422  main.F90
gcclassic          0000000000406B92  Unknown               Unknown  Unknown
libc-2.17.so       00002AACE8244555  __libc_start_main     Unknown  Unknown
gcclassic          0000000000406AA9  Unknown               Unknown  Unknown
```

The top line with a valid routine name and line number printed is the routine that exited with an error (`error_mod.F90`, line 437). You might also have to look at the other listed files as well to get some more information about the error (e.g. `main.F90`, line 422).

27.7 Identify whether the error happens consistently

If your **GEOS-Chem** or **HEMCO** error always happens at the same model date and time, this could indicate corrupted meteorology or emissions input data files. In this case, you may be able to fix the issue simply by re-downloading the files to your disk space.

If the error happened only once, it could be caused by a network problem or other such transient condition.

27.8 Isolate the error to a particular operation

If you are not sure where a **GEOS-Chem** error is occurring, turn off operations (such as transport, chemistry, dry deposition, etc.) one at a time in the `geoschem_config.yml` configuration file, and rerun your simulation.

Similarly, if you are debugging a **HEMCO** error, turn off different emissions inventories and extensions one at a time in the `HEMCO_Config.rc` file, and rerun your simulation.

Repeating this process should eventually lead you to the source of the error.

27.9 Compile with debugging options

You can compile **GEOS-Chem** or **HEMCO** in debug mode. This will activate several additional error run-time error checks (such as looking for assignments that go outside of array bounds or floating point math errors) that can give you more insight as to where your simulation is dying.

Configure your code for debug mode with the **-DCMAKE_RELEASE_TYPE=Debug** option. From your run directory, type these commands:

```
cd build
cmake ../CodeDir -DCMAKE_RELEASE_TYPE=Debug -DRUNDIR=..
make -j
make -j install
cd ..
```

Attention: Compiling in debug mode will add a significant amount of computational overhead to your simulation. Therefore, we recommend to activate these additional error checks only in short simulations and not in long production runs.

27.10 Use a debugger

You can save yourself a lot of time and hassle by using a debugger such as **gdb** (the GNU debugger). With a debugger you can:

- Examine data when a program stops
- Navigate the stack when a program stops
- Set break points

To run **GEOS-Chem** or **HEMCO** in the **gdb** debugger, you should first *compile in debug mode*. This will turn on the `-g` compiler flag (which tells the compiler to generate symbolic information for debugging) and the `-O0` compiler flag (which shuts off all optimizations. Once the executable has been created, type one of the following commands, which will start **gdb**:

```
$ gdb gcclassic    # for GEOS-Chem Classic
$ gdb gchp         # for GCHP
$ gdb hemco        # for HEMCO standalone
```

At the **gdb** prompt, type one of these commands:

```
(gdb) run                    # for GEOS-Chem Classic or GCHP
(gdb) run HEMCO_sa_Config.rc  # for HEMCO standalone
```

With **gdb**, you can also go directly to the point of the error without having to re-run GEOS-Chem or HEMCO. When your GEOS-Chem or HEMCO simulation dies, it will create a **corefile** such as `core.12345`. The `12345` refers to the process ID assigned to your executable by the operating system; this number is different for each running process on your system.

Typing one of these commands:

```
$ gdb gcclassic core.12345          # for GEOS-Chem Classic
$ gdb gchp core.12345               # for GCHP
$ gdb hemco_standalone core.12345   # for HEMCO standalone
```

will open **gdb** and bring you immediately to the point of the error. If you then type at the `(gdb)` prompt:

```
(gdb) where
```

You will get a *traceback* listing.

To exit **gdb**, type `quit`.

27.11 Print it out if you are in doubt!

Add `print*,` statements to write values of variables in the area of the code where you suspect the error is occurring. Also add the `call flush(6)` statement to flush the output to the screen and/or log file immediately after printing. Maybe you will see something wrong in the output.

You can often detect numerical errors by adding debugging print statements into your source code:

1. Use `MINVAL` and `MAXVAL` functions to get the minimum and maximum values of an array:

   ```
   PRINT*, '### Min, Max: ', MINVAL( ARRAY ), MAXVAL( ARRAY )
   CALL FLUSH( 6 )
   ```

2. Use the `SUM` function to check the sum of an array:

   ```
   PRINT*, '### Sum of X : ', SUM( ARRAY )
   CALL FLUSH( 6 )
   ```

27.12 Use the brute-force method when all else fails

If the bug is difficult to locate, then comment out a large section of code and run your **GEOS-Chem** or **HEMCO** simulation again. If the error does not occur, then uncomment some more code and run again. Repeat the process until you find the location of the error. The brute force method may be tedious, but it will usually lead you to the source of the problem.

27.13 Identify poorly-performing code with a profiler

If you think your **GEOS-Chem** or **HEMCO** simulation is taking too long to run, consider using profiling tools to generate a list of the time that is spent in each routine. This can help you identify badly written and/or poorly-parallelized code. For more information, please see our Profiling GEOS-Chem wiki page.

CHAPTER

TWENTYEIGHT

MANAGE A DATA ARCHIVE WITH BASHDATACATALOG

If you need to download a large amount of input data for **GEOS-Chem** or **HEMCO** (e.g. in support of a large user group at your institution) you may find **bashdatacatalog** helpful.

28.1 What is bashdatacatalog?

The **bashdatacatalog** is a command-line tool (written by Liam Bindle) that facilitates synchronizing local data collections with a remote data source. With the **bashdatacatalog**, you can run queries on your local data collections to answer questions like "What files am I missing?" or "What files aren't bitwise identical to remote data?". Queries can include a date range, in which case collections with temporal assets are filtered-out accordingly. The **bashdatacatalog** can format the results of queries as: a URL download list, a Globus transfer list, an rsync transfer list, or simply a file list.

The **bashdatacatalog** was written to facilitate downloading input data for users of the GEOS-Chem atmospheric chemistry model. The canonical GEOS-Chem input data repository has >1 M files and >100 TB of data, and the input data required for a simulation depends on the model version and simulation parameters such as start and end date.

28.2 Usage instructions

For detailed instructions on using **bashdatacatalog**, please see the bashdatacatalog wiki on Github.

Also see our input-data-catalogs Github repository for comma-separated input lists of GEOS-Chem data, separated by model version.

CHAPTER

TWENTYNINE

ARCHIVE OUTPUT WITH THE HISTORY DIAGNOSTICS

29.1 Introduction

GEOS-Chem Classic and GCHP allow you to save various diagnostic fields to netCDF files via the **History** component. In the following sections you will learn how to schedule diagnostics for output using History.

Note: HEMCO has its own diagnostic archiving capability. Please see the HEMCO diagnostics chapter of The HEMCO User's Guide more information. Note that HEMCO diagnostics are configured from configuration file `HEMCO_Diagn.rc` for both GCHP and GEOS-Chem Classic but diagnostics are also specified in `HISTORY.rc` for GCHP only.

29.1.1 The HISTORY.rc configuration file

You can request GEOS-Chem diagnostics by editing the `HISTORY.rc` configuration file. This file lists the groups of diagnostic outputs (called **collections**), and the parameters for each collection (frequency of archival, mode of archiving, fields per collection, etc.). GEOS-Chem Classic will write netCDF files for each collection at the output intervals that you specify in `HISTORY.rc`. If using GCHP this is done by the MAPL History component also using configuration file `HISTORY.rc`.

Sample HISTORY.rc file

The following is a stripped-down `HISTORY.rc` file example for illustration purposes. The `HISTORY.rc` file that you will find in your GEOS-Chem run directory will contain more collections than what is shown below. This example is for GEOS-Chem Classic.

```
#============================================================================
# EXPID allows you to specify the beginning of the file path corresponding
# to each diagnostic collection.  For example:
#
#   EXPID: ./GEOSChem
#      Will create netCDF files whose names begin "GEOSChem",
#      in this run directory.
#
#   EXPID: ./OutputDir/GEOSChem
#      Will create netCDF files whose names begin with "GEOSChem"
#      in the OutputDir sub-folder of this run directory.
#
```

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```
#============================================================================
EXPID:  ./OutputDir/GEOSChem

#============================================================================
# %%%%% COLLECTION NAME DECLARATIONS %%%%%
#
# To disable a collection, place a "#" character in front of its name.
#============================================================================
COLLECTIONS: 'SpeciesConc',
             'SpeciesConcSubset',
             'ConcAfterChem',
::
#============================================================================
# %%%%% THE SpeciesConc COLLECTION %%%%%
#
# GEOS-Chem species concentrations (default = advected species)
#
# Available for all simulations
#============================================================================
SpeciesConc.template:           '%y4%m2%d2_%h2%n2z.nc4',
SpeciesConc.frequency:          00000000 060000
SpeciesConc.duration :          00000001 000000
SpeciesConc.format:             'CFIO',
SpeciesConc.mode:               'instantaneous',
SpeciesConc.fields:             'SpeciesConcVV_?ADV?',
                                'SpeciesConcMND_?ALL?',
::
#============================================================================
# %%%%% THE SpeciesConcSubset COLLECTION %%%%%
#
# Same as the SpeciesConc collection, but will subset data in the horizontal
# and vertical dimensions so that the netCDF diagnostic files will cover
# a smaller region of the globe.  This can save disk space and memory.
#
# NOTE: This capability will be available in GEOS-Chem "Classic" 12.5.0
# and later versions.
#
# Available for all simulations
#============================================================================
SpeciesConcSubset.template:     '%y4%m2%d2_%h2%n2z.nc4',
SpeciesConcSubset.frequency:    00000000 060000
SpeciesConcSubset.duration:     00000001 000000
SpeciesConcSubset.format:       'CFIO',
SpeciesConcSubset.mode:         'instantaneous',
SpeciesConcSubset.LON_RANGE:    -40.0 60.0,
SpeciesConcSubset.LAT_RANGE:    -10.0 50.0,
SpeciesConcSubset.levels:       1 2 3 4 5,
SpeciesConcSubset.fields:       'SpeciesConcVV_?ADV?',
::
#============================================================================
# %%%%% THE ConcAfterChem COLLECTION %%%%%
#
```

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```
# Concentrations of OH, HO2, O1D, O3P immediately after exiting the KPP solver
# or OH after the CH4 specialty-simulation chemistry routine.
#
# OH:       Available for all full-chemistry simulations and CH4 specialty sim
# HO2:      Available for all full-chemistry simulations
# O1D, O3P: Availalbe for full-chemistry simulations using UCX mechanism
#============================================================================
ConcAfterChem.template:         '%y4%m2%d2_%h2%n2z.nc4',
ConcAfterChem.format:           'CFIO',
ConcAfterChem.frequency:        00000100 000000,
ConcAfterChem.duration:         00000100 000000,
ConcAfterChem.mode:             'time-averaged',
ConcAfterChem.fields:           'OHconcAfterChem',
                                'HO2concAfterChem',
                                'O1DconcAfterChem',
                                'O3PconcAfterChem',
::
```

In this `HISTORY.rc` file, we are requesting three collections, or types of netCDF file output. The table below explains in more detail parameters shown in the `HISTORY.rc` file above.

EXPID

Thi `EXPID` parameter controls the filename prefix, which is set to `./OutputDir/GEOSChem` by default. This means that diagnostic files will be written to the `./OutputDir` directory of the GEOS-Chem run directory, and will start with the prefix `GEOSChem`.

> **Note:** Restart files are placed in the `./Restarts` subdirectory of the run directory instead of `./OutputDir`, which only contains diagnostic files.

COLLECTIONS

The `COLLECTIONS:` tag specifies all of the diagnostic **collections** that you wish to activate during a GEOS-Chem simulation. Each collection represents a group of diagnostic quantities that will be written to disk in netCDF file format. The collection name will be automatically added to the netCDF file name along with the date/or time.

Each GEOS-Chem run directory will ship with its own customized `HISTORY.rc` configuration file. Only the diagnostic collections pertaining to a particular GEOS-Chem simulation will be included in the corresponding `HISTORY.rc` file.

Each collection name must be bracketed by single quotes, and be followed by a comma.

To disable an entire diagnostic collection, simply put a `#` comment character in front of the collection name in the `COLLECTIONS:` section.

GEOS-Chem will expect to find a collection definition section for each of the activated collections listed under the `COLLECTIONS:` section. In other words, if you have `SpeciesConc` listed under `COLLECTIONS:`, but there is no further information provided about the `SpeciesConc` collection, then GEOS-Chem will halt with an error message.

Note: You are not limited to the collections that are pre-defined in the `HISTORY.rc` configuration file. You may create additional diagnostic collections to suit your research purposes.

SpeciesConc

Name of the first collection in this `HISTORY.rc` file.

SpeciesConc.template

Determines the date and time format for the *SpeciesConc* collection filename suffix, as described below:

- `%y4%m2%d2_%h2%n2z.nc4` prints `YYYYMMDD_hhmmz.nc4` to the end of each netCDF filename.
- `YYYYMMDD` is the date in year/month/day format;
- `hhmm` is the time in `hour:minutes` format.
- `z` denotes "Zulu", which is an abbreviation for UTC time.
- `.nc4` denotes that the data file is in the netCDF-4 format.

Note: For example, the complete file path for the *SpeciesConc* collection at 00:00 UTC on 2020/01/01 will be `./OutputDir/GEOSChem.SpeciesConc.20200101_0000z.nc4`, where:

- *EXPID* specifies the filename prefix (`./OutputDir/GEOSChem`).
- *SpeciesConc.template* specifies the format of the filename suffix (`.20200101_0000z.nc4`).

SpeciesConc.frequency

Determines how often the diagnostic quantities belonging to the *SpeciesConc* collection will be saved to a netCDF file. This can be specified as either `hhmmss` or `YYYYMMDD hhmmss`.

In the above example, data belonging to the collection will be written to the file every 6 hours. Because `SpeciesConc` is an instantaneous collection, no time-averaging will be performed.

SpeciesConc.format

For GCHP simulations only. This tag indicates the I/O library that will be used.

SpeciesConc.duration

Determines how often a new `SpeciesConc` netCDF file will be created. Uses the same format as histguide-configfile-sample-sc-freq:.

SpeciesConc.mode

Determines the averaging method for the `SpeciesConc` collection. Allowable values are:

- `instantaneous`: Archives instantaneous values at the interval specified by histguide-configfile-sample-sc-freq:.
- `time-averaged`: Archives values averaged over the interval specified by histguide-configfile-sample-sc-freq:.

SpeciesConc.fields

Lists the diagnostic quantities to be archived in the *SpeciesConc* collection. Some diagnostic quantities (e.g. concentrations, fluxes, masses) may also have an extra dimension, which represents species, size bins, reaction numbers, etc.

For example, to request the ozone species concentration (in mixing ratio units) you may use the field name `SpeciesConcVV_O3`. The species name is separated from the quantity name by a single underscore.

Note: For GCHP, each diagnostic field must be followed by the name of the ESMF gridded component that it is associated with. For arrays in GEOS-Chem objects State_Met, State_Chm, and State_Diag this is `'GCHPchem',`. A few diagnostics may also be output from the advection component of GCHP which has ESMF gridded component name `DYNAMICS`.

If you are using GEOS-Chem Classic,you may also use a *wildcard* to specify a given category of species. In the above example `SpeciesConcVV_?ADV?` refers to all advected species and `SpeciesConcVV_?ALL?` refers to all species (both advected and non-advected).

Note: GCHP does not allow the use of wildcards. Each diagnostic quantity must be listed individually.

:: separator

Signifies the end of the *SpeciesConc* definition section. The `::` may be placed at any column.

SpeciesConc.subset

Name of the second diagnostic collection specified in this sample `HISTORY.rc` configuration file. In this collection we will request output to be restricted to a subset of the horizontal grid.

The `.template`, `.frequency`, `.duration`, `:mode`, and `.fields` are described for the *SpeciesConc* collection above, so we will not repeat them here.

SpeciesConcSubset.LON_RANGE

Defines the longitude range (`min max`) where diagnostic data will be archived. Data outside of this range will be ignored. If this option is omitted, values at all longitudes (`-180 180`) will be included.

SpeciesConcSubset.LAT_RANGE

Defines the latitude range (`min max`) where diagnostic data will be archived. Data outside of this range will be ignored. If this option is omitted, values at all latitudes (`-90 90`) will be included.

SpeciesConcSubset.levels

Specifies the levels that you wish to be included in the diagnostic archiving. If omitted, data at all levels will be included.

Note: In GEOS-Chem Classic, all levels between the minimum and maximum level specified will be included in the diagnostic archival. This differs from the behavior in GCHP, which archives only the specified levels.

ConcAfterChem

Name of the third collection specified in this sample `HISTORY.rc` configuration file.

The `.template`, `.frequency`, `.duration`, `:mode`, and `.fields` are described for the *SpeciesConc* collection above, so we will not repeat them here.

ConcAftercChem.mode

In this example, the `ConcAfterChem.mode` setting indicates that the `ConcAfterChem` collection will contain ime-averaged data. The averaging interval is set in the `frequency` field.

29.1.2 Wildcards (GEOS-Chem Classic only)

For GEOS-Chem Classic diagnostic output, you can use the following wildcards with diagnostic quantities that have a species/bin/reaction dimension:

Wildcard	Description	Example
`?ADV?`	Advected species	`SpeciesConcVV_?ADV?`
`?AER?`	Aerosol species	`SpeciesConcVV_?AER?`
`?ALL?`	All species	`SpeciesConcVV_?ALL?`
`?DRY?`	Dry-deposited species	`SpeciesConcVV_?DRY?`
`?DRYALT?`	Species for the histguide-concabovechem collection	`SpeciesConcVV_?DRYALT`
`?DUSTBIN?`	Dust bin number	`AODdust550nm_?DUSTBIN?`
`?FIX?`	Fixed species in the KPP chemistry mechanism	`SpeciesConcVV_?FIX?`
`?GAS?`	Gas-phase species	`SpeciesConcVV_?GAS?`
`?HYG?`	Aerosol species that undergo hygroscopic growth - (e.g. black carbon)	`AODhyg550nm_?HYG?`
`?KPP?`	All species (fixed variable) in the KPP chemistry mechanism	*SpeciesConcVV_?KPP?*
`?LOS?`	Chemical loss species or familes	*SpeciesConcVV_?LOS?*
`?PHO?`	Photolyzed species	*SpeciesConcVV_?PHO?*
`?PRD?`	Chemical production species or families	`SpeciesConcVV_?PRD?`
`?RRTMG?`	RRTMG-computed fluxes	`RadAllSkywSurf_?RRTMG?`
`?RXN?`	KPP reaction rates	`RxnRate_?RXN?`
`?TOMASBIN?`	TOMAS size bins	`TomasH2SO4Mass_?TOMASBIN?`
`?UVFLX?`	UV flux bins	`UVFluxDiffuse_?UVFLX?`
`?VAR?`	Variable (i.e. active) species in the KPP mechanism	`SpeciesConcVV_?VAR?`
`?WET?`	Wet-deposited species	`SpeciesConcVV_?WET`

29.1.3 Prefixes

You may add any field from the `State_Met` and `State_Chm` objects to any diagnostic collection as well. These fields must be prefixed as described below:

Wildcard	Description	Example
`Chem_`	Request diagnostic output from the `State_Chm` object	`Chem_pHCloud`
`Met_`	Request diagnostic output from the `State_Met` object	`Met_SPHU`

29.1.4 File naming convention

As mentioned above, `SpeciesConc.template`, GEOS-Chem History files adhere to the following naming convention:

```
EXPID.collection-name.collection-template
```

e.g.

```
../OutputDir/GEOSChem.SpeciesConc.20200101_0000z.nc4
```

The duration tag of each collection in `HISTORY.rc` controls how often a new file will be written to disk, as we saw *above*:

```
SpeciesConc.duration:           00000001 000000     # Write a new file each day
SpeciesConcSubset.duration:     00000001 000000     # Write a new file each day
ConcAfterChem.duration:         00000100 000000     # Write a new file each month
```

Therefore, based on all of these settings in our example `HISTORY.rc` file, GEOS-Chem will write the following netCDF files to disk in the current run directory:

```
GEOSChem.SpeciesConc.20160101_0000z.nc4    GEOSChem.SpeciesConcSubset.20160101_0000z.nc4
GEOSChem.SpeciesConc.20160102_0000z.nc4    GEOSChem.SpeciesConcSubset.20160102_0000z.nc4
GEOSChem.SpeciesConc.20160103_0000z.nc4    GEOSChem.SpeciesConcSubset.20160102_0000z.nc4
GEOSChem.SpeciesConc.20160104_0000z.nc4    GEOSChem.SpeciesConcSubset.20160104_0000z.nc4
... etc ...

GEOSChem.ConcAfterChem.20160101_0000z.nc4
GEOSChem.ConcAfterChem.20160201_0000z.nc4
GEOSChem.ConcAfterChem.20160301_0000z.nc4
GEOSChem.ConcAfterChem.20160401_0000z.nc4
... etc ...
```

29.1.5 Vertical coordinates in netCDF files

All netCDF files produced by GEOS-Chem (i.e. diagnostic files and restart files) adhere to the *the COARDS netCDF convention*. for the lon, lat, and time dimensions.

For the vertical dimension, we have chosen to use the following coordinate variables to include in GEOS-Chem Classic output files, emulating the file format of the NCAR Community Earth System Model (CESM):

```
variables:
     double lev(lev) ;
         lev:long_name = "hybrid level at midpoints (1000*(A+B))" ;
         lev:units = "level" ;
         lev:positive = "down" ;\
         lev:standard_name = "atmosphere_hybrid_sigma_pressure_coordinate" ;
         lev:formula_terms = "a: hyam b: hybm p0: P0 ps: PS" ;
     double hyam(lev) ;
         hyam:long_name = "hybrid A coefficient at layer midpoints" ;
     double hybm(lev) ;
         hybm:long_name = "hybrid B coefficient at layer midpoints" ;
     double ilev(ilev) ;
         ilev:long_name = "hybrid level at interfaces (1000*(A+B))" ;
         ilev:units = "level" ;
         ilev:positive = "down" ;
         ilev:standard_name = "atmosphere_hybrid_sigma_pressure_coordinate" ;
         ilev:formula_terms = "a: hyai b: hybi p0: P0 ps: PS" ;
     double hyai(ilev) ;
         hyai:long_name = "hybrid A coefficient at layer interfaces" ;
     double hybi(ilev) ;
         hybi:long_name = "hybrid B coefficient at layer interfaces" ;
     double P0 ;
         P0:long_name = "reference pressure" ;
```

The lev variable is used for data that is placed on the midpoints between vertical levels. This is an "approximate" eta coordinate, which is close to 1 at the surface and close to zero at the atmosphere top.

```
lev = 0.99250002413, 0.97749990013, 0.962499776, 0.947499955, 0.93250006,
   0.91749991, 0.90249991, 0.88749996, 0.87249996, 0.85750006, 0.842500125,
   0.82750016, 0.8100002, 0.78750002, 0.762499965, 0.737500105, 0.7125001,
   0.6875001, 0.65625015, 0.6187502, 0.58125015, 0.5437501, 0.5062501,
   0.4687501, 0.4312501, 0.3937501, 0.3562501, 0.31279158, 0.26647905,
   0.2265135325, 0.192541016587707, 0.163661504087706, 0.139115, 0.11825,
   0.10051436, 0.085439015, 0.07255786, 0.06149566, 0.05201591, 0.04390966,
   0.03699271, 0.03108891, 0.02604911, 0.021761005, 0.01812435, 0.01505025,
   0.01246015, 0.010284921, 0.008456392, 0.0069183215, 0.005631801,
   0.004561686, 0.003676501, 0.002948321, 0.0023525905, 0.00186788,
   0.00147565, 0.001159975, 0.00090728705, 0.0007059566, 0.0005462926,
   0.0004204236, 0.0003217836, 0.00024493755, 0.000185422, 0.000139599,
   0.00010452401, 7.7672515e-05, 5.679251e-05, 4.0142505e-05, 2.635e-05,
   1.5e-05 ;
```

The lev variable may be used for quick plotting. To compute the actual pressure at the midpoint of the grid box (I,J,L), you will need to supply your own 2-D surface pressure field (e.g. saved from another diagnostic file):

```
Pmid = ( hyam(L) * PS(I,J) ) + hybm(L)
```

The ilev variable is used for data that is placed on vertical level edges or "interfaces" (hence the "i" in ilev). This is also an "approximate" eta coordinate.

```
ilev = 1, 0.98500004826, 0.969999752, 0.9549998, 0.94000011, 0.92500001,
   0.90999981, 0.89500001, 0.87999991, 0.86500001, 0.85000011, 0.83500014,
   0.82000018, 0.80000022, 0.77499982, 0.75000011, 0.7250001, 0.7000001,
   0.6750001, 0.6375002, 0.6000002, 0.5625001, 0.5250001, 0.4875001,
   0.4500001, 0.4125001, 0.3750001, 0.3375001, 0.28808306, 0.24487504,
   0.208152025, 0.176930008175413, 0.150393, 0.127837, 0.108663, 0.09236572,
   0.07851231, 0.06660341, 0.05638791, 0.04764391, 0.04017541, 0.03381001,
   0.02836781, 0.02373041, 0.0197916, 0.0164571, 0.0136434, 0.0112769,
   0.009292942, 0.007619842, 0.006216801, 0.005046801, 0.004076571,
   0.003276431, 0.002620211, 0.00208497, 0.00165079, 0.00130051, 0.00101944,
   0.0007951341, 0.0006167791, 0.0004758061, 0.0003650411, 0.0002785261,
   0.000211349, 0.000159495, 0.000119703, 8.934502e-05, 6.600001e-05,
   4.758501e-05, 3.27e-05, 2e-05, 1e-05 ;
```

To compute the actual pressure at the bottom and top edges of the grid box (I,J,L), you will need to supply your own 2-D surface pressure field (e.g. saved from another diagnostic file):

```
Pbot = ( hyai(L  ) * PS(I,J) ) + hybi(L  )
Ptop = ( hyai(L+1) * PS(I,J) ) + hybi(L+1)
```

GCHP history files contain simply the lev coordinate which is the level index of the model. Level 1 corresponds to surface for all diagnostics retrieved from GEOS-Chem arrays State_Met, State_Diag, and State_Chm. These include all diagnostics that have prefix `Met_` or `Chm_` as well as all other `GCHPchem` diagnostics that do not begin with `Emis`. Diagnostics that begin with `Emis` or that have gridded component name other than `GCHPchem` have Level 1 correspond to top-of-atmosphere.

29.2 Diagnostic collections

The diagnostic collections described in the sections below are used by default in GEOS-Chem simulations. You can create your own customized collections by modifying the `HISTORY.rc` file.

The only restriction is that you cannot mix data that is placed on grid box layer edges in the same collection as data placed on grid box layer centers. This violates the netCDF convention that all data variables have to be defined with the same vertical dimension.

Note: For diagnostic quantities that have a species/bin/reaction dimension, we will use the abbreviation `<name|wc>` to indicate a species/bin/reaction name or wildcard.

For example, `SpeciesConcVV_<name|wc>` means that the diagnostic quantity can be a single species (`SpeciesConcVV_O3`) or a wildcarded subset of species (`SpeciesConcVV_?ADV?`).

29.2.1 AdvFluxVert

The **AdvFluxVert** collection contains diagnostics for vertical transport in GEOS-Chem Classic advection. In practice, this collection is only used to obtain the vertical flux of O3 from GEOS-Chem Classic fullchem benchmark simulations. Most GEOS-Chem users will not need to activate this collection.

Sample definition section for HISTORY.rc

```
  AdvFluxVert.template:    '%y4%m2%d2_%h2%n2z.nc4',
  AdvFluxVert.frequency:   00000100 000000
  AdvFluxVert.duration:    00000100 000000
  AdvFluxVert.mode:        'time-averaged'
  AdvFluxVert.fields:      'AdvFluxVert_O3',
::
```

List of diagnostic fields in the AdvFluxVert collection

Diagnostic field	Description	Units	Wildcards
AdvFluxVert_<name|wc>	Vertical flux of species in advection	kg/s	?ADV?

29.2.2 AerosolMass

The **AerosolMass** collection contains diagnostics for aerosol mass and particulate matter from full-chemistry simulations.

Sample definition section for HISTORY.rc

```
  AerosolMass.template:       '%y4%m2%d2_%h2%n2z.nc4',
  AerosolMass.frequency:      00000100 000000
  AerosolMass.duration:       00000100 000000
  AerosolMass.mode:           'time-averaged'
  AerosolMass.fields:         'AerMassASOA    ',
                              'AerMassBC      ',
                              'AerMassINDIOL  ',
                              'AerMassISN1OA  ',
```

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```
                                'AerMassISOA    ',
                                'AerMassLVOCOA  ',
                                'AerMassNH4     ',
                                'AerMassNIT     ',
                                'AerMassOPOA    ',
                                'AerMassPOA     ',
                                'AerMassSAL     ',
                                'AerMassSO4     ',
                                'AerMassSOAGX   ',
                                'AerMassSOAIE   ',
                                'AerMassSOAME   ',
                                'AerMassSOAMG   ',
                                'AerMassTSOA    ',
                                'BetaNO         ',
                                'PM25           ',
                                'TotalBiogenicOA',
                                'TotalOA        ',
                                'TotalOC        ',
::
```

List of diagnostic fields in the AerosolMass collection

Diagnostic field	Description	Units
AerMassASOA[1]	Aerosol products of light aromatics + IVOC oxidation	$\mu g/m^3$
AerMassBC	Aerosol products of light aromatics + IVOC oxidation	$\mu g/m^3$
AerMassINDIOL[1]	Generic aerosol-phase organonitrate hydrolysis product	$\mu g/m^3$
AerMassISN10A[1]	Aerosol phase 2nd generation hydroxynitrates formed from ISOP + NO3 rxn pathway	$\mu g/m^3$
AerMassISOA[1]	Aerosol products of isoprene oxidation	$\mu g/m^3$
AerMassLVOCOA[1]	Aerosol-phase low-volatility non-IEPOX product of ISOPOOH (RIP) oxidation	$\mu g/m^3$
AerMassNH4	Ammonium	$\mu g/m^3$
AerMassNIT	Inorganic nitrate aerosol	$\mu g/m^3$
AerMassPOA[1]	Aerosols from SVOCs	$\mu g/m^3$
AerMassOPOA[1]	Aerosols products of POG oxidation	$\mu g/m^3$
AerMassSAL	Sea salt aerosol (SALA+SALC)	$\mu g/m^3$
AerMassSO4	Sulfate	$\mu g/m^3$
AerMassSOAGX[1]	Aerosol phase glyoxal	$\mu g/m^3$
AerMassSOAIE[1]	Aerosol phase IEPOX	$\mu g/m^3$
AerMassSOAME[1]	Aerosol phase IMAE	$\mu g/m^3$
AerMassSOAMG[1]	Aerosol phase methylglyoxal	$\mu g/m^3$
AerMassTSOA[1]	Aerosol products of terpene oxidation	$\mu g/m^3$
BetaNO[1]	NO branching ratio	$\mu g/m^3$
PM25	Particulate matter (d < 2.5 :math:{mu}m`)	$\mu g/m^3$
TotalBiogenicOA[2]	Sum of all organic aerosol	$\mu g/m^3$
TotalOA[1]	Sum of all organic aerosol	$\mu g/m^3$
TotalOC	Sum of all organic carbon	$\mu g/m^3$

[1] Only defined for fullchem simulations with complex SOA species.
[2] Defined for aerosol-only simulations or fullchem simulations.

Notes for the AerosolMass collection

29.2.3 Aerosols

The **Aerosols** collection contains diagnostics for aerosol optical depth and related quantities from full-chemistry simulations.

Note: Some diagnostic fields in the Aerosols collection may be computed at up to 3 wavelengths (`WL1`, `WL2`, `WL3`) as specified in this menu of the `geoschem_config.yml` file:

```
rrtmg_rad_transfer_model:
    ... etc ...
    aod_wavelengths_in_nm:
    - 550
```

For GEOS-Chem simulations that do not use the RRTMG radiative transfer model, you may specify only one wavelength `WL1`, which is set to a default value of 550 nm. For GEOS-Chem simulations using RRTMG, you may specify up to 2 more additional wavelengths (`WL2` and `WL3`). GEOS-Chem will replace the tokens `WL1`, `WL2`, `WL3` in diagnostic field names with the corresponding wavelength.

For example, these diagnostic fields:

```
AODHygWL1_BCPI
AODDustWL1_DST1
AODStratLiquidAerWL1
AODPolarStratCloudWL1
AODSOAfromAqIsopreneWL1
AODStratLiquidAerWL1
AODPolarStratCloudWL1
```

will be saved to the `GEOSChem.Aerosols.YYYYMMDD_hhmmz.nc4` file(s) under these names:

```
AODHyg550nm_BCPI
AODDust550nm_DST1
AODStratLiquidAer550nm
AODPolarStratCloud550nm
AODSOAfromAqIsoprene550nm
AODStratLiquidAer550nm
AODPolarStratCloud550nm
```

Sample definition section for HISTORY.rc

```
  Aerosols.template:    '%y4%m2%d2_%h2%n2z.nc4',
  Aerosols.frequency:   00000100 000000
  Aerosols.duration:    00000100 000000
  Aerosols.mode:        'time-averaged'
  Aerosols.fields:      'AODDust                      ',
                        'AODDustWL1_?DUSTBIN?         ',
                        'AODHygWL1_?HYG?              ',
                        'AODSOAfromAqIsopreneWL1      ',
                        'AODStratLiquidAerWL1         ',
                        'AODPolarStratCloudWL1        ',
                        'AerHygroscopicGrowth_?HYG?   ',
```

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```
                        'AerNumDensityStratLiquid     ',
                        'AerNumDensityStratParticulate',
                        'AerAqueousVolume             ',
                        'AerSurfAreaDust              ',
                        'AerSurfAreaHyg_?HYG?         ',
                        'AerSurfAreaStratLiquid       ',
                        'AerSurfAreaPolarStratCloud   ',
                        'Chem_AeroAreaMDUST1          ',
                        'Chem_AeroAreaMDUST2          ',
                        'Chem_AeroAreaMDUST3          ',
                        'Chem_AeroAreaMDUST4          ',
                        'Chem_AeroAreaMDUST5          ',
                        'Chem_AeroAreaMDUST6          ',
                        'Chem_AeroAreaMDUST7          ',
                        'Chem_AeroAreaSULF            ',
                        'Chem_AeroAreaBC              ',
                        'Chem_AeroAreaOC              ',
                        'Chem_AeroAreaSSA             ',
                        'Chem_AeroAreaSSC             ',
                        'Chem_AeroAreaBGSULF          ',
                        'Chem_AeroAreaICEI            ',
                        'Chem_AeroRadiMDUST1          ',
                        'Chem_AeroRadiMDUST2          ',
                        'Chem_AeroRadiMDUST3          ',
                        'Chem_AeroRadiMDUST4          ',
                        'Chem_AeroRadiMDUST5          ',
                        'Chem_AeroRadiMDUST6          ',
                        'Chem_AeroRadiMDUST7          ',
                        'Chem_AeroRadiSULF            ',
                        'Chem_AeroRadiBC              ',
                        'Chem_AeroRadiOC              ',
                        'Chem_AeroRadiSSA             ',
                        'Chem_AeroRadiSSC             ',
                        'Chem_AeroRadiBGSULF          ',
                        'Chem_AeroRadiICEI            ',
                        'Chem_WetAeroAreaMDUST1       ',
                        'Chem_WetAeroAreaMDUST2       ',
                        'Chem_WetAeroAreaMDUST3       ',
                        'Chem_WetAeroAreaMDUST4       ',
                        'Chem_WetAeroAreaMDUST5       ',
                        'Chem_WetAeroAreaMDUST6       ',
                        'Chem_WetAeroAreaMDUST7       ',
                        'Chem_WetAeroAreaSULF         ',
                        'Chem_WetAeroAreaBC           ',
                        'Chem_WetAeroAreaOC           ',
                        'Chem_WetAeroAreaSSA          ',
                        'Chem_WetAeroAreaSSC          ',
                        'Chem_WetAeroAreaBGSULF       ',
                        'Chem_WetAeroAreaICEI         ',
                        'Chem_WetAeroRadiMDUST1       ',
                        'Chem_WetAeroRadiMDUST2       ',
                        'Chem_WetAeroRadiMDUST3       ',
```

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```
                        'Chem_WetAeroRadiMDUST4       ',
                        'Chem_WetAeroRadiMDUST5       ',
                        'Chem_WetAeroRadiMDUST6       ',
                        'Chem_WetAeroRadiMDUST7       ',
                        'Chem_WetAeroRadiSULF         ',
                        'Chem_WetAeroRadiBC           ',
                        'Chem_WetAeroRadiOC           ',
                        'Chem_WetAeroRadiSSA          ',
                        'Chem_WetAeroRadiSSC          ',
                        'Chem_WetAeroRadiBGSULF       ',
                        'Chem_WetAeroRadiICEI         ',
                        'Chem_StatePSC                ',
                        'Chem_KhetiSLAN2O5H2O         ',
                        'Chem_KhetiSLAN2O5HCl         ',
                        'Chem_KhetiSLAClNO3H2O        ',
                        'Chem_KhetiSLAClNO3HCl        ',
                        'Chem_KhetiSLAClNO3HBr        ',
                        'Chem_KhetiSLABrNO3H2O        ',
                        'Chem_KhetiSLABrNO3HCl        ',
                        'Chem_KhetiSLAHOClHCl         ',
                        'Chem_KhetiSLAHOClHBr         ',
                        'Chem_KhetiSLAHOBrHCl         ',
                        'Chem_KhetiSLAHOBrHBr         ',
::
```

List of diagnostic fields in the Aerosols collection

Diagnostic field	Description	Units	Wildcard
AODDust[3]	Mineral dust optical depth @ WL1	1	
AODDustWL1_<name|wc>	AOD for each dust bin @ WL1	1	?DUSTBIN?
AODHygWL1_<name|wc>	AOD @ WL1 for aerosol species	1	?HYG?
AODSOAfromAqIsopreneWL1[4]	Optical depth of SOA from aqueous isoprene @ WL1	1	
AODStratLiquidAerWL1	Stratospheric liquid optical depth @ WL1	1	
AODPolarStratCloudWL1	Polar stratospheric cloud type 1a/2 optical depth @ WL1	1	
AerHygroscopicGrowth_<name|wc>	Hygroscopic growth of aerosol species	1	?HYG?
AerNumDensityStratLiquid	Stratospheric liquid aerosol number density	1/cm3	
AerNumDensityStratParticulate	Stratospheric particulate aerosol number density	1/cm3	
AerAqueousVolume	Aqueous aerosol volume	cm2/cm3	
AerSurfAreaDust	Surface area of mineral dust	cm2/cm3	

continues on next page

Table 1 – continued from previous page

Diagnostic field	Description	Units	Wildcard
AerSurfAreaHyg_<name|wc>	Surface area of aerosol species	cm2/cm3	?HYG?
AerSurfAreaStratLiquid	Stratospheric liquid surface area	cm2/cm3	
AerSurfaceAreaPolarStratCloud	Polar stratospheric cloud type 1a/2 surface area	cm2/cm3	
Chem_AeroAreaMDUST1[P]	Dry aerosol area for mineral dust (0.15 μm)	cm2/cm3	
Chem_AeroAreaMDUST2[P]	Dry aerosol area for mineral dust (0.25 μm)	cm2/cm3	
Chem_AeroAreaMDUST3[P]	Dry aerosol area for mineral dust (0.4 μm)	cm2/cm3	
Chem_AeroAreaMDUST4[P]	Dry aerosol area for mineral dust (0.8 μm)	cm2/cm3	
Chem_AeroAreaMDUST5[P]	Dry aerosol area for mineral dust (1.5 μm)	cm2/cm3	
Chem_AeroAreaMDUST6[P]	Dry aerosol area for mineral dust (2.5 μm)	cm2/cm3	
Chem_AeroAreaMDUST7[P]	Dry aerosol area for mineral dust (4.0 μm)	cm2/cm3	
Chem_AeroAreaSULF[Page 2	Dry aerosol area for sulfate aerosol	cm2/cm3	
Chem_AeroAreaBC[Page 229,	Dry aerosol area for black carbon	cm2/cm3	
Chem_AeroAreaOC[Page 229,	Dry aerosol area for organic carbon	cm2/cm3	
Chem_AeroAreaSSA[Page 229	Dry aerosol area for sea salt aerosol, accumulation mode	cm2/cm3	
Chem_AeroAreaSSC[Page 229	Dry aerosol area for sea salt aerosol, coarse mode	cm2/cm3	
Chem_AeroAreaBGSULF	Dry aerosol area for background stratospheric sulfate	cm2/cm3	
Chem_AeroAreaICEI	Dry aerosol area for irregular ice cloud	cm2/cm3	
Chem_AeroRadiMDUST1[P]	Dry aerosol radius for mineral dust (0.15 μm)	cm	
Chem_AeroRadiMDUST2[P]	Dry aerosol radius for mineral dust (0.25 μm)	cm	
Chem_AeroRadiMDUST3[P]	Dry aerosol radius for mineral dust (0.4 μm)	cm	
Chem_AeroRadiMDUST4[P]	Dry aerosol radius for mineral dust (0.8 μm)	cm	
Chem_AeroRadiMDUST5[P]	Dry aerosol radius for mineral dust (1.5 μm)	cm	
Chem_AeroRAdiMDUST6[I]	Dry aerosol radius for mineral dust (2.5 μm)	cm	
Chem_AeroRadiMDUST7[P]	Dry aerosol radius for mineral dust (4.0 μm)	cm	

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Table 1 – continued from previous page

Diagnostic field	Description	Units	Wildcard
Chem_AeroRadiSULF[Page 2]	Dry aerosol radius for sulfate aerosol	cm	
Chem_AeroRadiBC[Page 229,]	Dry aerosol radius for black carbon	cm	
Chem_AeroRadiOC[Page 229,]	Dry aerosol radius for organic carbon	cm	
Chem_AeroRadiSSA[Page 229]	Dry aerosol radius for sea salt aerosol, accumulation mode	cm	
Chem_AeroRadiSSC[Page 229]	Dry aerosol radius for sea salt aerosol, coarse mode	cm	
Chem_AeroRadiBGSULF	Dry aerosol radius for background stratospheric sulfate	cm	
Chem_AeroRadiICEI	Dry aerosol Radius for irregular ice cloud	cm	
Chem_WetAeroAreaMDUS	Wet aerosol area for mineral dust (0.15 μm)	cm2/cm3	
Chem_WetAeroAreaMDUS	Wet aerosol area for mineral dust (0.25 μm)	cm2/cm3	
Chem_WetAeroAreaMDUS	Wet aerosol area for mineral dust (0.4 μm)	cm2/cm3	
Chem_WetAeroAreaMDUS	Wet aerosol area for mineral dust (0.8 μm)	cm2/cm3	
Chem_WetAeroAreaMDUS	Wet aerosol area for mineral dust (1.5 μm)	cm2/cm3	
Chem_WetAeroAreaMDUS	Wet aerosol area for mineral dust (2.5 μm)	cm2/cm3	
Chem_AeroAreaMDUST7[P]	Dry aerosol area for mineral dust (4.0 μm)	cm2/cm3	
Chem_WetAeroAreaSULF[P]	Wet aerosol area for sulfate aerosol	cm2/cm3	
Chem_WetAeroAreaBC[Page]	Wet aerosol area for black carbon	cm2/cm3	
Chem_WetAeroAreaOC[Page]	Wet aerosol area for organic carbon	cm2/cm3	
Chem_WetAeroAreaSSA[Pag]	Wet aerosol area for sea salt aerosol, accumulation mode	cm2/cm3	
Chem_WetAeroAreaSSC[Pag]	Wet aerosol area for sea salt aerosol, coarse mode	cm2/cm3	
Chem_WetAeroAreaBGSU	Wet aerosol area for background stratospheric sulfate	cm2/cm3	
Chem_WetAeroAreaICEI	Wet aerosol area for irregular ice cloud	cm2/cm3	
Chem_WetAeroRadiMDUS	Wet aerosol radius for mineral dust (0.15 μm)	cm	
Chem_WetAeroRadiMDUS	Wet aerosol radius for mineral dust (0.25 μm)	cm	

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Table 1 – continued from previous page

Diagnostic field	Description	Units	Wildcard
Chem_WetAeroRadiMDUS	Wet aerosol radius for mineral dust (0.4 μm)	cm	
Chem_WetAeroRadiMDUS	Wet aerosol radius for mineral dust (0.8 μm)	cm	
Chem_WetAeroRadiMDUS	Wet aerosol radius for mineral dust (1.5 μm)	cm	
Chem_WetAeroRAdiMDU	Wet aerosol radius for mineral dust (2.5 μm)	cm	
Chem_WetAeroRadiMDUS	Wet aerosol radius for mineral dust (4.0 μm)	cm	
Chem_WetAeroRadiSULF[3]	Wet aerosol radius for sulfate aerosol	cm	
Chem_WetAeroRadiBC[3]	Wet aerosol radius for black carbon	cm	
Chem_WetAeroRadiOC[3]	Wet aerosol radius for organic carbon	cm	
Chem_WetAeroRadiSSA[3]	Wet aerosol radius for sea salt aerosol, accumulation mode	cm	
Chem_WetAeroRadiSSC[3]	Wet aerosol radius for sea salt aerosol, coarse mode	cm	
Chem_WetAeroRadiBGSU	Wet aerosol radius for background stratospheric sulfate	cm	
Chem_WetAeroRadiICEI	Wet aerosol Radius for irregular ice cloud	cm	
Chem_KhetiSLAN2O5H2C	Sticking coefficient for N2O5 + H2O rxn	1	
Chem_KhetiSLAN2O5HCl	Sticking coefficient for N2O5 + HCl rxn	1	
Chem_KhetiSLACLNO3H2	Sticking coefficient for ClNO3 + H2O rxn	1	
Chem_KhetiSLACLNO3HC	Sticking coefficient for ClNO3 + HCl rxn	1	
Chem_KhetiSLACLNO3HI	Sticking coefficient for ClNO3 + HBr rxn	1	
Chem_KhetiSLABRNO3H2	Sticking coefficient for BrNO3 + H2O rxn	1	
Chem_KhetiSLABRNO3HC	Sticking coefficient for BrNO3 + HCl rxn	1	
Chem_KhetiSLAHOCLHC	Sticking coefficient for HOCl + HCl rxn	1	
Chem_KhetiSLAHOCLHB	Sticking coefficient for HOCl + HBr rxn	1	
Chem_KhetiSLAHOBRHC	Sticking coefficient for HOBr + HCl rxn	1	
Chem_KhetiSLAHOBRHB	Sticking coefficient for HOBr + HBr rxn	1	

[3] Defined for aerosol-only and fullchem simulations.
[4] Only defined for fullchem simulation with complex SOA species.

Notes for the Aerosols colletion

29.2.4 BoundaryConditions

The **BoundaryConditions** diagnostic collection contains advected species concentrations (archived from a global simulation) that will be used by GEOS-Chen Classic nested-grid simulations as transport boundary conditions.

Sample definition section for HISTORY.rc

```
  BoundaryConditions.template:   '%y4%m2%d2_%h2%n2z.nc4',
  BoundaryConditions.frequency:  00000000 030000
  BoundaryConditions.duration:   00000100 000000
  BoundaryConditions.mode:       'instantaneous'
  BoundaryConditions.fields:     'SpeciesBC_?ADV?',
::
```

List of diagnostic fields in the BoundaryConditions collection

Diagnostic field	Description	Units	Wildcard
SpeciesBC_<nam	Advected species concentrations used as boundary conditions GEOS-Chem Classic nested-grid simulations	mol/mol dry air	?ADV?

29.2.5 Budget

The **Budget** diagnostic collection is a 2D diagnostic containing the mass tendencies per grid cell, in kg/s, for each species within a region of the column and across each GEOS-Chem component. The diagnostic is calculated by taking the difference in vertically summed column mass before and after major GEOS-Chem components.

There are three pre-defined column regions defined for this diagnostic: troposphere-only, PBL-only, and full column, as well as a user-defined column region. By post-processing this diagnostic you can calculate global mass change or mass change across regions by summing the diagnostic values for the relevant grid cells. You can also retrieve the mass change across a longer chunk of time by multiplying the time-averaged output by the number of seconds in the averaging period.

While there are seven major components in GEOS-Chem, there are only six implemented for the budget diagnostics: chemistry, mixing, convection, transport (GEOS-Chem Classic only), wet deposition, and combined emissions and dry deposition.

> **Attention:** Emissions and dry deposition components are combined together for this diagnostic because of the way they are applied at the same time. Furthermore, if using non-local PBL mixing then the emissions and dry deposition budget diagnostic will not capture all fluxes from these sources and sinks. This is because emissions and dry deposition tendencies below the PBL are applied within mixing instead. When using full mixing, however, mixing and emissions/dry deposition budget diagnostics are fully separated.

Sample definition section for HISTORY.rc

```
  Budget.template:     '%y4%m2%d2_%h2%n2z.nc4',
  Budget.frequency:    00000100 000000
```

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[5] This diagnostic is only for use with GEOS-Chem Classic.

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```
 Budget.duration:     00000100 000000
 Budget.mode:         'time-averaged'
 Budget.fields:       'BudgetChemistryFull_?ADV? ',
                      'BudgetChemistryPBL_?ADV?  ',
                      'BudgetChemistryTrop_?ADV? ',
                      'BudgetEmisDepFull_?ADV?   ',
                      'BudgetEmisDepTrop_?ADV?   ',
                      'BudgetEmisDepPBL_?ADV?    ',
                      'BudgetTransportFull_?ADV? ',
                      'BudgetTransportTrop_?ADV? ',
                      'BudgetTransportPBL_?ADV?  ',
                      'BudgetMixingFull_?ADV?    ',
                      'BudgetMixingTrop_?ADV?    ',
                      'BudgetMixingPBL_?ADV?     ',
                      'BudgetConvectionFull_?ADV?',
                      'BudgetConvectionTrop_?ADV?',
                      'BudgetConvectionPBL_?ADV? ',
                      'BudgetWetDepFull_?WET?    ',
                      'BudgetWetDepTrop_?WET?    ',
                      'BudgetWetDepPBL_?WET?     ',
::
```

List of diagnostic fields in the Budget collection

Diagnostic field	Mass tendency (kg/s) across ...	Wild-card
BudgetChemistryFull_<name|wc>	Chemistry (full atmosphere)	?ADV?
BudgetChemistryLevs1to35_<name|wc>[6]	Chemistry (fixed level range)	?ADV?
BudgetChemistryPBL_<name|wc>	Chemistry (PBL only)	?ADV?
BudgetChemistryTrop_<name|wc>	Chemistry (troposphere only)	?ADV?
BudgetConvectionFull_<name|wc>	Convection (full atmosphere)	?ADV?
BudgetConvectionLevs1to35_<name|wc>[6]	Convection (fixed level range)	?ADV?
BudgetConvectionPBL_<name|wc>	Convection (PBL only)	?ADV?
BudgetConvectionTrop_<name|wc>	Convection (troposphere only)	?ADV?
BudgetEmisDepFull_<name|wc>[7]	Emissions & dry deposition (full atmosphere)	?ADV?
BudgetEmisDepLevs1to35_<name|wc>[6Page 232, 7]	Emissions & dry deposition (fixed level range)	?ADV?
BudgetEmisDepPBL_<name|wc>[Page 232, 7]	Emissions & dry deposition (PBL only)	?ADV?
BudgetEmisDepTrop_<name|wc>[Page 232, 7]	Emissions & dry deposition (troposphere only)	?ADV?
BudgetMixingFull_<name|wc>[8]	PBL mixing (full atmosphere)	?ADV?
BudgetMixingLevs1to35_<name|wc>[6Page 232, 8]	PBL mixing (full atmosphere) (fixed level range)	?ADV?
BudgetMixingPBL_<name|wc>[Page 232, 8]	PBL mixing (PBL only)	?ADV?
BudgetMixingTrop_<name|wc>[Page 232, 8]	PBL mixing (troposphere only)	?ADV?
BudgetTransportFull_<name|wc>[9]	Transport (full attmosphere)	?ADV?
BudgetTransportLevs1to35_<name|wc>[6Page 232, 9]	Transport (fixed level range)	?ADV?
BudgetTransportPBL_<name|wc>[Page 232, 9]	Transport (PBL only)	?ADV?
BudgetTransportTrop_<name|wc>[Page 232, 9]	Transport (troposphere only)	?ADV?
BudgetWetDepFull_<name|wc>	Wet deposition (full atmosphere)	?WET?
BudgetWetDepLevs1to35_<name|wc>[6]	Wet deposition (fixed level range)	?WET?
BudgetWetDepPBL_<name|wc>	Wet deposition (PBL only)	?WET

[6] These diagnostic quantities allow you to compute mass tendencies in a fixed level range. The lower level and upper level of the range is specified

Notes for the Budget collection

29.2.6 Carbon

The **Carbon** collection contains diagnostic fields specific to the GEOS-Chem carbon gases simulation.

Sample definition section for HISTORY.rc

```
  Carbon.template:    '%y4%m2%d2_%h2%n2z.nc4',
  Carbon.frequency:   00000100 000000
  Carbon.duration:    00000100 000000
  Carbon.mode:        'time-averaged'
  Carbon.fields:      'OHconcAfterChem',
                      'ProdCOfromCH4  ',
                      'ProdCOfromNMVOC',
                      'ProdCO2fromCO  ',
::
```

List of diagnostic fields in the Carbon collection

Diagnostic field	Description	Units
OHconcAfterChem	OH concentration immediately after chemistry	molec/cm3
ProdCOfromCH4	Production of CO from CH4	molec/cm3
ProdCOfromNMVOC	Production of CO from non-methane VOCs	molec/cm3
ProdCO2fromCO	Production of CO2 from CO oxidation	molec/cm3

29.2.7 CH4

The **CH4** collection contains diagnostics for loss of CH4 and OH concentration for the CH4 simulation.

> **Attention:** This simulation is slated to be replaced by the GEOS-Chem carbon gases simulation. when this happens, the CH4 collection will be replaced by the *Carbon* collection.

Sample definition section for HISTORY.rc

```
  CH4.template:    '%y4%m2%d2_%h2%n2z.nc4',
  CH4.frequency:   00000100 000000
  CH4.duration:    00000100 000000
  CH4.mode:        'time-averaged'
  CH4.fields:      'OHconcAfterChem   ',
                   'LossCH4byClinTrop ',
                   'LossCH4byOHinTrop ',
                   'LossCH4inStrat    ',
::
```

List of diagnostic fields in the CH4 collection

in the diagnostic name (`LevsXtoY`). Levels 1 to 35 (surface to approximately the tropopause) are the default settings.

[7] The emissions and dry deposition budget diagnostics will not capture all fluxes if using the non-local PBL mixing scheme since these tendencies are applied within mixing in `vdiff_mod.F90` below the PBL. When using full mixing, however, mixing and emissions/dry deposition are fully separated.

[8] The mixing budget diagnostics includes the application of emissions and dry deposition below the PBL if using the non-local PBL mixing scheme (vdiff).

[9] GEOS-Chem Classic only

Diagnostic field	Description	Units
LossCH4byClinTrop	Loss of CH4 by raction with Cl in the troposphere	kg/s
LossCH4byOHinTrop	Loss of CH4 by raction with OH in the troposphere	kg/s
LossCH4inStrat	Loss of CH4 in the stratosphere	kg/s
OHconcAfterChem	OH concentration after chemistry	kg/s

29.2.8 CloudConvFlux

The **CloudConvFlux** collection contains diagnostics for mass fluxes in cloud convection.

Sample definition section for HISTORY.rc

```
  CloudConvFlux.template:     '%y4%m2%d2_%h2%n2z.nc4',
  CloudConvFlux.frequency:    00000100 000000
  CloudConvFlux.duration:     00000100 000000
  CloudConvFlux.mode:         'time-averaged'
  CloudConvFlux.fields:       'CloudConvFlux_?ADV?',
::
```

List of diagnostic fields in the CloudConvFlux collection

Diagnostic field	Description	Units	Wildcards
CloudConvFlux_<name|wc>	Mass change due to cloud convection	kg/s	?ADV? ?GAS? ?WET?

29.2.9 CO

The **CO** collection contains diagnostic fields for the GEOS-Chem tagged CO simulation.

Attention: The tagged CO simulation is slated to be replaced by the GEOS-Chem carbon gases simulation. When this happens, the CO collection will be replaced with the *Carbon* collection.

```
  CO.template:   '%y4%m2%d2_%h2%n2z.nc4',
  CO.frequency:  00000100 000000
  CO.duration:   00000100 000000
  CO.mode:       'time-averaged'
  CO.fields:     'ProdCOfromCH4  ',
                 'ProdCOfromNMVOC',
::
```

List of diagnostic fields in the CO collection

Diagnostic field	Description	Units
ProdCOfromCH4	Production of CO from CH4	kg/s
ProdCOfromNMVOC	Production of CO from non-methane VOCs	kg/s

29.2.10 CO2

The **CO2** collection contains diagnostic outputs from the GEOS-Chem CO2 simulation.

> **Attention:** The CO2 simulation is slated to be replaced by the new GEOS-Chem carbon gases simulation. When this happens, the CO2 collection will be replaced with the *Carbon* collection.

Note: Several other diagnostics for the CO2 simulation are archived via HEMCO diagnostics.

Sample definition section for HISTORY.rc

```
  CO2.template:    '%y4%m2%d2_%h2%n2z.nc4',
  CO2.frequency:   00000100 000000
  CO2.duration:    00000100 000000
  CO2.mode:        'time-averaged'
  CO2.fields:      'ProdCO2fromCO',
::
```

List of diagnostic fields in the CO2 collection

Diagnostic field	Description	Units
ProdCO2fromCO	Chemical production of CO2 from CO oxidation	kg/m2/s

29.2.11 ConcAboveSfc

The **ConcAboveSfc** diagnostic collection uses dry deposition quantities (surface resistance, dry deposition velocity) to compute the species concentration of O3 and HNO3 at a given altitude (such as 10 m) above the surface. This will facilitate comparison between GEOS-Chem and observational networks (e.g. CASTNET), which often place instruments above the canopy at approx. 10m height.

> **Attention:** If dry deposition is turned off in your simulation, then you must disable this collection, or else your run will stop with an error.

Sample definition section for HISTORY.rc

```
ConcAboveSfc.template:      '%y4%m2%d2_%h2%n2z.nc4',
ConcAboveSfc.mode:          'instantaneous'
ConcAboveSfc.fields:        'DryDepRaALT1              ',
                            'DryDepVelForALT1_?DRYALT?',
                            'SpeciesConcALT1_?DRYALT? ',
::
```

List of diagnostic fields in the ConcAboveSfc collection

Diagnostic field	Description	Units	Wild-card
DryDepRaALT1[10]	Dry deposition aerodynamic resistance at ALT1 meters above the surface	s/cm	
DryDepVelForALT1_<name|wc>	Dry deposition velocity of species tagged with the ?DRYALT?wildcard	cm/s	?DRYALT?
SpeciesConcALT1_<name|wc>[11]	Concentration of species tagged with the ?DRYALT? wildcard	mol/mol dry air	?DRYALT?

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Notes about the ConcAboveSfc collection

29.2.12 ConcAfterChem

The **ConcAfterChem** collection contains diagnostics for OH, HO2, etc. species immediately upon exiting the chemical solver.

Sample definition section for HISTORY.rc

```
 ConcAfterChem.template:     '%y4%m2%d2_%h2%n2z.nc4',
 ConcAfterChem.frequency:    00000100 000000
 ConcAfterChem.duration:     00000100 000000
 ConcAfterChem.mode:         'time-averaged'
 ConcAfterChem.fields:       'OHconcAfterChem ',
                             'HO2concAfterChem',
                             'O1DconcAfterChem',
                             'O3PconcAfterChem',
                             'O3concAfterChem ',
                             'RO2concAfterChem',
::
```

List of diagnostic fields in the ConcAfterChem collection

Diagnostic field	Description	Units
HO2concAfterChem	HO2 immediately after exiting the chemical solver	mol/mol
O1DconcAfterChem	O1D immediately after exiting the chemical solver	molec/cm3
O3concAfterChem	O3 immediately after exiting the chemical solver	molec/cm3
O3PconcAfterChem	O3P immediately after exiting the chemical solver	molec/cm3
OHconcAfterChem	OH immediately after exiting the chemical solver	molec/cm3
RO2concAfterChem	RO2 immediately after exiting the chemical solver	molec/cm3

[10] Replace `ALT1` with the altitude in meters above the surface at which you would like these quantities computed. For example: `DryDepVelFor10m_?DRYALT?`, etc.

[11] Currently the `?DRYALT?` species are O3 and HNO3.

29.2.13 DryDep

The **DryDep** collection contains diagnostics for the flux and velocity of each species lost to dry-deposition.

Sample definition section for HISTORY.rc

```
  DryDep.template:     '%y4%m2%d2_%h2%n2z.nc4',
  DryDep.frequency:    00000100 000000
  DryDep.duration:     00000100 000000
  DryDep.mode:         'time-averaged'
  DryDep.fields:       'DryDepVel_?DRY?',
                       'DryDepMix_?DRY?',
                       'DryDepChm_?DRY?',
                       'DryDep_?DRY?   ',
::
```

List of diagnostic fields in the DryDep collection

Diagnostic field	Description	Units	Wildcard
DryDep_<name|wc>	Total dry deposition flux	molec/cm2/s	?DRY?
DryDepChm_<name|wc>	Dry deposition flux (computed in chemistry)	molec/cm2/s	?DRY?
DryDepMix_<name|wc>	Dry deposition flux (computed in the PBL)	molec/cm2/s	?DRY?
DryDepVel_<name|wc>	Dry deposition velocity	cm/s	?DRY?

29.2.14 JValues

The **JValues** collection contains diagnostics for photolysis rates for various chemical species, obtained from the photolysis mechanism.

Sample definition section for HISTORY.rc

```
  JValues.template:          '%y4%m2%d2_%h2%n2z.nc4',
  JValues.frequency:         00000100 000000
  JValues.duration:          00000100 000000
  JValues.mode:              'time-averaged'
  JValues.fields:            'Jval_?PHO?',
                             'JvalO3O1D ',
                             'JvalO3O3P ',
::
```

List of diagnostic fields in the JValues collection

Diagnostic field	Description	Units	Wildcard
Jval_<name|wc>	Photolysis rates	1/s	?PHO?
JvalO3O1D	Photolysis rate of O3 $\rightarrow$ O1D	1/s	
JvalO3O3P	Photolysis rate of O3 $\rightarrow$ O3P	1/s	

29.2.15 KppARDiags

The **KppARDiags** collection contains diagnostics for the KPP Rosenbrock solver with mechanism auto-reduction. You may leave this collection disabled unless you are interested in assessing the solver's performance.

Sample definition section for HISTORY.rc

```
 KppARDiags.template:        '%y4%m2%d2_%h2%n2z.nc4',
 KppARDiags.frequency:       00000100 000000
 KppARDiags.duration:        00000100 000000
 KppARDiags.mode:            'time-averaged'
 KppARDiags.fields:          'KppAutoReducerNVAR',
                             'KppAutoReduceThres',
                             'KppcNONZERO       ',
::
```

List of diagnostic fields in the KppARDiags collection

Diagnostic field	Description	Units
KppAutoReducerNVAR	Number of species (rNVAR) in the auto-reduced mechanism	count
KppAutoReduceThres	Auto-reduction threshold	molec/cm3/s
KppcNONZERO	Number of nonzero elements (cNONZERO) in LU decomposition in the auto-reduced mechanism	count

29.2.16 KppDiags

The **KppDiags** collection contains KPP solver diagnostics. You may leave this collection disabled unless you are interested in assessing the solver's performance.

Sample definition section for HISTORY.rc

```
 KppDiags.template:   '%y4%m2%d2_%h2%n2z.nc4',
 KppDiags.frequency:  00000100 000000
 KppDiags.duration:   00000100 000000
 KppDiags.mode:       'time-averaged'
 KppDiags.fields:     'KppIntCounts',
                      'KppJacCounts',
                      'KppTotSteps ',
                      'KppAccSteps ',
                      'KppRejSteps ',
                      'KppLuDecomps',
                      'KppSubsts   ',
                      'KppSmDecomps',
::
```

List of diagnostic fields in the KppDiags collection

Diagnostic field	Description	Units
KppAccSteps	Number of accepted integration timesteps	count
KppIntCounts	Number of times the function to be evaluated was called from within the integrator	count
KppJacCounts	Number of times the Jacobian matrix was constructed	count
KppLuDecomps	Number of LU decompositions performed	count
KppNegatives	Number of negative values	count
KppNegatives0	Number of negative values except on the first timestep	count
KppSmDecomps[12]	Number of singular matrix decompositions performed	count
KppSubsts	Number of matrix substitutions performed (both forward & backward substitutions)	count
KppRejSteps	Number of rejected integration timesteps	count
KppTime[13]	Time spent within the integrator	s
KppTotSteps	Total number of integration timesteps	count

29.2.17 LevelEdgeDiags

The **LevelEdgeDiags** collection contains diagnostics for quantities (mostly met fields) that are defined on the vertical edges of each grid box. According to the COARDS convention, all of the data variables in a netCDF file must be defined with the same vertical dimension.

Sample definition section for HISTORY.rc

```
 LevelEdgeDiags.template:    '%y4%m2%d2_%h2%n2z.nc4',
 LevelEdgeDiags.frequency:   00000100 000000
 LevelEdgeDiags.duration:    00000100 000000
 LevelEdgeDiags.mode:        'time-averaged'
 LevelEdgeDiags.fields:      'Met_CMFMC   ',
                             'Met_PEDGE   ',
                             'Met_PEDGEDRY',
                             'Met_PFICU   ',
                             'Met_PFILSAN ',
                             'Met_PFLCU   ',
                             'Met_PFLLSAN ',
::
```

List of diagnostic fields in the LevelEdgeDiags collection

Diagnostic field	Description	Units
Met_CMFMC	Upward moist convective mass flux	kg/m2/s
Met_PEDGE	Surface pressure at level edges (based on moist air)	hPa
Met_PEDGEDRY	Surface pressure at level edges (based on dry air)	hPa
Met_PFICU	3d flux of ice convective precipitation	kg/m2/s
Met_PFILSAN	3d flux of ice non-convective precipitation	kg/m2/s
Met_PFLCU	3d flux of liquid convective precipitation	kg/m2/s
Met_PFLLSAN	3d flux of liquid non-convective precipitation	kg/m2/s

[12] For Rosenbrock solvers, KppSmDecomps will be zero everywhere, because the Rosenbrock method utilizes LU decomposition instead of singular matrix decomposition.

[13] KppTime will likely not be identical between two successive simulations, as the time spent in the integrator will depend on local cluster conditions.

29.2.18 MercuryChem

The **MercuryChem** collection contains concentrations and prod/loss diagnostic outputs for the GEOS-Chem mercury simulation.

Sample definition section for HISTORY.rc

```
  MercuryChem.template:    '%y4%m2%d2_%h2%n2z.nc4',
  MercuryChem.frequency:   ${RUNDIR_HIST_TIME_AVG_FREQ}
  MercuryChem.duration:    ${RUNDIR_HIST_TIME_AVG_DUR}
  MercuryChem.mode:        'time-averaged'
  MercuryChem.fields:      'HgBrAfterChem  ',
                           'HgClAfterChem  ',
                           'HgOHAfterChem  ',
                           'HgBrOAfterChem ',
                           'HgClOAfterChem ',
                           'HgOHOAfterChem ',
                           'Hg2GToHg2P     ',
                           'Hg2PToHg2G     ',
                           'Hg2GasToHg2StrP',
                           'Hg2GasToSSA    ',
::
```

List of diagnostic fields in the MercuryChem collection

Diagnostic field	Description	Units
Hg2GToHg2P	Hg2 gas transferred to Hg2P	molec/cm3/s
Hg2GasToHg2StrP	Hg2 gas transferred to Hg2StrP	molec/cm3/s
Hg2GasToSSA	Hg2 gas transferred to sea salt aerosol	molec/cm3/s
Hg2PToHg2G	Hg2P transferred to Hg2 gas	molec/cm3/s
HgBrAfterChem	HgBr concentration immediately after chemistry	mol/mol
HgBrOAfterChem	HgBrO concentration immediately after chemistry	mol/mol
HgClAfterChem	HgCl concentration immediately after chemistry	mol/mol
HgClOAfterChem	HgClO concentration immediately after chemistry	mol/mol
HgOHAfterChem	HgOH concentration immediately after chemistry	mol/mol
HgOHOAfterChem	HgOHO concentration immediately after chemistry	mol/mol

29.2.19 MercuryEmis

The **MercuryEmis** collection contains emission diagnostics for the GEOS-Chem mercury simulation.

Note: Several other mercury emission diagnostics are archived via HEMCO diagnostics.

Sample definition section for HISTORY.rc

```
  MercuryEmis.template:   '%y4%m2%d2_%h2%n2z.nc4',
  MercuryEmis.frequency:  00000100 000000
  MercuryEmis.duration:   00000100 000000
  MercuryEmis.mode:       'time-averaged'
  MercuryEmis.fields:     'EmisHg0land ',
                          'EmisHg0ocean',
```

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```
                          'EmisHg0soil ',
                          'EmisHg0snow ',
::
```

List of diagnostic fields in the MercuryEmis collection

Diagnostic field	Description	Units
EmisHg0land	Re-emission of Hg0 from land	kg/s
EmisHg0ocean	Emissions of Hg0 from oceans	kg/s
EmisHg0snow	Emission of Hg0 from snowpack	kg/s
EmisHg0soil	Emissions of Hg0 from soils	kg/s

29.2.20 MercuryOcean

The **MercuryOcean** collection contains diagnostics from the mercury ocean model, used in the GEOS-Chem mercury simulation.

Sample definition section for HISTORY.rc

```
  MercuryOcean.template:    '%y4%m2%d2_%h2%n2z.nc4',
  MercuryOcean.frequency:   00000000 040000
  MercuryOcean.duration:    00000000 040000
  MercuryOcean.mode:        'time-averaged'
  MercuryOcean.fields:      'FluxHg0fromAirToOcean   ',
                            'FluxHg0fromOceanToAir   ',
                            'FluxHg2HgPfromAirToOcean',
                            'FluxHg2toDeepOcean      ',
                            'FluxOCtoDeepOcean       ',
                            'MassHg0inOcean          ',
                            'MassHg2inOcean          ',
                            'MassHgPinOcean          ',
                            'MassHgTotalInOcean      ',
::
```

List of diagnostic fields in the MercuryOcean collection

Diagnostic field	Description	Units
FluxHg0fromAirToOcean	Deposition flux of Hg0 from the atmosphere to the ocean	kg/s
FluxHg0fromOceanToAir	Volatization flux of Hg0 from the ocean to the atmosphere	kg/s
FluxHg2HgPfromAirToOcean	Deposition flux of Hg2 + HgP from atmosphere to ocean	kg/s
FluxHg2toDeepOcean	Flux of Hg2 sunk to the deep ocean	kg/s
MassHg0inOcean	Total mass of oceanic Hg0	kg
MassHg2inOcean	Total mass of oceanic Hg2	kg
MassHgPinOcean	Total mass of oceanic HgP	kg
MassHgTotalInOcean	Total mass of all organic mercury	kg

29.2.21 Metrics

The **Metrics** collection contains diagnostics for computing OH metrics from a GEOS-Chem full chemistry simulation (needed for benchmarking).

To compute the OH metrics, you must run the Python script `metrics.py` that ships with each fullchem or CH4 run directory.

Sample definition section for HISTORY.rc

```
  Metrics.template:    '%y4%m2%d2_%h2%n2z.nc4',
  Metrics.frequency:   'End',
  Metrics.duration:    'End',
  Metrics.mode:        'time-averaged'
  Metrics.fields:      'AirMassColumnFull       ',
                       'LossOHbyCH4columnTrop   ',
                       'LossOHbyMCFcolumnTrop   ',
                       'OHwgtByAirMassColumnFull',
::
```

List of diagnostic fields in the Metrics collection

Diagnostic field	Description	Units
AirMassColumnFull	Air mass column (full atmosphere)	kg
LossOHbyCH4columnTrop	Loss rate of CH4 by OH (tropospheric column sums)	molec/cm3
LossOHbyMCFcolumnTrop	Loss rate of CH4 by CH3CCl3 aka MCF (tropospheric column sums)	molec/cm3
OHwgtByAirMassColumn-Full	Airmass-weighted OH concentration (full atmosphere column sums)	kg air/kg OH/m3

29.2.22 ProdLoss

The **ProdLoss** collection contains chemical production and loss rates.

Sample definition section for HISTORY.rc

```
  ProdLoss.template:   '%y4%m2%d2_%h2%n2z.nc4',
  ProdLoss.frequency:  00000100 000000
  ProdLoss.duration:   00000100 000000
  ProdLoss.mode:       'time-averaged'
  ProdLoss.fields:     'Prod_?PRD?                  ',
                       'ProdBCPIfromBCPO            ',
                       'ProdOCPIfromOCPO            ',
                       'ProdHMSfromSO2andHCHOinCloud',
                       'ProdSO2andHCHOfromHMSinCloud',
                       'ProdSO4fromHMSinCloud       ',
                       'ProdSO4fromH2O2inCloud      ',
                       'ProdSO4fromO2inCloudMetal   ',
                       'ProdSO4fromO3inCloud        ',
                       'ProdSO4fromO3inSeaSalt      ',
                       'ProdSO4fromHOBrInCloud      ',
                       'ProdSO4fromSRO3             ',
                       'ProdSO4fromSRHObr           ',
```

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```
                        'ProdSO4fromO3s              ',
                        'Loss_?LOS?                  ',
                        'LossHNO3onSeaSalt           ',
                        'ProdCOfromCH4               ',
                        'ProdCOfromNMVOC             ',
::
```

List of diagnostic fields in the ProdLoss collection

Diagnostic field	Description	Units	Wild-card
Loss_<name|wc>	Chemical loss for a given species or family	molec/cm3	?LOS?
LossHNO3onSeaSalt[16]	L(HNO3) on sea salt aerosols	kg S/s	
Prod_<name|wc>	Chemical production for a given species or family	molec/cm3	?PRD?
ProdBCPIfromBCPO[16]	Production of hydrophilic BC from hydrophobic BC	kg	
ProdCOfromCH4[17]	P(CO) from CH4	molec/cm3	
ProdCOfromNMVOC[17]	P(CO) from NMVOCs SO3– loss by OH	molec/cm3	
ProdOCPIfromOCPO[16]	Production of hydrophilic OC from hydrophobic OC	kg	
ProdMSAfromDMS[15]	P(MSA) from DMS	kg S/s	
ProdNIT-fromHNO3uptakeOnDust[14]	P(NIT) from HNO3 uptake on dust aerosols	kg N/s	
ProdSO2fromDMS[15]	Total P(SO2) from DMS	kg S/s	
ProdSO2fromDMSandNO3[15]	P(SO2) from DMS + NO3	kg S/s	
ProdSO2fromDMSandOH[15]	P(SO2) from DMS + OH	kg S/s	
ProdSO2fromOxidationOnDust[14]	P(SO2) from DMS+OH on dust aerosols	kg S/s	
ProdSO4fromGasPhase[15]	P(SO4) in gas phase	kg S/s	
ProdSO4fromH2O2inCloud[16]	P(SO4) from aqueous oxidation of H2O2 in clouds	kg S/s	
ProdSO4fromHOBrinCloud[17]	P(SO4) from aqueous oxidation of HOBr in clouds	kg S/s	
ProdSO4fromO2inCloudMetal[16]	P(SO4) from aqueous oxidation of O2 from metals in cloud	kg S/s	
ProdSO4fromO3inCloud[16]	P(SO4) from aqueous oxidation of O3 in clouds	kg S/s	
ProdSO4fromO3inSeaSalt[16]	P(SO4) from O3 in sea salt	kg S/s	
ProdSO4fromO3s[16]	P(SO4) from aqueous phase SO3– loss by OH	kg S/s	
ProdSO4fromSRHOBR[17]	P(SO4) from sulfur production rate of HOBr + O3	kg S/s	
ProdSO4fromSRO3[16]	P(SO4) from sulfur production rate of O3	kg S/s	
ProdSO4fromUptakeOfH2SO4g[14]	P(SO4) from H2SO4 uptake on dust aerosols	kg S/s	

[16] Defined for aerosol-only and fullchem simulations.
[17] Only defined for fullchem simulations.
[15] Only defined for the aerosol-only simulation.
[14] Only defined for fullchem simulation with aciduptake on dust.

Notes for the ProdLoss collection

29.2.23 RadioNuclide

The **RadioNuclide** collection contains diagnostic outputs for radionuclide species in the GEOS-Chem TransportTracers simulation.

Note: Emissions of Rn222, Be7, and Be10 species are archived to diagnostic output by HEMCO diagnostics, and are thus not contained in this collection.

Sample definition section for HISTORY.rc

```
  RadioNuclide.template:    '%y4%m2%d2_%h2%n2z.nc4',
  RadioNuclide.format:      'CFIO',
  RadioNuclide.frequency:   00000100 000000
  RadioNuclide.duration:    00000100 000000
  RadioNuclide.mode:        'time-averaged'
  RadioNuclide.fields:      'PbFromRnDecay  ',
                            'RadDecay_Rn222 ',
                            'RadDecay_Pb210 ',
                            'RadDecay_Pb210s',
                            'RadDecay_Be7   ',
                            'RadDecay_Be7s  ',
                            'RadDecay_Be10  ',
                            'RadDecay_Be10s ',
::
```

List of diagnostic fields in the RadioNuclide collection

Diagnostic field	Description	Units
PbFromRnDecay	Pb^{210} created from radioactive decay	kg/s
RadDecay_Be7	Loss of Be^{7} due to radioactive decay	kg/s
RadDecay_Be7s	Loss of Be^{7} (produced in the stratosphere) due to radioactive decay	kg/s
RadDecay_Be10	Loss of Be^{10} due to radioactive decay	kg/s
RadDecay_Be10s	Loss of Be^{10} (produced in the stratosphere) due to radioactive decay	kg/s
RadDecay_Pb210	Loss of Pb^{210} due to radioactive decay	kg/s
RadDecay_Pb210s	Loss of Pb^{210} (produced in the stratosphere) due to radioactive decay	kg/s
RadDecay_Rn222	Loss of Rn^{222} due to readioactive decay	kg/s

29.2.24 Restart

The **Restart** diagnostic collection contains fields for saving out to the GEOS-Chem Classic restart file. This type of diagnostic output is used in all GEOS-Chem Classic simulations; therefore, we have listed Restart first in the `HISTORY.rc` files that ship with each GEOS-Chem run directory. Note that GCHP restart files are not handled by the MAPL History component and therefore do not appear in `HISTORY.rc`.

Note: The restart file will be created in the `Restarts/` subdirectory of the run directory, not in `OutputDir/`.

Sample definition section for HISTORY.rc

```
  Restart.filename:   './GEOSChem.Restart.%y4%m2%d2_%h2%n2z.nc4',
  Restart.frequency:  'End',
  Restart.duration:   'End',
  Restart.mode:       'instantaneous'
  Restart.fields:     'SpeciesRst_?ALL?   ',
                      'Chem_H2O2AfterChem ',
                      'Chem_SO2AfterChem  ',
                      'Chem_DryDepNitrogen',
                      'Chem_WetDepNitrogen',
                      'Chem_KPPHvalue     ',
                      'Met_DELPDRY        ',
                      'Met_PS1WET         ',
                      'Met_PS1DRY         ',
                      'Met_SPHU1          ',
                      'Met_TMPU1          ',
::
```

List of diagnostic fields in the Restart collection

Diagnostic field	Description	Units
Chm_DryDepNitro	Dry deposited nitrogen	molec/cm2/s
Chm_H2O2AfterCl	Concentration of H2O2 after sulfate chemistry	v/v
Chm_KPPHvalue	H-value for Rosenbrock solver	unitless
Chm_SO2AfterChe	Concentration of SO2 after sulfate chemistry	v/v
Chm_StatePSC	Polar stratospheric cloud type	count
Chm_WetDepNitro	Wet deposited nitrogen	molec/cm2/s
Met_DELPDRY	Delta-pressure across grid box (dry air)	hPa
Met_PS1WET	Wet surface pressure at dt start	hPa
Met_PS1DRY	Dry surface pressure at dt start	hPa
Met_SPHU1	Instantaneous specific humidity at time=T	g kg-1
Met_TMPU1	Instantaneous temperature at time=T	K
SpeciesRst_?ALL?	Instantaneous chemical species concentrations for use in starting subsequent GEOS-Chem simulations	mol/mol dry air

29.2.25 RRTMG

The **RRTMG** collection contains radiative flux diagnostics computed by the RRTMG radiative transfer model. You can leave this collection disabled unless your simulation uses RRTMG.

Note: You may compute RRTMG diagnostic quantities at up to 3 wavelengths (`WL1`, `WL2`, `WL3`). Specify the wavelengths in this menu of the `geoschem_config.yml` file:

```
rrtmg_rad_transfer_model:
    activate: true
    aod_wavelengths_in_nm:
    - 550 700 1000
    ... etc ...
```

GEOS-Chem will replace the tokens `WL1`, `WL2`, `WL3` in diagnostic field names with the corresponding wavelength. For example:

```
RadAODWL1_SU
RadAODWL2_SU
RadAODWL3_SU
```

will be saved to the `GEOSChem.RRTMG.YYYYMMDD_hhmmz.nc4` file(s) under these names:

```
RadAOD550nm_SU
RadAOD700nm_SU
RadAOD1000nm_SU
```

Sample definition section for HISTORY.rc

```
#============================================================================
# %%%%% THE RRTMG COLLECTION %%%%%
#
# Outputs for different species from the RRTMG radiative transfer model:
# (See http://wiki.geos-chem.org/Coupling_GEOS-Chem_with_RRTMG)
#
#    0=BA (Baseline    )  1=O3 (Ozone          )   2=ME (Methane   )
#    3=SU (Sulfate     )  4=NI (Nitrate        )   5=AM (Ammonium  )
#    6=BC (Black carbon)  7=OA (Organic aerosol)   8=SS (Sea Salt  )
#    9=DU (Mineral dust) 10=PM (All part. matter) 12=ST (Strat aer., UCX only)
#
# NOTES:
# (1) Only request diagnostics you need to reduce the overall run time.
# (2) The ?RRTMG? wildcard includes all output except ST (strat aerosols).
#     However, if ST is included explicitly for one diagnostic then it
#     will be included for all others that use the wildcard.
# (3) Only enable ST if running with UCX.
# (4) Optics diagnostics have a reduced set of output species (no BASE, O3, ME)
#============================================================================
  RRTMG.template:    %y4%m2%d2_%h2%n2z.nc4',
  RRTMG.frequency:   00000100 000000
  RRTMG.duration:    00000100 000000
  RRTMG.mode:        time-averaged'
  RRTMG.fields:      'RadClrSkyLWSurf_?RRTMG?',
                     'RadAllSkyLWSurf_?RRTMG?',
                     'RadClrSkySWSurf_?RRTMG?',
                     'RadAllSkySWSurf_?RRTMG?',
                     'RadClrSkyLWTOA_?RRTMG? ',
                     'RadAllSkyLWTOA_?RRTMG? ',
                     'RadClrSkySWTOA_?RRTMG? ',
                     'RadAllSkySWTOA_?RRTMG? ',
                     'RadAODWL1_?RRTMG?      ',
                     'RadAsymWL1_?RRTMG?     ',
::
```

List of diagnostic fields in the RRTMG collection

Diagnostic field	Description	Units	Wildcard
DynHeating	Dynamic heating rate in baseline simulation	K/day	?RRTMG?
DtRad	Temperature change due to radiative heating	K	?RRTMG?
RadAODWL1_<name|wc>	Aerosol optical depth computed @ WL1	1	?RRTMG?
RadAODWL2_<name|wc>	Aerosol optical depth computed @ WL2	1	?RRTMG?
RadAODWL3_<name|wc>	Aerosol optical depth computed @ WL3	1	?RRTMG?
RadAsymWL1_<name|wc>	Asymmetry parameter computed @ WL1	1	?RRTMG?
RadAsymWL2_<name|wc>	Asymmetry parameter computed @ WL2	1	?RRTMG?
RadAsymWL3_<name|wc>	Asymmetry parameter computed @ WL3	1	?RRTMG?
RadAllSkyLWSurf_<name|wc>	All-sky longwave radiation at the surface	W/m2	?RRTMG?
RadAllSkyLWTOA_<name|wc>	All-sky longwave radiation at top-of-atmosphere	W/m2	?RRTMG?
RadAllSkyLWTrop_<name|wc>	All-sky longwave radiation at the tropopause	W/m2	?RRTMG?
RadAllSkySWSurf_<name|wc>	All-sky shortwave radiation at the surface	W/m2	?RRTMG?
RadAllSkySWTOA_<name|wc>	All-sky shortwave radiation at top-of-atmosphere	W/m2	?RRTMG?
RadAllSkySWTrop_<name|wc>	All-sky shortwave radiation at the tropopause	W/m2	?RRTMG?
RadClrSkyLWSurf_<name|wc>	Clear-sky longwave radiation at the surface	W/m2	?RRTMG?
RadClrSkyLWTOA_<name|wc>	Clear-sky longwave radiation at top-of-atmosphere	W/m2	?RRTMG?
RadClrSkyLWTrop_<name|wc>	Clear-sky longwave radiation at the tropopause	W/m2	?RRTMG?
RadClrSkySWSurf_<name|wc>	Clear-sky shortwave radiation at the surface	W/m2	?RRTMG?
RadClrSkySWTOA_<name|wc>	Clear-sky shortwave radiation at top-of-atmosphere	W/m2	?RRTMG?
RadClrSkySWTrop_<name|wc>	Clear-sky shortwave radiation at the tropopause	W/m2	?RRTMG?
RadSSAWL1_<name|wc>	Single-scattering albedo computed @ WL1	1	?RRTMG?
RadSSAWL2_<name|wc>	Single-scattering albedo computed @ WL2	1	?RRTMG?
RadSSAWL3_<name|wc>	Single-scattering albedo computed @ WL3	1	?RRTMG?

29.2.26 RxnConst

The **RxnConst** collection contains reaction rate constants from the KPP solver.

```
  # It is best to list individual reactions to avoid using too much memory.
  # Reactions should be listed as "RxnConst_EQnnn", where nnn is the reaction
  # index as listed in KPP/fullchem/gckpp_Monitor.F90 (pad zeroes as needed).
  #
  # The units of reaction rate constants vary according to the number of reactants
  # in the reaction.
  #
  # Available for the fullchem simulations.
  RxnConst.template:   '%y4%m2%d2_%h2%n2z.nc4',
  RxnConst.frequency:  ${RUNDIR_HIST_TIME_AVG_FREQ}
  RxnConst.duration:   ${RUNDIR_HIST_TIME_AVG_DUR}
  RxnConst.mode:       'time-averaged'
  RxnConst.fields:     'RxnConst_EQ001                          ',
                       'RxnConst_EQ002                          ',
::
```

List of diagnostic fields in the RxnRate collection

Units are

Diagnostic field	Description	Units	Wildcard
RxnConst_EQnnn[18]	Rate constant for KPP reaction nnn	[19]	?RXN?

Notes for the RxnRates collection

29.2.27 RxnRates

The **RxnRates** collection contains reaction rates (aka equation rates) from the chemical mechanism (as computed by the KPP-generated solver code). For example, in the case of the NO + O_3 → NO_2 + O_2 reaction the returned quantity is k[NO][O_3] in molec/cm^3/s.

Here is a sample definition section for the RxnRates collection.

Sample definition section for HISTORY.rc

```
#
# It is best to list individual reactions to avoid using too much memory.
# Reactions should be listed as "RxnRate_EQnnn", where nnn is the reaction
# index as listed in KPP/fullchem/gckpp_Monitor.F90,
# KPP/carbon/gckpp_Monitor.F90, and KPP/Hg/gckpp_monitor.F90
# (pad zeroes as needed)
#
RxnRates.template:   '%y4%m2%d2_%h2%n2z.nc4',
RxnRates.frequency:  00000000 010000
RxnRates.duration:   00000000 010000
RxnRates.mode:       'time-averaged'
RxnRates.fields:     'RxnRate_EQ001                          ',
                     'RxnRate_EQ002                          ',
::
```

List of diagnostic fields in the RxnRate collection

Diagnostic field	Description	Units	Wildcard
RxnRate_EQnnn[20]	Rate for KPP reaction nnn	molec/cm3/s	?RXN?

Notes for the RxnRates collection

29.2.28 SatDiagn

The **SatDiagn** collection contains diagnostic quantities that will be sampled within a specified local time range. This is to mimic the overpass sampling times of sun-synchronus satellite instruments.

Tip: Set the the hours (local time) for the averaging interval with:

```
SatDiagn.hrrange:    11.98 15.02
```

Sample definition section for HISTORY.rc

[18] See the `gckpp_Monitor.F90` file to get a numbered list of reactions.
[19] Units are `{ (cm3/molec)**(nreactants-1) }/s`
[20] See the `gckpp_Monitor.F90` file to get a numbered list of reactions.

```
 SatDiagn.template:   '%y4%m2%d2_%h2%n2z.nc4',
 SatDiagn.frequency:  00000001 000000
 SatDiagn.duration:   00000100 000000
 SatDiagn.hrrange:    11.98 15.02
 SatDiagn.mode:       'time-averaged'
 SatDiagn.fields:     'SatDiagnConc_O3      ',
                      'SatDiagnOH           ',
                      'SatDiagnRH           ',
                      'SatDiagnAirDen       ',
                      'SatDiagnBoxHeight    ',
                      'SatDiagnPEdge        ',
                      'SatDiagnTROPP        ',
                      'SatDiagnPBLHeight    ',
                      'SatDiagnPBLTop       ',
                      'SatDiagnTAir         ',
                      'SatDiagnGWETROOT     ',
                      'SatDiagnGWETTOP      ',
                      'SatDiagnPARDR        ',
                      'SatDiagnPARDF        ',
                      'SatDiagnPRECTOT      ',
                      'SatDiagnSLP          ',
                      'SatDiagnSPHU         ',
                      'SatDiagnTS           ',
                      'SatDiagnPBLTOPL      ',
                      'SatDiagnMODISLAI     ',
                      'SatDiagnWetLossLS_   ',
                      'SatDiagnWetLossConv_ ',
                      'SatDiagnJval_        ',
                      'SatDiagnJvalO3O1D    ',
                      'SatDiagnJvalO3O3P    ',
                      'SatDiagnDryDep_      ',
                      'SatDiagnDryDepVel_   ',
                      'SatDiagnOHreactivity ',
                      'SatDiagnColEmis_     ',
                      'SatDiagnSurfFlux_    ',
                      'SatDiagnProd_?PRD?   ',
                      'SatDiagnLoss_?LOS?   ',
                      'SatDiagnRxnRate_EQnnn',
::
```

List of diagnostic fields in the SatDiagn collection

Diagnostic field	Description	Units	Wildcards
SatDiagnAirDen	Air density	molec/cm3	
SatDiagnBoxHeight	Grid box height	m	
SatDiagnColEmis_<name|wc>	Column emissions	kg/m2/s	?ADV?
SatDiagnConc_<name|wc>	Dry mixing ratio of species	mol/mol	?ADV?
SatDiagnDryDep_<name|wc>	Dry deposition flux of species	molec/cm2/s	?DRY?
SatDiagnDryDepVel_<name|wc>	Dry deposition velocity of species	cm/s	?DRY?
SatDiagnGWETROOT	Root zone soil moisture	1	
SatDiagnGWETTOP	Topsoil moisture (or	1	

continues on next page

Table 2 – continued from previous page

Diagnostic field	Description	Units	Wildcards
SatDiagnJVal_<name|wc>	Photolysis rate	1/s	?PHO?
SatDiagnJvalO3O1D	Photolysis rate for O3 → O1D	1/s	
SatDiagnJvalO3O3P	Photolysis rate for O3 → O1D	1/s	
SatDiagnLoss_<name|wc>	Chemical loss of species or families	molec/cm3/s	?LOS?
SatDiagnMODISLAI	MODIS daily LAI	m2/m2	
SatDiagnOH	OH number density	molec/cm3	
SatDiagnOHreactivity	OH reactivity	1/s	
SatDiagnPARDF	Diffuse photosynthetically active radiation	W/m2	
SatDiagnPARDR	Direct photosynthetically active radiation	W/m2	
SatDiagnPBLHeight	PBL Height	m	
SatDiagnPBLTop	PBL Top	m	
SatDiagnPBLTOPL	PBL top height	level	
SatDiagnPRECTOT	Total precipitation at surface	mm/day	
SatDiagnProd_<name|wc>	Chemical production of species or families	molec/cm3/s	?PRD?
SatDiagnRH	Relative humidity	%	
SatDiagnRxnRate_EQnnn	Rate for chemical reaction `nnn`	molec/cm3/s	?RXN?
SatDiagnSLP	Sea level pressure	hPa	
SatDiagnSPHU	Specific humidity interpolated to current time	g H2O/kg air	
SatDiagnSurfFlux_<name|wc>	Total surface fluxes (emis - drydep) from surface to top of PBL	kg/m2/s	?ADV?
SatDiagnTAir	Air temperature	K	
SatDiagnTROPP	Tropopause pressure	hPa	
SatDiagnTS	Surface temperature at 2m	K	
SatDiagnWetLossConv_<name|wc>	Loss of soluble species in convective updrafts	kg/s	?WET?
SatDiagnWetLossLS_<name|wc>	Loss of soluble species in large-scale precipitation	kg/s	?WET?

29.2.29 SatDiagnEdge

The **SatDiagn** collection contains diagnostic quantities (placed on level edges) that will be sampled within a specified local time range. This is to mimic the overpass sampling times of sun-synchronus satellite instruments.

Tip: Set the the hours (local time) for the averaging interval with:

```
SatDiagn.hrrange:    11.98 15.02
```

Sample definition section for HISTORY.rc

```
  SatDiagnEdge.template:      '%y4%m2%d2_%h2%n2z.nc4',
  SatDiagnEdge.frequency:     00000001 000000
  SatDiagnEdge.duration:      00000100 000000
  SatDiagnEdge.hrrange:       11.98 15.02
  SatDiagnEdge.mode:          'time-averaged'
  SatDiagnEdge.fields:        'SatDiagnConc_PEDGE',
::
```

List of diagnostic fields in the SatDiagnEdge collection

Diagnostic field	Description	Units
SatDiagnPEDGE	Pressure at grid box edges	hPa

29.2.30 SpeciesConc

The **SpeciesConc** diagnostic collection contains species concentrations.

Sample definition section for HISTORY.rc

```
  SpeciesConc.template:       '%y4%m2%d2_%h2%n2z.nc4',
  SpeciesConc.format:         'CFIO',
  SpeciesConc.frequency:      00000100 000000
  SpeciesConc.duration:       00000100 000000
  SpeciesConc.mode:           'time-averaged'
  SpeciesConc.fields:         'SpeciesConcVV_?ALL?',
                              'SpeciesConcMND_?ALL?',
::
```

List of diagnostic fields in the SpeciesConc collection

Diagnostic field	Description	Units	Wildcards
SpeciesConcMND_<name|wc>	Species concentration	molec/cm3	can be used with all wildcards
SpeciesConcVV_<name|wc>	Species concentration	mol/mol dry air	can be used with all wildcards

29.2.31 StateChm

The '"StateChm '" collection contains quantities from State_Chm, the Chemistry State object (other than the species concentrations, which are stored in the SpeciesConc collection).

Sample definition section for HISTORY.rc

```
  StateChm.template:    '%y4%m2%d2_%h2%n2z.nc4',
  StateChm.frequency:   00000100 000000
  StateChm.duration:    00000100 000000
  StateChm.mode:        'time-averaged'
  StateChm.fields:      'Chem_phSav      ', 'GIGCchem',
                        'Chem_HplusSav   ', 'GIGCchem',
                        'Chem_WaterSav   ', 'GIGCchem',
                        'Chem_SulRatSav  ', 'GIGCchem',
                        'Chem_NaRatSav   ', 'GIGCchem',
                        'Chem_AcidPurSav ', 'GIGCchem',
                        'Chem_BiSulSav   ', 'GIGCchem',
                        'Chem_pHCloud    ', 'GIGCchem',
                        'Chem_SSAlk',      ', 'GIGCchem',
                        'Chem_HSO3AQ     ', 'GIGCchem',
                        'Chem_SO3AQ      ', 'GIGCchem',
                        'Chem_fupdateHOBr', 'GIGCchem',
::
```

List of diagnostic fields in the StateChm collection

Diagnostic field	Description	Units
Chm_AcidPurSav	ISORROPIA acidpur concentration	M
Chm_BiSulSav	ISORROPIA bisulfate general acid concentration	M
Chm_fupdateHOBr	Correction factor for HOBr removal by SO2 grid box (wet air)	mol/L
Chm_HplusSav	ISORROPIA H+ concentration	M
Chm_HSO3AQ	Cloud bisulfite concentration	mol/L
Chm_NaRatSav	ISORROPIA Na+ concentration	M
Chm_phCloud	Cloud pH	1
Chm_phSav	ISORROPIA aerosol pH	1
Chm_SO3AQ	Cloud sulfite concentration	mol/L
Chm_SulRatSav	ISORROPIA sulfate concentration	M
Chm_SSalk	Sea salt alkalinity	
Chm_WaterSav	ISORROPIA aerosol water	$\mu g/m3$

29.2.32 StateMet

The **StateMet** collection contains met fields and other derived quantities that are carried in the State_Met object.

Sample definition section for HISTORY.rc

```
StateMet.template:    '%y4%m2%d2_%h2%n2z.nc4',
StateMet.frequency:   00000100 000000
StateMet.duration:    00000100 000000
StateMet.mode:        'time-averaged'
StateMet.fields:      'Met_AD         ',
                      'Met_AIRDEN     ',
                      'Met_AIRVOL     ',
                      'Met_ALBD       ',
                      'Met_AREAM2     ',
                      'Met_AVGW       ',
                      'Met_BXHEIGHT   ',
                      'Met_ChemGridLev',
                      'Met_CLDF       ',
                      'Met_CLDFRC     ',
                      'Met_CLDTOPS    ',
                      'Met_DELP       ',
                      'Met_DQRCU      ',
                      'Met_DQRLSAN    ',
                      'Met_DTRAIN     ',
                      'Met_EFLUX      ',
                      'Met_FRCLND     ',
                      'Met_FRLAKE     ',
                      'Met_FRLAND     ',
                      'Met_FRLANDIC   ',
                      'Met_FROCEAN    ',
                      'Met_FRSEAICE   ',
                      'Met_FRSNO      ',
                      'Met_GWETROOT   ',
                      'Met_GWETTOP    ',
                      'Met_HFLUX      ',
                      'Met_LAI        ',
```

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```
                        'Met_LWI        ',
                        'Met_PARDR      ',
                        'Met_PARDF      ',
                        'Met_PBLTOPL    ',
                        'Met_PBLH       ',
                        'Met_PHIS       ',
                        'Met_PMID       ',
                        'Met_PMIDDRY    ',
                        'Met_PRECANV    ',
                        'Met_PRECCON    ',
                        'Met_PRECLSC    ',
                        'Met_PRECTOT    ',
                        'Met_PS1DRY     ',
                        'Met_PS1WET     ',
                        'Met_PS2DRY     ',
                        'Met_PS2WET     ',
                        'Met_PSC2WET    ',
                        'Met_PSC2DRY    ',
                        'Met_QI         ',
                        'Met_QL         ',
                        'Met_OMEGA      ',
                        'Met_OPTD       ',
                        'Met_REEVAPCN   ',
                        'Met_REEVAPLS   ',
                        'Met_SLP        ',
                        'Met_SNODP      ',
                        'Met_SNOMAS     ',
                        'Met_SPHU       ',
                        'Met_SPHU1      ',
                        'Met_SPHU2      ',
                        'Met_SUNCOS     ',
                        'Met_SUNCOSmid  ',
                        'Met_SWGDN      ',
                        'Met_T          ',
                        'Met_TAUCLI     ',
                        'Met_TAUCLW     ',
                        'Met_THETA      ',
                        'Met_TMPU1      ',
                        'Met_TMPU2      ',
                        'Met_TO3        ',
                        'Met_TropHt     ',
                        'Met_TropLev    ',
                        'Met_TropP      ',
                        'Met_TS         ',
                        'Met_TSKIN      ',
                        'Met_TV         ',
                        'Met_U          ',
                        'Met_U10M       ',
                        'Met_USTAR      ',
                        'Met_UVALBEDO   ',
                        'Met_V          ',
                        'Met_V10M       ',
```

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```
                        'Met_Z0          ',
::
```

List of diagnostic fields in the StateMet collection

Diagnostic field	Description	Units
Met_AD	Dry air mass	kg
Met_AIRDEN	Dry air density	kg/m3
Met_AIRVOL	Grid box volume, dry air	m3
Met_ALBD	Surface albedo	1
Met_AREAM2	Grid box area	m2
Met_AVGW	Water vapor volume mixing ratio	vol H2O/vol d
Met_BXHEIGHT	Grid box height	m
Met_ChemGridLev	Chemistry grid level	1
Met_CLDF	3-D cloud fraction	
Met_CLDFRC	Column cloud fraction	1
Met_CLDTOPS	Maximum cloud top height	1
Met_DELP	Delta-pressure between top and bottom edges of grid box (wet air)	hPa
Met_DQRCU	Convective precipitation production rate (dry air)	kg/kg/s
Met_DTRAIN	Detrainment flux	kg/m2/s
Met_EFLUX	Latent heat flux	W/m2
Met_FRCLND	Olson land fraction	1
Met_FRLAKE	Fraction of grid box covered by lakes	1
Met_FRLAND	Fraction of grid box covered by land	1
Met_FRLANDIC	Fraction of grid box covered by land ice	1
Met_FROCEAN	Fraction of grid box covered by ocean	1
Met_FRSEAICE	Fraction of grid box covered by sea ice	1
Met_FRSNO	Fraction of grid box covered by snow	1
Met_GWETROOT	Root soil moisture	1
Met_GWETTOP	Topsoil moisture	1
Met_HFLUX	Sensible heat flux	W/m2
Met_LAI	Leaf area index from met field archive	m2/m2
Met_LWI	Land-water-ice indices	1
Met_PARDF	Diffuse photosynthetically active radiation	W/m2
Met_PARDR	Diffuse photosynthetically active radiation	W/m2
Met_PBLTOPL	PBL top layer	1
Met_PBLH	PBL height	m
Met_PHIS	Surface geopotential height	m
Met_PMID	Pressure at midpoint of model layers, defined as arithmetic average of edge pressures (wet air)	hPa
Met_PMIDDRY	Pressure at midpoint of model layers, defined as arithmetic average of edge pressures (dry air)	hPa
Met_PRECANV	Anvil precipitation (at surface)	mm/day
Met_PRECCON	Convective precipitation (at surface)	mm/day
Met_PRECLSC	Large-scale precipitation (at surface)	mm/day
Met_PRECTOT	Total precipitation (at surface)	mm/day
Met_PS1DRY	Instantaneous surface pressure at start of 3-hr met field interval (dry air)	hPa
Met_PS2DRY	Instantaneous surface pressure at end of 3-hr met field interval (dry air)	hPa
Met_PSC2DRY	Surface pressure interpolated to current time (dry air)	hPa
Met_PS1WET	Instantaneous surface pressure at start of 3-hr met field interval (wet air)	hPa
Met_PS2WET	Instantaneous surface pressure at end of 3-hr met field interval (wet air)	hPa
Met_PSC2WET	Surface pressure interpolated to current time (wet air)	hPa
Met_QI	Ice mixing ratio (dry air)	kg/kg dry air

continues on next

Table 3 – continued from previous page

Diagnostic field	Description	Units
Met_QL	Liquid water mixing ratio (dry air)	kg/kg dry air
Met_OMEGA	Updraft velocity	Pa/s
Met_OPTD	Visible optical depth	1
Met_REEVAPCN	Evaporation of convective precipitation (dry air)	kg/kg/s
Met_REEVAPLS	Evaporation of large-scale + anvil precipitation (dry air)	kg/kg/s
Met_SLP	Sea level pressure	hPa
Met_SNODP	Snow depth	m
Met_SNOMAS	Snow mass	kg/m2
Met_SPHU1	Instantaneous specific humidity at start of 3 hr met field interval (wet air)	kg/kg
Met_SPHU2	Instantaneous specific humidity at end of 3-hr met field interval (wet air)	kg/kg
Met_SPHU	Specific humidity interpolated to current time (wet air)	g H2O/kg air
Met_SUNCOS	Cosine of solar zenith angle at current time	1
Met_SUNCOSMID	Cosine of solar zenith angle at midpoint of chemistry timestep	1
Met_SWGDN	Incident shortwave radiation at ground	W/m2
Met_TAUCLI	Visible optical depth of ice clouds	1
Met_TAUCLW	Visible optical depth of water clouds	1
Met_THETA	Potential temperature	K
Met_TMPU1	Instantaneous temperature at start of 3-hr met field interval	K
Met_TMPU2	Instantaneous temperature at end of 3-hr met field interval	K
Met_T	Temperature interpolated to current time	K
Met_TO3	Total overhead ozone column	Dobsons
Met_TropHt	Tropopause height	u
Met_TropLev	Tropopause level	1
Met_TROPP	Tropopause pressure	hPa
Met_TS	Surface temperature	K
Met_TSKIN	Surface skin temperature	K
Met_U	East-west ccomponent of wind	m/s
Met_U10M	East-west component of wind at 10 m height above surface	m/s
Met_USTAR	Friction velocity	m/s
Met_UVALBEDO	Ultraviolet surface albedo	1
Met_V	North-south ccomponent of wind	m/s
Met_V10M	North-south component of wind at 10 m height above surface	m/s
Met_Z0	Surface roughness height	m
FracOfTimeInTrop	Fraction of time spent in the troposphere	1

29.2.33 StratBM

The **StratBM** collection contains diagnostic fields for GEOS-Chem 10-year stratospheric benchmark simulations. Unless you are involved with benchmarking GEOS-Chem, you may leave this collection deactivated.

Sample definition section for the StratBM collection

```
StratBM.template:       '%y4%m2%d2_%h2%n2z.nc4',
StratBM.frequency:      00000000 010000
StratBM.duration:       00000001 000000
StratBM.mode:           'time-averaged'
StratBM.fields:         'SpeciesConcVV_NO2                ',
                        'SpeciesConcVV_O3                 ',
                        'SpeciesConcVV_ClO                ',
                        'Met_PSC2WET                      ',
```

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```
                          'Met_BXHEIGHT                          ',
                          'Met_AIRDEN                            ',
                          'Met_AD                                ',
::
```

List of diagnostic fields in the StateMet collection

Diagnostic field	Description	Units
Met_AD	Dry air mass	kg
Met_AIRDEN	Dry air density	kg/m3
Met_BXHEIGHT	Grid box height	m
Met_PSC2WET	Surface pressure interpolated to current time (wet air)	hPa
SpeciesConcVV_ClO	ClO concentration	mol/mol dry air
SpeciesConcVV_NO2	NO2 concentration	mol/mol dry air
SpeciesConcVV_O3	O3 concentration	mol/mol dry air

29.2.34 Tomas

The **TOMAS** collection contains diagnostic fields for fullchem simulations with TOMAS aerosol microphysics.

```
  Tomas.template:       '%y4%m2%d2_%h2%n2z.nc4',
  Tomas.format:         'CFIO',
  Tomas.timestampStart: .true.
  Tomas.monthly:        0
  Tomas.frequency:      010000
  Tomas.duration:       010000
  Tomas.mode:           'time-averaged'
  Tomas.fields:         'TomasH2SO4mass_?TOMASBIN?         ',
                        #-----------------------------------------------
                        # NOTE: for GEOS-Chem Classic you can use the
                        # ?TOMASBIN? wildcard.  For GCHP you will need
                        # to list each diagnostic field individually
                        # such as is shown below:
                        #'TomasH2SO4mass_bin01              ',
                        #'TomasH2SO4mass_bin02              ',
                        #'TomasH2SO4mass_bin03              ',
                        #'TomasH2SO4mass_bin04              ',
                        #'TomasH2SO4mass_bin05              ',
                        #'TomasH2SO4mass_bin06              ',
                        #'TomasH2SO4mass_bin07              ',
                        #'TomasH2SO4mass_bin08              ',
                        #'TomasH2SO4mass_bin09              ',
                        #'TomasH2SO4mass_bin10              ',
                        #'TomasH2SO4mass_bin11              ',
                        #'TomasH2SO4mass_bin12              ',
                        #'TomasH2SO4mass_bin13              ',
                        #'TomasH2SO4mass_bin14              ',
                        #'TomasH2SO4mass_bin15              ',
                        #-----------------------------------------------
                        'TomasH2SO4number_?TOMASBIN?       ',
```

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```
                        'TomasCOAGmass_?TOMASBIN          ',
                        'TomasCOAGnumber_?TOMASBIN?       ',
                        'TomasNUCRATEFN                   ',
                        'TomasNUCLmass_?TOMASBIN?         ',
                        'TomasNUCLnumber_?TOMASBIN?       ',
                        'TomasNUCRATEnumber_?TOMASBIN?    ',
                        'TomasAQOXmass_?TOMASBIN?         ',
                        'TomasAQOXnumber_?TOMASBIN?       ',
                        'TomasMNFIXmass_?TOMASBIN?        ',
                        'TomasMNFIXnumber_?TOMASBIN?      ',
                        'TomasMNFIXh2so4mass_?TOMASBIN?   ',
                        'TomasMNFIXh2so4number_?TOMASBIN? ',
                        'TomasMNFIXcoagmass_?TOMASBIN?    ',
                        'TomasMNFIXcoagnumber_?TOMASBIN?  ',
                        'TomasMNFIXaqoxmass_?TOMASBIN?    ',
                        'TomasMNFIXaqoxnumber_?TOMASBIN?  ',
                        'TomasMNFIXezwat1number_?TOMASBIN?',
                        'TomasMNFIXezwat2mass_?TOMASBIN?  ',
                        'TomasMNFIXezwat2number_?TOMASBIN?',
                        'TomasMNFIXezwat3mass_?TOMASBIN?  ',
                        'TomasMNFIXezwat3number_?TOMASBIN?',
                        'TomasMNFIXcheck1mass_?TOMASBIN?  ',
                        'TomasMNFIXcheck1number_?TOMASBIN?',
                        'TomasMNFIXcheck2mass_?TOMASBIN?  ',
                        'TomasMNFIXcheck2number_?TOMASBIN?',
                        'TomasMNFIXcheck3mass_?TOMASBIN?  ',
                        'TomasMNFIXcheck3number_?TOMASBIN?',
                        'TomasSOAmass_?TOMASBIN?          ',
                        'TomasSOAnumber_?TOMASBIN?        ',
::
```

List of diagnostic fields for the Tomas collection

Diagnostic field	Description	Units	Wildcard
TomasAQOX-mass_<name|wc>	TomasAQOX mass rate	kg/kg/s	21
TomasAQOXnum-ber_<name|wc>	TomasAQOX number rate	#/kg/s	Page 257, 21
TomasCOAG-mass_<name|wc>	TOMASCOAG mass rate	kg/kg/s	Page 257, 21
TomasCOAGnum-ber_<name|wc>	TomasCOAG number rate	#/kg/s	Page 257, 21
TomasH2SO4mass_<name|	TomasH2SO4 mass rate	kg/kg/s	Page 257, 21
TomasH2SO4number_<nan	TomasH2SO4 number rate	#/kg/s	Page 257, 21
TomasMNFIX	Tomas error rate	1	Page 257, 21
TomasMNFIX-mass_<name|wc>	TomasMNFIX mass rate	kg/kg/s	Page 257, 21
TomasMNFIXnum-ber_<name|wc>	TomasMNFIX number rate	#/kg/s	Page 257, 21
TomasMNFIXaqox-mass_<name|wc>	TOMASMNFIXAQOX mass rate	kg/kg/s	Page 257, 21

continues on next page

Table 4 – continued from previous page

Diagnostic field	Description	Units	Wildcard
TomasMNFIXaqoxnumber_ <name|wc>	TOMASMNFIXAQOX number rate	#/kg/s	Page 257, 21
TomasMNFIXcoagmass_<name|wc>	TomasMNFIXCOAG mass rate	kg/kg/s	[21]
TomasMNFIXcoagnumber_<name|wc>	TomasMNFIXCOAG number rate	#/kg/s	[21]
TomasMNFIXcheck1mass_<name|wc>	TOMASMNFIXCHECK1 mass rate	kg/kg/s	[21]
TomasMNFIXcheck1number_<name|wc>	TOMASMNFIXCHECK1 number rate	#/kg/s	[21]
TomasMNFIXcheck2mass_<name|wc>	TOMASMNFIXCHECK2 mass rate	kg/kg/s	[21]
TomasMNFIXcheck2number_<name|wc>	TOMASMNFIXCHECK2 number rate	#/kg/s	[21]
TomasMNFIXcheck3mass_<name|wc>	TOMASMNFIXCHECK3 mass rate	kg/kg/s	[21]
TomasMNFIXcheck3number_<name|wc>	TOMASMNFIXCHECK3 number rate	#/kg/s	[21]
TomasMNFIXezwat1mass_<name|wc>	TOMASMNFIXEZWAT1 mass rate	kg/kg/s	[21]
TomasMNFIXezwat1number_<name|wc>	TOMASMNFIXEZWAT1 number rate	#/kg/s	[21]
TomasMNFIXezwat2mass_<name|wc>	TOMASMNFIXEZWAT2 mass rate	kg/kg/s	[21]
TomasMNFIXezwat2number_<name|wc>	TOMASMNFIXEZWAT2 number rate	#/kg/s	[21]
TomasMNFIXezwat3mass_<name|wc>	TOMASMNFIXEZWAT3 mass rate	kg/kg/s	[21]
TomasMNFIXezwat3number_<name|wc>	TOMASMNFIXEZWAT3 number rate	#/kg/s	[21]
TomasMNFIXh2so4mass_<name|wc>	TomasMNFIXH2SO4 mass rate	kg/kg/s	[21]
TomasMNFIXh2so4number_<name|w	TomasMNFIXH2SO4 number rate	#/kg/s	[21]
TomasNUCL	Tomas nucleation rate	1	[21]
TomasNUCLmass_<name|wc>	TomasNUCL mass rate	kg/kg/s	[21]
TomasNUCLnumber_<name|wc>	TomasNUCL number rate	#/kg/s	[21]
TomasSOA	TomasSOA rate	1	[21]
TomasSOAmass_<name|wc>	TomasSOA mass rate	kg/kg/s	[21]
TomasSOAnumber_<name|wc>	TomasSOA number rate	#/kg/s	[21]

[21] This diagnostic field can use the ?TOMASBIN? wildcard (for GEOS-Chem Classic only).

Notes for the Tomas collection

29.2.35 UVFlux

The **UVFlux** diagnostic contains diffuse, direct, and net UV fluxes at each of the photolysis wavelength bins.

Sample definition section for HISTORY.rc

```
  UVFlux.template:    '%y4%m2%d2_%h2%n2z.nc4',
  UVFlux.frequency:   00000100 000000
  UVFlux.duration:    00000100 000000
  UVFlux.mode:        'time-averaged'
  UVFlux.template:    'UVFluxDiffuse_?UVFLX?',
                      'UVFluxDirect_?UVFLX? ',
                      'UVFluxNet_?UVFLX?    ',
::
```

List of diagnostic fields in the UvFlux collection

Diagnostic field	Description	Units	Wildcards
UVFluxDiffuse_<name|wc>	Diffuse UV flux in wavelength bin	W/m2	?UVFLX?
UVFluxDirect_<name|wc>	Direct UV flux in wavelength bin	W/m2	?UVFLX?
UVFluxNet_<name|wc>	Net UV flux in wavelength bin	W/m2	?UVFLX?

29.2.36 WetLossConv

The **WetLossConv** collection contains diagnostics fluxes of soluble species lost to wet scavenging in convective updrafts.

Sample definition section for HISTORY.rc

```
  WetLossConv.template:    '%y4%m2%d2_%h2%n2z.nc4',
  WetLossConv.frequency:   00000100 000000
  WetLossConv.duration:    00000100 000000
  WetLossConv.mode:        'time-averaged'
  WetLossConv.fields:      'WetLossConv_?WET?    ',
                           'WetLossConvFrac_?WET?',
::
```

List of diagnostic fields in the WetLossConv collection

Diagnostic field	Description	Units	Wildcard
WetLossConv_<name|wc>	Loss of soluble species scavenged by cloud updrafts in moist convection	kg/s	?WET?
WetLossConvFrac_<name|wc>	Fraction of species scavenged by cloud updrafts in moist convection	1	?WET?

29.2.37 WetLossLS

The **WetLossLS** collection contains diagnostics fluxes of soluble species lost to rainout and washout in large-scale wet deposition.

Sample definition section for HISTORY.rc

```
  WetLossLS.template:     '%y4%m2%d2_%h2%n2z.nc4',
  WetLossLS.frequency:    00000100 000000
  WetLossLS.duration:     00000100 000000
  WetLossLS.mode:         'time-averaged'
  WetLossLS.fields:       'WetLossLS_?WET?',
::
```

List of diagnostic fields in the WetLossLS collection

Diagnostic field	Description	Units	Wildcard
WetLossLS_<name|wc>	Loss of soluble species in large-scale precipitation	kg/s	?WET?

29.3 Adding new History diagnostics

To add your own diagnostics we recommend that you find a similar existing diagnostic and use its implementation as a template. Most of the work is done in `Headers/state_diag_mod.F90`. Briefly, the following updates to that file are essential for adding in your own netCDF diagnostics:

1. Declare diagnostic array at top of module.
2. Set diagnostic array pointer to null in `Zero_State_Diag` subroutine.
3. Create a section in `Init_State_Diag` subroutine to allocate and register the array.
4. Deallocate the diagnostic array in subroutine `Cleanup_State_Diag`.
5. Add an `IF` block for the diagnostic within subroutine `Get_Metadata_State_Diag` to define its metadata, making sure to list the diagnostic name with all capital letters.

Good diagnostics to use as templates are `SpeciesConcVV` for 3-dimensional arrays that are for all species and `DryDepVel` for 2-dimensional arrays that are for a subset of species. If your diagnostic is not per species then `AODDust` is a good diagnostic to look at. Search the file `Headers/state_diag_mod.F90` for any of these strings to find all instances of code related to their implementation.

Note that information about the dimensions and species collection the diagnostic will include must be specified when allocating the array in `Init_State_Diag` and in `Get_Metadata_State_Diag`. In the latter subroutine the `Rank` is the integer number of dimensions of the diagnostic (not including species) and the `TagID` string, if any, specifies the species collection to output the diagnostic per. Each `TagID` is defined in subroutine Get_TagInfo. Each TagID string can also be used as a wildcard within `HISTORY.rc` to simplify diagnostic name specification (for GEOS-Chem Classic only).

Once you have implemented your diagnostic in `Headers/state_diag_mod.F90`, try adding it to HISTORY.rc and running. You should get your diagnostic output in the netCDF output file as all zeros. The next step is to populate the array with whatever value you want to output. You should do this by passing the `State_Diag` array to the location where you want to set the values. Then write code to fill the array. A simple test of your understanding is to initially set values to a constant other than zero and see if the output matches what you set the arrays to.

For additional help implementing your own GEOS-Chem diagnostics please contact the GEOS-Chem Support Team.

CHAPTER

THIRTY

WORK WITH NETCDF FILES

On this page we provide some useful information about working with data files in netCDF format.

30.1 Useful tools

There are many free and open-source software packages readily available for visualizing and manipulating netCDF files.

cdo

Climate Data Operators: Highly-optimized command-line tools for manipulating and analyzing netCDF files. Contains features that are especially useful for Earth Science applications.

See: https://code.zmaw.de/projects/cdo

GCPy

GEOS-Chem Python toolkit: Python package for visualizing and analyzing GEOS-Chem output. Used for creating the GEOS-Chem benchmark plots. Also contains some useful routines for creating single-panel plots and multi-panel difference plots, as well as file regridding utilities.

See: https://gcpy.readthedocs.io

ncdump

Generates a text representation of netCDF data and can be used to quickly view the variables contained in a netCDF file. **ncdump** is installed to the `bin/` folder of your netCDF library distribution.

See: https://www.unidata.ucar.edu/software/netcdf/workshops/2011/utilities/Ncdump.html

nco

netCDF operators: Highly-optimized command-line tools for manipulating and analyzing netCDF files.

See: http://nco.sourceforge.net

ncview

Visualization package for netCDF files. **Ncview** has limited features, but is great for a quick look at the contents of netCDF files.

See: http://meteora.ucsd.edu/~pierce/ncview_home_page.html

netcdf-scripts

Our repository of useful netCDF utility scripts for GEOS-Chem.

See: https://github.com/geoschem/netcdf-scripts

Panoply

Java-based data viewer for netCDF files. This package offers an alternative to ncview. From our experience, Panoply works nicely when installed on the desktop, but is slow to respond in the Linux environment.

See: https://www.giss.nasa.gov/tools/panoply/

xarray

Python package that lets you read the contents of a netCDF file into a data structure. The data can then be further manipulated or converted to numpy or dask arrays for further procesing.

See: https://xarray.readthedocs.io

Some of the tools listed above, such as **ncdump** and **ncview** may come pre-installed on your system. Others may need to be installed or loaded (e.g. via the **module load** command). Check with your system administrator or IT staff to see what is available on your system.

30.2 Examine the contents of a netCDF file

An easy way to examine the contents of a netCDF file is to use **ncdump** as follows:

```
$ ncdump -ct GEOSChem.SpeciesConc.20190701_0000z.nc4
```

You will see output similar to this:

```
netcdf GEOSChem.SpeciesConc.20190701_0000z {
dimensions:
    time = UNLIMITED ; // (1 currently)
    lev = 72 ;
    ilev = 73 ;
    lat = 46 ;
    lon = 72 ;
    nb = 2 ;
variables:
    double time(time) ;
        time:long_name = "Time" ;
        time:units = "minutes since 2019-07-01 00:00:00" ;
        time:calendar = "gregorian" ;
        time:axis = "T" ;
    double lev(lev) ;
        lev:long_name = "hybrid level at midpoints ((A/P0)+B)" ;
        lev:units = "level" ;
        lev:axis = "Z" ;
        lev:positive = "up" ;
        lev:standard_name = "atmosphere_hybrid_sigma_pressure_coordinate" ;
        lev:formula_terms = "a: hyam b: hybm p0: P0 ps: PS" ;
    double ilev(ilev) ;
        ilev:long_name = "hybrid level at interfaces ((A/P0)+B)" ;
        ilev:units = "level" ;
        ilev:positive = "up" ;
        ilev:standard_name = "atmosphere_hybrid_sigma_pressure_coordinate" ;
        ilev:formula_terms = "a: hyai b: hybi p0: P0 ps: PS" ;
    double lat_bnds(lat, nb) ;
        lat_bnds:long_name = "Latitude bounds (CF-compliant)" ;
```

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```
        lat_bnds:units = "degrees_north" ;
    double lat(lat) ;
        lat:long_name = "Latitude" ;
        lat:units = "degrees_north" ;
        lat:axis = "Y" ;
        lat:bounds = "lat_bnds" ;
    double lon_bnds(lon, nb) ;
        lon_bnds:long_name = "Longitude bounds (CF-compliant)" ;
        lon_bnds:units = "degrees_east" ;
    double lon(lon) ;
        lon:long_name = "Longitude" ;
        lon:units = "degrees_east" ;
        lon:axis = "X" ;
        lon:bounds = "lon_bnds" ;
    double hyam(lev) ;
        hyam:long_name = "hybrid A coefficient at layer midpoints" ;
        hyam:units = "hPa" ;
    double hybm(lev) ;
        hybm:long_name = "hybrid B coefficient at layer midpoints" ;
        hybm:units = "1" ;
    double hyai(ilev) ;
        hyai:long_name = "hybrid A coefficient at layer interfaces" ;
        hyai:units = "hPa" ;
    double hybi(ilev) ;
        hybi:long_name = "hybrid B coefficient at layer interfaces" ;
        hybi:units = "1" ;
    double P0 ;
        P0:long_name = "reference pressure" ;
        P0:units = "hPa" ;
    float AREA(lat, lon) ;
        AREA:long_name = "Surface area" ;
        AREA:units = "m2" ;
    float SpeciesConcVV_RCOOH(time, lev, lat, lon) ;
        SpeciesConc_RCOOH:long_name = "Dry mixing ratio of species RCOOH" ;
        SpeciesConcVV_RCOOH:units = "mol mol-1 dry" ;
        SpeciesConcVV_RCOOH:averaging_method = "time-averaged" ;
    float SpeciesConcVV_O2(time, lev, lat, lon) ;
        SpeciesConcVV_O2:long_name = "Dry mixing ratio of species O2" ;
        SpeciesConcVV_O2:units = "mol mol-1 dry" ;
        SpeciesConcVV_O2:averaging_method = "time-averaged" ;
    float SpeciesConcVV_N2(time, lev, lat, lon) ;
        SpeciesConcVV_N2:long_name = "Dry mixing ratio of species N2" ;
        SpeciesConcVV_N2:units = "mol mol-1 dry" ;
        SpeciesConcVV_N2:averaging_method = "time-averaged" ;
    float SpeciesConcVV_H2(time, lev, lat, lon) ;
        SpeciesConcVV_H2:long_name = "Dry mixing ratio of species H2" ;
        SpeciesConcVV_H2:units = "mol mol-1 dry" ;
        SpeciesConcVV_H2:averaging_method = "time-averaged" ;
    float SpeciesConcVV_O(time, lev, lat, lon) ;
        SpeciesConcVV_O:long_name = "Dry mixing ratio of species O" ;
        SpeciesConcVVO:units = "mol mol-1 dry" ;
```

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```
     ... etc ...

// global attributes:
            :title = "GEOS-Chem diagnostic collection: SpeciesConc" ;
            :history = "" ;
            :format = "not found" ;
            :conventions = "COARDS" ;
            :ProdDateTime = "" ;
            :reference = "www.geos-chem.org; wiki.geos-chem.org" ;
            :contact = "GEOS-Chem Support Team (geos-chem-support@g.harvard.edu)" ;
            :simulation_start_date_and_time = "2019-07-01 00:00:00z" ;
            :simulation_end_date_and_time = "2019-07-01 01:00:00z" ;
data:

 time = "2019-07-01 00:30" ;

 lev = 0.99250002413, 0.97749990013, 0.962499776, 0.947499955, 0.93250006,
    0.91749991, 0.90249991, 0.88749996, 0.87249996, 0.85750006, 0.842500125,
    0.82750016, 0.8100002, 0.78750002, 0.762499965, 0.737500105, 0.7125001,
    0.6875001, 0.65625015, 0.6187502, 0.58125015, 0.5437501, 0.5062501,
    0.4687501, 0.4312501, 0.3937501, 0.3562501, 0.31279158, 0.26647905,
    0.2265135325, 0.192541016587707, 0.163661504087706, 0.139115, 0.11825,
    0.10051436, 0.085439015, 0.07255786, 0.06149566, 0.05201591, 0.04390966,
    0.03699271, 0.03108891, 0.02604911, 0.021761005, 0.01812435, 0.01505025,
    0.01246015, 0.010284921, 0.008456392, 0.0069183215, 0.005631801,
    0.004561686, 0.003676501, 0.002948321, 0.0023525905, 0.00186788,
    0.00147565, 0.001159975, 0.00090728705, 0.0007059566, 0.0005462926,
    0.0004204236, 0.0003217836, 0.00024493755, 0.000185422, 0.000139599,
    0.00010452401, 7.7672515e-05, 5.679251e-05, 4.0142505e-05, 2.635e-05,
    1.5e-05 ;

 ilev = 1, 0.98500004826, 0.969999752, 0.9549998, 0.94000011, 0.92500001,
    0.90999981, 0.89500001, 0.87999991, 0.86500001, 0.85000011, 0.83500014,
    0.82000018, 0.80000022, 0.77499982, 0.75000011, 0.7250001, 0.7000001,
    0.6750001, 0.6375002, 0.6000002, 0.5625001, 0.5250001, 0.4875001,
    0.4500001, 0.4125001, 0.3750001, 0.3375001, 0.28808306, 0.24487504,
    0.208152025, 0.176930008175413, 0.150393, 0.127837, 0.108663, 0.09236572,
    0.07851231, 0.06660341, 0.05638791, 0.04764391, 0.04017541, 0.03381001,
    0.02836781, 0.02373041, 0.0197916, 0.0164571, 0.0136434, 0.0112769,
    0.009292942, 0.007619842, 0.006216801, 0.005046801, 0.004076571,
    0.003276431, 0.002620211, 0.00208497, 0.00165079, 0.00130051, 0.00101944,
    0.0007951341, 0.0006167791, 0.0004758061, 0.0003650411, 0.0002785261,
    0.000211349, 0.000159495, 0.000119703, 8.934502e-05, 6.600001e-05,
    4.758501e-05, 3.27e-05, 2e-05, 1e-05 ;

 lat = -89, -86, -82, -78, -74, -70, -66, -62, -58, -54, -50, -46, -42, -38,
    -34, -30, -26, -22, -18, -14, -10, -6, -2, 2, 6, 10, 14, 18, 22, 26, 30,
    34, 38, 42, 46, 50, 54, 58, 62, 66, 70, 74, 78, 82, 86, 89 ;

 lon = -180, -175, -170, -165, -160, -155, -150, -145, -140, -135, -130,
    -125, -120, -115, -110, -105, -100, -95, -90, -85, -80, -75, -70, -65,
    -60, -55, -50, -45, -40, -35, -30, -25, -20, -15, -10, -5, 0, 5, 10, 15,
```

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```
    20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95, 100, 105,
    110, 115, 120, 125, 130, 135, 140, 145, 150, 155, 160, 165, 170, 175 ;
}
```

You can also use **ncdump** to display the data values for a given variable in the netCDF file. This command will display the values in the SpeciesRst_O3 variable to the screen:

```
$ ncdump -v SpeciesConc_O3 GEOSChem.SpeciesConc.20190701_0000z.nc4 | less
```

Or you can redirect the output to a file:

```
$ ncdump -v SpeciesConc_O3 GEOSChem.SpeciesConc.20190701_0000z.nc4 > log
```

30.3 Read the contents of a netCDF file

30.3.1 Read data with Python

The easiest way to read a netCDF file is to use the xarray Python package.

```
#!/usr/bin/env python

# Imports
import numpy as np
import xarray as xr

# Read a restart file into an xarray Dataset object
ds = xr.open_dataset("GEOSChem.SpeciesConc.20190701_0000z.nc4")

# Print the contents of the DataSet
print(ds)

# Print units of data
print(f"\nUnits of SpeciesRst_O3: {ds['SpeciesConc_O3'].units}")

# Print the sum, max, and min of the data
# NOTE .values returns a numpy ndarray so that we can use
# other numpy functions like np.sum() on the data
print(f"Sum of SpeciesRst_O3: {np.sum(ds['SpeciesConc_O3'].values)}")
print(f"Max of SpeciesRst_O3: {np.max(ds['SpeciesConc_O3'].values)}")
print(f"Min of SpeciesRst_O3: {np.min(ds['SpeciesConc_O3'].values)}")
```

This above script will print the following output:

```
<xarray.Dataset>
Dimensions:               (ilev: 73, lat: 46, lev: 72, lon: 72, nb: 2, time: 1)
Coordinates:
  * time                  (time) datetime64[ns] 2019-07-01T00:30:00
  * lev                   (lev) float64 0.9925 0.9775 ... 2.635e-05 1.5e-05
  * ilev                  (ilev) float64 1.0 0.985 0.97 ... 3.27e-05 2e-05 1e-05
  * lat                   (lat) float64 -89.0 -86.0 -82.0 ... 82.0 86.0 89.0
```

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```
  * lon                   (lon) float64 -180.0 -175.0 -170.0 ... 170.0 175.0
Dimensions without coordinates: nb
Data variables: (12/315)
    lat_bnds              (lat, nb) float64 ...
    lon_bnds              (lon, nb) float64 ...
    hyam                  (lev) float64 ...
    hybm                  (lev) float64 ...
    hyai                  (ilev) float64 ...
    hybi                  (ilev) float64 ...
    ...                    ...
    SpeciesConc_AONITA    (time, lev, lat, lon) float32 ...
    SpeciesConc_ALK4      (time, lev, lat, lon) float32 ...
    SpeciesConc_ALD2      (time, lev, lat, lon) float32 ...
    SpeciesConc_AERI      (time, lev, lat, lon) float32 ...
    SpeciesConc_ACTA      (time, lev, lat, lon) float32 ...
    SpeciesConc_ACET      (time, lev, lat, lon) float32 ...
Attributes:
    title:                           GEOS-Chem diagnostic collection: Species...
    history:
    format:                          not found
    conventions:                     COARDS
    ProdDateTime:
    reference:                       www.geos-chem.org; wiki.geos-chem.org
    contact:                         GEOS-Chem Support Team (geos-chem-suppor...
    simulation_start_date_and_time:  2019-07-01 00:00:00z
    simulation_end_date_and_time:    2019-07-01 01:00:00z

Units of SpeciesRst_O3: mol mol-1 dry
Sum of SpeciesRst_O3: 0.4052325189113617
Max of SpeciesRst_O3: 1.01212954177754e-05
Min of SpeciesRst_O3: 3.758645839013752e-09
```

30.3.2 Read data from multiple files in Python

The xarray package will also let you read data from multiple files into a single Dataset object. This is done with the open_mfdataset (open multi-file-dataset) function as shown below:

```
#!/usr/bin/env python

# Imports
import xarray as xr

# Create a list of files to open
filelist = [
    'GEOSChem.SpeciesConc.20160101_0000z.nc4',
    'GEOSChem.SpeciesConc_20160201_0000z.nc4',
    ...
]

# Read a restart file into an xarray Dataset object
ds = xr.open_mfdataset(filelist)
```

30.4 Determining if a netCDF file is COARDS-compliant

All netCDF files used as input to GEOS-Chem and/or HEMCO must adhere to the *COARDS netCDF conventions*. You can use the isCoards script (from our netcdf-scripts repository at GitHub) to determine if a netCDF file adheres to the COARDS conventions.

Run the `isCoards` script at the command line on any netCDF file, and you will receive a report as to which elements of the file do not comply with the COARDS conventions.

```
$ isCoards myfile.nc

================================================================================
Filename: myfile.nc
================================================================================

The following items adhere to the COARDS standard:
--------------------------------------------------------------------------------
-> Dimension "time" adheres to standard usage
-> Dimension "lev" adheres to standard usage
-> Dimension "lat" adheres to standard usage
-> Dimension "lon" adheres to standard usage
-> time(time)
-> time is monotonically increasing
-> time:axis = "T"
-> time:calendar = "gregorian"
-> time:long_name = "Time"
-> time:units = "hours since 1985-1-1 00:00:0.0"
-> lev(lev)
-> lev is monotonically decreasing
-> lev:axis = "Z"
-> lev:positive = "up"
-> lev:long_name = "GEOS-Chem levels"
-> lev:units = "sigma_level"
-> lat(lat)
-> lat is monotonically increasing
-> lat:axis = "Y"
-> lat:long_name = "Latitude"
-> lat:units = "degrees_north"
-> lon(lon)
-> lon is monotonically increasing
-> lon:axis = "X"
-> lon:long_name = "Longitude"
-> lon:units = "degrees_east"
-> OH(time,lev,lat,lon)
-> OH:long_name = "Chemically produced OH"
-> OH:units = "kg/m3"
-> OH:long_name = 1.e+30f
-> OH:missing_value = 1.e+30f
-> conventions: "COARDS"
-> history: "Mon Apr  3 08:26:19 2017"
-> title: "COARDS/netCDF file created by BPCH2COARDS (GAMAP v2-17+)"
-> format: "NetCDF-3"
```

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```
The following items DO NOT ADHERE to the COARDS standard:
--------------------------------------------------------------------------------
-> time[0] != 0 (problem for GCHP)

The following optional items are RECOMMENDED:
--------------------------------------------------------------------------------
-> Consider adding the "references" global attribute
```

30.5 Edit variables and attributes

As discussed *in the preceding section*, you may find that you need to edit your netCDF files for COARDS-compliance. Below are several useful commands for editing netCDF files. Many of these commands utilize the *nco* and *cdo* utilities.

1. Display the header and coordinate variables of a netCDF file, with the time variable displayed in human-readable format. Also show status of file *compression and/or chunking*.

```
$ ncdump -cts file.nc
```

2. *Compress a netCDF file*. This can considerably reduce the file size!

```
# No deflation
$ nccopy -d0 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc

# Minimum deflation (good for most applications)
$ nccopy -d1 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc

# Medium deflation
$ nccopy -d5 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc

# Maximum deflation
$ nccopy -d9 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

3. Change variable name from `SpeciesConc_NO` to `NO`:

```
$ ncrename -v SpeciesConc_NO,NO myfile.nc
```

4. Set all missing values to zero:

```
$ cdo setemisstoc,0 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

5. Add/change the `long_name` attribute of the vertical coordinate (`lev`) to `GEOS-Chem levels`. This will ensure that HEMCO recognizes the vertical levels of the input file as GEOS-Chem model levels.

```
$ ncatted -a long_name,lev,o,c,"GEOS-Chem levels" myfile.nc
```

6. Add/change the `axis` and `positive` attributes of the vertical coordinate (`lev`):

```
$ ncatted -a axis,lev,o,c,"Z" myfile.nc
$ ncatted -a positive,lev,o,c,"up" myfile.nc
```

7. Add/change the `units` attribute of the latitude (`lat`) coordinate to `degrees_north`:

```
$ ncatted -a units,lat,o,c,"degrees_north" myfile.nc
```

8. Convert the `units` attribute of the CHLA variable from `mg/m3` to `kg/m3`

```
$ ncap2 -v -s "CHLA=CHLA/1000000.0f" myfile.nc tmp.nc
$ ncatted -a units,CHLA,o,c,"kg/m3" tmp.nc
$ mv tmp.nc myfile.nc
```

9. Add/change the `references`, `title`, and `history` global attributes

```
$ ncatted -a references,global,o,c,"www.geos-chem.org; wiki.geos-chem.org" myfile.nc
$ ncatted -a history,global,o,c,"Tue Mar  3 12:18:38 EST 2015" myfile.nc
$ ncatted -a title,global,o,c,"XYZ data from ABC source" myfile.nc
```

10. Remove the `references` global attribute:

```
$ ncatted -a references,global,d,, myfile.nc
```

11. Add a `time` dimension to a file that does not have one:

```
$ ncap2 -h -s 'defdim("time",1);time[time]=0.0;time@long_name="time";
↪time@calendar="standard";time@units="days since 2007-01-01 00:00:00"' -O myfile.
↪nc tmp.nc
$ mv tmp.nc myfile.nc
```

12. Add a `time` dimension to a variable:

```
# Assume myVar has lat and lon dimensions to start with
$ ncap2 -h -s 'myVar[$time,$lat,$lon]=myVar;' myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

13. Make the `time` dimension unlimited:

```
$ ncks --mk_rec_dmn time myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

14. Change the file reference date and time (i.e. `time:units`) from 1 Jan 1985 to 1 Jan 2000:

```
$ cdo setreftime,2000-01-01,00:00:00 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

15. Shift all time values ahead or back by 1 hour in a file:

```
# Shift ahead 1 hour
$ cdo shifttime,1hour myfile.nc tmp.nc
$ mv tmp.nc myfile.nc

# Shift back 1 hour
$ cdo shiftime,-1hour myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

16. Set the date of all variables in the file. (Useful for files that have only one time point.)

```
$ cdo setdate,2019-07-02 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

Tip: The following **cdo** commands are similar to **cdo setdate**, but allow you to manipulate other time variables:

```
$ cdo settime,03:00:00 ...  # Sets time to 03:00 UTC
$ cdo setday,26, ...        # Sets day of month to 26
$ cdo setmon,10, ...        # Sets month to 10 (October)
$ cdo setyear,1992, ...     # Sets year to 1992
```

See the cdo user manual for more information.

---

17. Change the `time:calendar` attribute:

    GEOS-Chem and HEMCO cannot read data from netCDF files where:

```
time:calendar = "360_day"
time:calendar = "365_day"
time:calendar = "noleap"
```

    We recommend converting the calendar used in the netCDF file to the `standard` netCDF calendar with these commands:

```
$ cdo setcalendar,standard myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

18. Change the type of the `time` coordinate from `int` to `double`:

```
$ ncap2 -s 'time=double(time)' myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

30.6 Concatenate netCDF files

There are a couple of ways to concatenate multiple netCDF files into a single netCDF file, as shown in the sections below.

30.6.1 Concatenate with the netCDF operators

You can use the **ncrcat** utility (from *nco*) to concatenate the individual netCDF files into a single netCDF file.

Let's assume we want to combine 12 monthy data files (e.g. `month_01.nc`, `month_02.nc`, .. `month_12.nc` into a single file called `annual_data.nc`.

First, make sure that each of the `month_*nc` files has an unlimited `time` dimension. Type this at the command line:

```
$ ncdump -ct month_01.nc | grep "time"
```

Then you should see this as the first line in the output:

```
time = UNLIMITED ; // (1 currently)
```

This indicates that the time dimension is unlimited. If on the other hand you see this output:

```
time = 1 ;
```

Then it means that the time dimension is fixed. If this is the case, you will have to use the **ncks** command to make the time dimension unlimited, as follows:

```
$ ncks --mk_rec_dmn time month_01.nc tmp.nc
$ mv tmp.nc month_01.nc
... etc for the other files ...
```

Then use **ncrcat** to combine the monthly data along the time dimension, and save the result to a single netCDF file:

```
$ ncrcat -h0 month_*nc annual_data.nc
```

You may then discard the `month_*.nc` files if so desired.

30.6.2 Concatenate with Python

You can use the xarray Python package to create a single netCDF file from multiple files. Click HERE to view a sample Python script that does this.

30.7 Regrid netCDF files

The following tools can be used to regrid netCDF data files (such as GEOS-Chem restart files and GEOS-Chem diagnostic files.

30.7.1 Regrid with cdo

cdo includes several tools for regridding netCDF files. For example:

```
# Apply conservative regridding
$ cdo remapcon,gridfile infile.nc outfile.nc
```

For `gridfile`, you can use the files here. Also see this reference.

Issue with cdo remapdis regridding tool

GEOS-Chem user **Bram Maasakkers** wrote:

> I have noticed a problem regridding GEOS-Chem diagnostic file to 2x2.5 using **cdo** version 1.9.4. When I use:
>
> ```
> $ cdo remapdis,geos.2x25.grid GEOSChem.Restart.4x5.nc GEOSChem.Restart.2x25.nc
> ```
>
> The last latitudinal band (-89.5) remains empty and gets filled with the standard missing value of cdo, which is really large. This leads to immediate problems in the methane simulation as enormous concentrations enter the domain from the South Pole. For now I've solved this problem by just using bicubic interpolation

```
$ cdo remapbic,geos.2x25.grid GEOSChem.Restart.4x5.nc GEOSChem.Restart.2x25.nc
```

You can also use conservative regridding:

```
$ cdo remapcon,geos.2x25.grid GEOSChem.Restart.4x5.nc GEOSChem.Restart.2x25.nc
```

30.7.2 Regrid with GCPy

GCPy (the GEOS-Chem Python Toolkit) has contains file regridding utilities that allow you to regrid from lat/lon to cubed-sphere grids (and vice versa). Regridding weights can be generated on-the-fly, or can be archived and reused. For detailed instructions, please see the please see the GCPy Regridding documentation.

30.7.3 Regrid with nco

nco also includes several regridding utilities. See the Regridding section of the NCO User Guide for more information.

30.7.4 Regrid with xarray

The xarray Python package has a built-in capability for 1-D interpolation. It wraps the SciPy interpolation module. This functionality can also be used for vertical regridding.

30.7.5 Regrid with xESMF

xESMF is a universal regridding tool for geospatial data, which is written in Python. It can be used to regrid data not only on cartesian grids, but also on cubed-sphere and unstructured grids.

Note: **xESMF** only handles horizontal regridding.

30.8 Crop netCDF files

If needed, a netCDF file can be cropped to a subset of the globe with the **nco** or **cdo** utilities (cf. *Useful tools*).

For example, **cdo** has a **selbox** operator for selecting a box by specifying the lat/lon bounds:

```
$ cdo sellonlatbox,lon1,lon2,lat1,lat2 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

See the cdo guide for more information.

30.9 Add a new variable to a netCDF file

You have a couple of options for adding a new variable to a netCDF file (for example, when having to add a new species to an existing GEOS-Chem restart file).

1. You can use **cdo** and **nco** utilities to copy the data from one variable to another variable. For example:

```
#!/bin/bash

# Extract field SpeciesRst_PMN from the original restart file
cdo selvar,SpeciesRst_PMN initial_GEOSChem_rst.4x5_standard.nc NPMN.nc4

# Rename selected field to SpeciesRst_NPMN
ncrename -h -v SpeciesRst_PMN,Species_Rst_NPMN NMPN.nc4

# Append new species to existing restart file
ncks -h -A -M NMPN.nc4 initial_GEOSChem_rst.4x5_standard.nc
```

2. **Sal Farina** wrote a simple Python script for adding a new species to a netCDF restart file:

```
#!/usr/bin/env python

import netCDF4 as nc
import sys
import os

for nam in sys.argv[1:]:
    f = nc.Dataset(nam,mode='a')
    try:
        o = f['SpeciesRst_OCPI']
    except:
        print "SpeciesRst_OCPI not defined"
    f.createVariable('SpeciesRst_SOAP',o.datatype,dimensions=o.dimensions,fill_
↪value=o._FillValue)
    soap = f['SpeciesRst_SOAP']
    soap[:] = 0.0
    soap.long_name= 'SOAP species'
    soap.units =  o.units
    soap.add_offset = 0.0
    soap.scale_factor = 1.0
    soap.missing_value = 1.0e30
    f.close()
```

3. Bob Yantosca wrote this Python script to insert a fake species into GEOS-Chem Classic and GCHP restart files (13.3.0)

```
#!/usr/bin/env python
"""
Adds an extra DataArray for into restart files:
Calling sequence:
    ./append_species_into_restart.py
"""
# Imports
import gcpy.constants as gcon
```

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```
import xarray as xr
from xarray.coding.variables import SerializationWarning
import warnings

# Suppress harmless run-time warnings (mostly about underflow or NaNs)
warnings.filterwarnings("ignore", category=RuntimeWarning)
warnings.filterwarnings("ignore", category=UserWarning)
warnings.filterwarnings("ignore", category=SerializationWarning)

def main():
    """
    Appends extra species to restart files.
    """
    # Data vars to skip
    skip_vars = gcon.skip_these_vars
    # List of dates
    file_list = [
        'GEOSChem.Restart.fullchem.20190101_0000z.nc4',
        'GEOSChem.Restart.fullchem.20190701_0000z.nc4',
        'GEOSChem.Restart.TOMAS15.20190701_0000z.nc4',
        'GEOSChem.Restart.TOMAS40.20190701_0000z.nc4',
        'GCHP.Restart.fullchem.20190101_0000z.c180.nc4',
        'GCHP.Restart.fullchem.20190101_0000z.c24.nc4',
        'GCHP.Restart.fullchem.20190101_0000z.c360.nc4',
        'GCHP.Restart.fullchem.20190101_0000z.c48.nc4',
        'GCHP.Restart.fullchem.20190101_0000z.c90.nc4',
        'GCHP.Restart.fullchem.20190701_0000z.c180.nc4',
        'GCHP.Restart.fullchem.20190701_0000z.c24.nc4',
        'GCHP.Restart.fullchem.20190701_0000z.c360.nc4',
        'GCHP.Restart.fullchem.20190701_0000z.c48.nc4',
        'GCHP.Restart.fullchem.20190701_0000z.c90.nc4'
    ]
    # Keep all netCDF attributes
    with xr.set_options(keep_attrs=True):
        # Loop over dates
        for f in file_list:
            # Input and output files
            infile = '../' + f
            outfile = f
            print("Creating " + outfile)

            # Open input file
            ds = xr.open_dataset(infile, drop_variables=skip_vars)
            # Create a new DataArray from a given species (EDIT ACCORDINGLY)
            if "GCHP" in infile:
                dr = ds["SPC_ETO"]
                dr.name = "SPC_ETOO"
            else:
                dr = ds["SpeciesRst_ETO"]
                dr.name = "SpeciesRst_ETOO"

            # Update attributes (EDIT ACCORDINGLY)
```

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```
            dr.attrs["FullName"] = "peroxy radical from ethene"
            dr.attrs["Is_Gas"] = "true"
            dr.attrs["long_name"] = "Dry mixing ratio of species ETOO"
            dr.attrs["MW_g"] = 77.06
            # Merge the new DataArray into the Dataset
            ds = xr.merge([ds, dr], compat="override")

            # Create a new file
            ds.to_netcdf(outfile)

            # Free memory by setting ds to a null dataset
            ds = xr.Dataset()

if __name__ == "__main__":
    main()
```

30.10 Chunk and deflate a netCDF file to improve I/O

We recommend that you **chunk** the data in your netCDF file. Chunking specifies the order in along which the data will be read from disk. The Unidata web site has a good overview of why chunking a netCDF file matters.

For GEOS-Chem with the high-performance option (aka GCHP), the best file I/O performance occurs when the file is split into one chunk per level (assuming your data has a lev dimension). This allows each individual vertical level of data to be read in parallel.

You can use the **nccopy** command of *nco* to do the chunking. For example, say you have a netCDF file called `myfile.nc` with these dimensions:

```
dimensions:
        time = UNLIMITED ; // (12 currently)
        lev = 72 ;
        lat = 181 ;
        lon = 360 ;
```

Then you can use the **nccopy** command to apply the optimal chunking along levels:

```
$ nccopy -c lon/360,lat/181,lev/1,time/1 -d1 myfile.nc tmp.nc
$ mv tmp.nc myfile.nc
```

This will create a new file called `tmp.nc` that has the proper chunking. We then replace `myfile.nc` with this temporary file.

You can specify the chunk sizes that will be applied to the variables in the netCDF file with the **-c** argument to **nccopy**. To obtain the optimal chunking, the `lon` chunksize must be identical to the number of values along the longitude dimension (e.g. `lon/360` and the `lat` chunksize must be equal to the number of points in the latitude dimension (e.g. `lat/181`).

We also recommend that you **deflate** (i.e. compress) the netCDF data variables at the same time you apply the chunking. Deflating can substantially reduce the file size, especially for emissions data that are only defined over the land but not over the oceans. You can deflate the data in a netCDF file by specifying the -d argumetnt to nccopy. There are 10 possible deflation levels, ranging from 0 (no deflation) to 9 (max deflation). For most purposes, a deflation level of 1 (**d1**) is sufficient.

The GEOS-Chem Support Team has created a Perl script named nc_chunk.pl (contained in the netcdf-scripts repository at GitHub) that will automatically chunk and compress data for you.

```
$ nc_chunk.pl myfile.nc    # Chunk netCDF file
$ nc_chunk.pl myfile.nc 1  # Chunk and compress file using deflate level 1
```

You can use the **ncdump -cts myfile.nc** command to view the chunk size and deflation level in the file. After applying the chunking and compression to myfile.nc, you would see output such as this:

```
dimensions:
        time = UNLIMITED ; // (12 currently)
        lev = 72 ;
        lat = 181 ;
        lon = 360 ;
variables:
        float PRPE(time, lev, lat, lon) ;
                PRPE:long_name = "Propene" ;
                PRPE:units = "kgC/m2/s" ;
                PRPE:add_offset = 0.f ;
                PRPE:scale_factor = 1.f ;
                PRPE:_FillValue = 1.e+15f ;
                PRPE:missing_value = 1.e+15f ;
                PRPE:gamap_category = "ANTHSRCE" ;
                PRPE:_Storage = "chunked" ;
                PRPE:_ChunkSizes = 1, 1, 181, 360 ;
                PRPE:_DeflateLevel = 1 ;
                PRPE:_Endianness = "little" ;\
        float CO(time, lev, lat, lon) ;
                CO:long_name = "CO" ;
                CO:units = "kg/m2/s" ;
                CO:add_offset = 0.f ;
                CO:scale_factor = 1.f ;
                CO:_FillValue = 1.e+15f ;
                CO:missing_value = 1.e+15f ;
                CO:gamap_category = "ANTHSRCE" ;
                CO:_Storage = "chunked" ;
                CO:_ChunkSizes = 1, 1, 181, 360 ;
                CO:_DeflateLevel = 1 ;
                CO:_Endianness = "little" ;\
```

The attributes that begin with a _ character are "hidden" netCDF attributes. They represent file properties instead of user-defined properties (like the long name, units, etc.). The "hidden" attributes can be shown by adding the **-s** argument to **ncdump**.

CHAPTER

THIRTYONE

PREPARE COARDS-COMPLIANT NETCDF FILES

On this page we discuss how you can generate netCDF data files in the proper format for HEMCO and and GEOS-Chem.

31.1 The COARDS netCDF standard

The Harmonized Emissions Compionent (HEMCO) reads data stored in the netCDF file format, which is a common data format used in atmospheric and climate sciences. NetCDF files contain **data arrays** as well as **metadata**, which is a description of the data.

Several netCDF conventions have been developed in order to facilitate data exchange and visualization. The Cooperative Ocean Atmosphere Research Data Service (COARDS) standard defines regular conventions for naming dimensions as well as the attributes describing the data. You will find more information about these conventions in the sections below. HEMCO requires its input data to be adhere to the COARDS standard.

Our *our "Work with netCDF files" supplemental guide* contains detailed instructions on how you can check a netCDF file for COARDS compliance.

31.2 COARDS dimensions

The **dimensions** of a netCDF file define how many grid boxes there are along a given direction. While the COARDS standard does not require any specific n

ames for dimensions, accepted practice is to use these names for rectilinear grids:

`time`
: Specifies the number of points along the time (`T`) axis.

  The *`time`* dimension must always be specified. When you create the netCDF file, you may declare *`time`* to be `UNLIMITED` and then later define its size. This allows you to append further time points into the file later on.

`lev`
: Specifies the number of points along the vertical level (`Z`) axis.

  This dimension may be omitted none of the data arrays in the netCDF file have a vertical dimension.

`lat`
: Specifies the number of points along the latitude (`Y`) axis.

`lon`
: Specifies the number of points along the longitude (`X`) axis.

Note: For non-rectilinear grids (e.g. cubed-sphere), the *lat* and *lon* dimensions may be named NY and NX instead.

31.3 COARDS coordinate vectors

Coordinate vectors (aka **index variables** or **axis variables**) are 1-dimensional arrays that define the values along each axis.

The only COARDS requirement for coordinate vectors are these:

1. Each coordinate vector must be given the same name as the dimension that is used to define it.
2. All of the values contained within a coordinate vector must be either monotonically increasing or monotonically decreasing.

31.3.1 time

A COARDS-compliant *time* coordinate vector will have these features:

```
dimensions
        time = UNLIMITED ; // (12 currently)
. . .
variables
        double time(time) ;
                time:long_name = "time" ;
                time:units = "hours since 2010-01-01 00:00:00" ;
                time:calendar = "standard" ;
                time:axis = "T";
```

Note: The above was generated by the **ncdump** command.

As you can see, *time* is an 8-byte floating point (aka REAL*8 with 12 time points.

The *time* coordinate vector has following attributes:

time:long_name

A detailed description of the contents of this array. This is usually set to time or Time.

time:units

Specifies the number of hours, minutes, seconds, etc. that has elapsed with respect to a reference datetime YYYY-MM-DD hh:mn:ss. Set this to one of the folllowing values:

- "days since YYYY-MM-DD hh:mn:ss"
- "hours since YYYY-MM-DD hh:mn:ss"
- "minutes since YYYY-MM-DD hh:mn:ss"
- "seconds since YYYY-MM-DD hh:mn:ss"

Tip: We recommend that you choose the reference datetime to correspond to the first time value in the file (i.e. time(0) = 0).

time:calendar

Specifies the calendar used to define the time system. Set this to one of the following values:

standard

Synonym for *gregorian*.

gregorian

Selects the Gregorian calendar system.

time:axis

Identifies the axis (X,Y,Z,T) corresponding to this coordinate vector. Set this to T.

Special considerations for time vectors

1. We recommend that index variables (such as time) be declared with type float or double. GCHP cannot parse files with that have index variables of type int.
2. We have noticed that netCDF files having a *time:units* reference datetime prior to 1900/01/01 00:00:00 may not be read properly when using HEMCO or GCHP within an ESMF environment. We therefore recommend that you use reference datetime values after 1900 whenever possible.
3. Weekly data must contain seven time slices in increments of one day. The first entry must represent Sunday data, regardless of the real weekday of the assigned datetime. It is possible to store weekly data for more than one time interval, in which case the first weekday (i.e. Sunday) must hold the starting date for the given set of (seven) time slices.

   - For instance, weekly data for every month of a year can be stored as 12 sets of 7 time slices. The reference datetime of the first entry of each set must fall on the first day of every month, and the following six entries must be increments of one day.

   Currently, weekly data from netCDF files is not correctly read in an ESMF environment.

31.3.2 lev

A COARDS-compliant *lev* coordinate vector will have these features:

```
dimensions:
        lev = 72 ;
. . .
variables:
        double lev(lev) ;
                lev:long_name = "level" ;
                lev:units = "level" ;
                lev:positive = "up" ;
                lev:axis = "Z" ;
```

Here, *lev* is an 8-byte floating point (aka REAL*8) with 72 levels.

The *lev* coordinate vector has the following attributes:

lev:long_name

A detailed description of the contents of this array. You may set this to values such as:

- "level"
- "GEOS-Chem levels"

- "Eta centers"
- "Sigma centers"

lev:units

(Required) Specifies the units of vertical levels. Set this to one of the following:

- "levels"
- "eta_level"
- "sigma_level"

Important: If you set long_name: to level as well, then HEMCO will be able to regrid between GEOS-Chem vertical grids.

---

lev:axis

Identifies the axis (X,Y,Z,T) corresponding to this coordinate vector. Set this to Z.

lev:positive

Specifies the direction in which the vertical dimension is indexed. Set this to one of these values:

- "up" (Level 1 is the surface, and level indices increase upwards)
- "down" (Level 1 is the atmosphere top, and level indices increase downwards)

For emisisons and most other data sets, you can set *lev:positive* to "up".

Important: GCHP and the NASA GEOS-ESM use a vertical grid where *lev:positive* is "down".

Additional considerations for lev vectors:

When using GEOS-Chem or HEMCO in a non-ESMF environment, data is interpolated onto the simulation levels if the input data is on vertical levels other than the HEMCO model levels (see HEMCO vertical regridding).

Data on non-model levels must be on a hybrid sigma pressure coordinate system. In order to properly determine the vertical pressure levels of the input data, the file must contain the surface pressure values and the hybrid coefficients (a, b) of the coordinate system. Furthermore, the level variable must contain the attributes standard_name and formula_terms (the attribute positive is recommended but not required). A header excerpt of a valid netCDF file is shown below:

```
float lev(lev) ;
    lev:standard_name = "atmosphere_hybrid_sigma_pressure_coordinate" ;
    lev:units = "level" ;
    lev:positive = "down" ;
    lev:formula_terms = "ap: hyam b: hybm ps: PS" ;
float hyam(nhym) ;
    hyam:long_name = "hybrid A coefficient at layer midpoints" ;
    hyam:units = "hPa" ;
float hybm(nhym) ;
    hybm:long_name = "hybrid B coefficient at layer midpoints" ;
    hybm:units = "1" ;
float time(time) ;
    time:standard_name = "time" ;
```

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```
    time:units = "days since 2000-01-01 00:00:00" ;
    time:calendar = "standard" ;
float PS(time, lat, lon) ;
    PS:long_name = "surface pressure" ;
    PS:units = "hPa" ;
float EMIS(time, lev, lat, lon) ;
    EMIS:long_name = "emissions" ;
    EMIS:units = "kg m-2 s-1" ;
```

31.3.3 lat

A COARDS-compliant *lat* coordinate vector will have these features:

```
dimensions:
        lat = 181 ;
variables:``
        double lat(lat) ;
                lat:long_name = "Latitude" ;
                lat:units = "degrees_north" ;
                lat:axis = "Y" ;
```

Here, *lat* is an 8-byte floating point (aka `REAL*8`) with 181 values.

The *lat* coordinate vector has the following attributes:

lat:long_name

A detailed description of the contents of this array. Set this to `Latitude`.

lat:units

Specifies the units of latitude. Set this to `degrees_north`.

lat:axis

Identifies the axis `(X,Y,Z,T)` corresponding to this coordinate vector. Set this to `Y`.

31.3.4 lon

A COARDS-compliant *lat* coordinate vector will have these features:

```
dimensions:
        lon = 360 ;
variables:``
        double lon(lon) ;
                lon:long_name = "Longitude" ;
                lon:units = "degrees_east" ;
                lon:axis = "X" ;
```

Here, *lon* is an 8-byte floating point (aka `REAL*8`) with 360 values.

The *lon* coordinate vector has following attributes:

lon:long_name

A detailed description of the contents of this array. Set this to `Longitude`.

lon:units

Specifies the units of latitude. Set this to `degrees_east`.

lon:axis

Identifies the axis `(X,Y,Z,T)` corresponding to this coordinate vector. Set this to `X`.

Longitudes may be represented modulo 360. For example, -180, 180, and 540 are all valid representations of the International Dateline and 0 and 360 are both valid representations of the Prime Meridian. Note, however, that the sequence of numerical longitude values stored in the netCDF file must be monotonic in a non-modulo sense.

Practical guidelines:

1. If your grid begins at the International Dateline (-180°), then place your longitudes into the range -180..180.
2. If your grid begins at the Prime Meridian (0°), then place your longitudes into the range 0..360.

31.4 COARDS data arrays

A COARDS-compliant netCDF file may contain several **data arrays**. In our example file shown above, there are two data arrays:

```
dimensions:
        time = UNLIMITED ; // (12 currently)
        lev = 72 ;
        lat = 181 ;
        lon = 360 ;
variables:``
        float PRPE(time, lev, lat, lon) ;
                PRPE:long_name = "Propene" ;
                PRPE:units = "kgC/m2/s" ;
                PRPE:add_offset = 0.f ;
                PRPE:missing_value = 1.e+15f ;
        float CO(time, lev, lat, lon) ;``
                CO:long_name = "CO" ;
                CO:units = "kg/m2/s" ;
                CO:_FillValue = 1.e+15f ;
                CO:missing_value = 1.e+15f ;
```

These arrays contain emissions for species tracers PRPE (lumped < C3 alkenes) and CO.

31.4.1 Attributes for data arrays

long_name

Gives a detailed description of the contents of the array.

units

Specifies the units of data contained within the array. SI units are preferred.

Special usage for HEMCO:

- Use `kg/m2/s` or `kg m-2 s-1` for emission fluxes of species
- Use `kg/m3` or `kg m-3` for concentration data;
- Use `1` for dimensionless data instead of `unitless`. HEMCO will recognize `unitless`, but it is non-standard and not recommended.

missing_value

Specifies the value that should represent missing data. This should be set to a number that will not be mistaken for a valid data value.

_FillValue

Synonym for *missing_value*. It is recommended to set both *missing_value* and *_FillValue* to the same value. Some data visualization packages look for one but not the other.

31.4.2 Ordering of the data

2D and 3D array variables in netCDF files must have specific dimension order. If the order is incorrect you will encounter netCDF read error "start+count exceeds dimension bound". You can check the dimension ordering of your arrays by using the **ncdump** command as shown below:

```
$ ncdump file.nc -h
```

Be sure to check the dimensions listed next to the array name rather than the ordering of the dimensions listed at the top of the **ncdump** output.

The following dimension orders are acceptable:

```
array(time,lat,lon)
array(time,lat,lon,lev)
```

The rest of this section explains why the dimension ordering of arrays matters.

When you use **ncdump** to examine the contents of a netCDF file, you will notice that it displays the dimensions of the data in the opposite order with respect to Fortran. In our sample file, **ncdump** says that the CO and PRPE arrays have these dimensions:

```
CO(time,lev,lat,lon)
PRPE(time,lev,lat,lon)
```

But if you tried to read this netCDF file into GEOS-Chem (or any other program written in Fortran), you must use data arrays that have these dimensions:

```
CO(lon,lat,lev,time)
PRPE(lon,lat,lev,time)
```

Here's why:

Fortran is a **column-major** language, which means that arrays are stored in memory by columns first, then by rows. If you have declared an arrays such as:

```
INTEGER            :: I, J, L, T
INTEGER, PARAMETER :: N_LON  = 360
INTEGER, PARAMETER :: N_LAT  = 181
INTEGER, PARAMETER :: N_LEV  = 72
INTEGER, PARAMTER  :: N_TIME = 12
REAL*4             :: CO  (N_LON,N_LAT,N_LEV,N_TIME)
REAL*4             :: PRPE(N_LON,N_LAT,N_LEV,N_TIME)
```

then for optimal efficiency, the leftmost dimension (`I`) needs to vary the fastest, and needs to be accessed by the innermost DO-loop. Then the next leftmost dimension (`J`) should be accessed by the next innermost DO-loop, and so on. Therefore, the proper way to loop over these arrays is:

```
DO T = 1, N_TIME
DO L = 1, N_LEV
DO J = 1, N_LAT
DO I = 1, N_LON
   CO  (I,J,L,N) = ...
   PRPE(I,J,L,N) = ...
ENDDO
ENDDO
ENDDO
ENDDO
```

Note that the `I` index is varying most often, since it is the innermost DO-loop, then `J`, `L`, and `T`. This is opposite to how a car's odometer reads.

If you loop through an array in this fashion, with leftmost indices varying fastest, then the code minimizes the number of times it has to load subsections of the array into cache memory. In this optimal manner of execution, all of the array elements sitting in the cache memory are read in the proper order before the next array subsection needs to be loaded into the cache. But if you step through array elements in the wrong order, the number of cache loads is proportionally increased. Because it takes a finite amount of time to reload array elements into cache memory, the more times you have to access the cache, the longer it will take the code to execute. This can slow down the code dramatically.

On the other hand, C is a **row-major** language, which means that arrays are stored by rows first, then by columns. This means that the outermost do loop (`I`) is varying the fastest. This is identical to how a car's odometer reads.

If you use a Fortran program to write data to disk, and then try to read that data from disk into a program written in C, then unless you reverse the order of the DO loops, you will be reading the array in the wrong order. In C you would have to use this ordering scheme (using Fortran-style syntax to illustrate the point):

```
DO I = 1, N_LON
DO J = 1, N_LAT
DO L = 1, N_LEV
DO T = 1, N_TIME
   CO(T,L,J,I)   = ...
   PRPE(T,L,J,I) = ...
ENDDO
ENDDO
ENDDO
ENDDO
```

Because **ncdump** is written in C, the order of the array appears opposite with respect to Fortran. The same goes for any other code written in a row-major programming language.

31.5 COARDS Global attributes

Global attributes are netCDF attributes that contain information about a netCDF file, as opposed to information about an individual data array.

From our example in the *Examine the contents of a netCDF file*, the output from **ncdump** showed that our sample netCDF file has several global attributes:

```
// global attributes:
            :Title = "COARDS/netCDF file containing X data"
            :Contact = "GEOS-Chem Support Team (geos-chem-support@as.harvard.edu)" ;
```

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```
            :References = "www.geos-chem.org; wiki.geos-chem.org" ;
            :Conventions = "COARDS" ;
            :Filename = "my_sample_data_file.1x1"
            :History = "Mon Mar 17 16:18:09 2014 GMT" ;
            :ProductionDateTime = "File generated on: Mon Mar 17 16:18:09 2014 GMT" ;
            :ModificationDateTime = "File generated on: Mon Mar 17 16:18:09 2014 GMT" ;
            :VersionID = "1.2" ;
            :Format = "NetCDF-3" ;
            :Model = "GEOS5" ;
            :Grid = "GEOS_1x1" ;
            :Delta_Lon = 1.f ;
            :Delta_Lat = 1.f ;
            :SpatialCoverage = "global" ;
            :NLayers = 72 ;
            :Start_Date = 20050101 ;
            :Start_Time = 00:00:00.0 ;
            :End_Date = 20051231 ;
            :End_Time = 23:59:59.99999 ;
```

Title (or title)

Provides a short description of the file.

Contact (or contact)

Provides contact information for the person(s) who created the file.

References (or references)

Provides a reference (citation, DOI, or URL) for the data contained in the file.

Conventions (or conventions)

Indicates if the netCDF file adheres to a standard (e.g. COARDS or CF).

Filename (or filename)

Specifies the name of the file.

History (or history)

Specifies the datetime of file creation, and of any subsequent modifications.

Note: If you edit the file with **nco** or **cdo**, then this attribute will be updated to reflect the modification that was done.

Format (or format)

Specifies the format of the netCDF file (such as `netCDF-3` or `netCDF-4`).

31.6 For more information

Please see our *Work with netCDF files* Supplemental Guide for more information about commands that you can use to combine, edit, or maniuplate data in netCDF files.

CHAPTER

THIRTYTWO

VIEW GEOS-CHEM SPECIES PROPERTIES

Properties for GEOS-Chem species are stored in the **GEOS-Chem Species Database**, which is a YAML file (`species_database.yml`) that is placed into each GEOS-Chem run directory.

View species properties from the current stable GEOS-Chem version:

- View properties for most GEOS-Chem species
- View properties for APM microphysics species
- View properties for TOMAS microphysics species
- View properties for Hg simulation species

32.1 Species properties defined

The following sections contain a detailed description of GEOS-Chem species properties.

32.1.1 Required default properties

All GEOS-Chem species should have these properties defined:

```
      Name:
        FullName: full name of the species
        Formula: chemical formula of the species
        MW_g: molecular weight of the species in grams
EITHER  Is_Gas: true
OR      Is_Aerosol: true
```

All other properties are species-dependent. You may omit properties that do not apply to a given species. GEOS-Chem will assign a "missing value" (e.g. `false`, `-999`, `-999.0`, or, `UNKNOWN`) to these properties when it reads the `species_database.yml` file from disk.

32.1.2 Identification

Name

Species short name (e.g. `ISOP`).

Formula

Species chemical formula (e.g. `CH2=C(CH3)CH=CH2`). This is used to define the species' `formula` attribute, which gets written to GEOS-Chem diagnostic files and restart files.

FullName

Species long name (e.g. `Isoprene`). This is used to define the species' `long_name` attribute, which gets written to GEOS-Chem diagnostic files and restart files.

Is_Aerosol

Indicates that the species is an aerosol (`true`), or isn't (`false`).

Is_Advected

Indicates that the species is advected (`true`), or isn't (`false`).

Is_DryAlt

Indicates that dry deposition diagnostic quantities for the species can be archived at a specified altitude above the surface (`true`), or can't (`false`).

Note: The `Is_DryAlt` flag only applies to species `O3` and `HNO3`.

Is_DryDep

Indicates that the species is dry deposited (`true`), or isn't (`false`).

Is_HygroGrowth

Indicates that the species is an aerosol that is capable of hygroscopic growth (`true`), or isn't (`false`).

Is_Gas

Indicates that the species is a gas (`true`), or isn't (`false`).

Is_Hg0

Indicates that the species is elemental mercury (`true`), or isn't (`false`).

Is_Hg2

Indicates that the species is a mercury compound with oxidation state +2 (`true`), or isn't (`false`).

Is_HgP

Indicates that the species is a particulate mercury compound (`true`), or isn't (`false`).

Is_Photolysis

Indicates that the species is photolyzed (`true`), or isn't (`false`).

Is_RadioNuclide

Indicates that the species is a radionuclide (`true`), or isn't (`false`).

32.1.3 Physical properties

Density
Density ($kg\ m^{-3}$) of the species. Typically defined only for aerosols.

Henry_K0
Henry's law solubility constant ($M\ atm^{-1}$), used by the default wet depositon scheme.

Henry_K0_Luo
Henry's law solubility constant ($M\ atm^{-1}$) used by the Luo *et al.* [2020] wet deposition scheme.

Henry_CR
Henry's law volatility constant (K) used by the default wet deposition scheme.

Henry_CR_Luo
Henry's law volatility constant (K) used by the Luo *et al.* [2020] wet deposition scheme.

Henry_pKa
Henry's Law pH correction factor.

MW_g
Molecular weight ($g\ mol^{-1}$) of the species.

Note: Some aerosol-phase species (such as MONITA and IONITA) are given the molar mass corresponding to the number of nitrogens that they carry, whereas gas-phase species (MONITS and MONITU) get the full molar mass of the compounds that they represent. This treatment has its origins in J. Fisher et al [2016].

Radius
Radius (m) of the species. Typically defined only for aerosols.

32.1.4 Dry deposition properties

DD_AeroDryDep
Indicates that dry deposition should consider hygroscopic growth for this species (`true`), or shouldn't (`false`).

Note: `DD_AeroDryDep` is only defined for sea salt aerosols.

DD_DustDryDep
Indicates that dry deposition should exclude hygroscopic growth for this species (`true`), or shouldn't (`false`).

Note: `DD_DustDryDep` is only defined for mineral dust aerosols.

DD_DvzAerSnow
Specifies the dry deposition velocity ($cm\ s^{-1}$) over ice and snow for certain aerosol species. Typically, `DD_DvzAerSnow = 0.03`.

DD_DvzAerSnow_Luo
Specifies the dry deposition velocity ($cm\ s^{-1}$) over ice and snow for certain aerosol species.

Note: `DD_DvzAerSnow_Luo` is only used when the Luo *et al.* [2020] wet scavenging scheme is activated.

DD_DvzMinVal

Specfies minimum dry deposition velocities ($cm\ s^{-1}$) for sulfate species (SO2, SO4, MSA, NH3, NH4, NIT). This follows the methodology of the GOCART model.

DD_DvzMinVal is defined as a two-element vector:

- DD_DvzMinVal(1) sets a minimum dry deposition velocity onto snow and ice.
- DD_DvzMinVal(2) sets a minimum dry deposition velocity over land.

DD_Hstar_Old

Specifies the Henry's law constant (K_0) that is used in dry deposition. This will be used to assign the HSTAR variable in the GEOS-Chem dry deposition module.

Note: The value of the DD_Hstar_old parameter was tuned for each species so that the dry deposition velocity would match observations.

DD_F0

Specifies the reactivity factor for oxidation of biological substances in dry deposition.

DD_KOA

Specifies the octanal-air partition coefficient, used for the dry deposition of species POPG.

Note: DD_KOA is only used in the POPs simulation.

32.1.5 Wet deposition properties

WD_Is_H2SO4

Indicates that the species is H2SO4 (true), or isn't (false). This allows the wet deposition code to perform special calculations when computing H2SO4 rainout and washout.

WD_Is_HNO3

Indicates that the species is HNO3 (true), or isn't (false). This allows the wet deposition code to perform special calculations when computing HNO3. rainout and washout.

WD_Is_SO2

Indicates that the species is SO2 (true), or isn't (false). This allows the wet deposition code to perform special calculations when computing SO2 rainout and washout.

WD_CoarseAer

Indicates that the species is a coarse aerosol (true), or isn't (false). For wet deposition purposes, the definition of coarse aerosol is radius > 1 μm.

WD_LiqAndGas

Indicates that the the ice-to-gas ratio can be computed for this species by co-condensation (true), or can't (false).

WD_ConvFacI2G

Specifies the conversion factor (i.e. ratio of sticking coefficients on the ice surface) for computing the ice-to-gas ratio by co-condensation, as used in the default wet deposition scheme.

Note: WD_ConvFacI2G only needs to be defined for those species for which WD_LiqAndGas is true.

WD_ConvFacI2G_Luo

Specifies the conversion factor (i.e. ratio of sticking coefficients on the ice surface) for computing the ice-to-gas ratio by co-condensation, as used in the Luo *et al.* [2020] wet deposition scheme.

Note: `WD_ConvFacI2G_Luo` only needs to be defined for those species for which `WD_LiqAndGas` is `true`, and is only used when the Luo *et al.* [2020] wet deposition scheme is activated.

WD_RetFactor

Specifies the retention efficiency R_i of species in the liquid cloud condensate as it is converted to precipitation. R_i < 1 accounts for volatization during riming.

WD_AerScavEff

Specifies the aerosol scavenging efficiency. This factor multiplies F, the fraction of aerosol species that is lost to convective updraft scavenging.

- `WD_AerScavEff = 1.0` for most aerosols.
- `WD_AerScavEff = 0.8` for secondary organic aerosols.
- `WD_AerScavEff = 0.0` for hydrophobic aerosols.

WD_KcScaleFac

Specifies a temperature-dependent scale factor that is used to multiply K (aka K_c), the rate constant for conversion of cloud condensate to precipitation.

`WD_KcScaleFac` is defined as a 3-element vector:

- `WD_KcScaleFac(1)` multiplies K when $T < 237$ kelvin.
- `WD_KcScaleFac(2)` multiplies K when $237 \leq T < 258$ kelvin
- `WD_KcScaleFac(3)` multiplies K when $T \geq 258$ kelvin.

WD_KcScaleFac_Luo

Specifies a temperature-dependent scale factor that is used to multiply K, aka K_c, the rate constant for conversion of cloud condensate to precipitation.

Used only in the Luo *et al.* [2020] wet deposition scheme.

`WD_KcScaleFac_Luo` is defined as a 3-element vector:

- `WD_KcScaleFac_Luo(1)` multiplies K when $T < 237$ kelvin.
- `WD_KcScaleFac_Luo(2)` multiplies K when $237 \leq T < 258$ kelvin.
- `WD_KcScaleFac_Luo(3)` multiplies K when $T \geq 258$ kelvin.

WD_RainoutEff

Specifies a temperature-dependent scale factor that is used to multiply F_i (aka `RAINFRAC`), the fraction of species scavenged by rainout.

`WD_RainoutEff` is defined as a 3-element vector:

- `WD_RainoutEff(1)` multiplies F_i when $T < 237$ kelvin.
- `WD_RainoutEff(2)` multiplies F_i when $237 \leq T < 258$ kelvin.
- `RainoutEff(3)` multiplies F_i when $T \geq 258$ kelvin.

This allows us to better simulate scavenging by snow and impaction scavenging of BC. For most species, we need to be able to turn off rainout when $237 \leq T < 258$ kelvin. This can be easily done by setting `RainoutEff(2) = 0`.

Note: For SOA species, the maximum value of `WD_RainoutEff` will be 0.8 instead of 1.0.

`WD_RainoutEff_Luo`

Specifies a temperature-dependent scale factor that is used to multiply F_i (aka `RAINFRAC`), the fraction of species scavenged by rainout. (Used only in the [Luo *et al.*, 2020] wet deposition scheme).

`WD_RainoutEff_Luo` is defined as a 3-element vector:

- `WD_RainoutEff_Luo(1)` multiplies F_i when $T < 237$ kelvin.
- `WD_RainoutEff_Luo(2)` multiplies F_i when $237 \leq T < 258$ kelvin.
- `RainoutEff_Luo(3)` multiplies F_i when $T \geq 258$ kelvin.

This allows us to better simulate scavenging by snow and impaction scavenging of BC. For most species, we need to be able to turn off rainout when $237 \leq T < 258$ kelvin. This can be easily done by setting `RainoutEff(2) = 0`.

Note: For SOA species, the maximum value of `WD_RainoutEff_Luo` will be 0.8 instead of 1.0.

32.1.6 Transport tracer properties

These properties are defined for species used in the TransportTracers simulation. We will refer to these species as **tracers**.

`Is_Tracer`

Indicates that the species is a transport tracer (`true`), or is not (`false`).

`Snk_Horiz`

Specifies the horizontal domain of the tracer sink term. Allowable values are:

`all`

The tracer sink term will be applied throughout the entire horizonatal domain of the simulation grid.

`lat_zone`

The tracer sink term will be applied only within the latitude range specified by *`Snk_Lats`*.

`Snk_Lats`

Defines the latitude range `[min_latitude, max_latitude]` for the tracer sink term. Will only be used if *`Snk_Horiz`* is set to `lat_zone`.

`Snk_Mode`

Specifies how the tracer sink term will be applied. Allowable values are:

`constant`

The tracer sink term is a constant value (specified by *`Snk_Value`*).

`efolding`

The tracer sink term has an e-folding decay constant (specified in *`Snk_Period`*).

`halflife`

A tracer sink term has a half-life (specified in *`Snk_Period`*).

`none`

The tracer does not have a sink term.

Snk_Period

Specifies the period (in days) for which the tracer sink term will be applied.

Snk_Value

Specifies a value for the tracer sink term.

Snk_Vert

Specifies the vertical domain of the tracer sink term. Allowable values are:

all

The tracer sink term will be applied throughout the entire vertical domain of the simulation grid.

boundary_layer

The tracer sink term will only be applied within the planetary boundary layer.

surface

The tracer sink term will only be applied at the surface.

troposphere

The tracer sink term will only be applied within the troposphere.

Src_Add

Specifies whether the tracer has a source term (`true`) or not (`false`).

Src_Horiz

Specifies the horizontal domain of the tracer source term. Allowable values are:

all

The tracer source term will be applied across the entire horizontal extent of the simulation grid.

lat_zone

The tracer source term will only be applied within the latitude range specified by *Src_Lats*.

Src_Lats

Defines the latitude range `[min_latitude, max_latitude]` for the tracer source term. Will only be applied if *Src_Horiz* is set to `lat_zone`.

Src_Mode

Describes the type of tracer source term. Allowable values are:

constant

The tracer source term is a constant value (specified by *Src_Value*).

decay_of_another_species

The tracer source term comes from the decay of another species (e.g. Pb210 source comes from Rn222 decay).

HEMCO

The tracer source term will be read from a file via HEMCO.

maintain_mixing_ratio

The tracer source term will be calculated as needed to maintain a constant mixing ratio at the surface.

none

The tracer does not have a source term.

Src_Unit

Specifies the unit of the source term that will be applied to the tracer.

ppbv

The source term has units of parts per billion by volume.

timestep

The source term has units of per emissions timestep.

Src_Value

Specifies a value for the tracer source term in *Src_Unit*.

Src_Vert

Specifies the vertical domain of the tracer source term. Allowable values are:

all

The tracer source term will be applied throughout the entire vertical domain of the simulation grid.

pressures

The tracer source term will only be applied within the pressure range specified in *Src_Pressures*.

stratosphere

The tracer source term will only be applied in the stratosphere.

troposphere

The tracer source term will only be applied in the troposphere.

surface

The tracer source term will only be applied at the surface.

Src_Pressures

Defines the pressure range `[min_pressure, max_pressure]`, in hPa for the tracer source term. Will only be used if *Src_Vert* is set to `pressures`.

Units

Specifies the default units of the tracers (e.g. `aoa`, `aoa_nh`, `aoa_bl` are carried in units `days`, while all other species in GEOS-Chem are `kg/kg dry air`).

Properties used by each transport tracer

The list below shows the various *transport tracer properties* that are used in the current TransportTracers simulation.

```
Is_Tracer
 - true                    : all

Snk_Horiz:
 - lat_zone                : aoa_nh
 - all                     : all others

Snk_Lats
 - 30 50                   : aoa_nh

Snk_Mode
 - constant                : aoa, aoa_bl, aoa_nh
 - efolding                : CH3I, CO_25
 - none                    : SF6
 - halflife                : Be7, Be7s, Be10, Be10s
```

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```
Snk_Period (days)
 - 5                        : CH3I
 - 25                       : CO_25
 - 50                       : CO_50
 - 90                       : e90, e90_n, e90_s
 - 11742.8                  : Pb210, Pb210s
 - 5.5                      : Rn222
 - 53.3                     : Be7, Be7s
 - 5.84e8                   : Be10, Be10s

Snk_Value
 - 0                        : aoa, aoa_bl, aoa_nh

Snk_Vert
 - boundary_layer           : aoa_bl
 - surface                  : aoa, aoa_nh
 - troposphere              : stOx
 - all                      : all others

Src_Add
 - false                    : Passive, stOx, st80_25
 - true                     : all others

Src_Horiz
 - lat_zone                 : e90_n, e90_s, nh_5, nh_50
 - all                      : all others

Src_Lats
 - [ 40.0,   91.0]          : e90_n
 - [-91.0,  -40.0]          : e90_s
 - [ 30.0,   50.0]          : nh_5, nh_50

Src_Mode
 - constant                 : aoa, aoa_bl, aoa_nh, nh_50, nh_5, st80_25
 - file2d                   : CH3I, CO_25, CO_50, Rn222, SF6  - HEMCO
 - file3d                   : Be10, Be7                       - HEMCO
 - maintain_mixing_ratio    : e_90, e90_n, e90_s
 - decay_of_another_species : Pb210, Pb210s

Src_Unit
 - ppbv                     : e90, e90_n, e90_s, st80_25
 - timestep                 : aoa, aoa_bl, aoa_nh

Src_Value
 - 1                        : aoa, aoa_bl, aoa_nh
 - 100                      : e90, e90_n, e90_s
 - 200                      : st80_25

Src_Vert
 - all                      : aoa, aoa_bl, aoa_nh, Pb210
 - pressures                : st80_25
 - stratosphere             : Be10s, Be7s, Pb210s, stOx
```

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```
 - surface                  : all others (not specified when Src_Mode: HEMCO)

Src_Pressures
 - [0, 80]                  : st80_25

Units
 - days                     : aoa, aoa_bl, aoa_bl
```

32.1.7 Other properties

BackgroundVV

If a restart file does not contain an global initial concentration field for a species, GEOS-Chem will attempt to set the initial concentration (in $vol\ vol^{-1}$ dry air) to the value specified in `BackgroundVV` globally. But if `BackgroundVV` has not been specified, GEOS-Chem will set the initial concentration for the species to $10^{-20} vol\ vol^{-1}$ dry air instead.

Note: Recent versions of GCHP may require that all initial conditions for all species to be used in a simulation be present in the restart file. See gchp.readthedocs.io for more information.

MP_SizeResAer

Indicates that the species is a size-resolved aerosol species (`true`), or isn't (`false`). Used only by simulations using either APM or TOMAS microphysics packages.

MP_SizeResNum

Indicates that the species is a size-resolved aerosol number (`true`), or isn't (`false`). Used only by simulations using either APM or TOMAS microphysics packages.

32.2 Access species properties in GEOS-Chem

In this section we will describe the derived types and objects that are used to store GEOS-Chem species properties. We will also describe how you can extract species properties from the GEOS-Chem Species Database when you create new GEOS-Chem code routines.

32.2.1 The Species derived type

The Species derived type (defined in module `Headers/species_mod.F90`) describes a complete set of properties for a single GEOS-Chem species. In addition to the fields mentioned in the preceding sections, the `Species` derived type also contains several species indices.

Table 1: Indices stored in the `Species` derived type

Index	Description
`ModelId`	Model species index
`AdvectId`	Advected species index
`AerosolId`	Aerosol species index
`DryAltId`	Dry dep species at altitude Id
`DryDepId`	Dry deposition species index
`GasSpcId`	Gas-phase species index
`HygGrthId`	Hygroscopic growth species index
`KppVarId`	KPP variable species index
`KppFixId`	KPP fixed spcecies index
`KppSpcId`	KPP species index
`PhotolId`	Photolyis species index
`RadNuclId`	Radionuclide index
`TracerId`	Transport tracer index
`WetDepId`	Wet deposition index

32.2.2 The SpcPtr derived type

The SpcPtr derived type (also defined in `Headers/species_mod.F90`) describes a container for an object of type *Species*.

```
TYPE, PUBLIC :: SpcPtr
   TYPE(Species), POINTER :: Info   ! Single entry of Species Database
END TYPE SpcPtr
```

32.2.3 The GEOS-Chem Species Database object

The GEOS-Chem Species database is stored in the `State_Chm%SpcData` object. It describes an array, where each element of the array is of type *SpcPtr* (which is a container for an object of type type *Species*.

```
TYPE(SpcPtr),  POINTER :: SpcData(:)   ! GC Species database
```

32.2.4 Species index lookup with Ind_()

Use function `Ind_()` (in module `Headers/state_chm_mod.F90`) to look up species indices by name. For example:

```
SUBROUTINE MySub( ..., State_Chm, ... )

   USE State_Chm_Mod, ONLY : Ind_

   ! Local variables
   INTEGER  :: id_O3, id_Br2, id_CO

   ! Find tracer indices with function the Ind_() function
   id_O3   = Ind_( 'O3'  )
   id_Br2  = Ind_( 'Br2' )
   id_CO   = Ind_( 'CO'  )
```

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```
   ! Print tracer concentrations
   print*, 'O3  at (23,34,1) : ', State_Chm%Species(id_O3 )%Conc(23,34,1)
   print*, 'Br2 at (23,34,1) : ', State_Chm%Species(id_Br2)%Conc(23,34,1)
   print*, 'CO  at (23,34,1) : ', State_Chm%Species(id_CO )%Conc(23,34,1)

   ! Print the molecular weight of O3 (obtained from the Species Database object)
   print*, 'Mol wt of O3 [g]: ', State_Chm%SpcData(id_O3)%Info%MW_g

END SUBROUTINE MySub
```

Once you have obtained the species ID (aka `ModelId`) you can use that to access the individual fields in the Species Database object. In the example above, we use the species ID for `O3` (stored in `id_O3`) to look up the molecular weight of `O3` from the Species Database.

You may search for other model indices with `Ind_()` by passing an optional second argument:

```
! Position of HNO3 in the list of advected species
AdvectId = Ind_( 'HNO3',  'A' )

! Position of HNO3 in the list of gas-phase species
AdvectId = Ind_( 'HNO3',  'G' )

! Position of HNO3 in the list of dry deposited species
DryDepId = Ind_( 'HNO3',  'D' )

! Position of HNO3 in the list of wet deposited species
WetDepId = Ind_( 'HNO3',  'W' )

! Position of HNO3 in the lists of fixed KPP, active, & overall KPP species
KppFixId = Ind_( 'HNO3',  'F' )
KppVarId = Ind_( 'HNO3',  'V' )
KppVarId = Ind_( 'HNO3',  'K' )

! Position of SALA in the list of hygroscopic growth species
HygGthId = Ind_( 'SALA',  'H' )

! Position of Pb210 in the list of radionuclide species
HygGthId = Ind_( 'Pb210', 'N' )

! Position of ACET in the list of photolysis species
PhotolId = Ind( 'ACET',   'P' )
```

`Ind_()` will return -1 if a species does not belong to any of the above lists.

Tip: For maximum efficiency, we recommend that you use `Ind_()` to obtain the species indices during the initialization phase of a GEOS-Chem simulation. This will minimize the number of name-to-index lookup operations that need to be performed, thus reducing computational overhead.

Implementing the tip mentioned above:

```
MODULE MyModule

  IMPLICIT NONE
  . . .

  ! Species ID of CO.  All subroutines in MyModule can refer to id_CO.
  INTEGER, PRIVATE :: id_CO

CONTAINS

  . . .  other subroutines  . . .

  SUBROUTINE Init_MyModule

    ! This subroutine only gets called at startup

    . . .

    ! Store ModelId in the global id_CO variable
    id_CO = Ind_('CO')

    . . .

  END SUBROUTINE Init_MyModule

END MODULE MyModule
```

32.2.5 Species lookup within a loop

If you need to access species properties from within a loop, it is better not to use the `Ind_()` function, as repeated name-to-index lookups will incur computational overhead. Instead, you can access the species properties directly from the GEOS-Chem Species Database object, as shown here.

```
SUBROUTINE MySub( ..., State_Chm, ... )

   !%%% MySub is an example of species lookup within a loop %%%

   ! Uses
   USE Precision_Mod
   USE State_Chm_Mod, ONLY : ChmState
   USE Species_Mod,   ONLY : Species

   ! Chemistry state object (which also holds the species database)
   TYPE(ChmState), INTENT(INOUT) :: State_Chm

   ! Local variables
   INTEGER                       :: N
   TYPE(Species),  POINTER       :: ThisSpc
   INTEGER                       :: ModelId,  DryDepId, WetDepId
   REAL(fp)                      :: Mw_g
   REAL(f8)                      :: Henry_K0, Henry_CR, Henry_pKa
```

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```
  ! Loop over all species
  DO N = 1, State_Chm%nSpecies

     ! Point to the species database entry for this species
     ! (this makes the coding simpler)
     ThisSpc   => State_Chm%SpcData(N)%Info

     ! Get species properties
     ModelId   =  ThisSpc%ModelId
     DryDepId  =  ThisSpc%DryDepId
     WetDepId  =  ThisSpc%WetDepId
     MW_g      =  ThisSpc%MW_g
     Henry_K0  =  ThisSpc%Henry_K0
     Henry_CR  =  ThisSpc%Henry_CR
     Henry_pKa =  ThisSpc%Henry_pKA


     IF ( ThisSpc%Is_Gas )
        ! ... The species is a gas-phase species
        ! ... so do something appropriate
     ELSE
        ! ... The species is an aerosol
        ! ... so do something else appropriate
     ENDIF

     IF ( ThisSpc%Is_Advected ) THEN
        ! ... The species is advected
        ! ... (i.e. undergoes transport, PBL mixing, cloud convection)
     ENDIF

     IF ( ThisSpc%Is_DryDep ) THEN
        ! ... The species is dry deposited
     ENDIF

     IF ( ThisSpc%Is_WetDep ) THEN
        ! ... The species is soluble and wet deposits
        ! ... it is also scavenged in convective updrafts
        ! ... it probably has defined Henry's law properties
     ENDIF

     ... etc ...

     ! Free the pointer
     ThisSpc =>  NULL()

   ENDDO

END SUBROUTINE MySub
```

CHAPTER

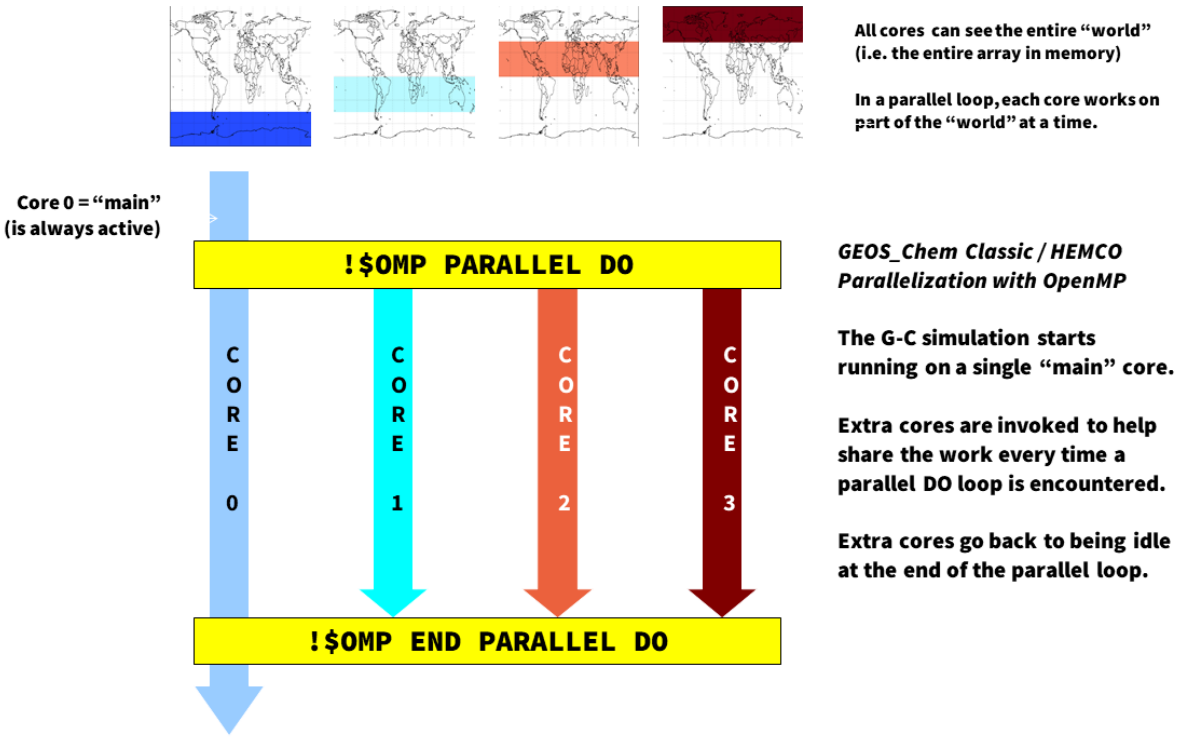
THIRTYTHREE

PARALLELIZE GEOS-CHEM AND HEMCO SOURCE CODE

Single-node paralellization in GEOS-Chem Classic and HEMCO is acheieved with OpenMP. OpenMP directives, which are included in every modern compiler, allow you to divide the work done in DO loops among several computational cores. In this Guide, you will learn more about how GEOS-Chem Classic and HEMCO utilize OpenMP.

33.1 Overview of OpenMP parallelization

Most GEOS-Chem and HEMCO arrays represent quantities on a geospatial grid (such as meteorological fields, species concentrations, production and loss rates, etc.). When we parallelize the GEOS-Chem and HEMCO source code, we give each computational core its own region of the "world" to work on, so to speak. However, all cores can see the entire "world" (i.e. the entire memory on the machine) at once, but is just restricted to working on its own region of the "world".



It is important to remember that OpenMP is **loop-level parallelization**. That means that only commands within selected DO loops will execute in parallel. GEOS-Chem Classic and HEMCO (when running within GEOS-Chem Classic, or as the HEMCO standalone) start off on a single core (known as the "main core"). Upon entering a parallel DO loop,

other cores will be invoked to share the workload within the loop. At the end of the parallel DO loop, the other cores return to standby status and the execution continues only on the "main" core.

One restriction of using OpenMP parallelization is that simulations may use only as many cores that share by the same memory. In practice, this limits GEOS-Chem Classic and HEMCO standalone simulations to using 1 node (typically less than 64 cores) of a shared computer cluster.

We should also note that GEOS-Chem High Performance (aka GCHP) uses a *different type of parallelization (MPI)*. This allows GCHP to use hundreds or thousands of cores across several nodes of a computer cluster. We encourage you to consider using GCHP for hour high-resolution simulations.

33.2 Example using OpenMP directives

Consider the following nested loop that has been parallelized with OpenMP directives:

```
!$OMP PARALLEL DO            &
!$OMP SHARED( A            ) &
!$OMP PRIVATE( I, J, B     ) &
!$OMP COLLAPSE( 2          ) &
!$OMP SCHEDULE( DYNAMIC, 4 )
DO J = 1, NY
DO I = 1, NX
   B = A(I,J)
   A(I,J) = B * 2.0
ENDDO
ENDDO
!$OMP END PARALLEL DO
```

This loop will assign different `(I,J)` pairs to different computational cores. The more cores specified, the less time it will take to do the operation.

Let us know look at the important features of this loop.

`!$OMP` `PARALLEL DO`

This is known as a **loop sentinel**. It tells the compiler that the following DO-loop is to be executed in parallel. The **clauses** following the sentinel specify further options for the parallelization. These clauses may be spread across multiple lines by using a continuation command (&) at the end of the line.

`!$OMP` `SHARED( A )`

This clause tells the compiler that all computational cores can write to `A` simultaneously. This is OK because each core will recieve a unique set of `(I,J)` pairs. Thus data corruption of the `A` array will not happen. We say that `A` is a **SHARED** variable.

Note: We recommend using the clause `!$OMP DEFAULT( SHARED )`, which will declare all varaiables as shared, unless they are explicitly placed in an `!$OMP PRIVATE` clause.

`!$OMP` `PRIVATE( I, J, B )`

Because different cores will be handling different `(I,J)` pairs, each core needs its own private copy of variables `I` and `J`. The compiler creates these temporary copies of these variables in memory "under the hood".

If the `I` and `J` variables were not declared `PRIVATE`, then all of the computational cores could simultaneously write to `I` and `J`. This would lead to data corruption. For the same reason, we must also place the variable `B` within the `!$OMP PRIVATE` clause.

`!$OMP COLLAPSE( 2 )`

By default, OpenMP will parallelize the outer loop in a set of nested loops. To gain more efficiency, we can vectorize the loop. "Under the hood", the compiler can convert the two nested loops over `NX` and `NY` into a single loop of size `NX * NY`, and then parallelize over the single loop. Because we wish to collapse 2 loops together, we use the `!$OMP COLLAPSE( 2 )` statement.

`!$OMP SCHEDULE( DYNAMIC, 4 )`

Normally, OpenMP will evenly split the domain to be parallelized (i.e. `(NX, NY)`) evenly between the cores. But if some computations take longer than others (i.e. photochemistry at the day/night boundary), this static scheduling may be inefficient.

The `SCHEDULE( DYNAMIC, 4 )` will send groups of 4 grid boxes to each core. As soon as a core finishes its work, it will immediately receive another group of 4 grid boxes. This can help to achieve better load balancing.

`!$OMP END PARALLEL DO`

This is a sentinel that declares the end of the parallel DO loop. It may be omitted. But we encourage you to include them, as defining both the beginning and end of a parallel loop is good programming style.

33.3 Environment variable settings for OpenMP

Please see Set environment variables for parallelization to learn which environment variables you must add to your login environment to control OpenMP parallelization.

33.4 OpenMP parallelization FAQ

Here are some frequently asked questions about parallelizing GEOS-Chem and HEMCO code with OpenMP:

33.4.1 How can I tell what should go into the !$OMP PRIVATE clause?

Here is a good rule of thumb:

> All variables that appear on the left side of an equals sign, and that have lower dimensionality than the dimensionality of the parallel loop must be placed in the `!$OMP PRIVATE` clause.

In the *example shown above*, `I`, `J`, and `B` are scalars, so their dimensionality is 0. But the parallelization occurs over two DO loops (`1..NY` and `1..NX`), so the dimensionality of the parallelization is 2. Thus `I`, `J`, and `B` must go inside the `!$OMP PRIVATE` clause.

Tip: You can also think of dimensionality as the number of indices a variable has. For example `A` has dimensionality 0, but `A(I)` has dimensionality 1, `A(I,J)` has dimensionality 2, etc.

33.4.2 Why do the !$OMP statements begin with a comment character?

This is by design. In order to invoke the parallel procesing commands, you must use a specific compiler command (such as `-openmp`, `-fopenmp`, or similar, depending on the compiler). If you omit these compiler switches, then the parallel processing directives will be considered as Fortran comments, and the associated DO-loops will be executed on a single core.

33.4.3 Do subroutine variables have to be declared PRIVATE?

Consider this subroutine:

```
SUBROUTINE mySub( X, Y, Z )

   ! Dummy variables for input
   REAL, INTENT(IN)  :: X, Y

   ! Dummy variable for output
   REAL, INTENT(OUT) :: Z

   ! Add X + Y to make Z
   Z = X + Y

END SUBROUTINE mySub
```

which is called from within a parallel loop:

```
INTEGER :: N
REAL    :: A, B, C

!$OMP PARALLEL DO           &
!$OMP DEFAULT( SHARED     ) &
!$OMP PRIVATE( N, A, B, C )
DO N = 1, nIterations

   ! Get inputs from some array
   A = Input(N,1)
   B = Input(N,2)

   ! Add A + B to make C
   CALL mySub( A, B, C )

   ! Save the output in an array
   Output(N) = C
ENDDO
!$OMP END PARALLEL DO
```

Using the *rule of thumb described above*, because `N`, `A`, `B`, and `C` are scalars (having dimensionality = 0), they must be placed in the `!$OMP PRIVATE` clause.

But note that the variables `X`, `Y`, and `Z` do not need to be placed within a `!$OMP PRIVATE` clause within subroutine `mySub`. This is because each core calls `mySub` in a separate thread of execution, and will create its own private copy of `X`, `Y`, and `Z` in memory.

33.4.4 What does the THREADPRIVATE statement do?

Let's modify the *above example* slightly. Let's now suppose that subroutine `mySub` from the prior example is now part of a Fortran-90 module, which looks like this:

```
MODULE myModule

  ! Module variable:
  REAL, PUBLIC :: Z

CONTAINS

  SUBROUTINE mySub( X, Y )

   ! Dummy variables for input
   REAL, INTENT(IN)  :: X, Y

   ! Add X + Y to make Z
   ! NOTE that Z is now a global variable
   Z  = X + Y

  END SUBROUTINE mySub

END MODULE myModule
```

Note that `Z` is now a global scalar variable with dimensionality = 0. Let's now use the same parallel loop (dimensionality = 1) as before:

```
! Get the Z variable from myModule
USE myModule, ONLY : Z

INTEGER :: N
REAL    :: A, B, C

!$OMP PARALLEL DO           &
!$OMP DEFAULT( SHARED     ) &
!$OMP PRIVATE( N, A, B, C )
DO N = 1, nIterations

   ! Get inputs from some array
   A = Input(N,1)
   B = Input(N,2)

   ! Add A + B to make C
   CALL mySub( A, B )

   ! Save the output in an array
   Output(N) = Z

ENDDO
!$OMP END PARALLEL DO
```

Because `Z` is now a global variable with lower dimensionality than the loop, we must try to place it within an `!$OMP PRIVATE` clause. However, `Z` is defined in a different program unit than where the parallel loop occurs, so we cannot

place it in an `!$OMP PRIVATE` clause for the loop.

In this case we must place `Z` into an `!$OMP THREADPRIVATE` clause within the module where it is declared, as shown below:

```
MODULE myModule

  ! Module variable:
  ! This is global and acts as if it were in a F77-style common block
  REAL, PUBLIC :: Z
  !$OMP THREADPRIVATE( Z )

  ... etc ...
```

This tells the computer to create a separate private copy of `Z` in memory for each core.

Important: When you place a variable into an `!$OMP PRIVATE` or `!$OMP THREADPRIVATE` clause, this means that the variable will have no meaning outside of the parallel loop where it is used. So you should not rely on using the value of `PRIVATE` or `THREADPRIVATE` variables elsewhere in your code.

Most of the time you won't have to use the `!$OMP THREADPRIVATE` statement. You may need to use it if you are trying to parallelize code that came from someone else.

33.4.5 Can I use pointers within an OpenMP parallel loop?

You may use pointer-based variables (including derived-type objects) within an OpenMP parallel loop. But you must make sure that you point to the target within the parallel loop section AND that you also nullify the pointer within the parallel loop section. For example:

INCORRECT:

```
! Declare variables
REAL, TARGET  :: myArray(NX,NY)
REAL, POINTER :: myPtr  (:    )

! Declare an OpenMP parallel loop
!$OMP PARALLEL DO                    ) &
!$OMP DEFAULT( SHARED                ) &
!$OMP PRIVATE( I, J, myPtr, ...etc... )
DO J = 1, NY
DO I = 1, NX

   ! Point to a variable.
   !This must be done in the parallel loop section.
   myPtr => myArray(:,J)

   . . . do other stuff . . .

ENDDO
!$OMP END PARALLEL DO

! Nullify the pointer.
```

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```
! NOTE: This is incorrect because we nullify the pointer outside of the loop.
myPtr => NULL()
```

CORRECT:

```
! Declare variables
REAL, TARGET  :: myArray(NX,NY)
REAL, POINTER :: myPtr  (:    )

! Declare an OpenMP parallel loop
!$OMP PARALLEL DO                    ) &
!$OMP DEFAULT( SHARED                ) &
!$OMP PRIVATE( I, J, myPtr, ...etc... )
DO J = 1, NY
DO I = 1, NX

   ! Point to a variable.
   !This must be done in the parallel loop section.
   myPtr => myArray(:,J)

   . . . do other stuff . . .

   ! Nullify the pointer within the parallel loop
   myPtr => NULL()

ENDDO
!$OMP END PARALLEL DO
```

In other words, pointers used in OpenMP parallel loops only have meaning within the parallel loop.

33.4.6 How many cores may I use for GEOS-Chem or HEMCO?

You can use as many computational cores as there are on a single node of your cluster. With OpenMP parallelization, the restriction is that all of the cores have to see all the memory on the machine (or node of a larger machine). So if you have 32 cores on a single node, you can use them. We have shown that run times will continue to decrease (albeit asymptotically) when you increase the number of cores.

33.4.7 Why is GEOS-Chem is not using all the cores I requested?

The number of threads for an OpenMP simulation is determined by the environment variable OMP_NUM_THREADS. You must define `OMP_NUM_THREADS` in your environment file to specify the desired number of computational cores for your simulation. For the `bash` shell, use4 this command to request 8 cores:

```
export OMP_NUM_THREADS=8
```

33.5 MPI parallelization

The *OpenMP parallelization* used by GEOS-Chem Classic and HEMCO standalone is an example of **shared memory parallelization** (also known as **serial parallelization**). As we have seen, we are restricted to using a single node of a computer cluster. This is because all of the cores need to talk with all of the memory on the node.

On the other hand, MPI (Message Passing Interface) parallelzation is an example of **distributed parallelization**. An MPI library installation is required for passing memory from one physical system to another (i.e. across nodes).

GEOS-Chem High Performance (GCHP) uses Earth System Model Framework (ESMF) and MAPL libraries to implement MPI parallelization. For detailed information, please see gchp.readthedocs.io.

CHAPTER

THIRTYFOUR

RUN NESTED-GRID SIMULATIONS

A **nested-grid simulation** is a GEOS-Chem Classic simulation running at the native horizontal resolution of the GEOS-FP (0.25° x 0.3125°) or MERRA-2 (0.5° x 0.6125°) meteorology fields over a subset of the globe. Nested-grid simulations use boundary conditions for transport that are archived from a global simulatoin.

Follow these steps to set up a GEOS-Chem Classic nested-grid simulation:

34.1 Run a global simulation to create boundary conditions

34.1.1 1. Download the GEOS-Chem source code

Download the GEOS-Chem Classic source code by *following these instructions*.

34.1.2 2. Create a global simulation run directory

Create a run directory for your global simulation by executing these commands:

```
$ cd /path/to/GCClassic/run   # or whatever you named the source code directory
$ ./createRunDir.sh
```

and then follow the prompts.

Tip: A 4° x 5° global simulation should be adequate for producing boundary condition output.

34.1.3 3. Activate the BoundaryConditions diagnostic collection

The `BoundaryConditions` diagnostic collection is deactivated by default in the *HISTORY.rc configuration file* that ships with the run directory. Activate this collection by removing the comment character (#) as shown below.

```
COLLECTIONS: 'Restart',
             'SpeciesConc',
             ... etc ...
             #'BoundaryConditions',    <== Remove the # sign in front
::
```

The `BoundaryConditions` collection will save out instantaneous concentrations of advected species every three hours to daily files. You may change those settings by modifying the BoundaryConditions collection section in the *HISTORY.rc* file.

Tip: If you wish to save disk space, Use the `.LON_RANGE` and `.LAT_RANGE` to reduce the size of the region in which the boundary conditions will be saved. The region in which the boundary condition is archived should be a little larger than the nested-grid simulation window.

```
#============================================================================
# %%%%% THE BoundaryConditions COLLECTION %%%%%
#
# GEOS-Chem boundary conditions for use in nested grid simulations
#
# Available for all simulations
#============================================================================
  BoundaryConditions.template:   '%y4%m2%d2_%h2%n2z.nc4',
  BoundaryConditions.format:     'CFIO',
  BoundaryConditions.frequency:  00000000 030000
  BoundaryConditions.duration:   00000001 000000
  BoundaryConditions.mode:       'instantaneous'
  BoundaryConditions.LON_RANGE:  -130.0 -60.0,
  BoundaryConditions.LAT_RANGE:   10.0 60.0,
  BoundaryConditions.fields:     'SpeciesBC_?ADV?             ', 'GIGCchem',
::
```

34.1.4 4. Configure the global simulation

Configure your global simulation by *changing settings in the relevant configuration files*. If you do not need the output from your global simulation, you may choose to turn off most of the diagnostic output in `HISTORY.rc` and `HEMCO_Diagn.rc`.

Tip: Turn off most diagnostic output in the *HISTORY.rc* and *HEMCO_Diagn.rc* files. This will minimize the run time and reduce the size of diagnostic ouptut.

34.1.5 5. Compile GEOS-Chem and run the global simulation

Follow the steps outlined in these sections to compile and run your GEOS-Chem global simulation.

1. *Compile the source code*
2. *Download input data* (e.g. do a dry-run and download data if necessary)
3. *Run your simulation*

Once your global simulation finishes, the boundary conditions files will be placed into the `OutputDir` subdirectory of your run directory. You should see files named `GEOSChem.BoundaryConditions.YYYYMMDD_0000z.nc4` (where `YYYYMMDD` are replaced by the simulation date) begin to appear in your run directory as your simulation runs. You will need to tell your nested-grid simulation where to find these files.

34.2 Set up your nested grid run directory

34.2.1 1. Create a nested-grid simulation run directory

Using the same GEOS-Chem Classic source code directory that *we downloaded above* follow these steps to *create a run directory* for your nested-grid simulation.

```
$ cd /path/to/GCClassic/run   # or whatever you named the source code directory
$ ./createRunDir.sh
```

Select the native resolution corresponding to your choice of meteorology. You will then be asked to specify which nested region you would like to use.

34.2.2 2. Configure your nested-grid simulation

Check the *run-directory configuration files* to make sure that you have the same chemistry, emissions, transport, etc. options selected as in the global simulation.

In *HEMCO_Config.rc*, make sure the `GC_BCs` option is set to `true` and update the `BC_` entry to point to your boundary condition files.

```
# ExtNr ExtName                 on/off  Species
0       Base                    : on    *
# ----- RESTART FIELDS ----------------------
    --> GC_RESTART              :       true
    --> GC_BCs                  :       true    <== make sure this is true
    --> HEMCO_RESTART           :       true
...
#==============================================================================
# --- GEOS-Chem boundary condition file ---
#==============================================================================
(((GC_BCs
* BC_  /path/to/your/GEOSChem.BoundaryConditions.$YYYY$MM$DD_$HH$MNz.nc4 SpeciesBC_?ADV?␣
↪ 1980-2023/1-12/1-31/0-23 RFY xyz 1 * - 1 1
)))GC_BCs
```

Activate your preferred diagnostics by changing the relevant settings in these configuration files:

1. *The HISTORY.rc configuration file*
2. *HEMCO_Diagn.rc*
3. *Planeflight.dat.YYYYMMDD*
4. *The ObsPack menu of geoschem_config.yml*

34.2.3 3. Copy the executable to the nested-grid run directory

You do not have to recompile GEOS-Chem Classic when changing grids. Therefore, you can copy the `gcclassic` executable from your *global simulation* run directory to your nested-grid run directory.

34.2.4 4. Run the nested-grid simulation

Follow the steps outlined in these sections to run your nested-grid simulation.

1. *Download input data* (e.g. do a dry-run and download data if necessary)
2. *Run your simulation*

34.3 Frequently asked questions

34.3.1 Can I run nested GEOS-Chem simulations on the AWS cloud?

Yes, you can run the nested grid simulations on AWS cloud. Please see the Running GEOS-Chem on AWS cloud online tutorial and contact the GEOS-Chem Support Team with any questions.

34.3.2 Can I save out boundary conditions for more than one nested grid in the same global run?

We recommend that you *generate boundary conditions* over the entire global domain (at 4° x 5° or 2° x 2.5°). Then these boundary conditions can be used as input to simulations on different nested domains.

34.3.3 How can I find which data are available for nested grid simulations?

You can browse the contents of the GEOS-Chem data portals by pointing your browser to one of the following links:

- *GEOS-Chem Input Data*
  - https://geos-chem.s3.amazonaws.com/index.html
- *GEOS-Chem Nested Input Data*
  - https://gcgrid.s3.amazonaws.com/index.html
- *GCAP 2.0 meteorology @ U. Rochester*
  - http://atmos.earth.rochester.edu/input/gc/ExtData/

34.3.4 Where can I find out more info about nested grid errors?

Please see the following Supplemental Guides:

1. *Understand what error messages mean*
2. *Debug GEOS-Chem and HEMCO errors*

34.3.5 I noticed abnormal concentrations at boundaries of the nested region. Is that normal?

If you see high tracer concentrations right at the boundary of your nested grid region, then this may be normal.

For nested grid simulations, we have to leave a "buffer zone" (i.e. typically 3 boxes along each boundary) in which the TPCORE advection is not applied. However, all other operations (chemistry, wetdep, drydep, convection, PBL mixing) will be applied. Therefore, in the "buffer zone", the concentrations will not be realistic because the advection is not allowed to transport the tracer out of these boxes.

In any case, the tracer concentrations in the "buffer zone" will get overwritten by the 2° x 2.5° or 4° x 5° boundary conditions at the specified time (usually every 3h).

Attention: You should exclude the boxes in the "buffer zone" from your scientific analysis.

The following diagram illustrates this:

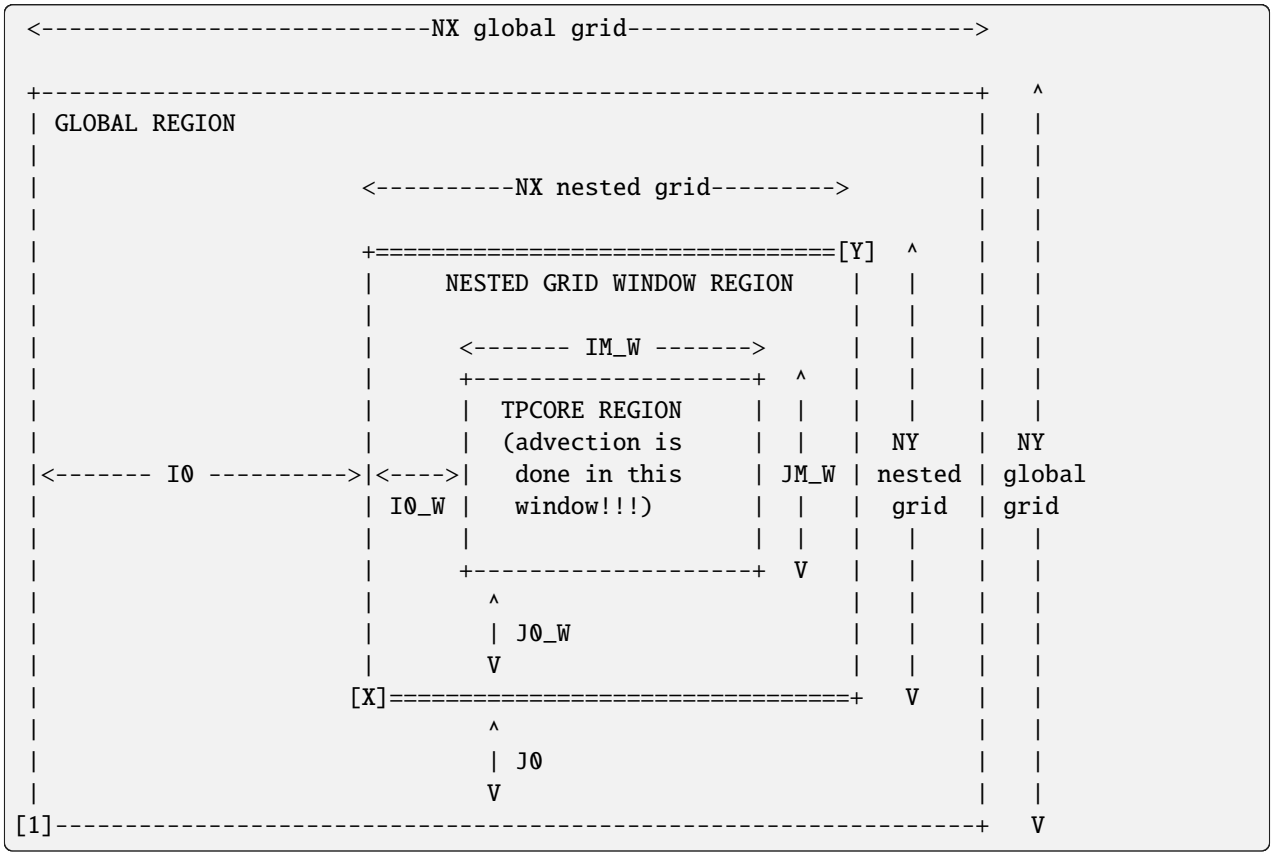

Diagram notes:

1. The outermost box (`GLOBAL REGION`) is the global grid size. This region has `NX global grid` boxes in longitude and `NY global grid` boxes in latitude. The origin of the `GLOBAL REGION`" is at the south pole, at the lower left-hand corner (point `[1]`).
2. The next innermost box (`NESTED GRID WINDOW REGION`) is the nested-grid window. This region has `NX nested grid` boxes in longitude and `NY nested grid` boxes in latitude. This is the size of the trimmed met fields that will be used for a "nested-grid" simulation.
3. The innermost region `TPCORE REGION` is the actual area in which **`TPCORE`** advection will be performed. Note

that this region is smaller ehan the NESTED GRID WINDOW REGION. It is set up this way since a cushion of grid boxes is needed for boundary conditions.

4. I0 is the longitude offset (# of boxes) and J0 is the latitude offset (# of boxes) which translate between the GLOBAL REGION and the NESTED GRID WINDOW REGION.

5. I0_W is the longitude offset (# of boxes), and J0_W is the latitude offset (# of boxes) which translate between the NESTED GRID WINDOW REGION and the TPCORE REGION. These define the thickness of the buffer zone mentioned above.

6. The lower left-hand corner of the NESTED GRID WINDOW REGION (point [X]) has longitude and latitude indices (I1_W, J1_W). Similarly, the upper right-hand corner (point [Y]) has longitude and latitude indices (I2_W, J2_W).

7. Note that if I0=0, J0=0, I0_W=0, J0_W=0, NX nested grid = NX global grid, NY nested grid = NY global grid specifies a global simulation. In this case the NESTED GRID WINDOW REGION totally coincides with the GLOBAL REGION.

8. In order for the nested-grid simulation to work we must save out concentrations over the NESTED GRID WINDOW REGION from a coarse model (e.g. 2° x 2.5° or 4° x 5°). These concentrations are copied along the edges of the NESTED GRID WINDOW REGION and are thus used as boundary conditions for **TPCORE**.

CHAPTER

THIRTYFIVE

UPDATE CHEMICAL MECHANISMS WITH KPP

This Guide demonstrates how you can use The Kinetic PreProcessor (aka KPP) to translate a chemical mechanism specification in plain text format to highly-optimized Fortran90 code for use with GEOS-Chem:

Attention: You must use at least KPP 3.2.0 with the current GEOS-Chem release series.

35.1 Using KPP: Quick start

35.1.1 1. Navigate to the KPP/custom folder within GEOS-Chem

The `KPP/custom` folder is intended for building customized mechanisms. (The standard mechanisms that ship with GEOS-Chem are contained in other folders named `KPP/fullchem` and `KPP/Hg`, but we will leave these alone.)

If you are using GEOS-Chem "Classic", type:

```
$ cd GCClassic/src/GEOS-Chem/KPP/custom
```

or if you are using GCHP, type:

```
$ cd GCHP/GCHP_GridComp/GEOSChem_GridComp/geos-chem/KPP/custom
```

35.1.2 2. Edit the chemical mechanism configuration files

The `KPP/custom` folder contains sample chemical mechanism specification files (*custom.eqn* and *custom.kpp*). These files define the chemical mechanism and are copies of the default **`fullchem`** mechanism configuration files found in the `KPP/fullchem` folder. (For a complete description of KPP configuration files, please see the documentation at kpp.readthedocs.io.)

You can edit these *custom.eqn* and *custom.kpp* configuration files to define your own custom mechanism (cf. *Using KPP: Reference section* for details).

Important: We recommend always building a custom mechanism from the `KPP/custom` folder, and to leave the other folders untouched. This will allow you to validate your modified mechanism against one of the standard mechanisms that ship with GEOS-Chem.

custom.eqn

The `custom.eqn` configuration file contains:

- List of active species
- List of inactive species
- Gas-phase reactions
- Heterogeneous reactions
- Photolysis reactions

custom.kpp

The `custom.kpp` configuration file is the main configuration file. It contains:

- Solver options
- Production and loss family definitions
- Functions to compute reaction rates
- Global definitions
- An **`#INCLUDE custom.eqn`** command, which tells **KPP** to look for chemical reaction definitions in *custom.eqn*.

Important: The symbolic link `gckpp.kpp` points to `custom.kpp`. This is necessary in order to generate Fortran files with the the naming convention `gckpp*.F90`.

35.1.3 3. Run the build_mechanism.sh script

Once you are satisfied with your custom mechanism specification you may now use KPP to build the source code files for GEOS-Chem.

Return to the top-level `KPP` folder from `KPP/custom`:

```
$ cd ..
```

There you will find a script named `build_mechanism.sh`, which is the driver script for running **KPP**. Execute the script as follows:

```
$ ./build_mechanism.sh custom
```

This will run the **KPP** executable (located in the folder `$KPP_HOME/bin`) `custom.kpp` configuration file (via symbolic link `gckpp.kpp`, It also runs a python script to generate code for the OH reactivity diagnostic. You should see output similar to this:

```
This is KPP-X.Y.Z.

KPP is parsing the equation file.
KPP is computing Jacobian sparsity structure.
KPP is starting the code generation.
KPP is initializing the code generation.
KPP is generating the monitor data:
```

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```
  - gckpp_Monitor
KPP is generating the utility data:
  - gckpp_Util
KPP is generating the global declarations:
  - gckpp_Main
KPP is generating the ODE function:
  - gckpp_Function
KPP is generating the ODE Jacobian:
  - gckpp_Jacobian
  - gckpp_JacobianSP
KPP is generating the linear algebra routines:
  - gckpp_LinearAlgebra
KPP is generating the utility functions:
  - gckpp_Util
KPP is generating the rate laws:
  - gckpp_Rates
KPP is generating the parameters:
  - gckpp_Parameters
KPP is generating the global data:
  - gckpp_Global
KPP is generating the driver from none.f90:
  - gckpp_Main
KPP is starting the code post-processing.

KPP has succesfully created the model "gckpp".

Reactivity consists of xxx reactions    # NOTE: xxx will be replaced by the actual number
Written to gckpp_Util.F90
```

where `X.Y.Z` denotes the **KPP** version that you are using.

If this process is successful, the `custom` folder will have several new files starting with `gckpp`:

```
$ ls gckpp*
gckpp_Function.F90    gckpp_Jacobian.F90       gckpp.log             gckpp_Precision.F90
gckpp_Global.F90      gckpp_JacobianSP.F90     gckpp_Model.F90       gckpp_Rates.F90
gckpp_Initialize.F90  gckpp.kpp@               gckpp_Monitor.F90     gckpp_Util.F90
gckpp_Integrator.F90  gckpp_LinearAlgebra.F90  gckpp_Parameters.F90
```

The `gckpp*.F90` files contain optimized Fortran-90 instructions for solving the chemical mechanism that you have specified. The `gckpp.log` file is a human-readable description of the mechanism. Also, `gckpp.kpp` is a symbolic link to the `custom.kpp` file.

A complete description of these KPP-generated files at kpp.readthedocs.io.

35.1.4 4. Recompile GEOS-Chem with your custom mechanism

GEOS-Chem will always use the default mechanism (which is named `fullchem`). To tell GEOS-Chem to use the `custom` mechanism instead, follow these steps.

Tip: GEOS-Chem Classic run directories have a subdirectory named `build` in which you can configure and build GEOS-Chem. If you don't have a build directory, you can add one to your run directory with **`mkdir build`**.

From the build directory, type:

```
$ cmake ../CodeDir -DMECH=custom -DRUNDIR=..
```

You should see output similar to this written to the screen:

```
-- General settings:
   * MECH:  fullchem  carbon  Hg  **custom**
```

This confirms that the custom mechanism has been selected.

Once you have configured **GEOS-Chem** to use the `custom` mechanism, you may build the exectuable. Type:

```
$ make -j
$ make -j install
```

The executable file (`gcclassic` or `gchp`, depending on which mode of GEOS-Chem that you are using) will be placed in the run directory.

35.2 Using KPP: Reference section

35.2.1 Adding species to a mechanism

List chemically-active (aka variable) species in the #DEFVAR section of `custom.eqn`, as shown below:

```
#DEFVAR
A3O2       = IGNORE; {CH3CH2CH2OO; Primary RO2 from C3H8}
ACET       = IGNORE; {CH3C(O)CH3; Acetone}
ACTA       = IGNORE; {CH3C(O)OH; Acetic acid}
...etc ...
```

The `IGNORE` tells KPP not to perform mass-balance checks, which would make GEOS-Chem execute more slowly.

List species whose concentrations do not change in the #DEFFIX section of `custom.eqn`, as shown below:

```
#DEFFIX
H2         = IGNORE; {H2; Molecular hydrogen}
N2         = IGNORE; {N2; Molecular nitrogen}
O2         = IGNORE; {O2; Molecular oxygen}
... etc ...
```

Species may be listed in any order, but we have found it convenient to list them alphabetically.

35.2.2 Adding reactions to a mechanism

Gas-phase reactions

List gas-phase reactions first in the #EQUATIONS section of `custom.eqn`.

```
#EQUATIONS
//
// Gas-phase reactions
//
...skipping over the comment header...
//
O3 + NO = NO2 + O2 :                          GCARR_ac(3.00E-12, -1500.0);
O3 + OH = HO2 + O2 :                          GCARR_ac(1.70E-12, -940.0);
O3 + HO2 = OH + O2 + O2 :                     GCARR_ac(1.00E-14, -490.0);
O3 + NO2 = O2 + NO3 :                         GCARR_ac(1.20E-13, -2450.0);
... etc ...
```

Gas-phase reactions: General form

No matter what reaction is being added, the general procedure is the same. A new line must be added to `custom.eqn` of the following form:

```
A + B = C + 2.000D : RATE_LAW_FUNCTION(ARG_A, ARG_B ...);
```

The denotes the reactants (A and B) as well as the products (C and D) of the reaction. If exactly one molecule is consumed or produced, then the factor can be omitted; otherwise the number of molecules consumed or produced should be specified with at least 1 decimal place of accuracy. The final section, between the colon and semi-colon, specifies the function `RATE_LAW_FUNCTION` and its arguments which will be used to calculate the reaction rate constant k. Rate-law functions are specified in the `custom.kpp` file.

For an equation such as the one above, the overall rate at which the reaction will proceed is determined by $k[A][B]$. However, if the reaction rate does not depend on the concentration of A or B, you may write it with a constant value, such as:

```
A + B = C + 2.000D : 8.95d-17
```

This will save the overhead of a function call.

Rates for two-body reactions according to the Arrhenius law

For many reactions, the calculation of k follows the Arrhenius law:

```
k = a0 * ( 300 / TEMP )**b0 * EXP( c0 / TEMP )
```

Important: In relation to Arrhenius parameters that you may find in scientific literature, a_0 represents the A term and c_0 represents $-E/R$ (not E/R, which is usually listed).

For example, the JPL chemical data evaluation), (Feb 2017) specifies that the reaction O3 + NO produces NO2 and O2, and its Arrhenius parameters are A = 3.0x10^-12 and E/R = 1500. To use the Arrhenius formulation above, we must specify $a_0 = 3.0e-12$ and $c_0 = -1500$.

To specify a two-body reaction whose rate follows the Arrhenius law, you can use the GCARR rate-law function, which is defined in gckpp.kpp. For example, the entry for the $O3 + NO = NO2 + O2$ reaction can be written as in custom.eqn as:

```
O3 + NO = NO2 + O2 : GCARR(3.00E12, 0.0, -1500.0);
```

Other rate-law functions

The gckpp.kpp file contains other rate law functions, such as those required for three-body, pressure-dependent reactions. Any rate function which is to be referenced in the custom.eqn file must be available in gckpp.kpp prior to building the reaction mechanism.

Making your rate law functions computationally efficient

We recommend writing your rate-law functions so as to avoid explicitly casting variables from REAL*4 to REAL*8. Code that looks like this:

```
REAL, INTENT(IN) :: A0, B0, C0
rate = DBLE(A0) + ( 300.0 / TEMP )**DBLE(B0) + EXP( DBLE(C0)/ TEMP )
```

Can be rewritten as:

```
REAL(kind=dp), INTENT(IN) :: A0, B0, C0
rate = A0 + ( 300.0d0 / TEMP )**B0 + EXP( C0/ TEMP )
```

Not only do casts lead to a loss of precision, but each cast takes a few CPU clock cycles to execute. Because these rate-law functions are called for each cell in the chemistry grid, wasted clock cycles can accumulate into a noticeable slowdown in execution.

You can also make your rate-law functions more efficient if you rewrite them to avoid computing terms that evaluate to 1. We saw above (cf. *Rates for two-body reactions according to the Arrhenius law*) that the rate of the reaction $O3+NO = NO2+O2$ can be computed according to the Arrhenius law. But because b0 = 0, term (300/TEMP)**b0 evaluates to 1. We can therefore rewrite the computation of the reaction rate as:

```
k = 3.0x10^-12 + EXP( 1500 / TEMP )
```

Tip: The EXP() and ** mathematical operations are among the most costly in terms of CPU clock cycles. Avoid calling them whenever necessary.

A recommended implementation would be to create separate rate-law functions that take different arguments depending on which parameters are nonzero. For example, the Arrhenius law function GCARR can be split into multiple functions:

1. GCARR_abc(a0, b0, c0): Use when a0 > 0 and b0 > 0 and c0 > 0
2. GCARR_ab(a0, b0): Use when a0 > 0 and b0 > 0
3. GCARR_ac(a0, c0): Use when a0 > 0 and c0 > 0

Thus we can write the O3 + NO reaction in custom.eqn as:

```
O3 + NO = NO2 + O2 : GCARR_ac(3.00d12, -1500.0d0);
```

using the rate law function for when both a0 > 0 and c0 > 0.

35.2.3 Heterogeneous reactions

List heterogeneous reactions after all of the gas-phase reactions in `custom.eqn`, according to the format below:

```
//
// Heterogeneous reactions
//
HO2 = O2 :                                  HO2uptk1stOrd( State_Het );           {2013/
↪03/22; Paulot2009; FP,EAM,JMAO,MJE}
NO2 = 0.500HNO3 + 0.500HNO2 :               NO2uptk1stOrdAndCloud( State_Het );
NO3 = HNO3 :                                NO3uptk1stOrdAndCloud( State_Het );
NO3 = NIT :                                 NO3hypsisClonSALA( State_Het );       {2018/
↪03/16; XW}
... etc ...
```

A simple example is uptake of HO2, specified as

```
HO2 = H2O : HO2uptk1stOrd( State_Het );
```

Note: KPP requires that each reaction have at least one product. In order to satisfy this requirement, you might need to set the product of your heterogeneous reaction to a dummy product or a fixed species (i.e. one whose concentration does not change with time).

The rate law function `NO2uptk1stOrd` is contained in the Fortran module `KPP/fullchem/fullchem_RateLawFuncs.F90`, which is symbolically linked to the `custom` folder. The `fullchem_RateLawFuncs.F90` file is inlined into `gckpp_Rates.F90` so that it can be used within the custom mechanism.

To implement an additional heterogeneous reaction, the rate calculation must be added to the `KPP/custom/custom.eqn` file. Rate calculations may be specified as mathematical expressions (using any of the variables contained in the `gckpp_Global.F90`)

```
SPC1 + SPC2 = SPC3 + SPC4: 8.0e-13 * TEMP_OVER_K300;  {Example}
```

or you may define a new rate law function in the `fullchem_RateLawFuncs.F90` such as:

```
SPC1 + SPC2 = SPC3 + SPC4: myNewRateFunction( State_Het ); {Example}
```

35.2.4 Photolysis reactions

List photolysis reactions after the heterogeneous reactions, as shown below.

```
//
// Photolysis reactions
//
O3 + hv = O + O2 :                          PHOTOL(2);      {2014/02/03; Eastham2014;␣
↪SDE}
O3 + hv = O1D + O2 :                        PHOTOL(3);      {2014/02/03; Eastham2014;␣
↪SDE}
O2 + hv = 2.000O :                          PHOTOL(1);      {2014/02/03; Eastham2014;␣
↪SDE}
... etc ...
NO3 + hv = NO2 + O :                        PHOTOL(12);     {2014/02/03; Eastham2014;␣
```

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```
↪SDE}
... etc ...
```

A photolysis reaction can be specified by giving the correct index of the `PHOTOL` array. This index can be determined by inspecting the file `FJX_j2j.dat`.

Tip: See the photolysis section of `geoschem_config.yml` to determine the path to the `cloudj_input_dir` folder in which the `FJX_j2j.dat` and `FJX_spec.dat` files are stored.

For example, one branch of the NO_3 photolysis reaction is specified in the `custom.eqn` file as

```
NO3 + hv = NO2 + O : PHOTOL(12)
```

Referring back to `FJX_j2j.dat` shows that reaction 12, as specified by the left-most index, is indeed $NO_3 = NO2 + O$:

```
12 NO3       PHOTON    NO2       O                          0.886 /NO3   /
```

If your reaction is not already in `FJX_j2j.dat`, you may add it there. You may also need to modify `FJX_spec.dat` (in the same folder ast `FJX_j2j.dat`) to include cross-sections for your species. Note that if you add new reactions to `FJX_j2j.dat` you will also need to set the parameter `JVN_` in Cloud-J module `Cloud-J/src/Core/cldj_cmn_mod.F90` to match the total number of entries.

If your reaction involves new cross section data, you will need to follow an additional set of steps. Specifically, you will need to:

1. Estimate the cross section of each wavelength bin (using the correlated-k method), and
2. Add this data to the `FJX_spec.dat` file.

For the first step, you can use tools already available on the Prather research group website. To generate the cross-sections used by Fast-JX, download the file UCI_fastJ_addX_73cx.tar.gz. You can then simply add your data to `FJX_spec.dat` and refer to it in `FJX_j2j.dat` as specified above. The following then describes how to generate a new set of cross-section data for the example of some new species MEKR:

To generate the photolysis cross sections of a new species, come up with some unique name which you will use to refer to it in the `FJX_j2j.dat` and `FJX_spec.dat` files - e.g. MEKR. You will need to copy one of the `addX_*.f` routines and make your own (say, `addX_MEKR.f`). Your edited version will need to read in whatever cross section data you have available, and you'll need to decide how to handle out-of-range information - this is particularly crucial if your cross section data is not defined in the visible wavelengths, as there have been some nasty problems in the past caused by implicitly assuming that the XS can be extrapolated (I would recommend buffering your data with zero values at the exact limits of your data as a conservative first guess). Then you need to compile that as a standalone code and run it; this will spit out a file fragment containing the aggregated 18-bin cross sections, based on a combination of your measured/calculated XS data and the non-contiguous bin subranges used by Fast-JX. Once that data has been generated, just add it to `FJX_spec.dat` and refer to it as above. There are examples in the addX files of how to deal with variations of cross section with temperature or pressure, but the main takeaway is that you will generate multiple cross section entries to be added to `FJX_spec.dat` with the same name.

Important: If your cross section data varies as a function of temperature AND pressure, you need to do something a little different. The acetone XS documentation shows one possible way to handle this; Fast-JX currently interpolates over either T or P, but not both, so if your data varies over both simultaneously then this will take some thought. The general idea seems to be that one determines which dependence is more important and uses that to generate a set of 3 cross sections (for interpolation), assuming values for the unused variable based on the standard atmosphere.

35.2.5 Adding production and loss families to a mechanism

Certain common families (e.g. PO_x, LO_x) have been pre-defined for you. You will find the family definitions near the top of the `custom.kpp` file (which is symbolically linked to `gckpp.kpp`):

```
#FAMILIES
POx : O3 + NO2 + 2NO3 + PAN + PPN + MPAN + HNO4 + 3N2O5 + HNO3 + BrO + HOBr + BrNO2 +␣
↪2BrNO3 + MPN + ETHLN + MVKN + MCRHN + MCRHNB + PROPNN + R4N2 + PRN1 + PRPN + R4N1 +␣
↪HONIT + MONITS + MONITU + OLND + OLNN + IHN1 + IHN2 + IHN3 + IHN4 + INPB + INPD + ICN␣
↪+ 2IDN + ITCN + ITHN + ISOPNOO1 + ISOPNOO2 + INO2B + INO2D + INA + IDHNBOO + IDHNDOO1␣
↪+ IDHNDOO2 + IHPNBOO + IHPNDOO + ICNOO + 2IDNOO + MACRNO2 + ClO + HOCl + ClNO2 +␣
↪2ClNO3 + 2Cl2O2 + 2OClO + O + O1D + IO + HOI + IONO + 2IONO2 + 2OIO + 2I2O2 + 3I2O3 +␣
↪4I2O4;
LOx : O3 + NO2 + 2NO3 + PAN + PPN + MPAN + HNO4 + 3N2O5 + HNO3 + BrO + HOBr + BrNO2 +␣
↪2BrNO3 + MPN + ETHLN + MVKN + MCRHN + MCRHNB + PROPNN + R4N2 + PRN1 + PRPN + R4N1 +␣
↪HONIT + MONITS + MONITU + OLND + OLNN + IHN1 + IHN2 + IHN3 + IHN4 + INPB + INPD + ICN␣
↪+ 2IDN + ITCN + ITHN + ISOPNOO1 + ISOPNOO2 + INO2B + INO2D + INA + IDHNBOO + IDHNDOO1␣
↪+ IDHNDOO2 + IHPNBOO + IHPNDOO + ICNOO + 2IDNOO + MACRNO2 + ClO + HOCl + ClNO2 +␣
↪2ClNO3 + 2Cl2O2 + 2OClO + O + O1D + IO + HOI + IONO + 2IONO2 + 2OIO + 2I2O2 + 3I2O3 +␣
↪4I2O4;
PCO : CO;
LCO : CO;
PSO4 : SO4;
LCH4 : CH4;
PH2O2 : H2O2;
```

Note: The PO_x, LO_x, PCO, and LCO families are used for computing budgets in the GEOS-Chem benchmark simulations. $PSO4$ is required for simulations using TOMAS aerosol microphysics.

To add a new prod/loss family, add a new line to the `#FAMILIES` section with the format

```
FAM_NAME : MEMBER_1 + MEMBER_2 + ... + MEMBER_N;
```

The family name must start with `P` or `L` to indicate whether KPP should calculate a production or a loss rate. You will also need to make a corresponding update to the *GEOS-Chem species database* (`species_database.yml`) in order to define the `FullName`, `Is_Gas`, and `MW_g`, and attributes. For example, the entries for family species `LCO` and `PCO` are:

```
LCO:
  FullName: Dummy species to track loss rate of CO
  Is_Gas: true
  MW_g: 28.01
PCO:
  FullName: Dummy species to track production rate of CO
  Is_Gas: true
  MW_g: 28.01
```

The maximum number of families allowed by KPP is currently set to 300. Depending on how many prod/loss families you add, you may need to increase that to a larger number to avoid errors in KPP. You can change the number for `MAX_FAMILIES` in `KPP/kpp-code/src/gdata.h` and then rebuild the KPP executable.

```
// - Many limits can be changed here by adjusting the MAX_* constants
// - To increase the max size of inlined code (F90_GLOBAL etc.),
```

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```
//   change MAX_INLINE in scan.h.
//
//   NOTES:
//   ------
//   (1) Note: MAX_EQN or MAX_SPECIES over 1023 causes a seg fault in CI build
//         -- Lucas Estrada, 10/13/2021
//
//   (2) MacOS has a hard limit of 65332 bytes for stack memory.  To make
//       sure that you are using this max amount of stack memory, add
//       "ulimit -s 65532" in your .bashrc or .bash_aliases script.  We must
//       also set smaller limits for MAX_EQN and MAX_SPECIES here so that we
//       do not exceed the avaialble stack memory (which will result in the
//       infamous "Segmentation fault 11" error).  If you are stll having
//       problems on MacOS then consider reducing MAX_EQN and MAX_SPECIES
//       to smaller values than are listed below.
//         -- Bob Yantosca (03 May 2022)
#ifdef MACOS
#define MAX_EQN        2000     // Max number of equations (MacOS only)
#define MAX_SPECIES    1000     // Max number of species   (MacOS only)
#else
#define MAX_EQN       11000     // Max number of equations
#define MAX_SPECIES    6000     // Max number of species
#endif
#define MAX_SPNAME       30     // Max char length of species name
#define MAX_IVAL         40     // Max char length of species ID ?
#define MAX_EQNTAG       32     // Max length of equation ID in eqn file
#define MAX_K          1000     // Max length of rate expression in eqn file
#define MAX_ATOMS        10     // Max number of atoms
#define MAX_ATNAME       10     // Max char length of atom name
#define MAX_ATNR        250     // Max number of atom tables
#define MAX_PATH        300     // Max char length of directory paths
#define MAX_FILES        20     // Max number of files to open
#define MAX_FAMILIES    300     // Max number of family definitions
#define MAX_MEMBERS     150     // Max number of family members
#define MAX_EQNLEN      300     // Max char length of equations
#define MAX_EQNLEN      200
```

Important: When adding a prod/loss family or changing any of the other settings in `gckpp.kpp`, you must *re-run KPP to produce new Fortran90 files for GEOS-Chem*.

Production and loss families are archived via the HISTORY diagnostics. For more information, please see the Guide to GEOS_Chem History diagnostics on the GEOS-Chem wiki.

35.2.6 Changing the numerical integrator

Several global options for **KPP** are listed at the top of the `gckpp.kpp` file:

```
#MINVERSION   3.2.0                  { Need this version of KPP or later          }
#INTEGRATOR   rosenbrock_autoreduce  { Use Rosenbrock integration method          }
#AUTOREDUCE   on                     { ... with autoreduce enabled but optional   }
#LANGUAGE     Fortran90              { Generate solver code in Fortran90 ...      }
#UPPERCASEF90 on                     { ... with .F90 suffix (instead of .f90)     }
#DRIVER       none                   { Do not create gckpp_Main.F90               }
#HESSIAN      off                    { Do not create the Hessian matrix           }
#MEX          off                    { MEX is for Matlab, so skip it              }
#STOICMAT     off                    { Do not create stoichiometric matrix        }
```

The #INTEGRATOR tag specifies the choice of numerical integrator that you wish to use with your chemical mechanism. The table below lists

Table 1: Integrators used for each KPP-based GEOS-Chem mechanism

Simulation	#INTEGRATOR setting	Integration method	#AUTOREDUCE setting
carbon	feuler	Forward Euler	N/A
custom	rosenbrock_autoreduce	RODAS3	on
fullchem	rosenbrock_autoreduce	RODAS3	on
Hg	rosenbrock	RODAS3	N/A

Attention: The auto-reduction option is activated but disabled by default in the GEOS-Chem carbon and fullchem mechanisms. You must activate the auto-reduction option in `geoschem_config.yml`.

If you wish to use a different integrator for research purposes, you may select from several more options.

The #LANGUAGE should be set to **Fortran90** and #UPPERCASEF90 should be set to **on**.

The #MINVERSION should be set to 3.2.0. This is the minimum KPP version you should be using with GEOS-Chem.

The other options should be left as they are, as they are not relevant to **GEOS-Chem**.

For more information about **KPP** settings, please see https://kpp.readthedocs.io.

CHAPTER

THIRTYSIX

USE THE KPP-STANDALONE BOX MODEL TO TEST CHEMICAL MECHANISMS

The **KPP-Standalone Box Model** takes a given set of initial conditions to replicate grid cell chemistry of 3D GEOS-Chem, GCHP, or GEOS-CF simulations. It reads an input file generated by the **KPP-Standalone Interface** that generates model output of the full chemical state of the grid cell. The full GEOS-Chem mechanism is run to replicate the chemistry of the specified grid cell.

The KPP-Standalone Box Model can be a useful tool for debugging chemical mechanisms or validating new chemistry reactions before adding them to an existing GEOS-Chem mechanism.

The current KPP-Standalone has been adapted from a box model used in Lin *et al.* [2023]. The GEOS-Chem Support Team has implemented the KPP-Standalone Box Model and KPP-Standalone Interface into GEOS-Chem 14.5.1 and later versions.

Note: The KPP-Standalone Box Model is currently compatible with the *fullchem* or *custom* chemistry mechanisms. But we hope to be able to extend this functionality to other mechanisms in the future.

36.1 Source code

36.1.1 KPP-Standalone Interface

The KPP-Standalone Interface source code is contained in the `GeosCore/kppsa_interface_mod.F90` module in the GEOS-Chem "science codebase" repository. The Interface code is used to archive the GEOS-Chem model state (at the locations and times that you choose) for input into the KPP-Standalone Box Model.

36.1.2 KPP-Standalone Box Model

The KPP-Standalone Box Model code is contained in the Git repository

- https://github.com/geos-chem/KPP-Standalone

This is our fork of the

- https://github.com/KineticPreProcessor/KPP-Standalone

repository, which is maintained by the Kinetic PreProcessor developers.

When you clone the GEOS-Chem Classic source code, the KPP-Standalone Box Model code will be copied into this folder:

- `GCClassic/src/GEOS-Chem/KPP/standalone`

Or if you clone the GCHP source code, the KPP-Standalone Box Model code will be copied into this folder:

- `gchp/src/GCHP_GridComp/GEOSChem_GridComp/geos-chem/KPP/standalone`.

The `KPP/standalone` folder contains the following files:

File	Description
`Beijing_L1_20190701_00` `txt`	Sample data file based on the GEOS-Chem 14.5.0 fullchem mechanism
`CMakeLists.txt`	CMake file used to build the KPP-Standalone Box Model executable
`kpp_standalone.F90`	KPP-Standalone Box Model source code
`kpp_standalone_init.` `F90`	Source code to read data files generated by the KPP-Standalone Interface into the KPP-Standalone Box Model
`python/`	Folder containing Python analysis & plotting scripts
`README.md`	README file from the KPP-Standalone GitHub repository

36.2 Usage instructions

1. Download the GEOS-Chem Classic or GCHP source code.
2. Navigate to the `run/` folder and create a run directory:

```
$ cd GCClassic/run     # If using GEOS-Chem Classic, or
$ cd gchp/run          # If using GCHP

$ ./createRunDir.sh
```

   Select the *fullchem* simulation (option 1) with any extra option (e.g. `standard`, `RRTMG`, etc.). Follow the prompts and provide the necessary information.

3. During the run directory creation, you will be asked if you wish to build KPP-Standalone. Type `y` and hit return, as shown below.

```
-------------------------------------------------------------
Do you want to build the KPP-Standalone Box Model? (y/n)
-------------------------------------------------------------
>>> y

>>>> REMINDER: You must compile with options: -DKPPSA=y <<<<

Created /path/to/your/fullchem/run/directory
```

4. Navigate to the run directory and configure the GEOS-Chem Classic or GCHP source code using CMake as you normally would. Then navigate to the build folder and apply option `-DKPPSA=y`:

```
$ cd build
$ cmake . -DKPPSA=y
$ make -j
$ make install
```

   The KPP-Standalone Box Model code will be compiled to an executable named `kpp_standalone`, which will be copied to the run directory along with the GEOS-Chem Classic or GCHP executable.

5. Open the `kpp_standalone_interface.yml` file (located in the run directory) in your favorite editor. The file will look similar to this:

```
---
# ============================================================================
# Configuration file for KPP standalone interface
#
# This file specifies at which locations we will archive the model
# state so that we can initialize KPP standalone box model simulations.
# ============================================================================

# -----------------------------------
# General settngs
# -----------------------------------
settings:
  activate: false                       # Main on/off switch
  start_output_at: [19000101, 000000]   # Save model state for KPP standalone
  stop_output_at:  [21000101, 000000]   # ... if between these 2 datetimes
  output_directory: "./OutputDir/"      # This directory should already exist
  levels:                               # Model levels to archive
    - 1
    - 2
    # ... etc. other levels not shown ...

# -----------------------------------
# Where to archive model state?
# -----------------------------------
active_cells:
  - Alert
  - Amazon
  - AtlanticOcean
  - Beijing
  # ... etc. other active_cells not shown ...

# -----------------------------------
# Active cell geographic coordinates
# -----------------------------------
locations:
  Alert:
    latitude: 82.5
    longitude: -62.3
  Amazon:
    latitude: -3.4653
    longitude: -62.2159
  AtlanticOcean:
    latitude: 34.707874
    longitude: -41.574755
  Beijing:
    latitude: 39.9042
    longitude: 116.4074
  # ... etc. other locations not shown ...
```

6. Edit the following entries under the `settings` section:

    1. Change `activate: false` to `activate: true`. This will turn on the KPP-Standalone Interface within

GEOS-Chem. By default the Interface is turned off.

2. Edit the `start_output_at` and `stop_output_at` entries to specify the time interval when the KPP-Standalone Interface will run. The KPP-Standalone Interface will archive the GEOS-Chem model state to disk at each chemistry timestep that occurs within the specified interval.

   Attention: We recommend that you only archive model state to disk for the time interval that you need. By default, the model state will be archived to disk at every chemistry timestep, which can cause your simulation to run much more slowly than normal.

   For example, if you wish to archive model state to disk only between `2019-01-01 00:00:00` and `2019-01-02 00:00:00`, edit these entries as shown below:

```
start_output_at: [20190101, 000000]  # Save model state for KPP standalone
stop_output_at:  [20190102, 000000]  # ... if between these 2 datetimes
```

3. If you wish, change the `output_directory` setting to specify where the files containing model state will be sent. By default, these files will be placed in the `OutputDir/` folder within the run directory.

4. Edit the `levels` setting to add or remove the model levels at which you wish to archive the GEOS-Chem model state.

7. Edit the `active_cells` section to define the names of sites where the KPP-Standalone Interface will archive the GEOS-Chem model state. The `kpp_standalone_interface.yml` file ships with several pre-defined active cells. You may keep these, remove them, and/or add new active cells as you please. The ordering of the active cell names does not matter.

8. Edit the `locations` section to add geographical coordinates for each of the `active_cells` that have been specified above. The ordering of the locations does not matter, but you must make sure that each active cell has a corresponding geographic location defined.

9. Run your GEOS-Chem Classic or GCHP simulation. Make sure that your simulation spans the time interval specified by the `start_output_at` and `stop_output_at` fields.

10. Once your simulation finishes, navigate to the directory specified by the `output_directory` field (which in our example is `./OutputDir`) and get a directory listing.

```
$ cd OutputDir   # Or whatever you specified for output_directory
$ ls -1
```

You should see several files ending in `*.txt`:

```
Alert_L1_20190701_0000.txt
Alert_L1_20190701_0020.txt
Alert_L1_20190701_0040.txt
Alert_L2_20190701_0000.txt
Alert_L2_20190701_0020.txt
Alert_L2_20190701_0040.txt
...
Amazon_L1_20190701_0000.txt
Amazon_L1_20190701_0020.txt
Amazon_L1_20190701_0040.txt
Amazon_L2_20190701_0000.txt
Amazon_L2_20190701_0020.txt
Amazon_L2_20190701_0040.txt
```

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```
...
AtlanticOcean_L1_20190701_0000.txt
AtlanticOcean_L1_20190701_0020.txt
AtlanticOcean_L1_20190701_0040.txt
AtlanticOcean_L2_20190701_0000.txt
AtlanticOcean_L2_20190701_0020.txt
AtlanticOcean_L2_20190701_0040.txt
...
Beijing_L1_20190701_0000.txt
Beijing_L1_20190701_0020.txt
Beijing_L1_20190701_0040.txt
Beijing_L2_20190701_0000.txt
Beijing_L2_20190701_0020.txt
Beijing_L2_20190701_0040.txt
...
... etc. for other sites & times ...
```

These files represent the GEOS-Chem model state at each active cell, model level, date and time. The format of these files is shown below (using the `Beijing_L1_20190701_0040.txt` as an example:

```
60
================================================================================

                  KPP Standalone Atmospheric Chemical State
File Description:
This file contains model output of the atmospheric chemical state
as simulated by the GEOS-Chem chemistry module in a 3D setting.
Each grid cell represents the chemical state of an individual location,
suitable for input into a separate KPP Standalone program which will
replicate the chemical evolution of that grid cell for mechanism analysis.
Note that the KPP Standalone will only use concentrations, rate constants,
and KPP-specific fields. All other fields are for reference. The first line
contains the number of lines in this header. If wanting to use this output
for other analysis, a Python class to read these fields is available by
request, contact Obin Sturm (psturm@usc.edu).

Generated by the GEOS-Chem Model
       (https://geos-chem.org/)
Using the KPP Standalone Interface
github.com/GEOS-ESM/geos-chem/tree/feature/psturm/kpp_standalone_interface
     With contributions from:
        Obin Sturm (psturm@usc.edu)
        Christoph Keller
        Michael Long
        Sam Silva

Meteorological and general grid cell metadata

Location:                                          Beijing
Timestamp:                                         2019/07/01 00:40
Longitude (degrees):                                  115.0000
Latitude (degrees):                                    38.0000
```

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```
GEOS-Chem Vertical Level:                              1
Pressure (hPa):                                  947.7906
Temperature (K):                                   300.29
Dry air density (molec/cm3):                   0.2273E+20
Water vapor mixing ratio (vol H2O/vol dry air):   0.9784E-02
Cloud fraction:                                0.0000E+00
Cosine of solar zenith angle:                  0.6833E+00

KPP Integrator-specific parameters

Init KPP Timestep (seconds):                     41.0561
Exit KPP Timestep (seconds):                     92.6195
Chemistry operator timestep (seconds):         1200.0000
Number of internal timesteps:                    15
ICNTRL integrator options used:
     1     0     4     0     0     0     1     0     0     0
     0     0     0   345    -1     0     0     0     0     0
RCNTRL integrator options used:
     0.000000     0.000000    41.056066     0.000000     0.000000
     0.000000     0.000000     0.000000     0.000000     0.000000
     0.000000     0.000000     0.000000     0.000050     0.000000
     0.000000     0.000000     0.000000     0.000000     0.000000

CSV data of full chemical state, including species concentrations,
rate constants (R) and instantaneous reaction rates (A).
All concentration units are in molec/cm3 and rates in molec/cm3/s.

================================================================================
Name,   Value,   Absolute Tolerance
CH2I2,  5.5790359988082701E+003,  1.00E-02
CH2IBr,  4.3058653390896252E+004,  1.00E-02
CH2ICl,  5.5586468566915649E+005,  1.00E-02
AERI,  1.0841371359954113E+007,  1.00E-02
AONITA,  1.0756986064207199E+009,  1.00E-02
...
R1   1,  3.9000149380783678E-020
R2,  1.9670377782305400E-007
R3,  1.6079592890328128E-008
R4,  7.2351790708373721E-022
...
A1,  4.6780159996820985E+003
A2,  4.6780159996820985E+003
A3,  4.6780159996820976E+003
A4,  5.1949221122605059E+003
```

The file header contains metadata about the meteorological conditions present at the site, as well as parameters used by the KPP solver. Species concentrations in $molecules\ cm^{-3}$ are listed along with the absolute tolerance value for each species. The number at the top of the header (`60`) indicates the number of lines to skip before the data begins. Data is saved to comma-separated variable (CSV) format.

Reaction rate constants (beginning with R) and instantaneous reaction rates (beginning with A) follow the species concentrations. These are archived in $molecules\ cm^{-3}\ s^{-1}$.

11. Run the KPP-Standalone Box Model for each of the active cells, model levels, dates, and times where the GEOS-

Chem model state has been archived.

```
$ ./kpp_standalone Beijing_L1_20190701_0040.txt Beijing_L1_20190701_0040.log
Processing sample: input/Beijing_L1_20190701_0040.txt
Number of internal timesteps (from 3D run):    15
Number of internal timesteps ( standalone):    15
Hexit (from 3D run):      92.62
Hexit ( standalone):      92.62
```

The first argument to `kpp_standalone` is the file containing the GEOS-Chem model state for a given active cell, level, date, and time.

The second argument is the log file (in our example, `Beijing_L1_20190701_0040.log`) containing the output of the KPP-Standalone Box Model. The log file will also be printed in CSV format.

The KPP-Standalone Box Model will print some statistics to the screen (aka "standard output" or "stdout"). Ideally the `Hexit` values should be pretty close to each other.

Your KPP-Standalone Box Model output should look similar to this:

```
43
================================================================================

KPP Standalone Output
This file contains the concentrations of all the chemical species
in a single grid cell of a GEOS-Chem 3D run as replicated by the
KPP Standalone. Concentrations before and after the operator timestep
are in CSV format, below.

Generated by the GEOS-Chem KPP Standalone:
https://github.com/KineticPreProcessor/KPP-Standalone

Input file used: Beijing_L1_20190701_0040.txt

Meteorological and general grid cell metadata

Location:                                          Beijing
Timestamp:                                         2019/07/01 00:40
Longitude (degrees):                                  115.0000
Latitude (degrees):                                    38.0000
GEOS-Chem Vertical Level:                               1
Pressure (hPa):                                       947.7906
Temperature (K):                                        300.29
Dry air density (molec/cm3):                        0.2273E+20
Water vapor mixing ratio (vol H2O/vol dry air):     0.9784E-02
Cloud fraction:                                     0.0000E+00
Cosine of solar zenith angle:                       0.6833E+00

KPP Integrator-specific parameters

Init KPP Timestep (seconds):                           41.0561
Exit KPP Timestep (seconds):                           92.6195
Chemistry operator timestep (seconds):               1200.0000
Number of internal timesteps:                           15
ICNTRL integrator options used:
```

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```
     1     0     4     0     0     0     1     0     0     0
     0     0     0   345    -1     0     0     0     0     0
RCNTRL integrator options used:
     0.000000     0.000000    41.056066     0.000000     0.000000
     0.000000     0.000000     0.000000     0.000000     0.000000
     0.000000     0.000000     0.000000     0.000050     0.000000
     0.000000     0.000000     0.000000     0.000000     0.000000

================================================================================
Species Name,Initial Concentration (molec/cm3),Final Concentration (molec/cm3)
CH2I2,  5.5790359988082701E+003,  2.8781775861340213E+000
CH2IBr,  4.3058653390896252E+004,  2.9971817468639663E+004
CH2ICl,  5.5586468566915649E+005,  5.0135868815135013E+005
AERI,  1.0841371359954113E+007,  1.0896017942806700E+007
AONITA,  1.0756986064207199E+009,  1.0756986064207199E+009
BUTDI,  2.0521956658716797E+010,  2.0526479192010277E+010
...
```

The header contains the same information as the corresponding input file containing model state archived from GEOS-Chem. The initial and final concentrations for each species are printed in $molecules\ cm^{-3}$. The number at the top of the header (`43`) indicates the number of lines to skip before the data begins.

12. **GCPy** (the GEOS-Chem Python Toolkit) contains scripts for plotting KPP-Standalone Box Model output. For usage instructions, please see the Visualizing KPP-Standalone box model output chapter of the GCPy documentation.

CHAPTER

THIRTYSEVEN

VIEW RELATED DOCUMENTATION

Table 1: **GEOS-Chem web, wiki and Youtube channel**

Site	Link
GEOS-Chem web site	geos-chem.org
GEOS-Chem wiki	wiki.geos-chem.org
Video tutorials on Youtube (various)	youtube.com/~geoschem

Table 2: **User manuals for GEOS-Chem and related software**

Software	Maintained by	Documentation and contact info
GEOS-Chem Classic	GCST	geos-chem.readthedocs.io
GCHP	GCST	gchp.readthedocs.io
HEMCO	GCST	hemco.readthedocs.io
GCPy (Python toolkit)	GCST	gcpy.readthedocs.io
WRF-GC (GEOS-Chem in WRF)	WRF-GC developers	wrf.geos-chem.org
KPP (The Kinetic PreProcessor)	KPP developers	kpp.readthedocs.io
IMI (Integrated Methane Inversion)	IMI developers	imi.readthedocs.io
CHEEREIO (Data assimilation & emissions inversions)	Drew Pendergrass (Harvard)	cheereio.readthedocs.io

Table 3: **Legacy documentation archives**

Legacy Code or Documentation	Archives
Unsupported versions (prior to 13.0.0)	geoschem.github.io/gcclassic-manpage-archive
GAMAP (superseded by GCPy)	geoschem.github.io/gamap-manual
Deprecated GEOS-Chem wiki content	GEOS-Chem Wiki archives

CHAPTER

THIRTYEIGHT

GEOS-CHEM VERSION HISTORY

For a list of updates by GEOS-Chem version, please see:

- CHANGELOG.md for the GEOS-Chem science codebase
- CHANGELOG.md for the GCClassic wrapper
- CHANGELOG.md for HEMCO

CHAPTER

THIRTYNINE

KNOWN BUGS AND ISSUES

Please see our Issue tracker on GitHub for a list of recent bugs and fixes.

39.1 Current bug reports

These bug reports (on GitHub) are currently unresolved. We hope to fix these in future releases.

Attention: It has been brought to our attention that the *RxnConst* and the *RxnRates* diagnostic collection may not be working as expected. We are currently investigating.

Important: The convection scheme used for GEOS-FP met generation changed from RAS to Grell-Freitas with impact on GEOS-FP meteorology files starting June 1, 2020, specifically enhanced vertical transport. In addition, there is a bug in convective precipitation flux following the switch where all values are zero. While this bug is automatically fixed by computing fluxes online for runs starting on or after June 1 2020, the fix assumes meteorology year corresponds to simulation year. Due to these issues we recommend splitting up GEOS-FP runs in time such that a single simulation does not run across June 1, 2020. Instead. set one run to stop on June 1 2020 and then restart a new run from there. If you wish to use a GEOS-FP meteorology year different from your simulation year please create a GEOS-Chem GitHub issue for assistance.

39.2 Bugs that have been resolved

These bugs (reported on GitHub) have been resolved.

CHAPTER

FORTY

CONTRIBUTING GUIDELINES

Thank you for looking into contributing to GEOS-Chem! GEOS-Chem is a grass-roots model that relies on contributions from community members like you. Whether you're new to GEOS-Chem or a longtime user, you're a valued member of the community, and we want you to feel empowered to contribute.

Updates to the GEOS-Chem model benefit both you and the entire GEOS-Chem community. You benefit through coauthorship and citations. Priority development needs are identified at GEOS-Chem users' meetings with updates between meetings based on GEOS-Chem Steering Committee (GCSC) input through Working Groups.

40.1 We use GitHub and ReadTheDocs

We use GitHub to host the GEOS-Chem Classic source code, to track issues, user questions, and feature requests, and to accept pull requests: https://github.com/geoschem/geos-chem. Please help out as you can in response to issues and user questions.

GEOS-Chem Classic documentation can be found at geos-chem.readthedocs.io.

40.2 When should I submit updates?

Submit bug fixes right away, as these will be given the highest priority. Please see **Support Guidelines** for more information.

Submit updates (code and/or data) for mature model developments once you have submitted a paper on the topic. Your Working Group chair can offer guidance on the timing of submitting code for inclusion into GEOS-Chem.

The practical aspects of submitting code updates are listed below.

40.3 How can I submit updates?

We use **GitHub Flow**, so all changes happen through pull requests. This workflow is described here.

As the author you are responsible for:

- Testing your changes
- Updating the user documentation (if applicable)
- Supporting issues and questions related to your changes

40.3.1 Process for submitting code updates

1. Contact your GEOS-Chem Working Group leaders to request that your updates be added to GEOS-Chem. They will will forward your request to the GCSC.
2. The GCSC meets quarterly to set GEOS-Chem model development priorities. Your update will be slated for inclusion into an upcoming GEOS-Chem version.
3. Create or log into your GitHub account.
4. Fork the relevant GEOS-Chem repositories into your Github account.
5. Clone your forks of the GEOS-Chem repositories to your computer system.
6. Add your modifications into a new branch off the **main** branch.
7. Add a sentence to the `CHANGELOG.md` file describing your update.
8. Test your update thoroughly and make sure that it works. For structural updates we recommend performing a difference test (i.e. testing against the prior version) in order to ensure that identical results are obtained).
9. Review the coding conventions and checklists for code and data updates listed below.
10. Create a pull request in GitHub.
11. The GEOS-Chem Support Team will add your updates into the development branch for an upcoming GEOS-Chem version. They will also validate your updates with benchmark simulations.
12. If the benchmark simulations reveal a problem with your update, the GCST will request that you take further corrective action.

40.3.2 Coding conventions

The GEOS-Chem codebase dates back several decades and includes contributions from many people and multiple organizations. Therefore, some inconsistent conventions are inevitable, but we ask that you do your best to be consistent with nearby code.

40.3.3 Checklist for submitting code updates

1. Use Fortran-90 free format instead of Fortran-77 fixed format.
2. Include thorough comments in all submitted code.
3. Include full citations for references at the top of relevant source code modules.
4. Check that you have updated the `CHANGELOG.md` file.
5. Remove extraneous code updates (e.g. testing options, other science).
6. Submit any related code or configuration files for GCHP along with code or configuration files for GEOS-Chem Classic.

40.3.4 Checklist for submitting data files

1. Choose a final file naming convention before submitting data files for inclusion to GEOS-Chem.
2. Make sure that all netCDF files adhere to the COARDS conventions.
3. Concatenate netCDF files to reduce the number of files that need to be opened. This results in more efficient I/O operations.
4. Chunk and deflate netCDF files in order to improve file I/O.
5. Include an updated HEMCO configuration file corresponding to the new data.
6. Include a README file detailing data source, contents, etc.
7. Include script(s) used to process original data.
8. Include a summary or description of the expected results (e.g. emission totals for each species).

Also follow these additional steps to ensure that your data can be read by GCHP:

1. All netCDF data variables should be of type `float` (aka `REAL*4`) or `double` (aka `REAL*8`).
2. Use a recent reference datetime (i.e. after `1900-01-01`) for the netCDF `time:units` attribute.
3. The first time value in each file should be 0, corresponding with the reference datetime.

40.4 How can I request a new feature?

We accept feature requests through issues on GitHub. To request a new feature, **open a new issue** and select the feature request template. Please include all the information that migth be relevant, including the motivation for the feature.

40.5 How can I report a bug?

Please see **Support Guidelines**.

40.6 Where can I ask for help?

Please see **Support Guidelines**.

CHAPTER

FORTYONE

SUPPORT GUIDELINES

GEOS-Chem support is maintained by the **GEOS-Chem Support Team (GCST)**, which is based jointly at Harvard University and Washington University in St. Louis.

We track bugs, user questions, and feature requests through **GitHub issues**. Please help out as you can in response to issues and user questions.

41.1 How to report a bug

We use GitHub to track issues. To report a bug, **open a new issue**. Please include your name, institution, and all relevant information, such as simulation log files and instructions for replicating the bug.

41.2 Where can I ask for help?

We use GitHub issues to support user questions. To ask a question, **open a new issue** and select the question template. Please include your name and institution in the issue.

41.3 What type of support can I expect?

We will be happy to assist you in resolving bugs and technical issues that arise when compiling or running GEOS-Chem. User support and outreach is an important part of our mission to support the International GEOS-Chem User Community.

Even though we can assist in several ways, we cannot possibly do everything. We rely on GEOS-Chem users being resourceful and willing to try to resolve problems on their own to the greatest extent possible.

If you have a science question rather than a technical question, you should contact the relevant GEOS-Chem Working Group(s) directly. But if you do not know whom to ask, you may open a new issue (See "Where can I ask for help" above) and we will be happy to direct your question to the appropriate person(s).

41.4 How to submit changes

Please see **Contributing Guidelines**.

41.5 How to request an enhancement

Please see **Contributing Guidelines**.

CHAPTER

FORTYTWO

EDITING THIS USER GUIDE

This user guide is generated with Sphinx. Sphinx is an open-source Python project designed to make writing software documentation easier. The documentation is written in a reStructuredText (it's similar to markdown), wh ich Sphinx extends for software documentation. The source for the documentation is the `docs/source` directory in top-level of the source code.

42.1 Quick start

To build this user guide on your local machine, you need to install Sphinx and its dependencies. Sphinx is a Python 3 package and it is available via **`pip`**. This user guide uses the Read The Docs theme, so you will also need to install `sphinx-rtd-theme`. It also uses the sphinxcontrib-bibtex and recommonmark extensions, which you'll need to install.

```
$ cd docs
$ pip install -r requirements.txt
```

To build this user guide locally, navigate to the `docs/` directory and make the `html` target.

```
$ make html
```

This will build the user guide in `docs/build/html`, and you can open `index.html` in your web-browser. The source files for the user guide are found in `docs/source`.

Note: You can clean the documentation with `make clean`.

42.2 Learning reST

Writing reST can be tricky at first. Whitespace matters, and some directives can be easily miswritten. Two important things you should know right away are:

- Indents are 3-spaces
- "Things" are separated by 1 blank line. For example, a list or code-block following a paragraph should be separated from the paragraph by 1 blank line.

You should keep these in mind when you're first getting started. Dedicating an hour to learning reST will save you time in the long-run. Below are some good resources for learning reST.

- reStructuredText primer: (single best resource; however, it's better read than skimmed)
- Official reStructuredText reference (there is *a lot* of information here)

- Presentation by Eric Holscher (co-founder of Read The Docs) at DjangoCon US 2015 (the entire presentation is good, but reST is described from 9:03 to 21:04)
- YouTube tutorial by Audrey Tavares

A good starting point would be Eric Holscher's presentations followed by the reStructuredText primer.

42.3 Style guidelines

Important: This user guide is written in semantic markup. This is important so that the user guide remains maintainable. Before contributing to this documentation, please review our style guidelines (below). When editing the source, please refrain from using elements with the wrong semantic meaning for aesthetic reasons. Aesthetic issues can be addressed by changes to the theme.

For **titles and headers**:

- Section headers should be underlined by # characters
- Subsection headers should be underlined by - characters
- Subsubsection headers should be underlined by ^ characters
- Subsubsubsection headers should be avoided, but if necessary, they should be underlined by " characters

File paths (including directories) occuring in the text should use the `:file:` role.

Program names (e.g. **`cmake`**) occuring in the text should use the `:program:` role.

OS-level commands (e.g. **`rm`**) occuring in the text should use the `:command:` role.

Environment variables occuring in the text should use the `:envvar:` role.

Inline code or code variables occuring in the text should use the `:code:` role.

Code snippets should use `.. code-block::` <language> directive like so

```
.. code-block:: python

   import gcpy
   print("hello world")
```

The language can be "none" to omit syntax highlighting.

For command line instructions, the "console" language should be used. The `$` should be used to denote the console's prompt. If the current working directory is relevant to the instructions, a prompt like `$~/path1/path2$` should be used.

Inline literals (e.g. the `$` above) should use the `:literal:` role.

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