Getting Started with GEOS-Chem 13.0.0
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.
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
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
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
Retire carbon-based units

<table>
<thead>
<tr>
<th>Species</th>
<th>Formula</th>
<th>MW in GC (g/mol)</th>
<th>Molecular Ratio</th>
<th>Actual MW (g/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACET</td>
<td>CH₃C(O)CH₃</td>
<td>12.0</td>
<td>3</td>
<td>58.09</td>
</tr>
<tr>
<td>ALD2</td>
<td>CH₃CHO</td>
<td>12.0</td>
<td>2</td>
<td>44.06</td>
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<tr>
<td>ALK4</td>
<td>&gt;= C₄ Alkanes</td>
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<td>58.12</td>
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<tr>
<td>BENZ</td>
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<tr>
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<td>30.08</td>
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<td>C₃H₈</td>
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<tr>
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<td>XYLE</td>
<td>C₈H₁₀</td>
<td>12.0</td>
<td>8</td>
<td>106.18</td>
</tr>
</tbody>
</table>
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'.
::
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

```yaml
# 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
```

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

GCHPctm

- ESMA_cmake
- ecbuild
- src

- GMAO_Shared
- FMS
- GCHPctm_GridComp
- GCHPctm.F90

- gFTL
  - MAPL
  - FVdycoreCubed_GridComp
  - GFDL_atmos_cubed_sphere

- gFTL-shared

- Interfaces/GCHP
  - gchp_chunk_mod.F90

- GEOS-Chem
- HEMCO

- Chem_GridComp
- GCHPctmEnv_GridComp

Credit: Lizzie Lundgren

KEY:
- Git Repository
- Git Repository as Submodule
- Driver File
- Directory
GCHPctm repository on Github

About

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

Readme

Releases

Create a new release
GCHPctm

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

CI statuses

<table>
<thead>
<tr>
<th>Pipeline</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Build Matrix (main)</td>
<td><img src="https://github.com/" alt="Azure Pipelines" /> succeeded</td>
</tr>
<tr>
<td>Quick Build (dev/gchp_13.0.0)</td>
<td><img src="https://github.com/" alt="Azure Pipelines" /> succeeded</td>
</tr>
</tbody>
</table>

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