GCHP v11-02 Tutorial

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Overview

1) What is GCHP and why use it?
2) Common Misconceptions
3) Useful Tips
4) Basic Tutorial
5) Introduction to GCHP Source Code
6) Resources

What is GCHP and why use it?

- GCHP features the same science as GEOS-Chem using the standard "classic" capability except:
  1. It operates on a cubed-sphere grid
  2. It is parallelized using a message-passing interface (MPI)
- GCHP improves upon GCC by:
  - Enabling more accurate transport
  - Providing efficient scaling making finer resolution global simulations possible

Common Misconceptions about GCHP

- I need a high performance compute cluster for GCHP
  - Not true! You can run GCHP on as little as one machine with 6 cores.
- I can only perform high-resolution runs with GCHP
  - Not true! GCHP can run at c24 resolution which is the cubed sphere equivalent of 4°x5°.
- I need met fields at the same resolution as my run
  - Not true! You may use GCHP with 2°x2.5° meteorology for up to at least c180 (0.5° res), although we recommend keeping the met resolution to no more than twice your run resolution equivalent to ensure quality output. If the met wind fields are too coarse relative to your internal resolution then polar divergence will occur.

Useful Tip #1: Grid Resolutions

- Cubed-sphere resolution “cN” means each of the six faces are divided into N x N grid cells.
- An easy rule-of-thumb for resolution mapping is to divide 90 by N to determine the approximate lat-lon degree resolution.

Standard lat-lon resolution	Approximate CS equivalent(s)
4° x 5°	c24
2° x 2.5°	c48
1° x 1.25°	c90
0.5° x 0.625° [1]	c180
0.25° x 0.3125° [2]	c360
0.125° x 0.15625°	c720 [3]

[1] Native resolution of MERRA-2 product from GMAO
[2] Native resolution of GEOS-FP product from GMAO
[3] Native cubed-sphere resolution of GEOS-5

Useful Tip #2: Resource Allocation

- Number of nodes and number of faces are independent
- Number of cores and number of faces are NOT independent
- Total number of cores must be divisible by number of faces (6)!
- How does it work?
  - Each NxN face is divided into NX x NY/6 segments, each comprised of approximately N/NX x N*6/NY cubed-sphere grid cells.
  - Each segment is processed by a single core
  - NX * NY must therefore equal the total number of cores
  - NX * NY/6 would ideally be square to minimize required communication between cores
- GCHP reads NX and NY from config file ‘GCHP.rc’.
- You should manually define them in script ‘runConfig.sh’ which will apply many user-configured parameters at run-time.
- More on this topic later in the presentation.

GCHP Tutorial

1. Download Source Code
2. Check Your Version
3. Create a Run Directory
4. Set Link to Source Code
5. Load Environment
6. Compile GCHP
7. Configure Run Settings
8. Run a Simulation
9. Analyze Output Data
10. Reuse a Run Directory

Step 1: Download Source Code

- You need two git repositories (repos) for source code:
  1. GEOS-Chem “classic” (GCC) code as your main directory
  2. GCHP code as a subdirectory within it

- Clone the repos from Github

```
git clone git@github.com:geoschem/geos-chem.git Code.gchp

cd Code.gchp

git clone git@github.com:geoschem/gchp.git GCHP

cd GCHP
```

- You may also fork the repositories and clone from your own Github account. This will enable you to do pull requests to submit model updates and bug fixes to the GEOS-Chem Support Team.

Step 2: Check Your Git Versions

- You can checkout any version from any of the git repos
- You must checkout compatible versions to compile and run
- The master branches will always be compatible, and will always be set to the last benchmarked version
- Check your branch from within each repo:
  - List branches with ‘git branch’. The branch you are on has an asterisk.
- To get an older version,
  - List tag names with ‘git tag’
  - Checkout a tag with ‘git checkout tags/*tagname*’
- Warnings:
  - Tag names may be slightly different in each repo
  - You are in “detached HEAD” mode when you checkout a tag. Create a new branch before editing files: ‘git checkout –b *newbranchname*’
- New to git? Git tutorials abound online. Or, check out the GCST git presentation posted on the GCHP wiki home page.

Step 3: Create a Run Directory

- You need one git repo for creating run directories
- Clone the repo from Github

```
git clone git@github.com:geoschem/geos-chem-unittest.git UT
```

- Checkout the version that matches your source code
- To create a run directory, modify UT/perl/CopyRunDirs.input:

```
#
# %%% Target directory and copy command %%%
#
   COPY_PATH      : {HOME}/GC/rundirs
   COPY_CMD       : cp -rfL
#
```

Set target directory

- Like GCC, each simulation has a different run directory
- Unlike GCC, simulation resolution is configurable at run-time

Set start and end dates

```
## ======= GCHP ========================================================
# gchp      -           -       benchmark       2013070100    2013080100    -
# gchp      -           -       standard        2013070100    2013070101    -
# gchp      -           -       RnPbBe          2013070100    2013070101    -
```

Uncomment simulation(s) of interest

Available GCHP Run Directories

- Run directories available in v11-02:
  1. Standard simulation
     - Use for full chemistry science simulations
     - Initial restart files are for July 1 and do not include HEMCO restart variables
  2. Rn-Pb-Be7 simulation
     - Use for Rn-Pb-Be7 and passive tracer simulations
     - Initial restart files are for January 1 and do not include HEMCO restart variables
  3. Benchmark simulation
     - Use for benchmarking only (turns on both complex and simple SOA)
     - Initial restart files are for July 1 and do include HEMCO restart variables
- All run directories include symbolic links to initial restart files for five resolutions: c24, c48, c90, c180, and c360.
- Like GCC, you should spin up the model to create your own restart files for production runs
- Unlike GCC, HEMCO restart variables are output in the same restart file as chemical species

GCHP Standard Run Directory

- README
- Data files (*.dat)
- Config files (*.rc, *.geos, *.nml)
- Utility scripts
  - setCodeDir
  - build.sh
  - runConfig.sh
  - gchp.run

- Makefile
- Symbolic links:
  - Restart files
  - Input data directories
  - Regridding files (tile files)
- Subdirectories
  - Env file examples
  - Output storage
  - Run script examples

```
OD ~/regal/gchp_standard $ ls
bashrcSamples/     HEMCO_Config.rc                          MetDir@
brc.dat            HEMCO_Diagn.rc                           org.dat
build.sh*          HISTORY.rc                               OutputDir/
CAP.rc             initial_GEOSChem_rst.c180_standard.nc@   README
ChemDataDir@       initial_GEOSChem_rst.c24_standard.nc@    runConfig.sh*
dust.dat           initial_GEOSChem_rst.c360_standard.nc@   runScriptSamples/
ExtData.rc         initial_GEOSChem_rst.c48_standard.nc@    setCodeDir*
FJX_j2j.dat        initial_GEOSChem_rst.c90_standard.nc@    so4.dat
FJX_spec.dat       input.geos                               soot.dat
fvcore_layout.rc   input.nml                                ssa.dat
GCHP.rc            jv_spec_mie.dat                          ssc.dat
gchp.run*          MainDataDir@                             TileFiles@
h2so4.dat          Makefile*
```

GCHP Environment Files: bashrcSamples Subdirectory

- Sample environment setup files are stored in the **`bashrcSamples`** subdirectory
- The sample files provided are mostly custom for the Harvard Odyssey compute cluster, but the ‘standalone’ file is more generic
- Examples for different compilers (ifort15, ifort17, and GNU) and MPI (OpenMPI and MVAPICH2) are included
- Use these files as examples to build ones for your own system
- Source your environment file prior to compiling and running
- You must use the same libraries during run-time that used during compilation
- Sourcing an env file is included in the run script ‘gchp.run’ but you must manually update its name to your own file

GCHP Run Config Files

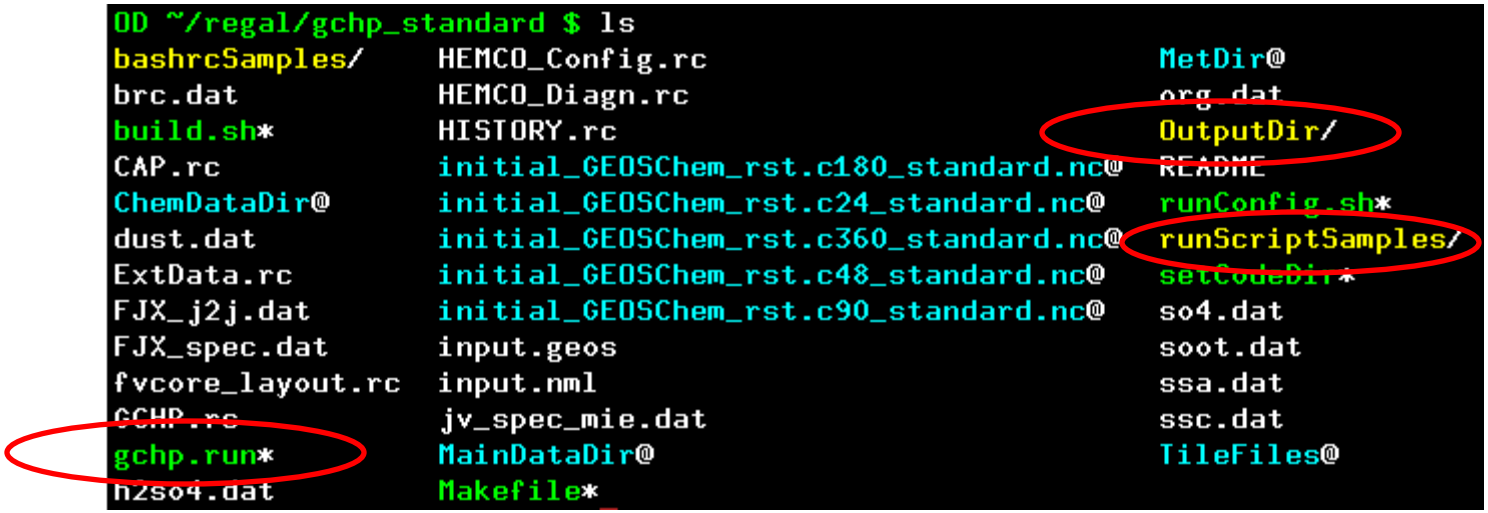
- In GCHP Only:
  - **`Cap.rc`**
    - start/end dates, and more
  - **`ExtData.rc`**
    - external data information
  - **`fvcore_layout.rc`**
    - transport-related settings
  - **`GCHP.rc`** / **`input.nml`**
    - general settings
  - **`HISTORY.rc`**
    - output data settings

- In GCHP and GCC:
  - **`HEMCO_Config.rc`**
  - **`HEMCO_Diagn.rc`**
  - **`input.geos`**
- **TIPS:**
  - Not all fields in **`input.geos`** and **`HEMCO_Config.rc`** are used
  - Some settings must be set in multiple files **(set once in runConfig.sh instead)**
  - None of these settings require recompiling

```
OD ~/regal/gchp_standard $ ls
bashrcSamples/      HEMCO_Config.rc                          MetDir@
brc.dat             HEMCO_Diagn.rc                           org.dat
build.sh*           HISTORY.rc                               OutputDir/
CAP.rc              initial_GEOSChem_rst.c180_standard.nc@   README
ChemDataDir@        initial_GEOSChem_rst.c24_standard.nc@    runConfig.sh*
dust.dat            initial_GEOSChem_rst.c360_standard.nc@   runScriptSamples/
ExtData.rc          initial_GEOSChem_rst.c48_standard.nc@    setCodeDir*
FJX_j2j.dat         initial_GEOSChem_rst.c90_standard.nc@    so4.dat
FJX_spec.dat        input.geos                               soot.dat
fvcore_layout.rc    input.nml                                ssa.dat
GCHP.rc             jv_spec_mie.dat                          ssc.dat
gchp.run*           MainDataDir@                             TileFiles@
h2so4.dat           Makefile*
```

GCHP Run Scripts and Output Directory

- **`OutputDir/`**
  - Where all GCHP diagnostic output configured in **`HISTORY.rc`** are saved
  - Restart file is NOT saved here
  - Do not remove or rename! GCHP will hang without an error message if OutputDir is missing.
- **`runScriptSamples/`**
  - SLURM:
    - **`gchp_slurm.run`**
  - Sun Grid Engine (SGE):
    - **`gchp_gridengine.run`**
  - Use these as examples for other job schedulers
- **`gchp.run`**
  - Copy of **`gchp_slurm.run`**

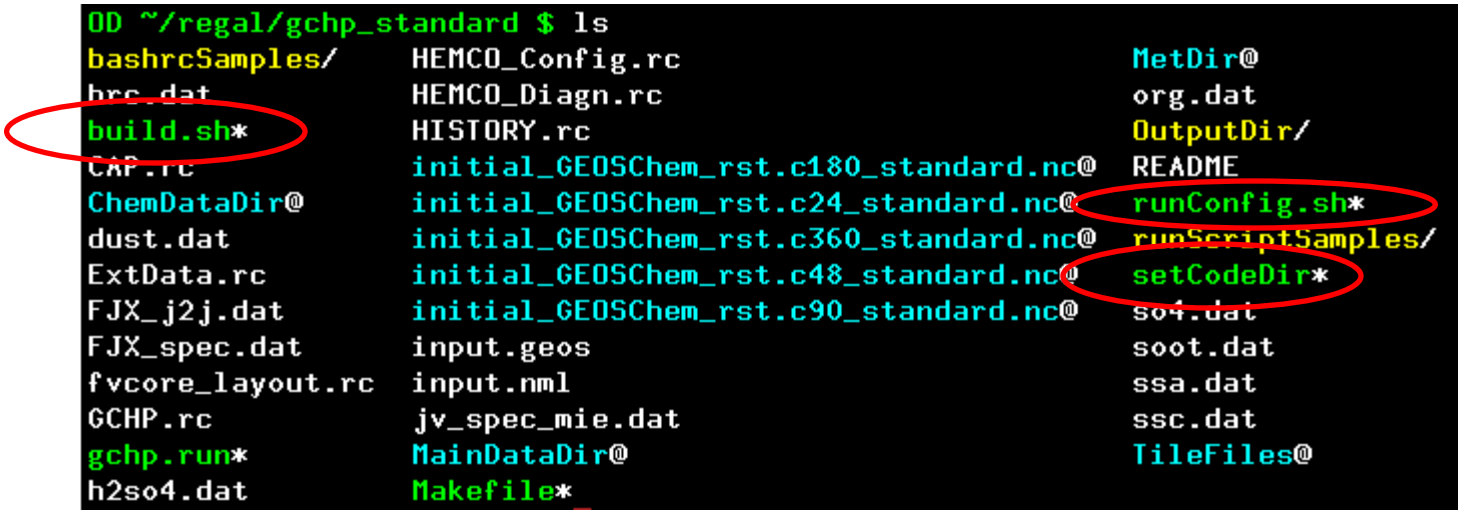


GCHP Utility Scripts

- **`setCodeDir`**
  - creates symbolic link to source code path
  - Pass full path (without links) as an argument
- **`build.sh`**
  - cleans and compiles code
  - executed in Makefile

- **`runConfig.sh`**
  - single location to update common run settings
  - overwrites config files
  - executed in run scripts

> 90% of GCHP errors are due to incorrect or inconsistent config file settings. Use bash script **`runConfig.sh`** to avoid common errors.



Step 4: Set Link to Source Code

- GCHP uses a symbolic link to source code called **`CodeDir`**
- Run bash shell script **`setCodeDir`** to set symbolic link:

```
OD ~/gchp_standard $ ./setCodeDir /n/home08/elundgren/Code.v11-02c_gchp/
CodeDir: symbolic link to `/n/home08/elundgren/Code.v11-02c_gchp/'
```

- Things to note:
  - Specify the path to the GEOS-Chem top-level directory, not the GCHP subdirectory
  - Do not include symbolic links in your source code path
  - Unlike GCC, do not edit the Makefile with your source code path

Step 5: Load GCHP Environment

- Set up your environment prior to compiling and/or running
- On Odyssey:

```
OD ~ $ source GCHP.ifort15_mvapich2_odyssey.bashrc
Loading modules for GCHP on Odyssey, please wait ...

Due to MODULEPATH changes the following have been reloaded:
  1) gd/2.0.28-fasrc01


Currently Loaded Modules:
  1) perl/5.10.1-fasrc04           4) intel/15.0.0-fasrc01   7) zlib/1.2.8-fasrc03
  2) perl-modules/5.10.1-fasrc12   5) gd/2.0.28-fasrc01      8) hdf5/1.8.12-fasrc12
  3) git/2.1.0-fasrc02             6) mvapich2/2.2-fasrc01   9) netcdf/4.1.3-fasrc09
```

- Elsewhere:
  - Create a **`.bashrc`** file based on sample files in the run directory
  - Using the libraries above is recommended but other combos are possible
    - OpenMPI
    - Intel MPI
    - Gfortran
    - Other NetCDF library versions

Step 6: Compile GCHP

- Like GCC, compile GCHP from the run directory using the Makefile

- First time compilation (30-60 min): **`make clean_compile`**
  - Warnings, error messages, and pauses are normal
  - Signs of successful compilation:
    - **“### GCHP compiled Successfully ###”**
    - The following files exist:
      - **GCHP/ESMF/esmf.install**
      - **GCHP/FVdycoreCubed_GridComp/fvdycore.install**
      - **GCHP/Shared/mapl.install**

- Subsequent compilation: **`make clean_standard`**
  - For updates to GC base code or GCHP top-level directory
  - Not for updates to GCHP subdirectories (e.g. GCHP/Shared)

Step 7: Configure Run Settings

- Use utility bash script **`runConfig.sh`** for select config settings:
  - Compute resources (e.g. # nodes and cores)
  - Internal grid resolution
  - Restart file
  - Simulation start/end times
  - Output diagnostic file frequency, duration, and mode
    - e.g. hourly (frequency) that is time-averaged (mode) and contained in daily files (duration)
  - Component on/off switches, including mixing scheme
  - Time-step intervals
  - Debug level for MAPL
- Manually change individual config files for all other settings
- Important things to understand about **`runConfig.sh`**
  - Run scripts execute **`runConfig.sh`** prior to executing **`geos`**
  - It overwrites **`input.geos`** and **`*.rc`** files (BEWARE!!!)
  - Does not updates **`HEMCO_Config.rc`** or **`Ext_Data.rc`** (yet)

runConfig.sh: Default Settings Part 1

```
#!/bin/bash

# runSettings.sh: Update select settings in *.rc and input.geos config files
#
# Usage: ./runSettings.sh
#
# E. Lundgren, 8/17/2017

############################
####  Configurables   ####
############################

#### COMPUTE RESOURCES
NUM_NODES=1
NUM_CORES_PER_NODE=6
NY=6                    # NY must be an integer and a multiple of 6
NX=1                    # NX*NY must equal total number of cores
                        # Choose NX and NY to optimize NX x NY/6 squareness
                        # within contraint of total # of CPUs
                        # e.g., (NX=2,NY=12) if 24 cores, (NX=4,NY=12) if 48

#### INPUT MET RESOLUTION
INPUT_MET_RES=placeholder # not yet implemented

### INTERNAL CUBED-SPHERE RESOLUTION
# Please note that lightning and dust emissions in GCHP are tuned to c24.
# Removing the online resolution dependency of lightning and dust by using
# offline lightning and dust emissions will be a future update. Until
# then, running at resolutions other than c24 will have degraded accuracy
# due to the resolution dependency of emissions. Please contact the GCST
# for more information.
CUBE_SPHERE_RES=24    # 24~4x5, 48~2x2.5, 90~1x1.25, 180~0.5x0.625

### INITIAL RESTART FILE
INITIAL_RESTART=default  # specify default or your own restart filename
```

See Useful Tip #2 at start of slides. Always check that your resources here match your run script settings!

Set simulation resolution

Set restart filename if not using symbolic links included in the run directory

runConfig.sh: Default Settings Part 2

```
#### SIMULATION TIMES
Start_Time="20130701 000000"
End_Time="20130701 010000"
Duration="00000000 010000"

#### OUTPUT
cs_frequency="010000"
cs_duration="010000"
cs_mode="'time-averaged'"
ll_frequency="010000"
ll_duration="010000"
ll_mode="'time-averaged'"

#### TURN COMPONENTS ON/OFF
Turn_on_Chemistry=T
Turn_on_emissions=T
Turn_on_Dry_Deposition=T
Turn_on_Wet_Deposition=T
Turn_on_Transport=T
Turn_on_Cloud_Conv=T
Turn_on_PBL_Mixing=T

#### TIMESTEPS
TransConv_Timestep_min=10
ChemEmis_Timestep_min=20

#### PBL MIXING
Use_nonlocal_PBL=T

#### DEBUG OPTIONS
MAPL_DEBUG_LEVEL=0    # 0 is none, output increases with higher values (to 20)
#GC_ND70="0 all"      # requires special handling; omit for now
```

Set simulation start and end times. Set duration to the difference, or multiples of the difference if doing segmented runs.

Set cubed-sphere file duration, data frequency, and mode, either "'time-averaged'" or "'instantaneous'". These update the "center" collection in HISTORY.rc. Ignore the "ll_" options.

Set high-level input.geos options

For MAPL debugging, set level as high as 20. Be aware this will come at great performance cost!

Step 8: Run GCHP (single node)

- Two run scripts are provided as examples of how to run GCHP:

```
OD ~/gchp_standard $ cd runScriptSamples/
OD ~/gchp_standard/runScriptSamples $ ls
gchp_gridengine.run*  gchp_slurm.run*
```

- Both run **`runConfig.sh`** prior to executing **`geos`**
- **`runConfig.sh`** will exit with an error if your settings do not make sense or if your restart file does not exist, thereby preventing GCHP from starting and hanging
- It is up to you, however, to check that your compute resource settings in your run script match those in **`runConfig.rc`**
- GCHP standard output is sent to a log called **`gchp.log`**
- You may change the log name in your run script.

Step 9: Analyze Output

- All GCHP output is in netCDF-4 format
- Two data outputs:
  - Restart file
    - Stored in top-level of run directory
    - Filename: **`gcchem_internal_checkpoint_c24.nc`** (configured in **`GCHP.rc`**)
    - Cubed-sphere grid
  - One or more diagnostic files
    - Output files are stored in **`OutputDir`**
    - File format: **`GCHP.{collection}.YYYYMMDD.nc4`**
    - Different files for each collection
    - Collections configured in **`HISTORY.rc`**
- Regrid from cubed sphere to lat-lon:
  - CSRegridTool (FORTRAN): https://bitbucket.org/sdeastham/csregridtool
  - CSRegrid (Matlab): https://bitbucket.org/gcst/csgrid
- Python tools are also available. Contact GCST for info.

Step 10: Reuse a Run Directory

- ‘make cleanup_output’:
  - Will clean your run directory (remove all output and logs)
  - Will NOT delete your executable and compile log
- You can also reuse your run directory without cleaning it. Beware that previous run files will be over-written.
- **To change meteorology resolution:**
  - Update paths in ExtData.rc
  - Change MetDir symbolic link target
- **To change run resolution:**
  - update **`runConfig.sh`**
- **To change # of cores and/or # of nodes:**
  - Remember to update **`runConfig.sh`** as well as your run script
  - Choose NX and NY such that NX by NY/6 is roughly square
  - See next slide for an example
- **See runConfig.sh for other run-time settings to play with**

GCHP with Multiple Nodes

- Example 1: 24 cores across 2 nodes
  - Run script:

```
#!/bin/bash

#SBATCH -n 24
#SBATCH -N 2
```

  - runConfig.sh:

```
#### COMPUTE RESOURCES
NUM_NODES=2
NUM_CORES_PER_NODE=12
NY=12                  # NY must be an integer and a multiple of 6
NX=2                   # NX*NY must equal total number of cores
                       # Choose NX and NY to optimize NX x NY/6 squareness
                       # within contraint of total # of CPUs
                       # e.g., (NX=2,NY=12) if 24 cores, (NX=4,NY=12) if 48
```

- Example 2: 48 cores across 3 nodes
  - Run script:
    - –n 48
    - –N 3
  - runConfig.sh:
    - NUM_NODES=3
    - NUM_CORES_PER_NODE=16
    - NY=12
    - NX=4

GCHP Source Code: ESMF, MAPL, FVdycore

ESMF and transport directories: these are compiled once and then you shouldn't need to touch them

```
OD ~/Code.v11-02/GCHP $ ls
Chem_GridCompMod.F90      GIGC_Connections.H            HEMCO_Includes_BeforeRun.H
ESMF/                     gigc_diagnostics_mod.F90      Includes_After_Dyn.H
FVdycoreCubed_GridComp/   gigc_finalization_mod.F90     Includes_After_Run.H
gchp_utils.F90            GIGC_GridCompMod.F90          Includes_Before_Dyn.H
gc_land_interface.F90     gigc_initialization_mod.F90   Includes_Before_Run.H
GCSA-HowTo.docx           GIGC.mk                       Makefile
GEOSChem.F90              gigc_mpi_wrap.F90             Registry/
GEOS_ctmEnvGridComp.F90   gigc_test_utils.F90           Shared/
GEOS_HyCoords.H           gigc_type_mod.F*
gigc_chunk_mod.F90        HEMCO_Includes_AfterRun.H
```

MAPL is stored here. It is also compiled once. Most run directory issue errors will point you here.

```
OD ~ $ cd Code.v11-02/GCHP/Shared/
OD ~/Code.v11-02/GCHP/Shared $ ls
Chem_Base/     CVS/          GFDL_fms/    GMAO_hermes/    GMAO_pilgrim/  MAPL_cfio/
Chem_Shared/   GEOS_Shared/  GMAO_etc/    GMAO_mpeu/      GNUmakefile*
Config/        GEOS_Util/    GMAO_gfio/   GMAO_perllib/   MAPL_Base/
```

Especially here.

GCHP Source Code: MAPL_Base

Error messages may lead you here…

Resource setup or time issues

Input data issues

Output data issues

Tile file issues (lat-lon <-> CS)

```
OD ~/Code.v11-02/GCHP/Shared/MAPL_Base $ ls
allgather.H                 MAPL_Cap.F90                MAPL_SatVapor.F90
allgatherv.H                MAPL_CFIO.F90               MAPL_ShmemMod.F90*
allreducemax.H*             MAPL_CFIOServer.F90         MAPL_SimpleBundleMod.F90
allreducemin.H*             MAPL_Comms.P90              MAPL_Sort.F90
allreducesum.H*             MAPL_Constants.F90          mapl_stub.pl*
arraygather.H               MAPL_ErrLog.h               MAPL_stubs.F90
arraygatherRcvCnt.H         MAPL_ErrLogMain.h           MAPL_sun_uc.P90
arrayscatter.H              MAPL_Exceptions.h           mapl_tree.py
arrayscatterRcvCnt.H        MAPL_ExtDataGridCompMod.F90 MAPL_VarSpecMod.F90
bcast.H                     MAPL_GenericCplComp.F90     mapl_vlist.py*
c_mapl_locstream_F.c        MAPL_Generic.F90            memuse.c*
CubeToLatLon.F90            MAPL_Generic.h              overload.macro*
CVS/                        MAPL_Hash.F90               Python/
eqsat.H                     MAPL_HeapMod.F90            qsatice.H
eqsat_verification.dat      MAPL_HistoryGridComp.F90    qsatlqu.H
esatice.H                   MAPL_HorzTransform.F90      read_parallel.H
esatlqu.H                   MAPL_InterpMod.F90          recv.H
ESMFL_Mod.P90               MAPL_IO.P90                 red_ma.pl*
gather.H                    MAPL_LoadBalance.F90        Sample_ExtData.rc
GetPointer.H                MAPL_LocStreamMod.F90       scatter.H
getrss.c                    MAPL_MaxMinMod.F90          send.H
GNUmakefile*                MAPL_MemUtils.F90*          sendrecv.H
hash.c                      MAPL_Mod.F90                sort.c
hinterp.F                   MAPL_NewArthParser.F90*     sun.H
HorzBinning.F90             MAPL_NominalOrbitsMod.F90   tests/
mapl_acg.pl*                MAPL_OrbGridCompMod.F90     TeX/
MAPL_Base.F90               MAPL_OrbGridComp.rc         tstqsat.F90
MAPL_base.mk*               MAPL_Profiler.F90           write_parallel.H
```

Review your run directory setup before trying to change MAPL code!

Resources

- GCHP Links:
  - Main Wiki Page
  - Online Tutorial
  - v11-02: new features, benchmarks, open and resolved issues
  - Working Group and Users

- Other Useful Links:
  - Interactive construction of a cubed-sphere grid
  - GMAO MAPL User's Guide (info may be outdated)
  - GEOS-5 wiki page for ExtData (info may be outdated)