GEOS-CHEM (v14.2.0) Notes

By Li Fangzhou

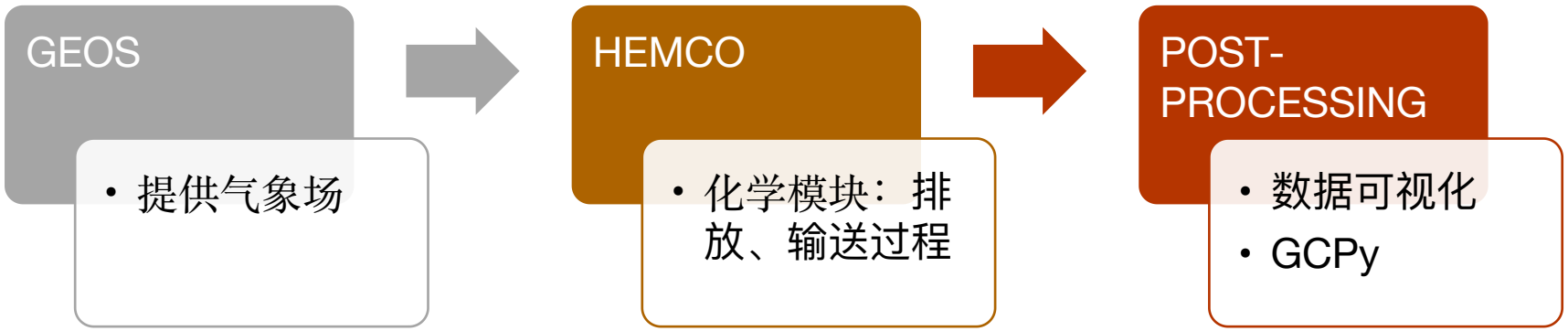
2023-09-20

OUTLINE

1. GEOS-CHEM模式简介
2. 安装环境
3. 安装步骤 - 下载及编译
   - 3.1 建立一个新实验
   - 3.2 编译及运行
4. 调参 – Configuration
5. 数据准备
   - 5.1 数据准备 – dry run
   - 筛选缺失数据 - check.py
   - 5.2 数据准备 – bashdatacatalog

1. GEOS-Chem模式简介

- 全球大气化学模型：https://geoschem.github.io/
- 2023.03 最新版本14.1.1
- **GCC: GEOS-CHEM-Classic，单节点多核并行/openMP**
- GCHP: GEOS-CHEM High Performance，多节点并行计算/MPI



2. 安装环境

- Unix系统
- 内存
  - 8-15G (4◦×5◦)
  - 30-40G （更高精度模拟）
- 软件&编译器
  - FORTRAN, C, C++, intel (推荐), GCC
  - Git
  - Cmake
  - GNU Make

Tips 测试通过版本:

Git 1.8.3.1

Cmake 3.17.5

GCC/gfortran 11.2.1

netCDF-c 4.3.3.1

Netcdf-fortran 4.4.2

3. 安装步骤 – 下载&编译

- **Step 1**

  用git下载GEOS-CHEM代码

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

  Tips: 默认文件名为GCClassic，注意保留软链接

- **Step 2**

  为模拟实验建立独立的目录

  ```
  cd GCClassic/run && ./createRunDir.sh
  ```

  然后按提示选择需要的设置 **（详见3.1）**

- **Step 3**

  继续编译**（详见3.2）**或者上传到服务器（服务器网络不支持git的情况下）再继续下一步

- **上传**

  ```
  rsync –P –e ‘ssh –p 2022’ –l –r GCClassic fzli@211.71.49.13:/share/home/fzli
  ```

  Tips: 注意要指定端口，选择断点续传，以及保留软链接

3.1 建立一个新实验

6.2 Example: Create a full-chemistry simulation run directory

第一次使用会有一个注册流程
（询问姓名单位等等）

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
```

到run目录下

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
```

选择化学模块

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

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

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

额外的模块

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)
```

选择气象场数据集

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
```

选择模拟精度
选项3代表有嵌套

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
```

选择嵌套的范围（optional）

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)
```

选择垂直精度/层数

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:
---------------------------------------------------------
```

输入你的目录位置

You can enter an absolute path (such as `$HOME/myusername/` followed by **ENTER)** .

You can 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.
---------------------------------------------------------
```

给目录起一个名字
（也会有default名字）

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_fullchem
```

or if you are creating a nested grid simulation:

不自定义命名情况下的default名字

```
-- Using default directory name gc_05x0625_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.

|br|
```

11. The last menu will prompt you with:

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

是否用github debug

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.

```
carol$ ll

    30 Sep 11 15:40 CodeDir -> /Users/carol/Desktop/GCClassic
    96 Sep 11 15:42 CreateRunDirLogs
546556 Sep 11 15:40 HEMCO_Config.rc
 11619 Sep 11 15:40 HEMCO_Config.rc.gmao_metfields
 51819 Sep 11 15:40 HEMCO_Diagn.rc
 43518 Sep 11 15:40 HISTORY.rc
    64 Sep 11 15:40 OutputDir
   469 Sep 11 15:40 README.md
    64 Sep 11 15:40 Restarts
  2816 Sep 11 15:40 archiveRun.sh
    96 Sep 11 15:42 build
   797 Sep 11 15:40 cleanRunDir.sh
 23186 Sep 11 15:40 download_data.py
  1800 Sep 11 15:40 download_data.yml
  9727 Sep 11 15:40 geoschem_config.yml
  7238 Sep 11 15:40 getRunInfo
 11307 Sep 11 15:40 metrics.py
    75 Sep 11 15:40 runScriptSamples -> /Users/carol/Desktop/
GCClassic/runScriptSamples
 93118 Sep 11 15:40 species_database.yml
```

主目录的软连接

生成log日志文件的档案库

清理上一次run生成的文件

3.2 编译及运行

1) cd run
2) ./createRunDir.sh
3) cd ~/gc_merra2_fullchem/build
4) cmake ../CodeDir -DRUNDIR=..
5) make -j 4 4是核数，也可以是其他数字
6) make install （生成**gccclassic**即为成功）
7) 重新编译之前记得 rm -r build && mkdir build && cd build
8) 查询编译情况：build_info
9) 运行即 ./gccclassic （详见6）
10) 如果你选了fullchemistry以外的module，就在第四步加上编译选项，比如开启RRTMG：

cmake ../CodeDir -DRUNDIR=.. -DRRTMG="ON"

```
lrwxrwxrwx. 1 lfz lfz       27 Sep 12 10:38 CodeDir -> /mnt/lfz/GEOSCHEM/GC-14.1
.1
drwxrwxr-x. 2 lfz lfz     4096 Sep 12 10:39 CreateRunDirLogs
-rw-rw-r--. 1 lfz lfz   546532 Sep 12 10:38 HEMCO_Config.rc
-rw-rw-r--. 1 lfz lfz    11595 Sep 12 10:38 HEMCO_Config.rc.gmao_metfields
-rw-r--r--. 1 lfz lfz    51819 Sep 12 10:38 HEMCO_Diagn.rc
-rw-rw-r--. 1 lfz lfz    43518 Sep 12 10:38 HISTORY.rc
drwxrwxr-x. 2 lfz lfz     4096 Sep 12 10:38 OutputDir
-rw-r--r--. 1 lfz lfz      469 Sep 12 10:38 README.md
drwxrwxr-x. 2 lfz lfz     4096 Sep 12 10:38 Restarts
-rwxr--r--. 1 lfz lfz     2816 Sep 12 10:38 archiveRun.sh
drwxrwxr-x. 7 lfz lfz     4096 Sep 12 15:38 build
drwxrwxr-x. 2 lfz lfz     4096 Sep 12 15:38 build_info
-rwxr--r--. 1 lfz lfz      797 Sep 12 10:38 cleanRunDir.sh
-rwxr-xr-x. 1 lfz lfz    23186 Sep 12 10:38 download_data.py
-rw-r--r--. 1 lfz lfz     1800 Sep 12 10:38 download_data.yml
-rwxr-xr-x. 1 lfz lfz 23019240 Sep 12 15:34 gcclassic
-rw-rw-r--. 1 lfz lfz     9703 Sep 12 10:38 geoschem_config.yml
-rwxr-xr-x. 1 lfz lfz     7238 Sep 12 10:38 getRunInfo
-rwxr--r--. 1 lfz lfz    11307 Sep 12 10:38 metrics.py
lrwxrwxrwx. 1 lfz lfz       72 Sep 12 10:38 runScriptSamples -> /mnt/lfz/GEOSCHE
M/GC-14.1.1/src/GEOS-Chem/run/GCClassic/runScriptSamples
-rw-r--r--. 1 lfz lfz    93118 Sep 12 10:38 species_database.yml
```

4. 调参- Configuration

- GEOS-Chem 14.0.0之前版本是修改 input.geos 文件，之后为

```
#============================================================
# 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
```

模拟类型，其他包括aerosol/CH4/CO2/Hg/POPs/etc.

起始时间

数据位置

气象场数据源，MERRA2包括1980至今的数据

变量定义列表

是否打印debug

是否打印每个过程的运算时间

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]
```

空间精度

时间精度

经度范围

中心是否设置为180

维度范围

南北极的格点精度为其他地方格点精度的一半

是否嵌套

维度范围嵌套的比例，依次为北，南，东，西

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

时间步长

输送，云对流，大气边界层混合过程，湿沉降
global模拟建议600，嵌套建议300以下

化学，排放过程
global模拟建议1200
嵌套建议600以下

RRTMG model，辐射转换过程，仅在fullchemistry模式下启用

Chemistry

化学模块设置

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

  chemistry:
    activate: true
    linear_chemistry_aloft:
      activate: true
      use_linoz_for_O3: true
    active_strat_H2O:
      activate: true
      use_static_bnd_cond: true
    gamma_HO2: 0.2

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

是否开启化学模块

线性化学计算（仅fullchemistry开启）是否运用在平流层和中间层

true – Linoz stratospheric ozone chemistry （模式计算）
false – synthetic flux of ozone （简化合成过程）

模拟的水汽是否与湿度场交互

true – 静态边界条件 （不随时间变化）
false – 非静态边界条件

Convection

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

  # .. preceding sub-sections omitted ...

  convection:
    activate: true

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

云对流过程开启

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 ...
```

干沉降过程开启

CO2浓度对植物气孔阻力的影响

单位ppb

10m以上用这个浓度

Wet deposition

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

  # .. preceding sub-sectio

  wet_deposition:
    activate: true
```

湿沉降过程开启

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 ...
```

大气边界层混合开启

true – 非局地混合参数化方案（非均匀混合）
false – 默认方案，均匀混合

Photolysis

光化学模块（仅fullchemistry和Hg模式有效）

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

数据路径

FAST-JX光化学参数化方案中，是否用模式输出的O3

FAST-JX光化学参数化方案中，是否用气象场中的O3

FAST-JX光化学参数化方案中，是否用TOMS-SBUV库中的O3

硝酸盐气溶胶的光解过程

RRTMG radiative transfer model

RRTMG - 辐射参数化方案

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

气溶胶光学属性的波长设置（unit：nm）

长短波辐射

是否输出Clear sky（无云天空）/全天空模式下的通量计算值

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 ...
```

平流方案选取，数字代表不同的方案，对应经度，维度，垂直三个方向

惰性的，仅输送，并不发生化学反应

Carbon aerosols

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

  carbon:
    activate: true                    碳气溶胶开启
    brown_carbon: false               黑碳BC
    enhance_black_carbon_absorption:  外层的coating引起的吸收效应
```

```
      activate: true
      hydrophilic: 1.5        亲水性黑碳的吸收性参数
      hydrophobic: 1.0

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

Complex SOA

The `aerosols:complex_SOA` section contains settings for

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

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

  complex_SOA:
    activate:  true
    semivolatile_POA: false

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

复杂二次气溶胶参数化方案开启
（fullchemistry中只有benchmar模式启用，其他模式关闭）

半挥发性有机气溶胶是否开启

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 ...
```

沙尘

开启的话，考虑沙尘酸性吸收过程中产生的硝酸盐，硫酸盐气溶胶增加12个变量

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 ...
```

海盐气溶胶

Accumulation/coarse mode粒径范围设置

海洋有机气溶胶，开启的话增加两个额外的变量

Stratospheric aerosols

平流层气溶胶

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

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

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

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

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

Sulfate aerosols

硫酸盐气溶胶

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
```

5. 数据准备

数据种类	获取方式
初始条件场输入数据 — Restart files 气象场数据 化学场数据 污染排放数据	1. dry run (详见5.1) 2. Bashdatacatalog （详见5.2）

5.1 数据准备 – dry run

- configure完成后执行

  ./gcclassic −dryrun >& log.dryrun

- 然后下载本次实验所需的所有数据，如果已经存在将跳过

  ./download.py log.dryrun washu

- 如果不想下载，只生成数据list

  ./download.py log.dryrun −skip

  数据list文件将生成，名为`log.dryrun.unique`

  并且生成自动下载数据的执行文件`auto_generated_download_script.sh`

- 用check.py检查缺失文件，把需要补充的文件列在`log.dryrun.unique.2`

```python
import os


# 读取包含文件路径的文件
file_path = "log.dryrun.unique"  # 替换为你的文件路径
with open(file_path, "r") as file:
    lines = file.readlines()


# 检查每一行文件路径是否存在，如果存在就删除该行
updated_lines = []
for line in lines:
    file_path = line.strip()  # 移除行尾的换行符和空格
    if not os.path.exists(file_path):
        updated_lines.append(line)


# 将更新后的内容写回文件
file_path = "log.dryrun.unique.2"
with open(file_path, "w") as file:
    file.writelines(updated_lines)


print("已删除存在的文件路径行。")
```

5.2 数据准备 - bashdatacatalog

1） 安装bashdatacatalog

- 自动安装

  bash <(curl -s https://raw.githubusercontent.com/LiamBindle/bashdatacatalog/main/install.sh)

  服务器上不行

- 手动安装

```
$ git clone https://github.com/LiamBindle/bashdatacatalog.git     # 下载安装包
$ export PATH=$PATH:$(pwd)/bashdatacatalog/bin
# add bin/ to your $PATH  (可以加入环境变量文件)
```

2） 选取对应版本的csv脚本文件：http://geoschemdata.wustl.edu/ExtData/DataCatalogs/

其中，MeteorologicalInputs.csv 不同版本的geoschem共用

批量下载csv：git clone --recurse-submodules https://github.com/geoschem/input-data-catalogs.git

3） 生成用于wget的下载文件url.txt

```
bashdatacatalog-fetch *csv  (一共要读四个csv)
bashdatacatalog-list -am -f url *.csv >& url_1411.txt (1411表示为GEOSCHEM版本为14.1.1)
wget -x -c -i url_1411.txt (-x保留相对路径，-c开启断点续传，-i接txt，逐一读取下载路径)
mv geoschemdata.wustl.edu 14-1-1 (建议把父文件夹名改为GEOSCHEM版本名字)
```

5.2 数据准备 - bashdatacatalog

1） 写一个bash脚本wget.sh

```
#!/bin/bash
while read file; do
        wget -x -c -i ${file} -b
done < url.txt
```

(url.txt文件由bashdatacatalog生成)

运行脚本

```
nohup ./wget.sh &
```

2）写一个python批量下载（详见下一页）

```python
import os
import requests
from bs4 import BeautifulSoup
from urllib.parse import urljoin
import subprocess

months = ["01","02","03","04","05","06","07","08", "09", "10", "11", "12"]

# 目标网站的URL
base_url = "http://geoschemdata.wustl.edu/ExtData/GEOS_2x2.5/MERRA2/2006/"
download_dir = "ExtData/GEOS_2x2.5/MERRA2/2006/"
os.makedirs(download_dir, exist_ok=True)

for month in months:
# 构建每个月份的URL
month_url = urljoin(base_url, month + "/")

# 发起HTTP请求并获取页面内容
response = requests.get(month_url)
soup = BeautifulSoup(response.text, "html.parser")

# 创建一个目录来存储下载的文件
month_folder = os.path.join(download_dir, month)
os.makedirs(month_folder, exist_ok=True)

# 遍历页面上的链接
for link in soup.find_all("a"):
href = link.get("href")
```

6. sbatch执行GEOSCHEM

1）写一个sh文件：

```
#!/bin/bash


#SBATCH -c 8
#SBATCH -N 1
#SBATCH -t 0-12:00
#SBATCH -p batch

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
export LD_LIBRARY_PATH=~/local/lib:$LD_LIBRARY_PATH

srun -c $OMP_NUM_THREADS time -p ./gcclassic >> GC.log
```

2）提交后台作业

```
sbatch filename.sh
```

3) 查看运行结果

- ✓ slurm.out没有Err
- ✓ GC.log没有ERROR，结尾处出现”END OF GEOSCHEM”
- ✓ 生成文件
  - ✓ OutputDir/GEOSChem*.nc4
  - ✓ OutputDir/HEMCO*.nc
  - ✓ End Time的Restart文件
  - ✓ GEOSChem.Restart.YYYYMMDD_hhmmz.nc4
  - ✓ HEMCO_restart.YYYYMMDDhh.nc

7. 嵌套实验 – nested simulation

1）需要建立两个独立实验，第一个实验先跑一个global的边界层，跑的时候需要把HISTORY.rc中的BoundaryConditions打开

```
COLLECTIONS: 'Restart',
             'SpeciesConc',
             'Budget',
             'AerosolMass',
             'Aerosols',
             'CloudConvFlux',
             'ConcAfterChem',
             'DryDep',
             'JValues',
             'JValuesLocalNoon',
             'LevelEdgeDiags',
             'ProdLoss',
             'StateChm',
             'StateMet',
             'WetLossConv',
             'WetLossLS',
             'Transport',
             'BoundaryConditions',
::
```

7. 嵌套实验 – nested simulation

2）第二个实验跑嵌套的内层，在geoschemconfig.yml文件中设置经纬度范围

```
%%% GRID MENU %%%        :
Grid resolution          : 0.25x0.3125
Longitude min/max        : -130.0 -60.0
Latitude  min/max        :   9.75  60.0
 Half-sized polar boxes?: F
Number of levels         : 47
Nested grid simulation? : T
 Buffer zone (N S E W ) :  3  3  3  3
```

3）打开HEMCO_Config.rc中的BC选项，并且修改边界层文件的路径

```
# ExtNr ExtName                on/off  Species
0       Base                   : on    *
# ----- RESTART FIELDS ----------------------
    --> GC_RESTART             :       true
    --> GC_BCs                 :       true
    --> HEMCO_RESTART          :       true

...

#==============================================================================
# --- GEOS-Chem boundary condition file ---
#==============================================================================
(((GC_BCs
* BC_   $ROOT/SAMPLE_BCs/v2019-05/tropchem/GEOSChem.BoundaryConditions.$YYYY$MM$DD_$HH$MNz.nc4 SpeciesBC_?ADV?  1980-2019/1-12/1-31/0-23 RFY xyz 1 * - 1 1
)))GC_BCs
```

4）然后就可以正常运行gcclassic了

Bugs – MAC OS

1. GCClassic/src/GEOS-Chem/run/GCClassic/init_rd.sh: line 25: realpath: command not found

   brew install coreutils

2. The following sample restart provided for this simulation was not found:

GEOSCHEM/ExtData/GEOSCHEM_RESTARTS/GC_14.0.0/GEOSChem.Restart.fullchem.20190701_0000z.nc4

3. bogon:build carol$ cmake ../CodeDir -DRUNDIR=..

   dyld[87103]: Library not loaded: '@rpath/librhash.0.dylib'

   Referenced from: '/opt/miniconda3/bin/cmake’

   ln -s librhash.1.dylib librhash.0.dylib

4. **gfortran: error:** unrecognized argument in option '**-mcmodel=medium**‘

   gfortran: note: valid arguments to '**-mcmodel=**' are: large small tiny

   fortran版本太新

Bugs – CENTOS

1. Counldn't find one or more of NetCDF's files! The following files/directories weren't found:

NETCDF_F_LIBRARY: Path to "libnetcdff.so"

NETCDF_F90_INCLUDE_DIR: Directory containing "netcdf.mod"

NETCDF_F77_INCLUDE_DIR: Directory containing "netcdf.inc”

Netcdf和GC必须同一个版本gcc编译

Netcdf必须支持fortran

2. installing netcdf-fortran 4.4.2 (https://artifacts.unidata.ucar.edu/service/rest/repository/browse/downloads-netcdf-fortran/4.4.2/)

Error: Type mismatch between actual argument at (1) and actual argument at (2) (REAL(4)/REAL(8)).

netcdf4_func.f90:720:75:

configure with:

export FCFLAGS="-w -fallow-argument-mismatch -O2"

Bugs – CENTOS

3. HEMCO ERROR: Cannot find file for current simulation time: ./Restarts/GEOSChem.Restart.20000201_0000z.nc4 - Cannot get field SPC_ACET.

vi HEMCO_Config_rc

找到SPC的一行，把EFYO改为CYS或者EY

4. Min and Max of each species in BC file [mol/mol]

   HEMCO ERROR: not enough time slices: BC_BCPI

跑嵌套的时候BoundaryCondition必须是3小时一次，如果时间精度更粗的话，就会出出现已上报错。

5. 如果同时选取同类型排放源（e.g.CEDS和EDGAR均为global anthropogenic emission inventory）,model会怎么处理?

需要查阅Hier属性,变量行最后一个数字，例如EDGAR，是”2“，CEDS是”5“，所以优先了CEDS。但是EDGAR补充了DICE_AFRICA部分

Hier

Emission hierarchy. Used to prioritize emission fields within the same emission category. Emissions of higher hierarchy overwrite lower hierarchy data. Fields are only considered within their defined domain, i.e. regional inventories are only considered within their mask boundaries.

```
#==============================================================================
(((EDGARv43
0   EDGAR_SOAP_POW $ROOT/EDGARv43/v2016-11/EDGAR_v43.CO.POW.0.1x0.1.nc   emi_co   1970-2010/1/1/0 C xy kg/m2/s SOAP 1201/26/52/280   1 2
```