GEOS-Chem Classic

Release 14.1.1

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

KEY REFERENCES

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

References

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).

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 $4° \times 5°$ "standard" simulation

- 8-15 GB RAM

For the $2° \times 2.5°$ "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 14 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. $1° \times 1.25°$ or higher resolution) global simulations
- Running high-resolution (e.g. $0.25° \times 0.3125°$ or $0.5° \times 0.625°$
- Running $2° \times 2.5°$ 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
$1° \times 1.25°$	Global	~30
$2° \times 2.5°$	Global	~110
$0.5° \times 0.625°$	Nested Asia (aka AS)	~115
$0.5° \times 0.625°$	Nested Europe (aka EU)	~58
$0.5° \times 0.625°$	Nested North America (aka NA)	~110

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

Resolution	Type	Size GB/yr
$1° \times 1.25°$	Global	~30
$2° \times 2.5°$	Global	~120
$0.25° \times 0.3125°$	Nested Asia (aka AS)	~175
$0.25° \times 0.3125°$	Nested Europe (aka EU)	~175
$0.25° \times 0.3125°$	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>.

Also see our *Input data for GEOS-Chem Classic* 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):

- 19.0.5.281
- 19.0.4
- 18.0.5
- 17.0.4
- 15.0.0
- 13.0.079
- 11.1.069

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

Tip: Intel 2021 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):

- 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

Best way to install: *With Spack*.

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: With Conda (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.

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.

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 required libraries*.

4.2 Sample environment file for GNU 10.2.0 compilers

Below is a sample environment file from the Harvard Cannon computer cluster. This file will load software libraries built with the GNU 10.2.0 compilers.

Save the code below (with any appropriate modifications for your own computer system) to a file named `~/gcclassic.gnu102.env`.

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

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```
#==============================================================================
# Modules (specific to Cannon @ Harvard)
#==============================================================================

# Remove previously-loaded modules
module purge

# Load modules for GNU Compilers v10.2.0
module load git/2.17.0-fasrc01
module load gcc/10.2.0-fasrc01
module load openmpi/4.1.0-fasrc01
module load netcdf-fortran/4.5.3-fasrc03
module load flex/2.6.4-fasrc01
module load cmake/3.17.3-fasrc01

#==============================================================================
# Environment variables
#==============================================================================

# Parallelization settings for GEOS-Chem Classic
export OMP_NUM_THREADS=8
export OMP_STACKSIZE=500m

# Make all files world-readable by default
umask 022

# Specify compilers
export CC=gcc
export CXX=g++
export FC=gfortran

# Netcdf variables for CMake
# NETCDF_HOME and NETCDF_FORTRAN_HOME are automatically
# defined by the "module load" commands on Cannon.
export NETCDF_C_ROOT=${NETCDF_HOME}
export NETCDF_FORTRAN_ROOT=${NETCDF_FORTRAN_HOME}

# Set memory limits to max allowable
ulimit -c unlimited              # coredumpsize
ulimit -l unlimited              # memorylocked
ulimit -u 50000                  # maxproc
ulimit -v unlimited              # vmemoryuse
ulimit -s unlimited              # stacksize

# List modules loaded
module list
```

Tip: Ask your sysadmin how to load software libraries. If you are using your institution's computer cluster, then chances are there will be a software module system installed, with commands similar to those listed above.

Then you can activate these seetings from the command line by typing:

```
$ . ~/gcclassic.gnu102.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 19 compilers

To load software libraries based on the Intel 19 compilers, we can start from our *GNU 10.2.0 environment file* and add the proper **module load** commands for Intel 19.

Add the code below (with the appropriate modifications for your system) into a file named ~/gcclassic.intel19.env.

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

#==============================================================================
# Modules (specific to Cannon @ Harvard)
#==============================================================================

# Remove previously-loaded modules
module purge

# Load modules for Intel compilers v19.0.4
module load git/2.17.0-fasrc01
module load intel/19.0.5-fasrc01
module load openmpi/4.0.1-fasrc01
module load netcdf-fortran/4.5.2-fasrc03
module load flex/2.6.4-fasrc01
module load cmake/3.17.3-fasrc01

#==============================================================================
# Environment variables
#==============================================================================

# Parallelization settings for GEOS-Chem Classic
export OMP_NUM_THREADS=8
export OMP_STACKSIZE=500m

# Make all files world-readable by default
umask 022

# Specify compilers
export CC=icc
export CXX=icpc
export FC=ifort

# Netcdf variables for CMake
# NETCDF_HOME and NETCDF_FORTRAN_HOME are automatically
# defined by the "module load" commands on Cannon.
export NETCDF_C_ROOT=${NETCDF_HOME}
export NETCDF_FORTRAN_ROOT=${NETCDF_FORTRAN_HOME}

# Set memory limits to max allowable
ulimit -c unlimited              # coredumpsize
ulimit -l unlimited              # memorylocked
```

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```
ulimit -u 50000                    # maxproc
ulimit -v unlimited                # vmemoryuse
ulimit -s unlimited                # stacksize

# List modules loaded
module list
```

Tip: Ask your sysadmin how to load software libraries. If you are using your institution's computer cluster, then chances are there will be a software module system installed, with commands similar to those listed above.

Then you can activate these settings from the command line by typing:

```
$ . ~/gcclassic.intel19.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:

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*.

Table 1: Environment variables that specify compilers

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

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=icc
export CXX=icpc
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 error after the TPCORE transport module is initialized. 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

DOWNLOAD SOURCE CODE

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

5.1 Source code repositories

The **`GEOS-Chem Classic`** source code is distributed into 3 Github repositories, 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 (aka CESM-GC)
- GEOS-Chem withn WRF (aka WRF-GC)

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

5.1.1 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
- Scripts to create GEOS-Chem integration tests
- Interfaces (i.e. the driver programs) for GEOS-Chem Classic, GCHP, etc.

5.1.2 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.

5.1.3 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**.

5.2 Download instructions

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

5.2.1 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`; and
3. Clones the *HEMCO* repo from GitHub to `GCClassic/src/HEMCO`.

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:

```
Cloning into 'GCClassic'...
remote: Enumerating objects: 2680, done.
remote: Counting objects: 100% (1146/1146), done.
remote: Compressing objects: 100% (312/312), done.
remote: Total 2680 (delta 858), reused 1099 (delta 825), pack-reused 1534
Receiving objects: 100% (2680/2680), 1.74 MiB | 13.16 MiB/s, done.
Resolving deltas: 100% (1411/1411), done.
Submodule 'docs/source/geos-chem-shared-docs' (https://github.com/geoschem/geos-chem-
↪shared-docs.git) registered for path 'docs/source/geos-chem-shared-docs'
Submodule 'src/GEOS-Chem' (https://github.com/geoschem/geos-chem.git) registered for␣
↪path 'src/GEOS-Chem'
Submodule 'src/HEMCO' (https://github.com/geoschem/hemco.git) registered for path
↪'src/HEMCO'
Cloning into '/local/ryantosca/GC/rundirs/epa-kpp/tmp/GCClassic/docs/source/geos-chem-
↪shared-docs'...
remote: Enumerating objects: 148, done.
remote: Counting objects: 100% (148/148), done.
remote: Compressing objects: 100% (103/103), done.
remote: Total 148 (delta 77), reused 116 (delta 45), pack-reused 0
Receiving objects: 100% (148/148), 162.29 KiB | 2.90 MiB/s, done.
Resolving deltas: 100% (77/77), done.
```

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```
Cloning into '/local/ryantosca/GC/rundirs/epa-kpp/tmp/GCClassic/src/GEOS-Chem'...
remote: Enumerating objects: 75574, done.
remote: Counting objects: 100% (410/410), done.
remote: Compressing objects: 100% (187/187), done.
remote: Total 75574 (delta 238), reused 364 (delta 216), pack-reused 75164
Receiving objects: 100% (75574/75574), 85.23 MiB | 30.59 MiB/s, done.
Resolving deltas: 100% (62327/62327), done.
Cloning into '/local/ryantosca/GC/rundirs/epa-kpp/tmp/GCClassic/src/HEMCO'...
remote: Enumerating objects: 3178, done.
remote: Counting objects: 100% (638/638), done.
remote: Compressing objects: 100% (195/195), done.
remote: Total 3178 (delta 476), reused 585 (delta 438), pack-reused 2540
Receiving objects: 100% (3178/3178), 2.24 MiB | 11.87 MiB/s, done.
Resolving deltas: 100% (2270/2270), done.
Submodule path 'docs/source/geos-chem-shared-docs': checked out
↪'228507857eb53740dacf4055ce9268aa8ccf520d'
Submodule path 'src/GEOS-Chem': checked out '7e51a0674aba638c8322fef493ac9251095e8cf4'
Submodule path 'src/HEMCO': checked out '4a66bae48f33e6dc22cda5ec9d4633192dee2f73'
Submodule 'docs/source/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 '/local/ryantosca/GC/rundirs/epa-kpp/tmp/GCClassic/src/HEMCO/docs/source/
↪geos-chem-shared-docs'...
remote: Enumerating objects: 148, done.
remote: Counting objects: 100% (148/148), done.
remote: Compressing objects: 100% (103/103), done.
remote: Total 148 (delta 77), reused 116 (delta 45), pack-reused 0
Receiving objects: 100% (148/148), 162.29 KiB | 3.00 MiB/s, done.
Resolving deltas: 100% (77/77), done.
Submodule path 'src/HEMCO/docs/source/geos-chem-shared-docs': checked out
↪'645401baa35b6a6838b9bedede309a01a311517f'
```

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

```
$ cd GCClassic
$ ls -CF src/*
```

and you will see output similar to this:

```
src/CMakeLists.txt  src/gc_classic_version.H@  src/main.F90@

src/GEOS-Chem:
APM/            CMakeScripts/  GeosUtil/  History/     lib/         ObsPack/   run/
AUTHORS.txt     doc/           GTMM/      Interfaces/  LICENSE.txt  PKUCPL/
bin/            GeosCore/      Headers/   ISORROPIA/   mod/         README.md
CMakeLists.txt  GeosRad/       help/      KPP/         NcdfUtil/    REVISIONS

src/HEMCO:
AUTHORS.txt  CMakeLists.txt  CMakeScripts/  LICENSE.txt  README.md  run/  src/
```

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

5.2.2 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
```

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.

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

5.2.3 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

SIX

CREATE A RUN DIRECTORY

We have greatly simplified run directory creation in GEOS-Chem Classic 13.0.0 and later versions. You no longer need to download the separate GEOS-Chem Unit Tester repository, but can create run directories from a script in the GEOS-Chem source code itself.

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

6.1 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

-----------------------------------------------------------
```

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```
What is the name of your principal invesigator?
(Enter 'self' if you are the principal investigator.)
-----------------------------------------------------------
>>> 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 Registraton` message, check your internet connection and try again. If the problem persists, open a new Github issue.

6.2 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
   ```

   You should see this output:

   ```
   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
   ```

and you should see this output:

```
HEMCO_Config.rc.templates/  geoschem_config.yml.templates/
HEMCO_Diagn.rc.templates/   getRunInfo*
HISTORY.rc.templates/       gitignore
README                      init_rd.sh*
archiveRun.sh*              runScriptSamples/
createRunDir.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. CH4
   4. CO2
   5. Hg
   6. POPs
   7. Tagged CH4
   8. Tagged CO
   9. Tagged O3
  10. TransportTracers
  11. Trace metals
  12. Carbon
>>>
```

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
```

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```
  5. Acid uptake on dust
  6. TOMAS
  7. APM
  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):

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

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

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
  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 (such as `$HOME/myusername/` followed by **ENTER)**.

You may also enter a relative path (such as `~/rundirs` followed by ENTER). In this case you will see that the `./createRunDir.sh` script will expand the path to:

```
Expanding to: /n/home09/myusername/rundirs |br|
|br|
```

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.

The script will display the following output:

```
-- 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:

```
-- This run directory has been set up for 20190701 - 20190801.
   You may modify these settings in input.geos.

-- The default frequency and duration of diagnostics is set to monthly.
   You may modify these 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.

12. The script will display the full path to the run directory. You can navigate there and then start editing the *GEOS-Chem configuration files*.

6.3 Example: Create a CH4 simulation run directory

The process of creating run directories for the GEOS-Chem specialty simulations is similar to that as listed in Example 1 above. However, the number of menus that you need to select from will likely be fewer than for the full-chemistry simulation. We'll use the methane simulation as an example.

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

   ```
   $ cd /path/to/your/GCClassic
   $ ls -CF
   ```

   You should see this output:

   ```
   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
   ```

   and you should see this output:

   ```
   HEMCO_Config.rc.templates/  geoschem_config.yml.templates/
   HEMCO_Diagn.rc.templates/   getRunInfo*
   HISTORY.rc.templates/       gitignore
   README                      init_rd.sh*
   archiveRun.sh*              runScriptSamples/
   createRunDir.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. CH4
      4. CO2
      5. Hg
      6. POPs
      7. Tagged CH4
   ```

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```
   8. Tagged CO
   9. Tagged O3
  10. TransportTracers
  11. Trace metals
  12. Carbon
>>>
```

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

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

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

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

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

6. 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
  5. Custom
>>>
```

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

7. 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**.

8. 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 (such as `$HOME/myusername/` followed by ENTER).

You may also enter a relative path (such as `~/rundirs` followed by ENTER). In this case you will see that the `./createRunDir.sh` script will expand the path to:

```
Expanding to: /n/home09/myusername/rundirs
```

9. 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_CH4
```

or if you are creating a nested grid simulation:

```
-- Using default directory name gc_05x0625_merra2_CH4
```

and then

```
-- This run directory has been set up for 20190701 - 20190801.
   You may modify these settings in input.geos.

-- The default frequency and duration of diagnostics is set to monthly.
   You may modify these settings in HISTORY.rc and HEMCO_Config.rc.
```

10. 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.

11. The script will display the full path to the run directory. You can navigate there and then start editing the *GEOS-Chem configuration files*.

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

6.4 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

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

SEVEN

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:

7.1 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.

7.1.1 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 ~/gc_merra2_fullchem
$ ls
archiveRun.sh*      GEOSChem.Restart.20190701_0000z.nc4   metrics.py
build/              getrunInfo*                           OutputDir/
cleanRunDir.sh*     HEMCO_Config.rc                       README
CodeDir@            HEMCO_Diagn.rc                        rundir.version
download_data.py*   HISTORY.rc                            runScriptSamples
download_data.yml   input.geos                            species_database.yml
```

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

7.1.2 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).

7.1.3 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:

```
-- The Fortran compiler identification is GNU 11.2.0
-- Detecting Fortran compiler ABI info
-- Detecting Fortran compiler ABI info - done
-- Check for working Fortran compiler: /n/home09/ryantosca/spack/var/spack/
↪environments/gc-classic/.spack-env/view/bin/gfortran - skipped
-- Checking whether /n/home09/ryantosca/spack/var/spack/environments/gc-classic/.
↪spack-env/view/bin/gfortran supports Fortran 90
-- Checking whether /n/home09/ryantosca/spack/var/spack/environments/gc-classic/.
↪spack-env/view/bin/gfortran supports Fortran 90 - yes
=================================================================
GCClassic X.Y.Z (superproject wrapper)
Current status: X.Y.Z
=================================================================
-- Found NetCDF: /n/home09/ryantosca/spack/opt/spack/linux-centos7-x86_64/gcc-8.3.0/
↪netcdf-fortran-4.5.3-tb3oqspkitgcbkcyp623tdq2al6gxmom/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:       /n/holyscratch01/jacob_lab/ryantosca/tests/test/test_cc
-- 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
  * BPCH_DIAG:    **ON**  OFF
  * USE_REAL8:    **ON**  OFF
  * SANITIZE:     ON  **OFF**
-- Components:
  * TOMAS:        ON  **OFF**
  * TOMAS_BINS:   **NA**  15  40
  * APM:          ON  **OFF**
  * RRTMG:        ON  **OFF**
```

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```
  * GTMM:          ON   **OFF**
  * HCOSA:         ON   **OFF**
  * LUO_WETDEP:    ON   **OFF**
=================================================================
HEMCO 3.6.0
Current status: A.B.C
=================================================================
=================================================================
GEOS-Chem 14.1.0 (science codebase)
Current status: T.U.V
=================================================================
Creating /n/holyscratch01/jacob_lab/ryantosca/tests/test/test_cc/CodeDir/src/GEOS-
↪Chem/Interfaces/GCClassic/gc_classic_version.H
-- Configuring done
-- Generating done
-- Build files have been written to: /n/holyscratch01/jacob_lab/ryantosca/tests/test/
↪test_cc/build
```

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

7.1.4 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.

BPCH_DIAG

Toggles the legacy binary punch diagnostics on.

Attention: This option is deprecated and will be removed soon. Most binary-punch format diagnostics have been replaced by *netCDF-based History diagnostics*.

Accepted values are:

y

Activate legacy binary-punch diagnostics.

n

Deactivate legacy binary-punch diagnostics. **(Default option)**

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)**

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)**

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.

7.1.5 Understand CMake output

As you can see from the example CMake output listed above, GEOS-Chem Classic contains code from 3 independent 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.

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*.

7.2 Compile with Make

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

7.2.1 Build the GEOS-Chem Classic executable

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

```
$ make -j
```

You will see output similar to this:

```
Scanning dependencies of target HeadersHco
Scanning dependencies of target Isorropia
Scanning dependencies of target KPP_FirstPass
[  1%] Building Fortran object src/HEMCO/src/Shared/Headers/CMakeFiles/HeadersHco.dir/
↪hco_inquireMod.F90.o
[  1%] Building Fortran object src/HEMCO/src/Shared/Headers/CMakeFiles/HeadersHco.dir/
↪hco_precision_mod.F90.o
[  1%] Building Fortran object src/HEMCO/src/Shared/Headers/CMakeFiles/HeadersHco.dir/
↪hco_charpak_mod.F90.o
[  3%] Building Fortran object src/GEOS-Chem/KPP/fullchem/CMakeFiles/KPP_FirstPass.
↪dir/gckpp_Monitor.F90.o
[  3%] Building Fortran object src/GEOS-Chem/KPP/fullchem/CMakeFiles/KPP_FirstPass.
↪dir/gckpp_Precision.F90.o
[  3%] Building Fortran object src/GEOS-Chem/KPP/fullchem/CMakeFiles/KPP_FirstPass.
↪dir/gckpp_Parameters.F90.o
[  3%] Linking Fortran static library libKPP_FirstPass.a
```

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```
[  3%] Built target KPP_FirstPass
Scanning dependencies of target Headers
[  3%] Building Fortran object src/GEOS-Chem/ISORROPIA/CMakeFiles/Isorropia.dir/
↪isorropiaII_main_mod.F.o
[  3%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/charpak_
↪mod.F90.o
[  3%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/
↪dictionary_m.F90.o
[  3%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/CMN_SIZE_
↪mod.F90.o
[  3%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/qfyaml_
↪mod.F90.o
[  4%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/CMN_O3_
↪mod.F90.o
[  6%] Building Fortran object src/GEOS-Chem/Headers/CMakeFiles/Headers.dir/
↪inquireMod.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.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.

7.2.2 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
```

and you will see output similar to this:

```
[  1%] Built target HeadersHco
[  3%] Built target KPP_FirstPass
[  3%] Built target Isorropia
[  4%] Built target JulDayHco
[ 13%] Built target Headers
[ 18%] Built target NcdfUtilHco
[ 19%] Built target JulDay
[ 19%] Built target GeosUtilHco
[ 25%] Built target NcdfUtil
[ 40%] Built target HCO
[ 46%] Built target GeosUtil
[ 56%] Built target HCOX
[ 59%] Built target Transport
[ 62%] Built target History
[ 63%] Built target ObsPack
[ 71%] Built target KPP
[ 71%] Built target HCOI_Shared
[ 98%] Built target GeosCore
[100%] Built target gcclassic
Install the project...
-- Install configuration: "Release"
-- Up-to-date: /home/ubuntu/gc_merra2_fullchem/build_info/CMakeCache.txt
-- Up-to-date: /home/ubuntu/gc_merra2_fullchem/build_info/summarize_build
-- Up-to-date: /home/ubuntu/gc_merra2_fullchem/gcclassic
```

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

```
$ cd ..
$ ls
CodeDir@                            cleanRunDir.sh*
GEOSChem.Restart.20190701_0000z.nc4 download_data.py*
HEMCO_Config.rc                     download_data.yml
HEMCO_Config.rc.gmao_metfields      gcclassic*
HEMCO_Diagn.rc                      geoschem_config.yml
HISTORY.rc                          getRunInfo*
OutputDir/                          metrics.py*
README                              runScriptSamples@
archiveRun.sh*                      rundirConfig/
build/                              species_database.yml
build_info/
```

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!

7.2.3 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.

7.3 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:

```
## Compiler Info
#  Family:   GNU
#  Version:  11.2.0
#  Which:    /path/to/gfortran

## Compiler Options (global)
-DCMAKE_Fortran_FLAGS=""
-DCMAKE_Fortran_FLAGS_DEBUG="-g"

## Compiler Options (GEOS-Chem)
-DGEOSChem_Fortran_FLAGS_GNU="-g;-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_DEBUG_GNU="-O0;-Wall;-Wextra;-Wconversion;-Warray-
↪temporaries;-fcheck=array-temps;-ffpe-trap=invalid,zero,overflow;-finit-real=snan;-
↪fcheck=bounds;-fcheck=pointer"
```

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```
## 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_DEBUG_GNU="-g;-gdwarf-2;-gstrict-dwarf;-O0;-Wall;-Wextra;-
↪Wconversion;-Warray-temporaries;-fcheck=array-temps;-ffpe-trap=invalid,zero,
↪overflow;-finit-real=snan;-fcheck=bounds;-fcheck=pointer;-fcheck=no-recursion"

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

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

CHAPTER

EIGHT

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.

8.1 Commonly-updated configuration files

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

8.1.1 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.

Note: 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.

Simulation settings

```
#============================================================================
# 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
  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).

You must *configure your build* with `-DMECH=carbon` in order to use this simulation.

> **Attention:** This simulation is still undergoing validation and testing. We therefore do not recommend using this simulation in the present version.

`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 `-DMECH=Hg` in order to use this simulation.

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

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

root_data_dir
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
Name of the meteorology product that will be used to drive GEOS-Chem Classic. 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.

debug_printout
Activates (`true`) or deactivates (`false`) debug print statements to the screen or log file.

use_gcclassic_timers
Activates (`true`) or deactivates (`false`) the GEOS-Chem Classic timers. If activated, information about how long each component of GEOS-Chem took to execute will be printed to the screen and/or *GEOS-Chem 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

```
#============================================================================
# Grid settings
#============================================================================
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 $4°\times5°$ GEOS-Chem Classic grid.

2.0x2.5
The global $2.0\circ\times2.5°$ GEOS-Chem Classic grid.

0.5x0.625
The global $0.5°\times0.625°$ GEOS-Chem Classic grid (*MERRA2* only). Can be used for global or nested simulations.

0.5x0.625
The global $0.25°\times0.3125°$ 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 centers), 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 centers), 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

```
#============================================================================
# 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:

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.

- Recommended value for global simulations: `600`
- Recommended value for nested simluations: `300` or smaller

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

- Recommended value for global simulations `1200`
- Recommended value for nested simulations `600` or smaller

radiation_timestep_in_s
Specifies the frequency at which the RRTMG radiative transfer model will be called (valid for *fullchem* simulations only).

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:
```

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```
    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
      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.* [[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:
    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:
    input_dir: /path/to/ExtData/CHEM_INPUTS/FAST_JX/v2021-10/
    overhead_O3:
      use_online_O3_from_model: true
      use_column_O3_from_met: true
      use_TOMS_SBUV_O3: false
    photolyze_nitrate_aerosol:
      activate: false
      NITs_Jscale_JHNO3: 0.0
      NIT_Jscale_JHNO2: 0.0
      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`* and *`Hg`* simultions.

input_dir
Specifies the path to the FAST_JX configuration file that contain information about species cross sections and quantum yields.

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 FAST-JX 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`.

RRTMG radiative transfer model

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

  # .. preceding sub-sections omitted ...

  rrtmg_rad_transfer_model:
    activate: false
    aod_wavelengths_in_nm:
      - 550
    longwave_fluxes: false
    shortwave_fluxes: false
    clear_sky_flux: false
    all_sky_flux: false

  # .. 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 FAST-JX photolysis mechanism 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`.

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 ...
    passive_species:
      PassiveTracer:
        long_name: Passive_tracer_for_mass_conservation_evaluation
        mol_wt_in_g: 1.0
        lifetime_in_s: -1
        default_bkg_conc_in_vv: 1.0e-7
      # ... etc more passive species ...

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

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

gcclassic_tpcore
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.

passive_species

Optional menu that allows you to specify **passive species**, which are excluded from undergoing chemical reactions.

Define passive species by providing the name of the species along with associated metadata fields. For example:

```
PassiveTracer:
  long_name: Passive_tracer_for_mass_conservation_evaluation
  mol_wt_in_g: 1.0
  lifetime_in_s: -1              # -1 indicates infinite lifetime!
  default_bkg_conc_in_vv: 1.0e-7
```

Each passive species must also be listed under *transported_species*.

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`:

Carbon aerosols

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

  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

  # ... 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
```

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```
    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* or HEMCO:

Obspack diagnostic

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
    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

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`*.

Legacy diagnostics

Attention: These diagnostics (in the older binary data format) are slated to be replaced by netCDF output in an upcoming version.

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

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

   gamap:
     diaginfo_dat_file: ./diaginfo.dat
     tracerinfo_dat_file: ./tracerinfo.dat

   ND51_satellite:
     activate: false
     output_file: ts_satellite.YYYYMMDD.bpch
     tracers:
       - 1
       - 2
       - 501
```

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```
    UTC_hour_for_write: 0
    averaging_period_in_LT: [9, 11]
    IMIN_and_IMAX_of_region: [1, 72]
    JMIN_and_JMAX_of_region: [1, 46]
    LMIN_and_LMAX_of_region: [1, 1]

  ND51b_satellite:
    # same format as ND51_satellite
```

The `extra_diagnostics:gamap` specify the paths where GEOS-Chem will create the `diaginfo.dat` and `tracerinfo.dat` files used by GAMAP.

The `extra_diagnostics:ND51_satellite` and `extra_diagnostics:ND51b_satellite` contain settings for the GEOS-Chem satellite timeseries diagnostics.. These will be replaced by *GEOS-Chem History diagnostics* (in netCDF format) in an upcoming version.

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:

  # ... 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 (cf. the Integrated Methane Inversion).

```
#============================================================================
# Settings specific to the CH4 simulation / Integrated Methane Inversion
#============================================================================
CH4_simulation_options:

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

  analytical_inversion:
    activate: true
    emission_perturbation: 1.0
    state_vector_element_number: 0
    use_emission_scale_factor: false
    use_OH_scale_factors: false
```

`activate`
Activates (`true`) or deactivates (`false`) the analytical inversion.

Default value: `true`

`activate`
Specifies a factor by which emissions at a grid box will be perturbed.

Default value: `1.0`

`state_vector_element_number`
Specifies the element of the state vector used for the inversion.

Default value: `0`

`use_emission_scale_factor`
Activates (`true`) or deactivates (`false`) scaling methane emissions by a fixed factor.

Default value: `false`

`use_emission_scale_factor`
Activates (`true`) or deactivates (`false`) scaling OH by a fixed factor.

Default value: `false`

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:
    fossil_fuel_emissions: true
    ocean_exchange: true
```

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```
    balanced_biosphere_exchange: true
    net_terrestrial_exchange: true
    ship_emissions: true
    aviation_emissions: true
    3D_chemical_oxidation_source: true

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

fossil_fuel_emissions
Activates (`true`) or deactivates (`false`) using CO_2 fossil fuel emissions as computed by HEMCO.

Default value: `true`

ocean_exchange
Activates (`true`) or deactivates (`false`) CO_2 ocean-air exchange.

Default value: `true`

balanced_biosphere_exchange
Activates (`true`) or deactivates (`false`) CO_2 balanced-biosphere exchange.

Default value: `true`

net_terrestrial_exchange
Activates (`true`) or deactivates (`false`) CO_2 net terrestrial exchange.

Default value: `true`

ship_emissions
Activates (`true`) or deactivates (`false`) CO_2 ship emissions as computed by HEMCO.

Default value: `true`

aviation_emissions
Activates (`true`) or deactivates (`false`) CO_2 aviation emissions as computed by HEMCO.

Default value: `true`

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 $2.0° \times 2.5°$.

```
#============================================================================
# Settings specific to the CO2 simulation
#============================================================================
CO2_simulation_options:

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

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```
  tagged_species:
    save_fossil_fuel_in_background: false
    tag_bio_and_ocean_CO2: false
    tag_land_fossil_fuel_CO2:
    tag_global_ship_CO2: false
    tag_global_aircraft_CO2: false
```

save_fossil_fuel_in_background
Activates (`true`) or deactivates (`false`) saving the CO_2 background.

Default value: `false`

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.

# .. following sub-sections omitted . . .

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`

8.1.2 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
Logfile:                     HEMCO.log
DiagnFile:                   HEMCO_Diagn.rc
DiagnPrefix:                 ./OutputDir/HEMCO_diagnostics
DiagnFreq:                   Monthly
Wildcard:                    *
Separator:                   /
Unit tolerance:              1
Negative values:             0
Only unitless scale factors: false
Verbose:                     0
Warnings:                    1

### 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
# ----- 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 ...
```

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```
# -----------------------------------------------------------------------------
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) ---
#==============================================================================
(((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 ###
```

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```
### END OF HEMCO INPUT FILE ###
```

8.1.3 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.

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. Units
7. 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.

8.1.4 HISTORY.rc

You can specify which GEOS-Chem Classic diagnostic outputs you would like to archive with the `HISTORY.rc` configuration file.

Sample HISTORY.rc diagnostic input file

A simplified `HISTORY.rc` file is shown below.

```
#============================================================================
# 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.
#
#============================================================================
EXPID:  ./OutputDir/GEOSChem
#==============================================================================
# %%%%% COLLECTION NAME DECLARATIONS %%%%%
#
# To disable a collection, place a "#" character in front of its name
#
# NOTE: These are the "default" collections for GEOS-Chem.
# But you can create your own custom diagnostic collections as well.
#==============================================================================
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 mode:               'instantaneous' ,
SpeciesConc.fields:             'SpeciesConcVV_?ADV?'
                                'SpeciesConcMND_?ADV?'
::
#==============================================================================
# %%%%% 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:    060000,
```

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```
SpeciesConcSubset.duration:     00000001 000000,
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?',
                                'SpeciesConcMND_?ADV?',
::
#==============================================================================
# %%%%% THE ConcAfterChem COLLECTION %%%%%
#
# 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.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 (`SpeciesConc`, `SpeciesConcSubset`, and `ConcAfterChem`). Each collection represents a set of netCDF files that will contain the same diagnostic fields.

Legend

`COLLECTIONS:`

List of **diagnostic collections** in the `HISTORY.rc` file.

To turn off a collection, place a comment character (`#`) before its name. For example:

```
COLLECTIONS:  #'SpeciesConc',
              'SpeciesConcSubset',
              'ConcAfterChem',
```

turns off the `SpeciesConc` collection.

`<collection-name>.template`

Determines the date and time format of the netCDF file names that will be created for diagnostic collection `<collection-name>`.

The string `%y4%m2%d2_%h2%n2z.nc4` will print `YYYYMMDD_hhmmz.nc4` to the end of each netCDF filename, where:

- `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.

`<collection-name>.frequency`

Determines how often the diagnostic fields belonging to collection `<collection-name>` collection will be written to a netCDF file. For example:

- `010000` schedules diagnostic archival each hour.
- `00000100 000000` schedules diagnostic output each month.
- `00000001 000000` (or `240000`) schedules diagnostic output each day.
- … etc. …

`<collection-name>.duration`

Determines how often a new netCDF file will be created for collection `<collection-name>`. For example:

- `010000` creates a new netCDF each hour.
- `00000100 000000` creates a new netCDF file each month. month.
- `00000001 000000` (or `240000`) creates a new netCDF file each day.

`<collection-name>.mode`

Determines the averaging method for collection `<collection-name>`. Accepted values are:

`instantaneous`

Data will be archived as instantaneous "snapshots" at the frequency specified in *`<collection-name>.frequency`*.

`time-averaged`

Data will be time-averaged with the frequency specified in *`<collection-name>.frequency`*.

`<collection-name>.fields`

A list of the diagnostic fields that will be included in collection `<collection-name>`.

A single underscore _ denotes a **species-based diagnostic field**. To request output for a single species, list the species name immediately after the underscore, such as:

```
SpeciesConc.fields:   'SpeciesConcVV_NO'
                      'SpeciesConcVV_O3'
                      'SpeciesConcVV_CO'
                      ... etc ...
::
```

You may also use a **wildcard** such as `?ADV?`, which requests all advected species:

```
SpeciesConc.fields:    'SpeciesConcVV_?ADV?'
                       ... etc ...
::
```

The complete wildcard list is shown below. Wildcards are case-insensitive.

- `?ADV?`: Only the advected species
- `?AER?`: Only the aerosol species
- `?ALL?`: All GEOS-Chem species
- `?DRYALT?`: Only the dry-deposited species whose concentrations we wish to archive at a given altitude above the surface. (In practice these are only O3 and HNO3.)
- `?DRY?`: Only the dry-deposited species
- `?FIX?`: Only the inactive (aka "fixed") species in the KPP chemical mechanism
- `?GAS?`: Only the gas-phase species

- `?HYG?`: Only aerosols that undergo hygroscopic growth (sulfate, BC, OC, SALA, SALC)
- `?LOS?`: Only chemical loss species or families
- `?KPP?`: Only the KPP species
- `?PHO?`: Only the photolyzed species
- `?VAR?`: Only the active (aka "variable") species in the KPP chemical mechanism
- `?WET?`: Only the wet-deposited species
- `?PRD?`: Only chemical production species or families
- `?DUSTBIN?`: Only the dust bin number
- `?PHOTOBIN?` Number of a given wavelength bin for FAST-JX photolysis

To include fields from the `State_Chm` object in collection `<collection-name>`, precede the field name with `Chem_`:

```
'Chem_phCloud',
... etc ...
```

To include fields from the `State_Met` object in collection `<collection-name>`, precede the field name with `Met_`:

```
'Met_T'.
'Met_PS',
'Met_SPHU',
... etc ...
```

Both `Chem_` and `Met_` specifiers are case-insensitive.

`<collection-name>.LON_RANGE`
: **Optional**. Restrict data fields of collection `<collection-name>` to the range `min_lon, max_lon`.

`<collection-name>.LAT_RANGE`
: **Optional**. Restrict data fields of collection `<collection-name>` to the range `min_lat, max_lat`.

`<collection-name>.levels`
: **Optional**. Restrict data fields of collection `<collection-name>` to the specified levels (e.g., `1,2,3,4,5` or `1-5`).

`::`
: Signifies the end of the definition section for collection `<collection-name>`.

All of the above-mentioned files are included in your *GEOS-Chem Classic run directory*.

8.2 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:

8.2.1 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.

```
# 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.

8.2.2 Photolysis and chemistry configuration files

Note: You won't need to edit these configuration files unless you are changing the photolysis and/or chemistry mechanisms used in your GEOS-Chem Classic simulation.

Photolysis configuration files

These are found in the `ExtData/CHEM_INPUTS/FAST_JX/` directory structure. Please see Input files for FAST-JX v7.0 for details.

Chemical mechanism configuration files

GEOS-Chem Classic 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 source code for GEOS-Chem Classic;
3. *Compile GEOS-Chem Classic* to create a new executable;
4. Start your GEOS-Chem Classic 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*

CHAPTER

NINE

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.

9.1 Input data for GEOS-Chem Classic

GEOS-Chem Classic reads (via HEMCO) several data files from disk during a simulation. These can be grouped into the following categories:

1. *Initial conditions input data* (aka *Restart files*)
2. *Chemistry input data*
3. *Emissions input data*
4. *Meteorology input data*

9.1.1 Data portals

Input data files for GEOS-Chem can be downloaded from one of the following portals:

`WashU`
The primary data portal for GEOS-Chem, geoschemdata.wustl.edu

`Amazon`
GEOS-Chem data on the Amazon cloud, s3://gcgrid

`Rochester`
Portal for the GCAP 2.0 meteorological data files, atmos.earth.rochester.edu

9.1.2 Initial conditions input data

Initial conditions include:

- Initial species concentrations (aka *Restart files*) used to start a GEOS-Chem simulation.

Download method	From portals
Dry run simulation	*WashU* *Amazon* *Rochester*
Run *bashdatacatalog* on the `InitialConditions.csv` file [1]	*WashU*
Direct data download (**FTP** or **wget**)	*WashU* *Amazon* *Rochester*
Globus, use endpoint **GEOS-Chem data (WashU)**	*WashU*

[1] We provide `InitialConditions.csv` files (for each GEOS-Chem version since 13.0.0) at our input-data-catalogs Github repository.

9.1.3 Chemistry input data

Chemistry input data includes:

- Quantum yields and cross sections for **FAST-JX** photolysis
- Climatology data for **Linoz**
- Boundary conditions for **UCX** stratospheric chemistry routines

Download method	From portals
Dry run simulation	*WashU* *Amazon* *Rochester*
Run *bashdatacatalog* on the `ChemistryInputs.csv` file [2]	*WashU*
Direct data download (**FTP** or **wget**)	*WashU* *Amazon* *Rochester*
Globus, use endpoint **GEOS-Chem data (WashU)**	*WashU*

[2] We provide `ChemistryInputs.csv` files (for each GEOS-Chem version since 13.0.0) at our input-data-catalogs Github repository.

9.1.4 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

Download method	From portals
Dry run simulation	*WashU Amazon Rochester*
Run *bashdatacatalog* on the `EmissionsInputs.csv` file [3]	*WashU*
Direct data download (**FTP** or **wget**)	*WashU Amazon Rochester*
Globus, use endpoint **GEOS-Chem data (WashU)**	*WashU*

[3] We provide `EmissionsInputs.csv` files (for each GEOS-Chem version since 13.0.0) at our input-data-catalogs Github repository.

9.1.5 Meteorology input data

As described previously, GEOS-Chem Classic be driven by the following meteorology products:

1. MERRA-2
2. GEOS-FP
3. GCAP 2.0

Download method	From portals
Dry run simulation	*WashU Amazon Rochester*
Run *bashdatacatalog* on the `MeteorologyInputs.csv` file [4]	*WashU*
Direct data download (**FTP** or **wget**)	*WashU Amazon Rochester*
Globus, use endpoint **GEOS-Chem data (WashU)**	*WashU*

[4] We provide a `MeteorologyInputs.csv` file at our input-data-catalogs Github repository.

9.2 Restart files

In the following chapers, you will learn about **restart files** and how they are used.

9.2.1 What is a restart file?

Restart files contain the initial conditions (cf. *Initial conditions input data*) for a GEOS-Chem simulation. GEOS-Chem simulations need two 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, 2016 is named: `GEOSChem.Restart.20160801_0000z.nc4`. The `z` indicates "Zulu" time, which is another name for UTC.

GEOS-Chem restart files are created in the top-level of your *GEOS-Chem run directory* directory (and NOT in the *`OutputDir/`* folder, which is where History diagnostic files are created.

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 top-level of your *GEOS-Chem run directory* directory (and NOT in the `OutputDir/` folder, which is where History diagnostic files are created. HEMCO restart files are created in the top-level of your GEOS-Chem run

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*

9.2.2 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_           ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 SpeciesRst_?ALL?    $YYYY/
↪$MM/$DD/$HH EFYO xyz 1 * - 1 1
* DELPDRY        ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Met_DELPDRY         $YYYY/
↪$MM/$DD/$HH EY   xyz 1 * - 1 1
* KPP_HVALUE     ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_KPPHvalue      $YYYY/
↪$MM/$DD/$HH EY   xyz 1 * - 1 1
* WETDEP_N       ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_WetDepNitrogen $YYYY/
↪$MM/$DD/$HH EY   xy  1 * - 1 1
* DRYDEP_N       ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_DryDepNitrogen $YYYY/
↪$MM/$DD/$HH EY   xy  1 * - 1 1
* SO2_AFTERCHEM  ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_SO2AfterChem   $YYYY/
↪$MM/$DD/$HH EY   xyz 1 * - 1 1
* H2O2_AFTERCHEM ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_H2O2AfterChem  $YYYY/
↪$MM/$DD/$HH EY   xyz 1 * - 1 1
* AEROH2O_SNA    ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_AeroH2OSNA     $YYYY/
↪$MM/$DD/$HH EY   xyz 1 * - 1 1
```

(continues on next page)

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```
* ORVCSESQ       ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_ORVCSESQ       $YYYY/
↪$MM/$DD/$HH EY   xyz 1 * - 1 1
* JOH            ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_JOH            $YYYY/
↪$MM/$DD/$HH EY   xy  1 * - 1 1
* JNO2           ./GEOSChem.Restart.$YYYY$MM$DD_$HH$MNz.nc4 Chem_JNO2           $YYYY/
↪$MM/$DD/$HH EY   xy  1 * - 1 1
* STATE_PSC      ./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

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: http://geoschemdata.wustl.edu/ExtData/GEOSCHEM_RESTARTS/.

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 13.0.0 10-year benchmark may be found at http://ftp.as.harvard.edu/gcgrid/geos-chem/10yr_benchmarks/13.0.0/GCClassic/restarts. We will also add restart files from the 14.0.0 10-year benchmark simulation shortly.

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 12/1/13, you could spin up the model for one year using the initial GEOS-FP restart file dated 7/1/13 and then use the new restart file to spin up the model for five additional months, from 7/1/13 to 12/1/13.

See also this discussion on our Github page for further guidance: https://github.com/geoschem/geos-chem/discussions/911.

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 ./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 TMPU1    from restart file
 Initialize SPHU1    from restart file
 Initialize PS1_WET  from restart file
 Initialize PS1_DRY  from restart file
 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.

For more information, please see our documentation about the Restart collection in GEOS-Chem History diagnostics. This documentation is currently on the GEOS-Chem wiki, but will be ported to ReadTheDocs in the near future.

9.2.3 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 the HEMCO diagnostics (at hemco.readthedocs.io) for more information about restart files and other diagnostic outpus from HEMCO.

9.3 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.

Tip: Another way to download and manage GEOS-Chem input data is with the *bashdatacatalog* tool.

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`*, *`CH4`*, *`TransportTracers`*, etc.)

In the following chapters, you will learn how to you can download data using the output from a dry-run simulation:

9.3.1 Execute a dry-run simulation

Follow the steps below to perform a GEOS-Chem Classic dry-run simulation:

Tip: Also be sure to watch our video tutorial Using the updated dry-run capability in GEOS-Chem 13.2.1 and later versions at our GEOS-Chem Youtube Channel, which will guide you through these steps.

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`*: Setthe end date and time for your simulation.
3. *`met_field`*: Check if the meteorology setting (*`GEOS-FP`*, *`MERRA2`*, *`GCAP2`*) is correct for your simulation.
4. *`root_data_dir`*: Make sure that the path to `ExtData` is correct.

`HISTORY.rc`

1. Set the frequency and duration for the *HISTORY diagnostic* collections 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*).

9.3.2 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 one of several GEOS-Chem mirror sites, which are described in the following sections.

Important: Before you use the `download_data.py` script, make sure to initialize a Conda environment by typing **`conda activate ENV-NAME`** (where 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.

Choose a data portal

You can download input data data from one of the following mirror sites:

The geoschemdata.wustl.edu mirror (aka WashU)

If you are using GEOS-Chem on your institutional computer cluster, we recommend that you **download data from the WashU (Washington University in St. Louis) mirror site** (http://geoschemdata.wustl.edu). This mirror, which is maintained by Randall Martin's group at WashU, is the main data mirror mirror for GEOS-Chem.

Tip: We have also set up a Globus endpoint named **GEOS-Chem data (WashU)** on the WashU mirror site. If you need to download many years of data, it may be faster to use Globus (particularly if your home institution supports it).

The s3://gcgrid mirror (aka Amazon)

If you are running GEOS-Chem Classic on the Amazon Web Services cloud, you can quickly **download the necessary data for your GEOS-Chem simulation from the :file:`s3://gcgrid` bucket** to the Elastic Block Storage (EBS) volume attached to your cloud instance.

Navigate to your GEOS-Chem Classic run directory and type:

```
$ ./download_data.py log.dryrun amazon
```

This will start the data download process using the `aws s3 cp` commands, which should execute much more quickly than if you were to download the data from Compute Canada. It will also produce the **log of unique data files**.

Important: Copying data from `s3://gcgrid` to the EBS volume of an Amazon EC2 cloud instance is always free. But if you download data from `s3://gcgrid` to your own computer system, you will incur an egress fee. **PROCEED WITH CAUTION!**

The atmos.earth.rochester.edu mirror (aka Rochester)

The U. Rochester site (which is maintained by Lee Murray's research there) contains the GCAP 2.0 met field data. This met field data is useful if you wish to perform simulations stretching back into the preindustrial period, or running into the future.

To download data from the Rochester mirror, type:

```
$ ./download_data.py log.dryrun rochester
```

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 washu
```

The `download_data.py` Python program is included in the *GEOS-Chem run directory* that you created. This Python program creates and executes a temporary bash script containing the appropriate `wget` commands to download the data files. (We have found that this is the fastest method.)

The `download_data.py` program will also 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       : 20160701 000000
!!! End Date         : 20160701 010000
!!! Simulation       : standard
!!! Meteorology      : GEOSFP
!!! Grid Resolution  : 4.0x5.0
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
./GEOSChem.Restart.20160701_0000z.nc4 --> /n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/
↪data/ExtData/GEOSCHEM_RESTARTS/v2018-11/initial_GEOSChem_rst.4x5_standard.nc
./HEMCO_Config.rc
./HEMCO_Diagn.rc
./HEMCO_restart.201607010000.nc
./HISTORY.rc
./input.geos
/n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/data/ExtData/CHEM_INPUTS/FAST_JX/v2019-10/
↪FJX_j2j.dat
/n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/data/ExtData/CHEM_INPUTS/FAST_JX/v2019-10/
↪FJX_spec.dat
/n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/data/ExtData/CHEM_INPUTS/FAST_JX/v2019-10/
↪dust.dat
/n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/data/ExtData/CHEM_INPUTS/FAST_JX/v2019-10/
↪h2so4.dat
/n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/data/ExtData/CHEM_INPUTS/FAST_JX/v2019-10/
↪jv_spec_mie.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

TEN

RUN YOUR SIMULATION

In the following chapters, you will learn how to run your GEOS-Chem Classic simulation on your computer system.

10.1 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 GEOS-Chem run script is provided for you in the GEOS-Chem Classic *run directory*. You can edit this script as necessary for your own computational system.

Navigate to your run directory. Then copy the `runScriptSamples/geoschem.run` sample run script into the run directory:

```
cp ./runScriptSamples/geoschem.run .
```

The `geoschem.run` script looks like this:

```
#!/bin/bash

#SBATCH -c 8
#SBATCH -N 1
#SBATCH -t 0-12:00
#SBATCH -p MYQUEUE
#SBATCH --mem=15000
#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)
###############################################################################

# 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 2>&1

# Exit normally
exit 0
```

The sample run script contains commands for the SLURM scheduler, which is used on many HPC sytems.

Note: If your computer system uses a different scheduler (such as LSF or PBS), then you can replace the SLURM-specific commands with commands for your scheduler. Ask your IT staff for more information.

Important commands in the run script are listed below:

#SBATCH `-c 8`
: Tells SLURM to request 8 computational 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 MYQUEUE`
: Tells SLURM to run GEOS-Chem Classic in the computational partition named `MYQUEUE`. Ask your IT staff for a list of the available partitions on your system.

#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).

srun `-c $OMP_NUM_THREADS`
: Tells SLURM to run the GEOS-Chem Classic executable using the number of cores specified in *`OMP_NUM_THREADS`*.

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`.

10.2 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.

10.2.1 First-time setup

1. Make sure that your computational environment meets all of the *hardware* and *software* requirements for GEOS-Chem Classic.

10.2.2 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: Prior to running with `GEOS-FP` met fields, please be aware of several caveats regarding that data stream. (cf. The GEOS-FP wiki page).

4. *Configure and build* the source code into an executable file.
5. Copy a sample *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*.
7. Be aware of *ways in which you can speed up your GEOS-Chem Classic simulations*.

10.3 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.

10.4 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 (`geoschem-int.sh`). 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

# 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
```

10.5 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 the following resources:

- *Debug GEOS-Chem and HEMCO errors*
- Guide to GEOS-Chem error messages
- Submitting GEOS-Chem support requests

10.6 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?*).

10.7 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. It has been shown that running GEOS-Chem with recommended timesteps from Philip *et al.* [[Philip et al., 2016]]. can increase run times by approximately a factor of 2. To speed up GEOS-Chem Classic simulations, users may choose to use any of the following options.

10.7.1 Use coarser timesteps

As *discussed previously*, the default timesteps for GEOS-Chem Classic are 600 seconds for dynamics, and 1200 seconds for chemistry and emissions. You can experiment with using coarser timesteps (such as 1800 seconds for dynamics and 3600 seconds for emissions & chemistry).

Attention: For nested-grid simulations, you might not be able to use coarser timesteps, or else the Courant limit in transport will be violated.

10.7.2 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.

10.7.3 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`.

CHAPTER

ELEVEN

VIEW OUTPUT FILES

In this chapter, you will learn more about the **output files** that are generated by GEOS-Chem Classic simulations.

11.1 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.

11.1.1 GEOS-Chem 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.

11.1.2 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.

11.1.3 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.

11.1.4 HEMCO log file

File name: `HEMCO.log`

Contains information about how emissions, met fields, and other relevant data are read from disk and processed by HEMCO for input into GEOS-Chem Classic.

11.1.5 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.

11.1.6 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.

11.2 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 *HISTORY.rc* 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* 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.CH4.YYYYMMDD_hhhmmz.nc4`	CH4	*CH4*
`GEOSChem.CloudConvFlux.YYYYMMDD_hhhmmz.nc4`	CloudConvFlux	All simulations
`GEOSChem.ConcAboveSfc.YYYYMMDD_hhhmmz.nc4`	ConcAboveSfc	*fullchem*
`GEOSChem.ConcAfterChem.YYYYMMDD_hhhmmz.nc4`	ConcAfterChem	*fullchem*
`GEOSChem.DryDep.YYYYMMDD_hhhmmz.nc4`	DryDep	All simulations with dry- depositing species
`GEOSChem.JValues.YYYYMMDD_hhhmmz.nc4`	JValues	*fullchem* *Hg*
`GEOSChem.KppDiags.YYYYMMDD_hhhmmz.nc4`	KppDiags	*fullchem* *Hg*
`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.POPs.YYYYMMDD_hhhmmz.nc4`	POPs	*POPs*
`GEOSChem.Metrics.YYYYMMDD_hhhmmz.nc4`	Metrics	*fullchem* *CH4*
`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.RxnRates.YYYYMMDD_hhhmmz.nc4`	RxnRates	*fullchem* *CH4* *Hg*
`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.WetLossConv.YYYYMMDD_hhhmmz.nc4`	WetLossConv	All simulations with wet-depositing species
`GEOSChem.WetLossLS.YYYYMMDD_hhhmmz.nc4`	WetLossLS	All simulations with wet-depositing species

11.3 Other diagnostic output files

11.3.1 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.

11.3.2 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.

11.3.3 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

TWELVE

DIAGNOSTICS REFERENCE

In the following chapters, you will learn about the types of diagnostic outputs you can generate with GEOS-Chem Classic.

12.1 GEOS-Chem History diagnostics

At present, our Guide to GEOS-Chem History diagnostics is still located on the GEOS-Chem wiki. We will be migrating this information over to ReadTheDocs very soon.

12.2 HEMCO diagnostics

Information about diagnostic output from HEMCO (the Harmonized Emissions Component) may be found on our HEMCO ReadTheDocs site.

12.3 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*.

Attention: 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.

12.3.1 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
NOy	Concentration of NOy family	v/v dry
GMAO_TEMP	Temperature	K

continues on next page

Table 1 – continued from previous page

Quantity	Description	Units
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
OBS	Value of the observation (if known), used to compare to model output

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  ...
    6    Sllb 20120630 1713   54.95 -112.45  876.13   1891.310 000061283 005 00015␣
↪00037  1.906E-006  2.942E+002  ...
```

Columns

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`

12.4 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.

12.4.1 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.

12.4.2 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 from NOAA (see https://www.esrl.noaa.gov/gmd/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 ;
                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 ;
```

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```
        ...
        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.

12.4.3 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" ;
```

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```
        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" ;
        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.

12.4.4 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
THIRTEEN

GEOS-CHEM CLASSIC FOLDER TREE

The tables below list the folders in which various components of GEOS-Chem and HEMCO reside.

13.1 GEOS-Chem folder tree

`GCClassic/src/GEOS-Chem`
Root folder for the GEOS-Chem "science codebase".

`GCClassic/src/GEOS-Chem/GTMM`
Contains the GTMM (Global Terrestrial Mercury Model) source code. (NOTE: This option has fallen into disuse.)

`GCClassic/src/GEOS-Chem/GeosCore`
Contains most GEOS-Chem modules & routines

`GCClassic/src/GEOS-Chem/GeosRad`
Contains the RRTMG radiative transfer model source code.

`GCClassic/src/GEOS-Chem/GeosUtil`
Contains GEOS-Chem utility modules & routines (for error handling, string handling, etc.)

`GCClassic/src/GEOS-Chem/Headers`
Contains modules for with derived-type definitions for state objects, fixed parameter settings, etc.

`GCClassic/src/GEOS-Chem/History`
Contains modules & routines for archiving GEOS-Chem diagnostics to netCDF-format output.

`GCClassic/src/GEOS-Chem/ISORROPIA`
Contains the ISORROPIA II source code, which is used for aerosol thermodynamical equilibrium computations.

`GCClassic/src/GEOS-Chem/KPP`
Main folder for chemical mechanisms built with KPP-for-GEOS-Chem.

`GCClassic/src/GEOS-Chem/NcdfUtil`
Contains modules & routines for netCDF file I/O.

`GCClassic/src/GEOS-Chem/ObsPack`
Contains modules & routines for generating GEOS-Chem diagnostic output at the same locations of NOAA ObsPack observational stations.

`GCClassic/src/GEOS-Chem/PKUCPL`
Contains the coupler code for the PKU 2-way nesting algorithm. (This option has fallen into disuse.)

`` `GEOS-Chem/Interfaces/GCClassic ``
Contains the GCClassic driver program (main.F90).

13.2 HEMCO folder tree

`GCClassic/src/HEMCO/src/Core`
Contains modules for reading, storing, and updating data.

`GCClassic/src/HEMCO/src/Extensions`
Contains modules for calculating emissions that depend on meterological variables or parameterizations.

`GCClassic/src/HEMCO/src/Interfaces`
Contains modules and routines for linking HEMCO to GEOS-Chem Classic and other external models.

`GCClassic/src/HEMCO/src/shared`
Contains various modules with utility routines (such as for netCDF I/O, regridding, string handling, etc.)

CHAPTER FOURTEEN

SAMPLE GEOS-CHEM RUN SCRIPTS

Here are some sample run scripts that you can adapt for your own purposes.

14.1 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:

14.1.1 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 my-queue_name
#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)
###############################################################################

# Load your bash-shell customizations
source ~/.bashrc

# Load software modules
# (this example is for GNU 10.2.0 compilers)
source ~/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
```

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.

14.1.2 Submitting jobs with Slurm

To schedule a **GEOS-Chem Classic** job with Slurm, use this command:

```
$ sbatch geoschem.run.slurm
```

14.2 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.

14.2.1 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.
export OMP_NUM_THREADS=$(nproc)

# 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
```

14.2.2 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

FIFTEEN

LOAD REQUIRED LIBRARIES

This supplemental guide describes the how to load the required software dependencies for **GEOS-Chem** and **HEMCO** into your computational environment.

15.1 On the Amazon Web Services Cloud

All of the required software libraries 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.

15.2 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 libraries.

Depending on your system's setup, there are a few different ways in which you can make these libraries available for use in your computational environment. These are described in the following sections:

15.2.1 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 IT staff. But in general, module managers succeed in ensuring that only well-tested compiler/software combinations are made available to users.

Example: Load modules for GNU compilers 8.2.0

If your computer system uses **lmod**, you can load software packages into your computational environment with **module load** commands, such as:

```
$ module purge
$ module load git/2.17.0-fasrc01
$ module load gcc/8.2.0-fasrc01
$ module load openmpi/3.1.1-fasrc01
$ module load netcdf/4.1.3-fasrc02
```

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```
$ module load perl/5.26.1-fasrc01
$ module load cmake/3.17.3-fasrc01
```

In this example (from the Harvard Cannon cluster), the version number and build identifier are part of the module name. This setup may differ on your system.

Tip: Consult your computer system documentation for more information on software package names.

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)

15.2.2 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 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:

```
$ spack load gcc@10.2.0
$ spack load netcdf-c%gcc@10.2.0
$ spack load netcdf-fortran%gcc@10.2.0
... etc ...
```

When loading a Spack-built library, you can specify its version number. For example, **`spack load gcc@10.2.0`** tells Spack to load the GNU Compiler Collection version 10.2.0.

You may also specify a library by the compiler it was built with. For example, **`spack load netcdf-fortran%gcc@10.2.0`** tells Spack to load the version of netCDF-Fortran that was built with GNU Compiler Collection version 10.2.0.

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
```

15.2.3 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.

15.2.4 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*.

BUILD LIBRARIES WITH SPACK

Here are some up-to-date instructions on installing a software stack for **GEOS-Chem Classic** or **HEMCO** with Spack.

Note: If you will be using GCHP, please see gchp.readthedocs.io for instructions on how to download required libraries with Spack.

16.1 Initial Spack setup

16.1.1 Install spack to your home directory

Spack can be installed with Git, as follows:

```
cd ~
$ git clone git@github.com:spack/spack.git
```

16.1.2 Initialize Spack

To initialize Spack type these commands:

```
$ export SPACK_ROOT=${HOME}/spack
$ source ${SPACK_ROOT}/spack/share/spack/setup-env.sh
```

16.1.3 Make sure the default compiler is in compilers.yaml

Tell Spack to search for compilers:

```
$ spack compiler find
```

You can confirm that the default compiler was found by inspecing `compilers.yaml` file with your favorite editor, e.g.:

```
$ emacs ~/.spack/linux/compilers.yaml
```

For example, the default compiler that was on my cloud instance was the GNU Compiler Collection 7.4.0. This collection contains C (**gcc**), C++ (:program`g++`), and Fortran (**gfortran**) compilers. These are specified in the `compiler.yaml` file as:

```
compilers:
- compiler:
    spec: gcc@7.4.0
    paths:
      cc: /usr/bin/gcc-7
      cxx: /usr/bin/g++-7
      f77: /usr/bin/gfortran-7
      fc: /usr/bin/gfortran-7
    flags: {}
    operating_system: ubuntu18.04
    target: x86_64
    modules: []
    environment: {}
    extra_rpaths: []
```

As you can see, the default compiler executables are located in the `/usr/bin` folder. This is where many of the system-supplied executable files are located.

16.2 Build the GCC 10.2.0 compilers

Let's build a newer compiler verion with Spack. In this case we'll build the GNU Compiler Collection 10.2.0 using the default compilers.

```
$ spack install gcc@10.2.0 target=x86_64 %gcc@7.4.0
$ spack load gcc%10.2.0
```

16.2.1 Update compilers.yaml

In order for Spack to use this new compiler to build other packages, the `compilers.yaml` file must be updated using these commands:

```
$ spack load gcc@10.2.0
$ spack compiler find
```

16.3 Install required libraries for GEOS-Chem

Now that we have installed a the GNU Compiler Collection 10.2.0, we can use it to build the required libraries for **`GEOS-Chem Classic`** and **`HEMCO`**.

16.3.1 HDF5

Now we can start installing libraries. First, let's install **`HDF5`**, which is a dependency of **`netCDF`**.

```
$ spack install hdf5%gcc@10.2.0 target=x86_64 +cxx+fortran+hl+pic+shared+threadsafe
$ spack load hdf5%gcc@10.2.0
```

The `+cxx+fortran+hl+pic+shared+threadsafe` specifies necessary options for building HDF5.

16.3.2 netCDF-Fortran and netCDF-C

Now that we have installed :program:, we may proceed to installing **netCDF-Fortran** (which will install **netCDF-C** as a dependency).

```
$ spack install netcdf-fortran%gcc@10.2.0 target=x86_64 ^
↪hdf5+cxx+fortran+hl+pic+shared+threadsafe
$ spack load netcdf-fortran%gcc@10.2.0
$ spack load netcdf-c%gcc@10.2.0
```

We tell Spack to use the same version of HDF5 that we just built by appending `^hdf5+cxx+fortran+hl+pic+shared+threadsafe` to the spack install command. Otherwise, Spack will try to build a new version of HDF5 with default options (which is not what we want).

16.3.3 ncview

Ncview is a convenient viewer for browsing netCDF files. Install it with:

```
$ spack install ncview%gcc@10.2.0 target=x86_64 ^
↪hdf5+cxx+fortran+hl+pic+shared+threadsafe
$ spack load ncview%gcc@10.2.0
```

16.3.4 nco (The netCDF Operators)

The netCDF operators (**nco**) are useful programs for manipulating netCDF files and attributes. Install (**nco**) with:

```
$ spack install nco%gcc@10.2.0 target=x86_64 ^
↪hdf5+cxx+fortran+hl+pic+shared+threadsafe
$ spack load nco%gcc@10.2.0
```

16.3.5 cdo (The Climate Data Operators)

The Climate Data Operators (**cdo**) are utilities for processing data in netCDF files.

```
$ spack install cdo%gcc@10.2.0 target=x86_64 ^
↪hdf5+cxx+fortran+hl+pic+shared+threadsafe
$ spack load cdo%gcc@10.2.0
```

16.3.6 flex

The **flex** library is a lexical parser. It is a dependency for The Kinetic PreProcessor (KPP).

```
$ spack install flex%gcc@10.2.0 target=x86_64
$ spack load flex%gcc10.2.0
```

gdb and cgdb

Gdb is the GNU Debugger. **Cgdb** is a visual, user-friendly interface for **gdb**.

```
$ spack install gdb@9.1%gcc@10.2.0 target=x86_64
$ spack load gdb%10.2.0

$ spack install cgdb%gcc@10.2.0 target=x86_64
$ spack load cgdb%gcc@10.2.0
```

cmake and gmake

Cmake and **gmake** are used to build source code into executables.

```
$ spack install cmake%gcc@10.2.0 target=x86_64
$ spack load cmake%gcc@10.2.0

$ spack install gmake%gcc@10.2.0 target=x86_64
$ spack load gmake%gcc@10.2.0
```

16.4 Installing optional packages

These packages are useful not strictly necessary for GEOS-Chem.

16.4.1 OpenJDK (Java)

Some programs might need the **openjdk** Java Runtime Environment:

```
$ spack install openjdk%gcc@10.2.0
$ spack load openjdk%gcc@10.2.0
```

16.4.2 TAU performance profiler

The Tuning and Analysis Utilities (;program:*tau*) lets you profile **GEOS-Chem** and **HEMCO** in order to locate computational bottlenecks:

```
$ spack install tau%gcc@10.2.0 +pthread+openmp~otf2
$ spack load tau%gcc@10.2.0
```

16.5 Loading Spack packages at startup

16.5.1 Creating an environment file for Spack

Once you have finished installing libraries with **Spack**, you can create an environment file to load the Spack libraries whenever you start a new Unix shell. Here is a sample environment file that can be used (or modified) to load the Spack libraries described above.

```
#==============================================================================
# %%%%% Clear existing environment variables %%%%%
#==============================================================================
unset CC
unset CXX
unset EMACS_HOME
unset FC
unset F77
unset F90
unset NETCDF_HOME
unset NETCDF_INCLUDE
unset NETCDF_LIB
unset NETCDF_FORTRAN_HOME
unset NETCDF_FORTRAN_INCLUDE
unset NETCDF_FORTRAN_LIB
unset OMP_NUM_THREADS
unset OMP_STACKSIZE
unset PERL_HOME

#==============================================================================
# %%%%% Load Spack packages %%%%%
#==============================================================================
echo "Loading gfortran 10.2.0 and related libraries ..."

# Initialize Spack
# In the examples above /path/to/spack was ${HOME}/spack
export SPACK_ROOT=/path/to/spack
source $SPACK_ROOT/share/spack/setup-env.sh

# List each Spack package that you want to load
# (add the backslash after each new package that you add)
pkgs=(                       \
  gcc@10.2.0                 \
  cmake%gcc@10.2.0           \
  openmpi%gcc@10.2.0         \
  netcdf-fortran%gcc@10.2.0 \
  netcdf-c%gcc@10.2.0        \
  hdf5%gcc@10.2.0            \
  gdb%gcc@10.2.0             \
  flex%gcc@10.2.0            \
  openjdk%gcc@10.2.0         \
  cdo%gcc@10.2.0             \
  nco%gcc@10.2.0             \
  ncview%gcc@10.2.0          \
  perl@5.30.3%gcc@10.2.0     \
  tau%gcc@10.2.0             \
)

# Load each Spack package
for f in ${pkgs[@]}; do
    echo "Loading $f"
    spack load $f
done

#==============================================================================
# %%%%% Settings for OpenMP parallelization %%%%%
#==============================================================================
```

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```
# Max out the stack memory for OpenMP
# Asking for a huge number will just give you the max availble
export OMP_STACKSIZE=500m

# By default, set the number of threads for OpenMP parallelization to 1
export OMP_NUM_THREADS=1

# Redefine number threads for OpenMP parallelization
# (a) If in a SLURM partition, set OMP_NUM_THREADS = SLURM_CPUS_PER_TASK
# (b) Or, set OMP_NUM_THREADS to the optional first argument that is passed
if [[ -n "${SLURM_CPUS_PER_TASK+1}" ]]; then
  export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
elif [[ "$#" -eq 1 ]]; then
  if [[ "x$1" != "xignoreeof" ]]; then
    export OMP_NUM_THREADS=${1}
  fi
fi
echo "Number of OpenMP threads: $OMP_NUM_THREADS"

#==============================================================================
# %%%%% Define relevant environment variables %%%%%
#==============================================================================

# Compiler environment variables
export FC=gfortran
export F90=gfortran
export F77=gfortran
export CC=gcc
export CXX=g++

# Machine architecture
export ARCH=`uname -s`

# netCDF paths
export NETCDF_HOME=`spack location -i netcdf-c%gcc@10.2.0`
export NETCDF_INCLUDE=${NETCDF_HOME}/include
export NETCDF_LIB=${NETCDF_HOME}/lib

# netCDF-Fortran paths
export NETCDF_FORTRAN_HOME=`spack location -i netcdf-fortran%gcc@10.2.0`
export NETCDF_FORTRAN_INCLUDE=${NETCDF_FORTRAN_HOME}/include
export NETCDF_FORTRAN_LIB=${NETCDF_FORTRAN_HOME}/lib

# Other important paths
export GCC_HOME=`spack location -i gcc@10.2.0`
export MPI_HOME=`spack location -i openmpi%gcc@10.2.0`
export TAU_HOME=`spack location -i tau%gcc@10.2.0`

#==============================================================================
# %%%%% Echo relevant environment variables %%%%%
#==============================================================================
echo
echo "Important environment variables:"
echo "CC  (C compiler)       : $CC"
echo "CXX (C++ compiler)     : $CXX"
echo "FC  (Fortran compiler) : $FC"
```

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```
echo "NETCDF_HOME            : $NETCDF_HOME"
echo "NETCDF_INCLUDE         : $NETCDF_INCLUDE"
echo "NETCDF_LIB             : $NETCDF_LIB"
echo "NETCDF_FORTRAN_HOME    : $NETCDF_FORTRAN_HOME"
echo "NETCDF_FORTRAN_INCLUDE : $NETCDF_FORTRAN_INCLUDE"
echo "NETCDF_FORTRAN_LIB     : $NETCDF_FORTRAN_LIB"
```

Save this to your home folder with a name such as `~/.spack_env`. The `.` in front of the name will make it a hidden file like your `.bashrc` or `.bash_aliases`.

16.5.2 Loading Spack-built libraries

Whenever you start a new Unix session (either by opening a terminal window or running a new job), your `.bashrc` and `.bash_aliases` files will be sourced, and the commands contained within them applied. You should then load the Spack modules by typing at the terminal prompt:

```
$ source ~/.spack.env
```

You can also add some code to your `.bash_aliases` so that this will be done automatically:

```
if [[ -f ~/.spack.env ]]; then
    source ~/.spack.env
fi
```

In either case, this will load the modules for you. You should see output similar to:

```
Loading gfortran 10.2.0 and related libraries ...
Loading gcc@10.2.0
Loading cmake%gcc@10.2.0
Loading openmpi%gcc@10.2.0
Loading netcdf-fortran%gcc@10.2.0
Loading netcdf-c%gcc@10.2.0
Loading hdf5%gcc@10.2.0
Loading gdb%gcc@10.2.0
Loading flex%gcc@10.2.0
Loading openjdk%gcc@10.2.0
Loading cdo%gcc@10.2.0
Loading nco%gcc@10.2.0
Loading ncview%gcc@10.2.0
Loading perl@5.30.3%gcc@10.2.0
Loading tau%gcc@10.2.0
Number of OpenMP threads: 1

Important environment variables:
CC   (C compiler)       : gcc
CXX  (C++ compiler)     : g++
FC   (Fortran compiler) : gfortran
NETCDF_HOME             : /net/seasasfs02/srv/export/seasasfs02/share_root/ryantosca/
↪spack/opt/spack/linux-centos7-x86_64/gcc-10.2.0/netcdf-c-4.7.4-
↪22bkbtqledcaipqc2zrgun4qes7kkm5q
NETCDF_INCLUDE          : /net/seasasfs02/srv/export/seasasfs02/share_root/ryantosca/
↪spack/opt/spack/linux-centos7-x86_64/gcc-10.2.0/netcdf-c-4.7.4-
↪22bkbtqledcaipqc2zrgun4qes7kkm5q/include
NETCDF_LIB              : /net/seasasfs02/srv/export/seasasfs02/share_root/ryantosca/
↪spack/opt/spack/linux-centos7-x86_64/gcc-10.2.0/netcdf-c-4.7.4-
↪22bkbtqledcaipqc2zrgun4qes7kkm5q/lib
```

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```
NETCDF_FORTRAN_HOME    : /net/seasasfs02/srv/export/seasasfs02/share_root/ryantosca/
↪spack/opt/spack/linux-centos7-x86_64/gcc-10.2.0/netcdf-fortran-4.5.3-
↪mtuoejjcl3ozbvd6prgqm44k5jre3hne
NETCDF_FORTRAN_INCLUDE : /net/seasasfs02/srv/export/seasasfs02/share_root/ryantosca/
↪spack/opt/spack/linux-centos7-x86_64/gcc-10.2.0/netcdf-fortran-4.5.3-
↪mtuoejjcl3ozbvd6prgqm44k5jre3hne/include
NETCDF_FORTRAN_LIB     : /net/seasasfs02/srv/export/seasasfs02/share_root/ryantosca/
↪spack/opt/spack/linux-centos7-x86_64/gcc-10.2.0/netcdf-fortran-4.5.3-
↪mtuoejjcl3ozbvd6prgqm44k5jre3hne/lib
```

Once you see this output, you can then start using programs that rely on these Spack-built libraries.

16.5.3 Setting the number of cores for OpenMP

If you type:

```
$ source ~/.spack.env
```

by itself, this will set the `OMP_NUM_THREADS` variable to 1. This variable sets the number of computational cores that OpenMP should use.

You can change this with, e.g.

```
source ~/.spack.env 6
```

which will set `OMP_NUM_THREADS` to 6. In this case, GEOS-Chem Classic (and other programs that use OpenMP parallelization) will parallelize with 6 cores.

If you are using the SLURM scheduler and are source `.spack.env` in your job script, then `OMP_NUM_THREADS` will be automatically set to `SLURM_CPUS_PER_TASK`, which is then number of cores requested. If you are not using SLURM then you should add e.g.

```
export OMP_NUM_THREADS=6
```

(or however many cores you have requested) in your SLURM job script.

CHAPTER

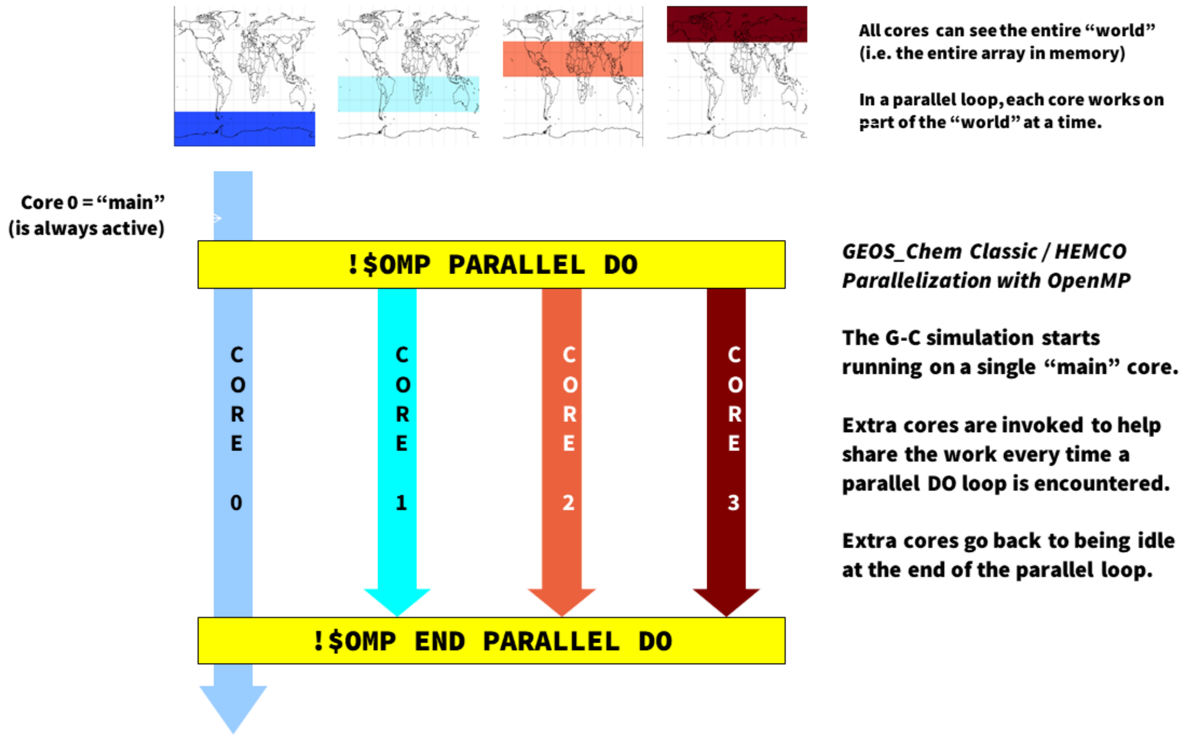
SEVENTEEN

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.

17.1 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".


All cores can see the entire "world" (i.e. the entire array in memory)
In a parallel loop, each core works on part of the "world" at a time.
Core 0 = "main" (is always active)
!$OMP PARALLEL DO
CORE 0
CORE 1
CORE 2
CORE 3
!$OMP END PARALLEL DO
GEOS_Chem Classic / HEMCO Parallelization with OpenMP
The G-C simulation starts running on a single "main" core.
Extra cores are invoked to help share the work every time a parallel DO loop is encountered.
Extra cores go back to being idle at the end of the parallel loop.

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.

17.2 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.

17.3 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.

17.4 OpenMP parallelization FAQ

Here are some frequently asked questions about parallelizing GEOS-Chem and HEMCO code with OpenMP:

17.4.1 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.

17.4.2 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.

17.4.3 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.

17.4.4 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
```

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```
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.

17.4.5 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.
! 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.
```

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```
   !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.

17.4.6 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.

17.4.7 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
```

17.5 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

EIGHTEEN

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.

18.1 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.

18.2 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

18.3 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.

18.4 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.

18.5 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
Negative values:             0
Only unitless scale factors: false
```

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```
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.

18.6 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).

18.7 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.

18.8 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.

18.9 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.

18.10 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`.

18.11 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 )
   ```

18.12 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.

18.13 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

NINETEEN

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.

19.1 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.

19.2 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

TWENTY

WORK WITH NETCDF FILES

On this page we provide some useful information about working with data files in netCDF format.

20.1 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.

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.

20.2 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)" ;
		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)" ;
```

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```
                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 SpeciesConc_RCOOH(time, lev, lat, lon) ;
                SpeciesConc_RCOOH:long_name = "Dry mixing ratio of species RCOOH" ;
                SpeciesConc_RCOOH:units = "mol mol-1 dry" ;
                SpeciesConc_RCOOH:averaging_method = "time-averaged" ;
        float SpeciesConc_O2(time, lev, lat, lon) ;
                SpeciesConc_O2:long_name = "Dry mixing ratio of species O2" ;
                SpeciesConc_O2:units = "mol mol-1 dry" ;
                SpeciesConc_O2:averaging_method = "time-averaged" ;
        float SpeciesConc_N2(time, lev, lat, lon) ;
                SpeciesConc_N2:long_name = "Dry mixing ratio of species N2" ;
                SpeciesConc_N2:units = "mol mol-1 dry" ;
                SpeciesConc_N2:averaging_method = "time-averaged" ;
        float SpeciesConc_H2(time, lev, lat, lon) ;
                SpeciesConc_H2:long_name = "Dry mixing ratio of species H2" ;
                SpeciesConc_H2:units = "mol mol-1 dry" ;
                SpeciesConc_H2:averaging_method = "time-averaged" ;
        float SpeciesConc_O(time, lev, lat, lon) ;
                SpeciesConc_O:long_name = "Dry mixing ratio of species O" ;
                SpeciesConc_O:units = "mol mol-1 dry" ;

                ... 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:
```

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```
 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,
    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
```

20.3 Read the contents of a netCDF file

20.3.1 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
  * 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
```

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```
    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
```

20.3.2 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:

```python
#!/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)
```

20.4 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
```

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```
-> 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"

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
```

20.5 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 coordinates (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 to 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
```

20.6 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.

20.6.1 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 -hO month_*nc annual_data.nc
```

You may then discard the month_*.nc files if so desired.

20.6.2 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.

20.7 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.

20.7.1 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
```

20.7.2 Regrid with nco

`nco` also includes several regridding utilities. See the Regridding section of the NCO User Guide for more information.

20.7.3 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.

20.7.4 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.

20.7.5 Regrid with gridspec and sparselt

Please see this chapter at gcpy.readthedocs.io for more information about this method of regridding.

20.8 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.

20.9 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)
```

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```
    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
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:
```

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```
            # 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)
            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()
```

20.10 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

TWENTYONE

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.

21.1 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 Co-operative 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.

21.2 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.

21.3 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.

21.3.1 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 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.
2. 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.

21.3.2 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” ;
    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” ;
```

21.3.3 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`.

21.3.4 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.

21.4 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.

21.4.1 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.

21.4.2 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.

21.5 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)" ;
            :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" ;
```

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```
            :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`).

21.6 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

TWENTYTWO

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

22.1 Species properties defined

The following sections contain a detailed description of GEOS-Chem species properties.

22.1.1 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.

22.1.2 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).

22.1.3 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.* [[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.* [[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.

Radius
Radius (m) of the species. Typically defined only for aerosols.

22.1.4 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.* [[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.

22.1.5 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.* [[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.* [[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.* [[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.

22.1.6 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.

22.2 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.

22.2.1 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
`WetDepId`	Wet deposition index

22.2.2 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
```

22.2.3 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
```

22.2.4 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'  )

   ! Print tracer concentrations
```

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```
   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.
```

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```
  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
```

22.2.5 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

   ! 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
```

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```
      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

TWENTYTHREE

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:

23.1 Using KPP: Quick start

23.1.1 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
```

23.1.2 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`.

23.1.3 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 172 reactions
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.map              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.map` 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.

23.1.4 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:
   * CUSTOMMECH:  fullchem  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.

23.2 Using KPP: Reference section

23.2.1 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.

23.2.2 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...
//
```

(continues on next page)

(continued from previous page)

```
O3 + NO = NO2 + O2 :                        GCARR(3.00E-12, 0.0, -1500.0);
O3 + OH = HO2 + O2 :                        GCARR(1.70E-12, 0.0, -940.0);
O3 + HO2 = OH + O2 + O2 :                   GCARR(1.00E-14, 0.0, -490.0);
O3 + NO2 = O2 + NO3 :                       GCARR(1.20E-13, 0.0, -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`.

23.2.3 Heterogeneous reactions

TODO Remove reference to HET array

List heterogeneous reactions after all of the gas-phase reactions in `custom.eqn`, according to the format below:

```
//
// Heterogeneous reactions
//
HO2 = O2 :                                       HET(ind_HO2,1);
↪{2013/03/22; Paulot2009; FP,EAM,JMAO,MJE}
NO2 = 0.500HNO3 + 0.500HNO2 :                    HET(ind_NO2,1);
NO3 = HNO3 :                                     HET(ind_NO3,1);
NO3 = NIT :                                      HET(ind_NO3,2);
↪{2018/03/16; XW}
... etc ...
```

Implementing new heterogeneous chemistry requires an additional step. For the reaction in question, a reaction should be added as usual, but this time the rate function should be given as an entry in the `HET` array. A simple example is uptake of HO2, specified as

```
HO2 = O2 : HET(ind_HO2,1);
```

Note that the product in this case, O2, is actually a fixed species, so no O2 will actually be produced. O2 is used in this case only as a dummy product to satisfy the KPP requirement that all reactions have at least one product. Here, `HET` is simply an array of pre-calculated rate constants. The rate constants in `HET` are actually calculated in `gckpp_HetRates.F90`.

To implement an additional heterogeneous reaction, the rate calculation must be added to this file. The following example illustrates a (fictional) heterogeneous mechanism which converts the species XYZ into CH2O. This reaction is assumed to take place on the surface of all aerosols, but not cloud droplets (this requires additional steps not shown here). Three steps would be required:

1. Add a new line to the `custom.eqn` file, such as `XYZ = CH2O : HET(ind_XYZ,1);`
2. Add a new function to `gckpp_HetRates.F90` designed to calculate the heterogeneous reaction rate. As a simple example, we can copy the function `HETNO3` and rename it `HETXYZ`. This function accepts two arguments: molecular mass of the impinging gas-phase species, in this case XYZ, and the reaction's "sticking coefficient" - the probability that an incoming molecule will stick to the surface and undergo the reaction in question. In the case of `HETNO3`, it is assumed that all aerosols will have the same sticking coefficient, and the function returns a first-order rate constant based on the total available aerosol surface area and the frequency of collisions
3. Add a new line to the function `SET_HET` in `gckpp_HetRates.F90` which calls the new function with the appropriate arguments and passes the calculated constant to `HET`. Example: assuming a molar mass of 93 g/mol, and a sticking coefficient of 0.2, we would write `HET(ind_XYZ, 1) = HETXYZ(93.0_fp, 0.2_fp)`

The function `HETXYZ` can then be specialized to distinguish between aerosol types, or extended to provide a second-order reaction rate, or whatever the user desires.

23.2.4 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;
↪ 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 :file:`geoschem_config.yml* to determine the folder in which `FJX_j2j.dat` is located.

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 GEOS-Chem module `Headers/CMN_FJX_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.

23.2.5 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 `gckpp.kpp` file:

```
#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.

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 KPP.

```
// - Many limits can be changed here by adjusting the MAX_* constants
// - To increase the max size of inlined code (F90_GLOBAL etc.),
//   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.

23.2.6 Changing the numerical integrator

Several global options for **KPP** are listed at the top of the `gckpp.kpp` file:

```
#MINVERSION   2.5.0
#INTEGRATOR   rosenbrock
#LANGUAGE     Fortran90
#UPPERCASEF90 on
#DRIVER       none
#HESSIAN      off
#MEX          off
#STOICMAT     off
```

The #INTEGRATOR tag specifies the choice of numerical integrator that you wish to use with your chemical mechanism. The Rosenbrock solver is used by default for the GEOS-Chem **fullchem** and **Hg** mechanisms. But 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 2.5.0. 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

TWENTYFOUR

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/c/geoschem

Table 2: **User manuals for GEOS-Chem and related software**

Software	Documentation
GEOS-Chem Classic	geos-chem.readthedocs.io
GCHP	gchp.readthedocs.io
HEMCO	hemco.readthedocs.io
GEOS-Chem on the cloud	geos-chem-cloud.readthedocs.io
WRF-GC (GEOS-Chem in WRF)	wrf.geos-chem.org
GCPy (Python toolkit)	gcpy.readthedocs.io
KPP (The Kinetic PreProcessor)	kpp.readthedocs.io
IMI (Integrated Methane Inversion)	imi.readthedocs.io
CHEEREIO (Data assimilation & emissions inversions)	cheereio.readthedocs.io

CHAPTER

TWENTYFIVE

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

TWENTYSIX

KNOWN BUGS AND ISSUES

Please see our Issue tracker on GitHub for a list of recent bugs and fixes.

26.1 Current bug reports

These bug reports (listed at GitHub) are currently unresolved. We hope to fix these in future releases.

CHAPTER

TWENTYSEVEN

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.

27.1 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.

27.2 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.

27.3 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

27.3.1 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. 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).
8. Review the coding conventions and checklists for code and data updates listed below.
9. Create a pull request in GitHub.
10. 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.
11. If the benchmark simulations reveal a problem with your update, the GCST will request that you take further corrective action.

27.3.2 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.

27.3.3 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. Remove extraneous code updates (e.g. testing options, other science).
5. Submit any related code or configuration files for GCHP along with code or configuration files for GEOS-Chem Classic.

27.3.4 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.

27.4 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.

27.5 How can I report a bug?

Please see **Support Guidelines**.

27.6 Where can I ask for help?

Please see **Support Guidelines**

CHAPTER

TWENTYEIGHT

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.

28.1 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.

28.2 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.

28.3 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).

28.4 How to submit changes

Please see **Contributing Guidelines**.

28.5 How to request an enhancement

Please see **Contributing Guidelines**.

CHAPTER

TWENTYNINE

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.

29.1 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`.

29.2 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.

29.3 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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INDEX