Getting Started with

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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	CH3C(O)CH3	12.0	3	58.09
ALD2	CH3CHO	12.0	2	44.06
ALK4	>= C4 Alkanes	12.0	4.3	58.12
BENZ	C6H6	12.0	6	78.12
C2H6	C2H6	12.0	2	30.08
C3H8	C3H8	12.0	3	44.11
EOH	C2H5OH	12.0	2	46.08
ISOP	CH2=C(CH3)CH=CH2	12.0	5	46.08
MEK	RC(O)R	12.0	4	72.11
PRPE	C3H6	12.0	3	42.09
TOLU	C7H8	12.0	7	92.15
XYLE	C8H10	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
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
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’

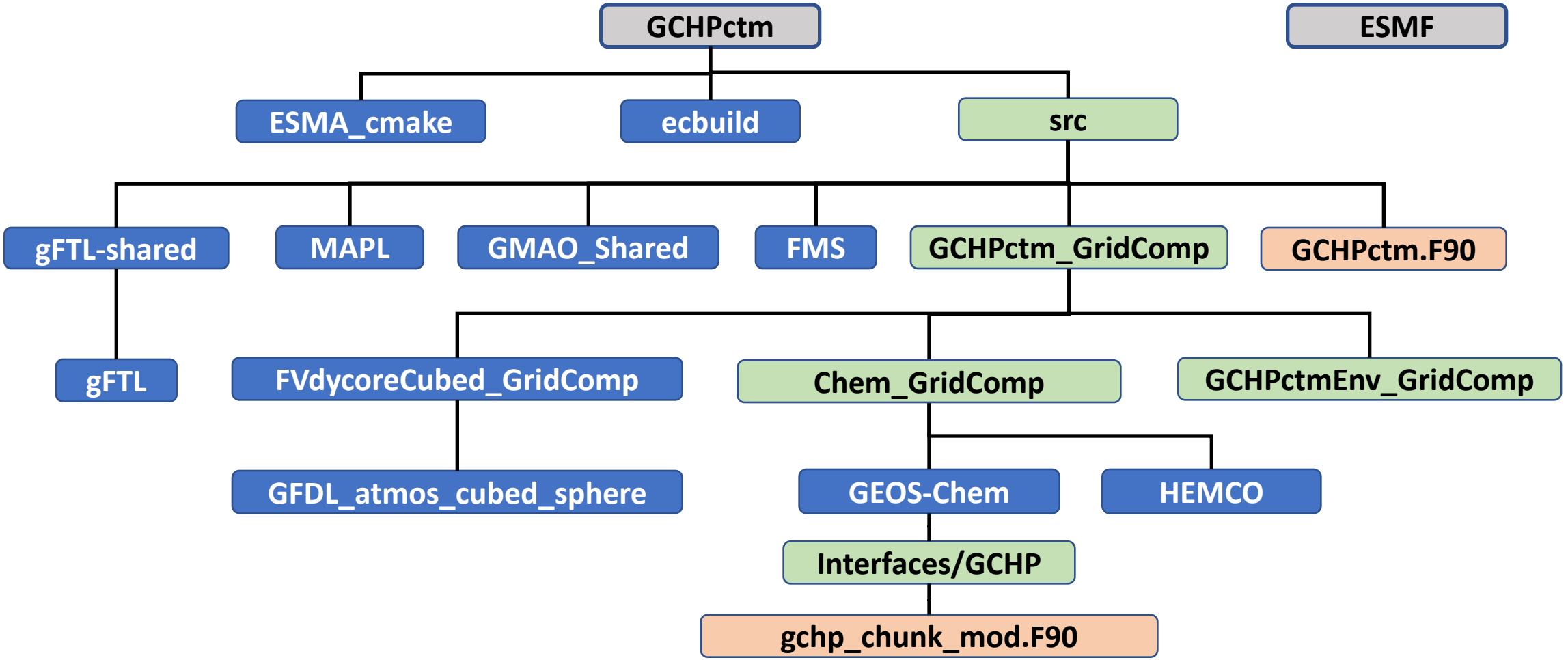
GEOS-Chem 13.0.0 Bug Fixes

- Heterogeneous chem fixes, performance improvements, clarification
- Fix UCX horizontal resolution issue when reading NOx coefficients
- Prevent divide-by-zero errors in UCX routine UCX_NOX
- Restore separate fertilizer NOx 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.

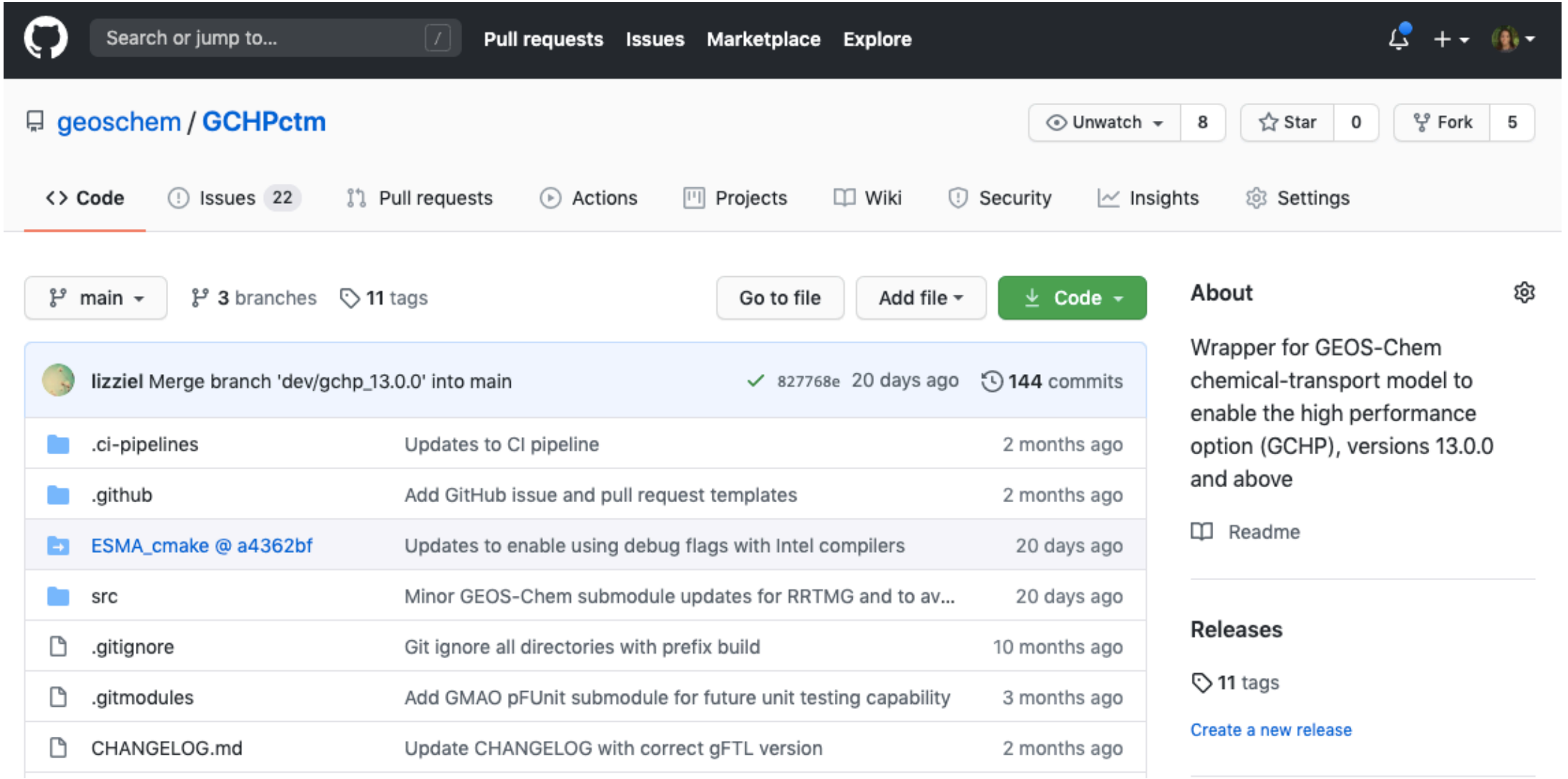
GCHP 13.0.0



Credit: Lizzie Lundgren

KEY: Git Repository | Git Repository as Submodule | Driver File | Directory

GCHPctm repository on Github



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