

Getting Started with

GE  **S - Chem 13.0.0**

Melissa Sulprizio
Jacob Group Meeting
23 September 2020

Fall Release

The GCST plans to simultaneously release:

- GEOS-Chem 13.0.0
- GCHP 13.0.0
- HEMCO 3.0.0
- GCPy 1.0.0

All will be major version releases involving significant structural changes and breaking backwards compatibility

GEOS-Chem 13.0.0

Structural changes for GCHP and HEMCO have necessitated changes within GEOS-Chem “Classic”

- GEOS-Chem classic wrapper to encompass GEOS-Chem, HEMCO, and shared utilities
 - This will allow for HEMCO to be easily interfaced into other models
 - A separate HEMCO repository will hopefully foster feedback and developments from users outside of the GEOS-Chem community

- Change build process to CMake and retire GNU Make
 - GCHPctm and HEMCO standalone now solely use CMake
 - CMake was added as an option to GNU Make in GEOS-Chem 12.6.0

GEOS-Chem 13.0.0

Structural changes for GCHP and HEMCO have necessitated changes within GEOS-Chem “Classic”

- Move run directory files to **run/** within the GEOS-Chem repository
 - The GEOS-Chem repository already included run directory files and setup scripts for GCHPctm and GEOS-GC
 - Storing run directory files separately in the GEOS-Chem Unit Test repository has been a source of error and confusion among users
 - Run directory updates will now be pegged to a GEOS-Chem version
 - A setup script walks the users through run time options

GEOS-Chem 13.0.0 Science Updates

- Update CEDS emissions for 1970-2017 (McDuffie et al., 2020)
- Update QFED emissions through July 2020
- Updated ODIAC CO₂ fossil fuel emissions through 2018
- Global Hg emissions from Streets et al. (2019) as option
- Global Hg emissions from EDGARv4.tox2 as option
- Global Fuel Exploitation Inventory for CH₄ from Scarpelli et al. (2019)
- Enable RRTMG in GCHP and fix RRTMG netCDF diagnostics

GEOS-Chem 13.0.0 Science Updates

➤ Retire tropchem chemistry mechanism

- KPP now only has one “fullchem” mechanism
 - Previously supported Standard, Tropchem, and SOA_SVPOA mechanisms
 - Other mechanisms will eventually be added (Hg, CH₄, CO₂)
- When creating run directories, users can choose their chemistry grid
 - Selecting “Troposphere+Stratosphere” will turn on UCX logical, chemistry will be solved up to stratopause, and above stratopause GMI prod/loss rates will be applied
 - Selecting “Troposphere only” will solve chemistry up to the tropopause and apply UCX prod/loss rates above that

GEOS-Chem 13.0.0 Science Updates

➤ Retire carbon-based units

| Species | Formula | MW in GC (g/mol) | Molecular Ratio | Actual MW (g/mol) |
|---------|--|------------------|-----------------|-------------------|
| ACET | CH ₃ C(O)CH ₃ | 12.0 | 3 | 58.09 |
| ALD2 | CH ₃ CHO | 12.0 | 2 | 44.06 |
| ALK4 | >= C4 Alkanes | 12.0 | 4.3 | 58.12 |
| BENZ | C ₆ H ₆ | 12.0 | 6 | 78.12 |
| C2H6 | C ₂ H ₆ | 12.0 | 2 | 30.08 |
| C3H8 | C ₃ H ₈ | 12.0 | 3 | 44.11 |
| EOH | C ₂ H ₅ OH | 12.0 | 2 | 46.08 |
| ISOP | CH ₂ =C(CH ₃)CH=CH ₂ | 12.0 | 5 | 46.08 |
| MEK | RC(O)R | 12.0 | 4 | 72.11 |
| PRPE | C ₃ H ₆ | 12.0 | 3 | 42.09 |
| TOLU | C ₇ H ₈ | 12.0 | 7 | 92.15 |
| XYLE | C ₈ H ₁₀ | 12.0 | 8 | 106.18 |

GEOS-Chem 13.0.0 Structural Updates

➤ Metrics diagnostic collection

```
#=====
# %%%% THE Metrics COLLECTION %%%%
#
# Diagnostics for chemistry metrics such as global mean OH concentration,
# MCF lifetime, and CH4 lifetime.
#
# This diagnostic collection should always be left on.
# Use the run-directory script ./metrics_fullchem.py to print results.
#
# Available for full-chemistry and CH4 simulations only.
#=====
Metrics.template:      '%y4%m2%d2_%h2%n2z.nc4',
Metrics.format:        'CFIO',
Metrics.frequency:     'End',
Metrics.duration:      'End',
Metrics.mode:          'time-averaged'
Metrics.fields:        'AirMassColumnFull           ', 'GIGCchem',
                      'LossOHbyCH4columnTrop      ', 'GIGCchem',
                      'LossOHbyMCFcolumnTrop      ', 'GIGCchem',
                      'OHwgtByAirMassColumnFull     ', 'GIGCchem',
::
#=====
```


GEOS-Chem 13.0.0 Structural Updates

➤ Metrics diagnostic collection

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

```
Simulation start : 2019-07-01 00:00:00z
```

```
Simulation end   : 2019-08-01 00:00:00z
=====
```

```
Mass-weighted mean OH concentration      = 11.57054057008 x 10^5 molec cm^-3
```

```
CH3CCl3 lifetime w/r/t tropospheric OH = 5.3626 years
```

```
CH4 lifetime w/r/t tropospheric OH      = 9.0299 years
```

GEOS-Chem 13.0.0 Structural Updates

➤ Conversion of species database from Fortran to YAML file

```
# GEOS-Chem Species Database (04 Aug 2020)
# Core species only (neglecting microphysics)
# NOTE: Anchors must be defined before any variables that reference them
A302:
  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
ACTA:
  DD_F0: 1.0
  DD_Hstar: 4.1e+3
:
```

GEOS-Chem 13.0.0 Structural Updates

- Reduction of memory for HISTORY diagnostics
- Remove HEMCO code from PBL mixing
- Initial modifications for CESM-GC
 - Restructuring of interface routines in HEMCO
 - Removing unused MAP_A2A regridding routines
- Enable a stretched grid capability in GCHP
- Rename 'master' branch in all repositories to 'main'

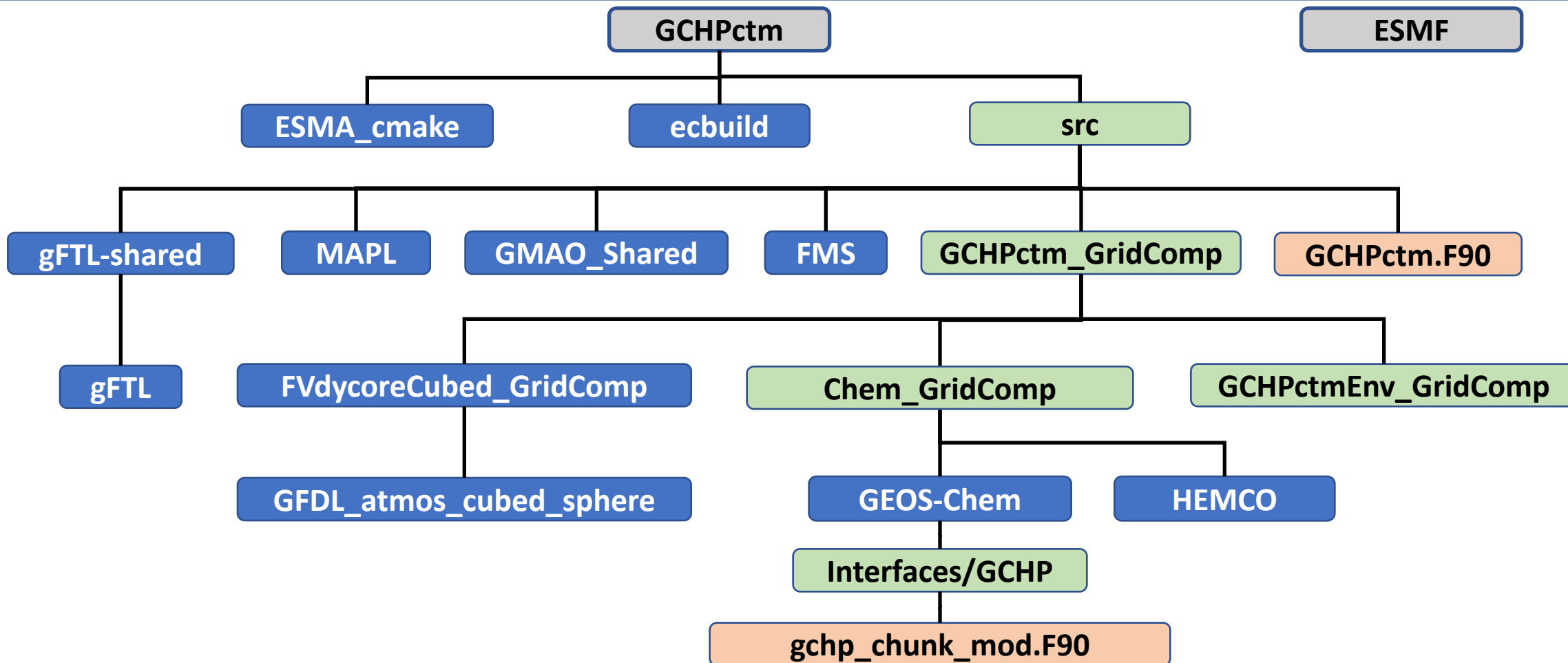
GEOS-Chem 13.0.0 Bug Fixes

- Heterogeneous chem fixes, performance improvements, clarification
- Fix UCX horizontal resolution issue when reading NO_x coefficients
- Prevent divide-by-zero errors in UCX routine UCX_NOX
- Restore separate fertilizer NO_x emissions diagnostic
- Fixes for typos:
 - Fix stratospheric loss in CH₄ simulation using 12.9.0
 - Fix for reading archived OH and Cl in CH₄ simulations
 - Update format statements in fast_jx_mod.F90 for 3 integers
 - Fix typo in mercury_mod.F for saving EmisHg0land
 - Fix species name typo in Init_HetInfo subroutine

GEOS-Chem 13.0.0 Demo

NOTE: An official tutorial will be made available through GEOS-Chem's YouTube channel when 13.0.0 is released.

GCHP 13.0.0



Credit: Lizzie Lundgren

KEY:

Git Repository

Git Repository as Submodule

Driver File

Directory

GCHPctm repository on Github

The screenshot shows the GitHub repository page for `geoschem/GCHPctm`. The repository has 8 unwatchers, 0 stars, and 5 forks. The navigation bar includes links for Code, Issues (22), Pull requests, Actions, Projects, Wiki, Security, Insights, and Settings. The repository is currently on the `main` branch, with 3 other branches and 11 tags. A recent commit by `lizziel` merged the `dev/gchp_13.0.0` branch into `main` 20 days ago, with 144 commits. The file list includes `.ci-pipelines`, `.github`, `ESMA_cmake @ a4362bf`, `src`, `.gitignore`, `.gitmodules`, and `CHANGELOG.md`.

Search or jump to... / Pull requests Issues Marketplace Explore

geoschem / GCHPctm Unwatch 8 Star 0 Fork 5

<> Code Issues 22 Pull requests Actions Projects Wiki Security Insights Settings

main 3 branches 11 tags Go to file Add file Code

lizziel Merge branch 'dev/gchp_13.0.0' into main ✓ 827768e 20 days ago 🕒 144 commits

| | | |
|-----------------------------------|--|---------------|
| <code>.ci-pipelines</code> | Updates to CI pipeline | 2 months ago |
| <code>.github</code> | Add GitHub issue and pull request templates | 2 months ago |
| <code>ESMA_cmake @ a4362bf</code> | Updates to enable using debug flags with Intel compilers | 20 days ago |
| <code>src</code> | Minor GEOS-Chem submodule updates for RRTMG and to av... | 20 days ago |
| <code>.gitignore</code> | Git ignore all directories with prefix build | 10 months ago |
| <code>.gitmodules</code> | Add GMAO pFUnit submodule for future unit testing capability | 3 months ago |
| <code>CHANGELOG.md</code> | Update CHANGELOG with correct gFTL version | 2 months ago |

About ⚙️

Wrapper for GEOS-Chem chemical-transport model to enable the high performance option (GCHP), versions 13.0.0 and above

[Readme](#)

Releases

11 tags


[Create a new release](#)

GCHPctm README.md

GCHPctm

Wrapper for GEOS-Chem chemical-transport model to enable the high performance option (GCHP).

CI statuses

| Pipeline | Status |
|-------------------------------|--|
| Build Matrix (main) |  Azure Pipelines succeeded |
| Quick Build (dev/gchp_13.0.0) |  Azure Pipelines succeeded |

Getting started

1. Set up your environment

Requirements:

- CMake (version 3.13 or greater)
- NetCDF-C, NetCDF-CXX, NetCDF-Fortran
- Fortran compiler (gfortran 8.3+, ifort 18+)
- MPI (C, C++, and Fortran)

Questions and Discussion