Getting Started with High Performance GEOS-Chem

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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:
 - It operates on a cubed-sphere grid
 - It is parallelized using a message-passing interface (MPI) implementation
- GCHP improves upon GCC by:
 - Enabling more accurate transport
 - Providing efficient scaling across many cores and multiple nodes

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 with c24, the cubed-sphere equivalent of 4°x5°.
- I need met fields at the same resolution as my run
 - Not true! GCHP can use 2°x2.5° met fields 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 segments.
- 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, c45
1° x 1.25°	c96, c90
0.5° x 0.625° ¹	c192, c180
0.25° x 0.3125° ²	c384, 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 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
- NX and NY are manually set in config file GCHP.rc but are overwritten by NX and NY of your choosing in utility script runConfig.rc. Setting them will soon be automatic.
- More on this topic later in the presentation.

GCHP Tutorial

- 1. Downloading Source Code
- 2. Create a Run Directory
- 3. Load Environment
- 4. Compiling GCHP
- 5. Configure Run
- 6. Run a Simulation
- 7. Analyze Output Data
- 8. Reusing a Run Directory

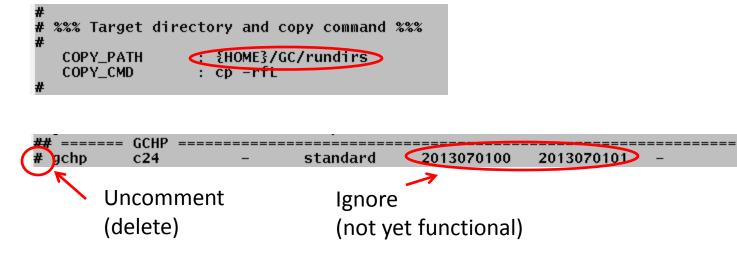
Step 1: Download Source Code

- You need two repositories for GCHP:
 - 1. GEOS-Chem "classic" (GCC) code as your main directory
 - 2. GCHP code as a subdirectory within it
- Use the GC and GCHP master branches

git clone -b master https://bitbucket.org/gcst/gc_bleeding_edge Code.v11-02_gchp
cd Code.v11-02_gchp
git clone -b master https://bitbucket.org/gcst/gchp GCHP

Step 2: Create a Run Directory

- Download a GCHP run directory from GEOS-Chem Unit Tester
- Use the UT_Bleeding_Edge master branch
 - If you have the repository already, check out the branch:
 - git pull
 - git checkout master
 - If you do not have the repository:
 - git clone -b master https:/bitbucket.org/gcst/ut_bleeding_edge UT
- Run directory set up for c24 (~4°x5°), 1 hour, standard simulation
- To download, modify UT/perl/CopyRunDirs.input:



GCHP Run Directory: Out-of-the-box Contents

- 1. Config files
- 2. Standard sim ***.dat** files
- 3. Sample .bashrc files
- 4. Sample run scripts
- 5. Utility bash scripts
- 6. Output data subdirectory
- 7. README
- 8. Makefile
- 9. Files to ignore:
 - getRunInfo
 - input.nml
 - HEMCO restart file (not used by GCHP)

WARNING: do not use the GCHP run directory out-of-the-box! Initial setup is required (more on this later).

OD ~/gchp_c24_standard \$ ls	
brc.dat	HEMCO_restart.201307010000.
build.sh*	HISTORY.rc
CAP.rc	initialSetup.sh*
dust.dat	input.geos
ExtData.rc	input.nml
FJX_j2j.dat	jv_spec_mie.dat
FJX_spec.dat	Makefile*
fvcore_layout.rc	org.dat
GCHP.gfortran_MVAPICH2.bashrc	OutputDir/
GCHP_gridengine.run*	README
GCHP.ifort13_openmpi_glooscap.bashrc	runConfig.sh*
GCHP.ifort15_mvapich2_odyssey.bashrc	so4.dat
GCHP.rc	soot.dat
GCHP_slurm.run*	ssa.dat
getRunInfo*	ssc.dat
h2so4.dat	validate*
HEMCO_Config.rc	

.nc

GCHP Run Directory: .bashrc Files

Three examples provided:

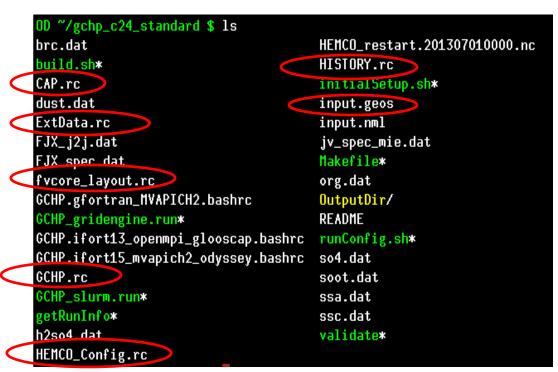
- For Odyssey (Harvard):
 - ifort15, MVAPICH2
 - gfortran, MVAPICH2
- For Glooscap (Dalhousie):
 ifort13, OpenMPI
- Other Systems
 - Use these as examples to build your own

	OD ~/gchp_c24_standard \$ ls	
	brc.dat	HEMCO_restart.201307010000.nc
	build.sh*	HISTORY.rc
	CAP.rc	initialSetup.sh*
	dust.dat	input.geos
	ExtData.rc	input.nml
	FJX_j2j.dat	jv_spec_mie.dat
	FJX_spec.dat	Makefile*
	fvcore_layout.rc	org.dat
<	GCHP.gfortran_MVAPICH2.bashrc	OutputDir/
	GCHP_gridengine.run*	README
	GCHP.ifort13_openmpi_glooscap.bashrc	<pre>wunConfig.sh*</pre>
	GCHP.ifort15_mvapich2_odyssey.bashrc	so4.dat
e).	GCHP.rc	soot.dat
	GCHP_slurm.run*	ssa.dat
	getRunInfo*	ssc.dat
	h2so4.dat	validate*
	HEMCO_Config.rc	

GCHP Run Directory: Config Files

- GCHP Specific:
 - Cap.rc
 - start/end dates, and more
 - ExtData.rc
 - external data information
 - fvcore_layout.rc
 - transport-related settings
 - GCHP.rc
 - general settings
 - HISTORY.rc
 - output data settings
- Same as GCC:
 - input.geos
 - HEMCO_Config.rc

• WARNINGS:



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

- Not all fields in input.geos and HEMCO_Config.rc are used.
- Some settings must be set in multiple files (use runConfig.sh for sanity!!!)

GCHP Run Directory: Run Scripts

Two examples provided:

- For Odyssey (Harvard):
 - GCHP_slurm.run
- For Glooscap (Dalhousie).
 GCHP_gridengine.run
- Other Systems
 - Use these as examples to build your own

OD ~/gchp_c24_standard \$ 1s	
brc.dat	HEMCO_restart.201307010000.nc
build.sh*	HISTORY.rc
CAP.rc	initialSetup.sh*
dust.dat	input.geos
ExtData.rc	input.nml
FJX_j2j.dat	jv_spec_mie.dat
FJX_spec.dat	Makefile*
fvcore_layout.rc	org.dat
GCHP.gfortran_MVAPICH2.bashrc	OutputDir/
GCHP_gridengine.run*	README
GCHP.iforti3_openmpi_glooscap.bashrc	runConfig.sh*
GCHP.ifort15_mvapich2_odyssey.bashrc	so4.dat
GCHP.rc	soot.dat
GCHP_slurm.run*	ssa.dat
getRun1nfo*	ssc.dat
h2so4.dat	validate*
HEMCO_Config.rc	

GCHP Run Directory: Output Data Storage

OutputDir/

- All GCHP output data configured in HISTORY.rc are saved here
- Restart file is not saved here
- Do not remove or rename!
 GCHP will hang without a helpful error message

OD ~/gchp_c24_standard \$ ls	
brc.dat	HEMCO_restart.201307010000.nc
build.sh*	HISTORY.rc
CAP.rc	initialSetup.sh*
dust.dat	input.geos
ExtData.rc	input.nml
FJX_j2j.dat	jv_spec_mie.dat
FJX_spec.dat	Makefile*
fvcore_layout.rc	org.dat
GCHP.gfortran_MVAPICH2.bashrc	OutputDir/
GCHP_gridengine.run*	DEADME
GCHP.ifort13_openmpi_glooscap.bashrc	runConfig.sh*
GCHP.ifort15_mvapich2_odyssey.bashrc	so4.dat
GCHP.rc	soot.dat
GCHP_slurm.run*	ssa.dat
getRunInfo*	ssc.dat
h2so4.dat	validate*
HEMCO_Config.rc	

GCHP Run Directory: Utility Scripts

- initialSetup.sh
 - creates symlinks to data
 - IMPORTANT: run once after rundir download

• 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

OD ~/gchp_c24_standard \$ 1s	
bre dat	HEMCO_restart.201307010000.nc
build.sh*	HISTORY.re
CAP_rc	initialSetup.sh*
dust.dat	input.geec
ExtData.rc	input.nml
FJX_j2j.dat	jv_spec_mie.dat
FJX_spec.dat	Makefile*
fvcore_layout.rc	org.dat
GCHP.gfortran_MVAPICH2.bashrc	OutputDir/
GCHP_gridengine.run*	READITE
GCHP.ifort13_openmpi_glooscap.baskrc	runConfig.sh*
GCHP.ifort15_mvapich2_odyssey.bashrc	S04.uai
GCHP.rc	soot.dat
GCHP_slurm.run*	ssa.dat
getRunInfo*	ssc.dat
h2so4.dat	validate*
HEMCO_Config.rc	

Step 3: One-time Run Directory Setup

- One-time setup of your run directory after downloading is required
- Run bash shell script initialSetup.sh to set symbolic links:
 - You will be prompted for your source code location (set as symlink CodeDir)
 - The rest is automatically set for you if on Odyssey (do manually elsewhere)
 - ChemDataDir ExtData/CHEM_INPUTS
 - MainDataDir ExtData/HEMCO
 - MetDir meteorology data
 - **TileFiles** ExtData/GCHP/TileFiles
 - initial_GEOSChem_rst.c24_standard.nc GCHP restart file at c24 (cubed-sphere equivalent of 4°x5°)
- Things to note:
 - Use path for your GC base code and 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
 - Config files assume **MetDir** points to 2°x2.5° GEOS-FP meteorology

Step 3: One-time Run Directory Setup

• Following initial setup, your run directory should look like this:

```
OD ~/gchp_c24_standard $ ./initialSetup.sh
Enter path to code directory:/n/home08/elundgren/Code.v11-02
Are you on Odyssey [y/n]? y
Thank you for using GCHP!
Go to http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_HP for documentation.
Send comments, issues, or questions to Lizzie Lundgren at elundgren@seas.harvard.edu.
OD ~/gchp_c24_standard $ 1s
                                      HISTORY rc
brc.dat
build.sh*
                                     initial_GEOSChem_rst.c24_standard.nc@
                                      initialSctup ch*
CAP.rc
ChemDataDir@
                                      input.geos
CodeDir@
                                      input.nml
                                      iv epec mie.dat
dusi.uat
                                      MainDataDir@
ExtData.rc
FJX_j2j.dat
                                      Makefile*
FJX_spec.dat
                                      MetDir@
fvcore_layout.rc
                                      org.uat
GCHP.gfortran_MVAPICH2.bashrc
                                      OutputDir/
GCHP_gridengine.run*
                                      README
GCHP.ifort13_openmpi_glooscap.bashrc
                                      runConfig.sh*
GCHP.ifort15_mvapich2_odyssey.bashrc
                                      so4.dat
GCHP.rc
                                      soot.dat
GCHP_slurm.run*
                                      ssa.dat
getRunInfo*
                                      sec.dat
h2so4.dat
                                      TileFiles@
HEMCO_Config.rc
                                      validate*
HEMCO_restart.201307010000.nc
```

Step 4: 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 2) perl-modules/5.10.1-fasrc12 3) git/2.1.0-fasrc02	 4) intel/15.0.0-fasrc01 5) gd/2.0.28-fasrc01 6) mvapich2/2.2-fasrc01 	 7) zlib/1.2.8-fasrc03 8) hdf5/1.8.12-fasrc12 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 or Intel MPI
 - Gfortran
 - Other NetCDF library versions

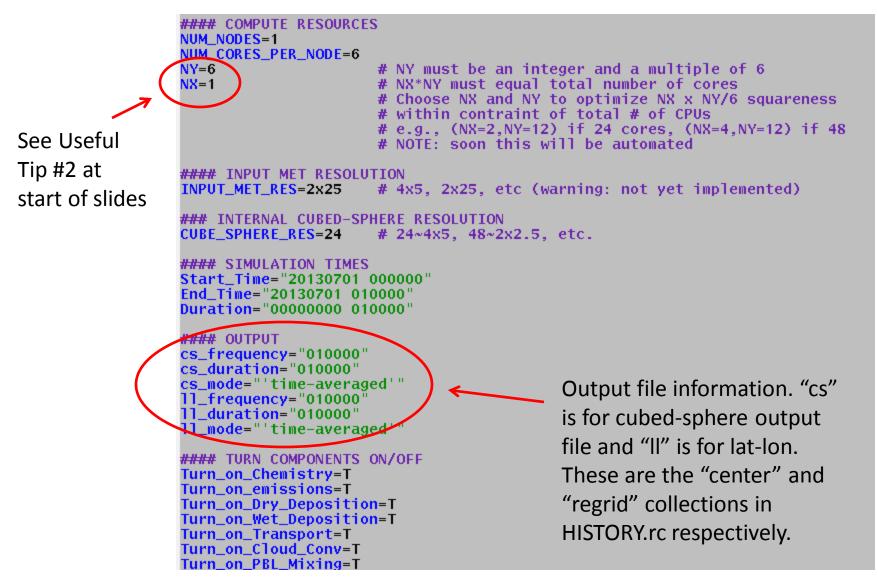
Step 5: Compile GCHP

- 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 6: Configure Run

- Use utility bash script runConfig.sh for select config settings
- If there is a setting you don't see in **runConfig.sh** (e.g. list of variables to include in output file set in **HISTORY.rc**) then you need to manually change it in the appropriate config file.
- Things to note about using runConfig.sh
 - Overwrites input.geos and *.rc files
 - Sample run scripts execute runConfig.sh prior to executing geos
 - Run scripts send summary of runConfig.sh settings to runConfig.log
 - HEMCO_Config.rc settings are not currently in runConfig.sh
 - Currently in development and design may change in the future!

runConfig.sh: Default Settings Part 1



runConfig.sh: Default Settings Part 2

DEBUG OPTIONS MAPL_DEBUG_LEVEL=0 #GC_ND70="0 all"

0 is none, output increases with higher values (to 20)
requires special handling; omit for now

TIMESTEPS
Transport_Timestep_min=10
Convect_Timestep_min=10
Emissions_Timestep_min=20
Chemistry_Timestep_min=20

GENERAL Use_variable_tropopause=T Type_of_simulation=3

PBL MIXING Use_nonlocal_PBL=T Starting here, the rest of the options in runConfig.sh (not all shown) overwrite settings in input.geos only

EMISSIONS
HEMCO_Input_file=HEMCO_Config.rc
ppt_MBL_BRO_Sim=F
Use_CH4_emissions=F
#sfc_BC_CH4=T # these need special handling since duplicate text in input.geos
#sfc_BC_OCS=T # omit for now
#sfc_BC_CCFCs=T
#sfc_BC_C1_species=T
#sfc_BC_Br_species=F
#sfc_BC_N20=T
initial_MR_strat_H20=T
CFC_emission_year=0
AEDOCOLS

AEROSOLS
Online_SULFATE_AEROSOLS=T
Online_CRYST_AQ_AEROSOLS=F
Online_CARBON_AEROSOLS=T
se_Brown_Carbon=F
Online_2dy_ORG_AEROSOLS=T
Semivolatile_POA=F
Online_DUST_AEROSOLS=T
Acidic_uptake=F

Step 7: Run GCHP (single node)

- Submit GCHP to slurm using a run script
- The most basic test is 6 cores on 1 node:

```
#!/bin/bash
#SBATCH -n 6
#SBATCH -N 1
#SBATCH -t 0-12:00
#SBATCH -p regal
#SBATCH --mem-per-cpu=6000
#SBATCH --mail-type=ALL
# Load environment
BASHRC=GCHP.ifort15_mvapich2_odyssey.bashrc
echo "WARNING: You are using environment settings in $BASHRC"
source SBASHRC
# Overwrite config files with settings in runConfig.sh
./runConfig.sh > runConfig.log
# Run GCHP
log="GCHP.log"
time srun -n $SLURM_NTASKS -N $SLURM_NNODES --mpi=pmi2 ./geos >> $log
```

• This requires the same compute resources set in runConfig.rc

Step 8: Analyze Output

- All GCHP output is in netCDF-4 format (hurray!)
- Three outputs:
 - Restart file
 - Stored in top-level of run directory
 - Filename: -gcchem_internal_checkpoint_c24.nc (configured in GCHP.rc)
 - Cubed-sphere grid
 - OutputDir/GCHP.regrid.YYYYMMDD.nc4
 - "regrid" collection configured in HISTORY.rc
 - Analogous to ND45 in GCC (species concentration diagnostic on lat/lon grid)
 - Not conservatively regridded from cubed-sphere and so we do not recommend using this data
 - OutputDir/GCHP.center.YYYYMMDD.nc4
 - "center" collection configured in HISTORY.rc
 - On the cubed-sphere grid at the run resolution and thus superior to "regrid"
 - Can be regridded from cubed-sphere to lat/lon using either of the following tools:
 - CSGrid Matlab package (https://bitbucket.org/gcst/csgrid)
 - GCPy Python package (<u>https://bitbucket.org/gcst/gcpy</u>)

Step 9: Rerunning

- You can reuse your GCHP run directory but MUST do the following prior to rerunning to avoid a seg fault: **make cleanup_output**
- Experiment with different run settings in runConfig.sh
- If changing # 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

Example: GCHP with Multiple Nodes

• Run script:

```
#!/bin/bash
#SBATCH -n 24
#SBATCH -N 2
#SBATCH -t 0-12:00
#SBATCH -p regal
#SBATCH --mem-per-cpu=6000
#SBATCH --mail-type=ALL
# Load environment
BASHRC=GCHP.ifort15_mvapich2_odyssey.bashrc
echo "WARNING: You are using environment settings in $BASHRC"
source SBASHRC
# Overwrite config files with settings in runConfig.sh
./runConfig.sh > runConfig.log
# Run GCHP
log="GCHP.log"
time srun -n $SLURM_NTASKS -N $SLURM_NNODES --mpi=pmi2 ./geos >> $log
```

• runConfig.sh:

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_OridCompNod.F90	GIGC_Connections.H	HEMCO_Includes_BeforeRun.H
	ESMF/	gigc_diagnostics_mod.F90	Includes_After_Dyn.H
_	FVdycoreCubed_GridComp/	<pre>gigc_finalization_mod.F90</pre>	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	<pre>gigc_type_mod.F*</pre>	
	gigc_chunk_mod.F90	HEMCO_Includes_AfterRun.H	

This is also compiled once. Most run directory issue errors will point you here.



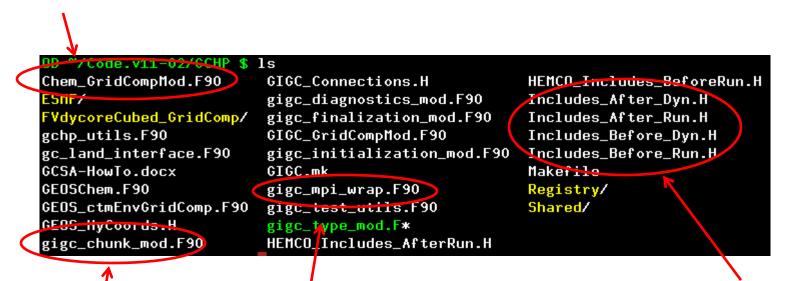
GCHP Source Code: MAPL

OD ~/Code.v11-02/GCHP/Shared/MAPL_Base \$ 1s			
	allgather.H	MAPL_Cap.F98	MAPL_SatVapor.F90
Error messages	allgatherv.H	MAPL_CEID_F90	MAPL_ShmemMod.F90*
e	allreducemax.H*	MAPL_CFIOServer.F90	MAPL_SimpleBundleMod.F90
may lead you	allreducemin.H*	MAPL_Comms.P90	MAPL_Sort.F90
here	allreducesum.H*	MAPL_Constants.F90	<pre>mapl_stub.pl*</pre>
nere	arraygather.H	MAPL_ErrLog.h	MAPL_stubs.F90
	arraygatherRcvCnt.H	MAPL_ErrLogMain.h	MAPL_sun_uc.P90
Decourse setup	arrayscatter.H	MAPL Exceptions.h	mapl_tree.py
Resource setup	arrayscatterRcvCnt.H	MAPL_ExtDataGridCompMod.F90	MAPL_VarSpecMod.F90
or time issues	bcast.H	MAPL_GenericCpiComp.F90	mapl_vlist.py*
	c_mapl_locstream_F.c	MAPL_Generic.F90	memuse.c*
	CubeTolatLon.F90	MAPL_Generic.h	overload.macro*
Input data	ers/	MAPL_Hash.F90	Python/
input data	eqsat.H	MAPL_HeapHou.F30	qsatice.H
issues	eqsat_verification.dat	MAPL_HistoryGridComp_E90	qsatlqu.H
	esatice.H	MAPL_HorzTransform.F90	read_parallel.H
	esatlqu.H	MAPL_InterpMod.F30	recv.H
Output data 🦯	ESMFL_Mod.P90	MAPL_I0.P90	red_ma.pl*
	gather.H	MAPL_LoadBalance.F90	Sample_ExtData.rc
issues	GetPointer.H	MAPL_LocStreamMod.F90	scatter.H
	getrss.c	MAPL_MaxMinMod.F90	send.H
	GNomakefile*	MAPL_MemUtils.F90*	sendrecv.H
Tile file issues 🦯	hash.c	MAPL_Mod.F90	sort.c
(lat log < > CS)	hinterp.F	MAPL_NewArthParser.F90*	sun.H
(lat-lon <-> CS)	HorzBinning.F90	MAPL_NominalOrbitsMod.F90	tests/
	<pre>mapl_acg.pl*</pre>	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!

GCHP Source Code: High-level GCHP

GCHP equivalent of main.F in that it is where the actions are executed



Module for init, run, and finalize methods called in Chem_GridCompMod.F90 (looks similar to main.F) Where Input_Opt variables are broadcast as constants to all cores Defines what import and internal states (full cubed_sphere arrays) are assigned to GEOS-Chem derived type objects to be processed per core (e.g. State_Met).

Resources

- GCHP Links:
 - <u>Main Wiki Page</u>
 - Online Tutorial
 - v11-02: new features, benchmarks, open and resolved issues
 - Working Group and Users
 - Timing Tests
- Other Useful Links:
 - Interactive construction of a cubed-sphere grid
 - FORTRAN tool for regridding between lat-lon and cubed-sphere
 - GMAO MAPL User's Guide (info may be outdated)
 - <u>GEOS-5 wiki page for ExtData (info may be outdated)</u>