GEOS-Chem Code Structure

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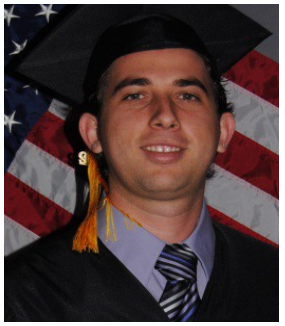

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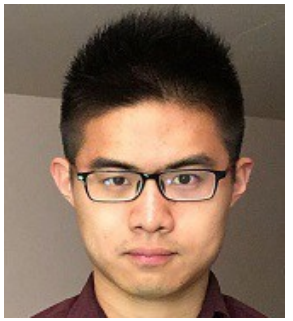


Jiawei Zhuang
(Harvard)

GCST supports the International GC User Community

User support (helpdesk)

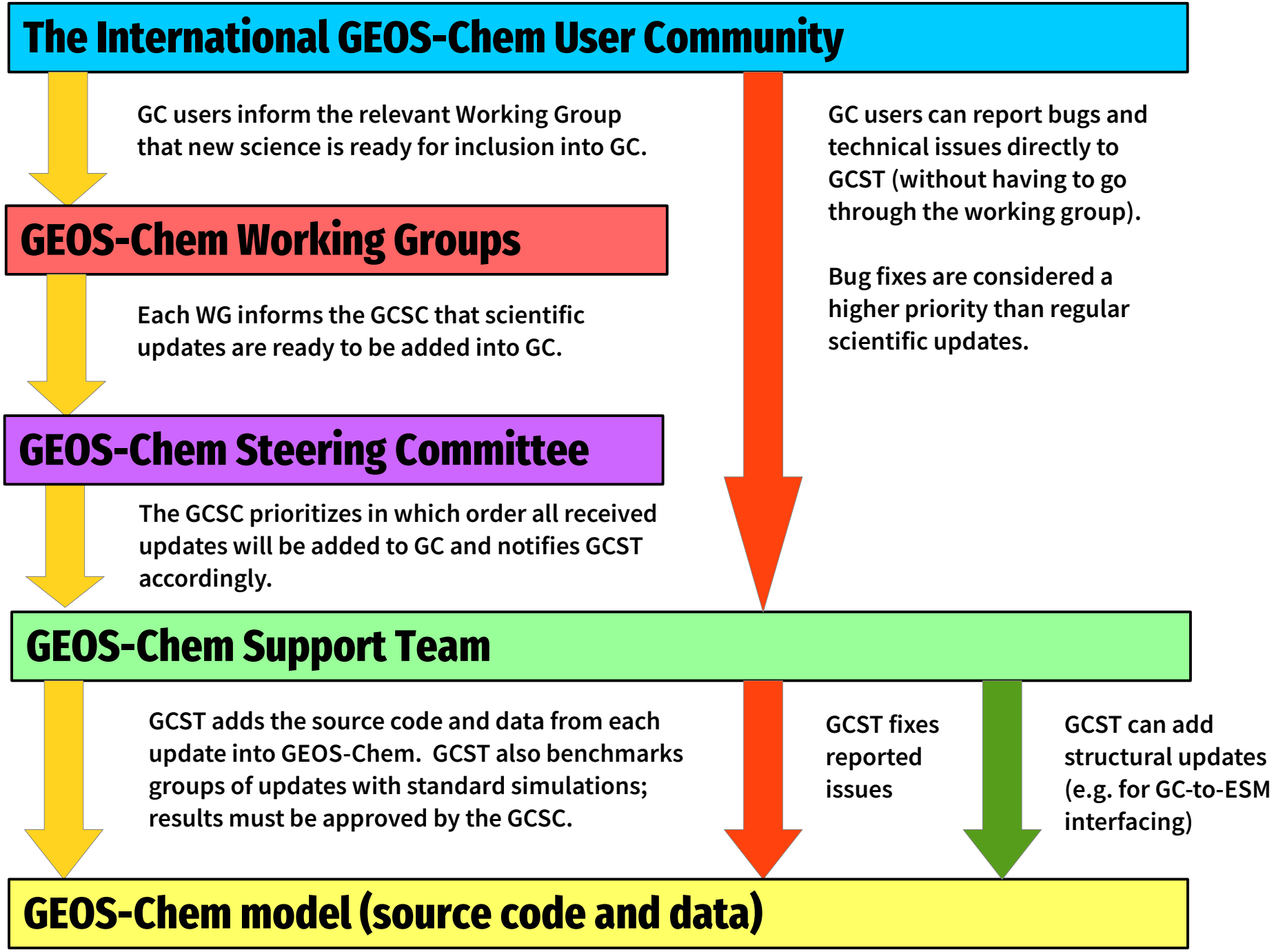
- Helping new users to get started with GC
- Assisting GC users in debugging their simulations
- Developing supporting software
- Distributing met fields & other data for input into GC
- Met field data archive: maintained by Dalhousie U.

Source code management & validation

- Accepting new GC science updates from the community
- Maintaining public code as Git repositories (on Github)
- Facilitating traceability for all updates made to GC
- Validating code updates with unit tests & difference tests
- Benchmarking GC versions with standard simulations

Documentation, communication, & education

- GC Web Site, Wiki, and Online User's Manual
- GC Adjoint wiki pages
- Quarterly e-Newsletters
- GC email lists (e.g. geos-chem@g.harvard.edu)
- Online tutorials


The International GEOS-Chem User Community
GC users inform the relevant Working Group that new science is ready for inclusion into GC.
GC users can report bugs and technical issues directly to GCST (without having to go through the working group).
Bug fixes are considered a higher priority than regular scientific updates.
GEOS-Chem Working Groups
Each WG informs the GCSC that scientific updates are ready to be added into GC.
GEOS-Chem Steering Committee
The GCSC prioritizes in which order all received updates will be added to GC and notifies GCST accordingly.
GEOS-Chem Support Team
GCST adds the source code and data from each update into GEOS-Chem. GCST also benchmarks groups of updates with standard simulations; results must be approved by the GCSC.
GCST fixes reported issues
GCST can add structural updates (e.g. for GC-to-ESM interfacing)
GEOS-Chem model (source code and data)

GEOS-Chem updates to facilitate interconnection with ESMs

2011-present
Our first case: NASA GEOS ESM

Recent GEOS-Chem updates

- Much work has been done to allow GC to interface with ESMs and to operate in HPC environments (via MPI)
  - Removal/replacement of legacy code (e.g. COMMON blocks)
  - Implementation of derived-type objects (aka state variables)
  - Species database (contains all species properties & metadata)
  - Flexible precision for floating-point real variables
    - Can toggle between 4-byte and 8-byte at compile time
  - HEMCO: A new emissions component
  - FlexChem: a clean implementation of the KPP solver package
  - Compatibility with GNU Fortran, open source compiler

State variables

- F90 allows for derived-type objects
  - Objects are custom variables that can hold many types of data
  - Objects can replace COMMON blocks and USE statements as a way to pass data between routines
- An object is essentially a “bucket of variables”
  - It's simple to add more fields to an object
  - Adding extra fields to an object does not require modifying argument lists in the routines where the object is passed
- GC now passes data between routines with objects

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt
    TYPE(MetState), INTENT(IN)    :: State_Met

! !INPUT/OUTPUT PARAMETERS:
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

This is the layout of a typical GEOS-Chem subroutine.

The use of state variables (F90 objects) allows us to drastically reduce the number of arguments that need to be passed.

Additional subroutine header comments have been omitted for the sake of brevity.

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt
    TYPE(MetState), INTENT(IN)    :: State_Met

! !INPUT/OUTPUT PARAMETERS:
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

am_I_Root

Uses type `LOGICAL`

Has value `.TRUE.` if the current CPU is the root core, or `.FALSE.` otherwise.

Can be used to restrict WRITE statemetnts (e.g. for debugging) to the root core.

Restricting WRITE statements to the root core can minimize I/O overhead when running in HPC environments (with MPI).

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt
    TYPE(MetState), INTENT(IN)    :: State_Met

! !INPUT/OUTPUT PARAMETERS:
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

Input_Opt

"Input Options" object

Uses type `OptInput`

Appears as read-only to all GEOS-Chem subroutines (except where it is populated).

Holds all of the on-off switches and input options that are read in from the main GEOS-Chem configuration file (`input.geos`).

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt
    TYPE(MetState), INTENT(IN)    :: State_Met

! !INPUT/OUTPUT PARAMETERS:
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

State_Met

"Meteorology State" object

Uses type MetState

Appears as read-only to all GEOS-Chem subroutines (except where it is populated).

Holds all meteorological fields that are read from disk, as well as fields that are derived from the input meteorology.

Any field of State_Met can be sent to netCDF diagnostic output.

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt
    TYPE(MetState), INTENT(IN)    :: State_Met

! !INPUT/OUTPUT PARAMETERS:
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

State_Chm

"Chemistry State" object

Uses type ChmState

Appears as read-write to all GEOS-Chem subroutines.

Holds:
(1) Species concentrations
(2) Arrays for aerosol properties
(3) The "species database".

Any field of State_Chm can be sent to netCDF diagnostic output.

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt
    TYPE(MetState), INTENT(INOUT) :: State_Met

! !INPUT/OUTPUT PARAMETERS:
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

State_Diag

"Diagnostic State" object

Uses type DgnState

Appears as read-write to all GEOS-Chem subroutines.

Holds arrays for quantities that will be sent to netCDF diagnostic output.

Arrays of State_Diag contain diagnostic quantities for a single timestep. Time-averaging is handled by the diagnostic routines of the parent model.

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt

! !INPUT/OUTPUT PARAMETERS:
    TYPE(MetState), INTENT(INOUT) :: State_Met
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

RC

"Return Code"

Uses type `INTEGER`

Returns `GC_SUCCESS` if the subroutine ended without errors.

Returns `GC_FAILURE` if an error is encountered.

`GC_SUCCESS` (which = 0) and `GC_FAILURE` (which = -1) are defined parameters in module `errcode_mod.F90`.

```
SUBROUTINE TYPICAL_GC_SUB( am_I_Root, Input_Opt,  State_Met,  &
                           State_Chm, State_Diag, RC          )
! !USES:
    USE Precision_Mod
    USE ErrCode_Mod
    USE Input_Opt_Mod,  ONLY : OptInput
    USE State_Chm_Mod,  ONLY : ChmState
    USE State_Diag_Mod, ONLY : DgnState
    USE State_Met_Mod,  ONLY : MetState

! !INPUT PARAMETERS:
    LOGICAL,        INTENT(IN)    :: am_I_Root
    TYPE(OptInput), INTENT(IN)    :: Input_Opt

! !INPUT/OUTPUT PARAMETERS:
    TYPE(MetState), INTENT(INOUT) :: State_Met
    TYPE(ChmState), INTENT(INOUT) :: State_Chm
    TYPE(DgnState), INTENT(INOUT) :: State_Diag

! !OUTPUT PARAMETERS:
    INTEGER,        INTENT(OUT)   :: RC

! LOCAL VARIABLES:
    REAL(fp)                      :: Var_Flex
    REAL(f4)                      :: Var_4byte
    REAL(f8)                      :: Var_8byte
```

fp, f4, f8

Fortran KIND parameters, stored in `precision_mod.F90`

fp = flexible precision. This is Set to `REAL*8` by default but can be toggled to `REAL*4` at compile time if so desired.

f4 = 4-byte (`REAL*4`) precision

f8 = 8-byte (`REAL*8`) precision

Most floating-point variables in GEOS-Chem are defined with **REAL(fp)**.

HEMCO[1]:
A new way to compute emissions
(and also pre-process non-emissions data)

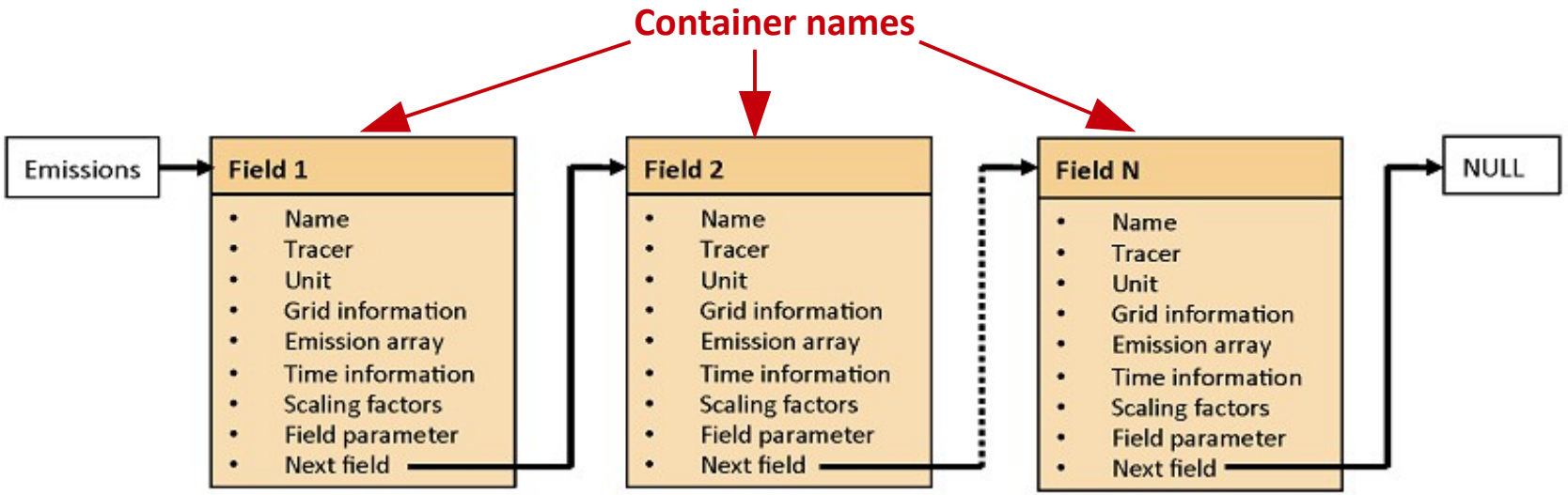
Introduced in 2015

[1]Harvard-NASA Emissions Component
cf, C. Keller et al, GMD, 7, 1409-1417, 2014.

HEMCO features

- Author: Christoph Keller (now at NASA/GMAO)
- Users can choose which emissions inventories and/or non-emissions data to include by editing the HEMCO configuration file.
- HEMCO reads data in their native resolution from netCDF format and regrids to the model resolution.
  - For non-Cartesian regridding (e.g. cubed-sphere), HEMCO can use the regridding capability supplied by the parent model (cf. “ExtData” module of NASA GEOS ESM).
- HEMCO stores data in its “linked list” structure.
- HEMCO applies scale factors, masks, other manipulations to data.
- Addition of new inventories or data sources via HEMCO is immediate.
- HEMCO can write the resultant emissions or data to netCDF format.
- See *The HEMCO User's Guide* for more information
  - http://wiki.geos-chem.org/The_HEMCO_Users_Guide

The emissions linked list in HEMCO



- List with all emission data
- Flexible length
- One variable ('Emissions') leads to all content
- Contains all information required to calculate the emissions

The heart and soul of HEMCO is the **linked list** structure. The linked list consists of multiple **containers**. Each **container** can store an **emissions inventory** (global or regional), a **non-emissions data set**, a **scale factor**, a **mask**, the **total computed emissions for a given species**, or a **diagnostic output**.

Courtesy of Christoph Keller

HEMCO online vs. HEMCO offline

- HEMCO can interface directly with GEOS-Chem
  - Which is the typical mode of operation for GC “Classic”.
  - But the I/O overhead can be substantial when if running at ¼ degree resolution in an HPC environment.
- HEMCO can also operate as a standalone model
  - Users can generate emissions with the HEMCO standalone for:
    - The same spatial resolution as the ESM that drives GC
    - Any temporal resolution (hourly, daily, monthly, etc.)
  - These resultant emissions can be simply read from disk.
  - This is the preferred mode of operation for e.g. GC in GEOS-ESM.

FlexChem:
A clean implementation of the KPP[1] chemical solver

Introduced in 2017

[1]KPP = Kinetic Pre-Processor
cf. A. Sandu & R. Sander, ACP., 6, 187-195, 2006

KPP features

- The Kinetic Pre-Processor (KPP) can create optimized code for solving a chemical mechanism:
  - Inputs
    - A list of chemical species
    - A list of reactions and coefficients
    - Functions for computing rate constants
    - Choice of a desired solver (e.g. Rosenbrock, Runge-Kutta, etc.)
  - Outputs:
    - Optimized source code (in C++, F77, F90, or Matlab) for solving the given chemical mechanism for adding into an external model.
  - GEOS-Chem uses the F90 modules produced by KPP.

Updating FlexChem mechanisms

1) Download and compile KPP source code from our repo:
   a) https://bitbucket.org/gcst/kpp; checkout GC_Updates branch
2) Update the following files:
   a) gckpp.kpp Global options, inlined rate functions, P/L families
   b) globchem.spc Species definitions
   c) globchem.eqn Reaction definitions, coefficients
3) Run the KPP executable to create F90 modules
4) Copy F90 modules to the `KPP/Custom` folder of GC
5) Compile GC with `CHEM=Custom` flag

See: wiki.geos-chem.org/FlexChem#Adding_chemical_mechanisms_in_FlexChem

Challenges for the near future

Challenges for model development

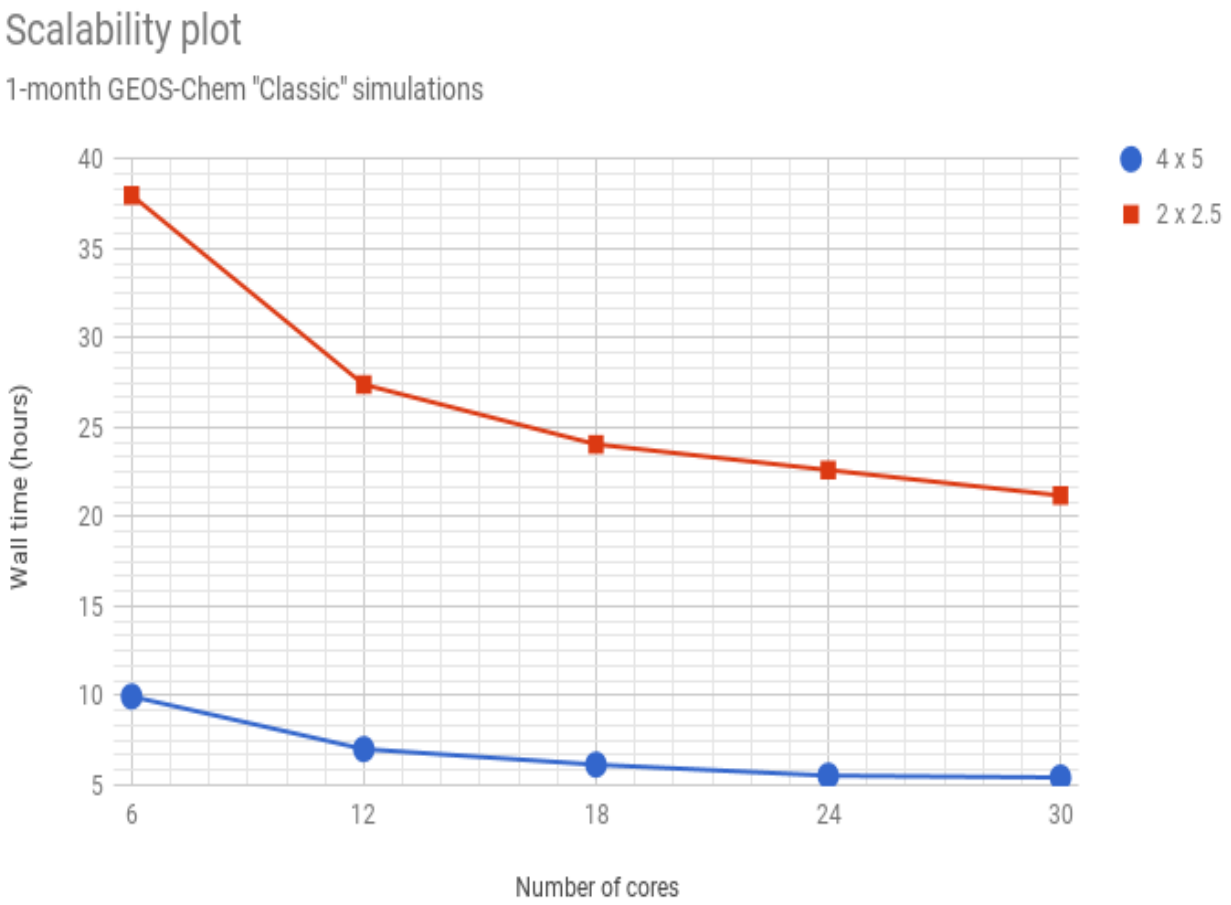
- Improving performance
  - We would like to make chemistry go faster.
  - We also know some operations (e.g. wetdep) do not scale well.
- Legacy code
  - While most data is now passed via objects, some legacy modules still rely on USE-associated arrays. Problematic for e.g GC-CESM.
  - Also, GC contains third-party code that is difficult to modify.
- Data
  - Using GC in a CTM mode at e.g. ¼° resolution requires lots of archived met data. Coupling to ESM may reduce data storage.

For more information

- All on the GEOS-Chem wiki (wiki.geos-chem.org):
  - HEMCO
  - Implementation of HEMCO in GEOS-Chem
  - The HEMCO User's Guide
  - FlexChem
  - GEOS-Chem species database
  - Physical properties of GEOS-Chem species
- Email the GEOS-Chem Support Team:
  - `geos-chem-support@as.harvard.edu`

Extra Slides
for reference

Current performance of GC “Classic”



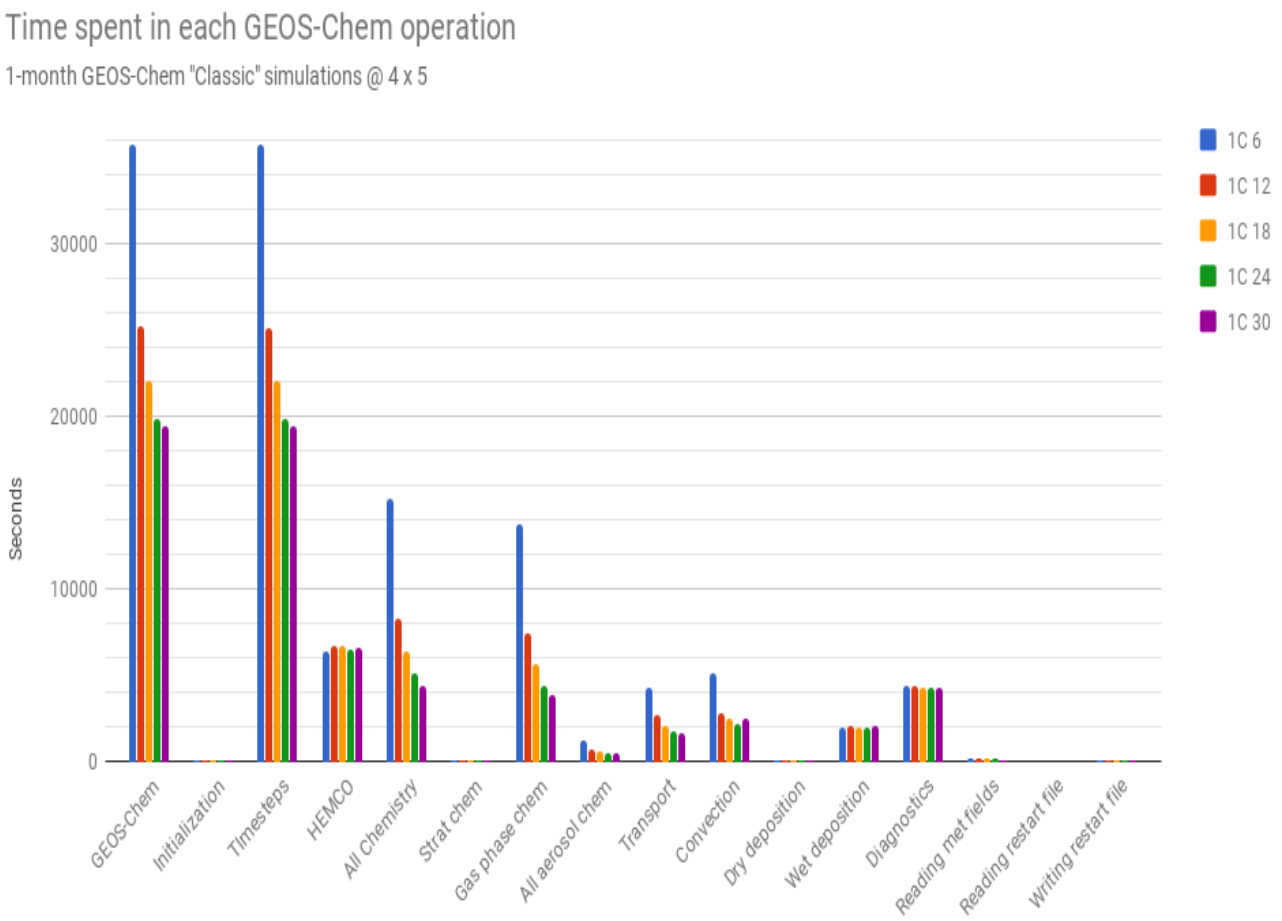
This plot represents several 1-month GC “Classic” simulations (done for the GCHP Paper).

Machine: Odyssey “shared” partition, where each node has 2 Intel Broadwell CPUs x 16 CPUs/node = 32 CPUs/node. Each node has 128 GB RAM. Network = FDR Infiniband.

Adding more cores to both the **2 x 2.5** and **4 x 5** runs results in increased run times (increasing asymptotically). We do not see the “turnover” as we did in Mat’s plot, where adding more cores results in slower runs.

The **4 x 5** run with 30 cores is about 2x as fast as with 6 cores.

Time spent in each GC operation – 4 x 5



Best scalability: Gas-phase chemistry (KPP solver). Speedup is about 3.5x when going from 6 -> 30 cores!

Transport and convection scale less well than KPP (speedup of about 2x).

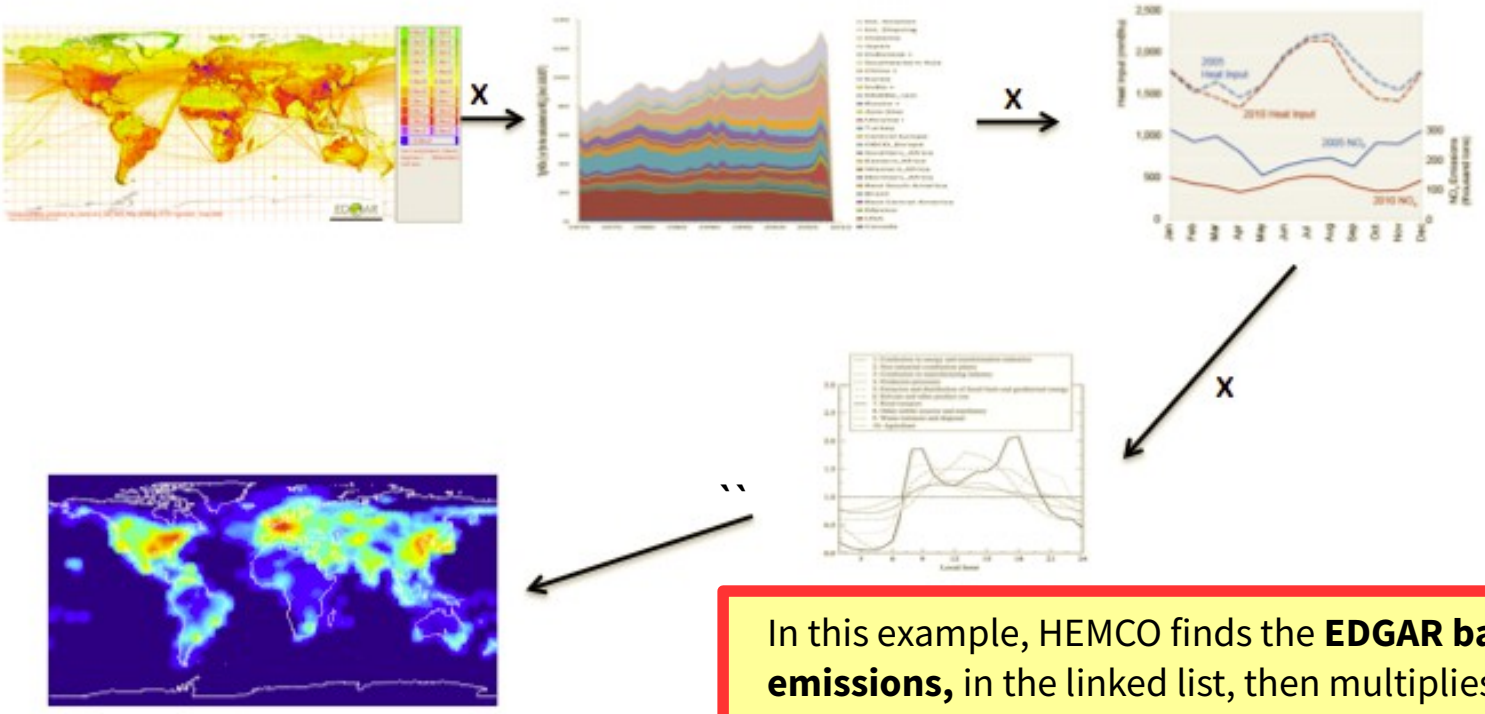
HEMCO + Diagnostics don't show much speedup. These involve disk I/O, which only operates on the main thread.

Wetdep also doesn't scale well; perhaps due to non-optimal loop ordering. We loop over each surface box, then over vertical boxes and species (IJLN). But the optimal ordering is to have the N loop on the outside (NLIJ), because this will step through the array in the order it is laid out in memory. (This reduces the number of memory accesses via the CPU cache.)

Everything else is in the noise.

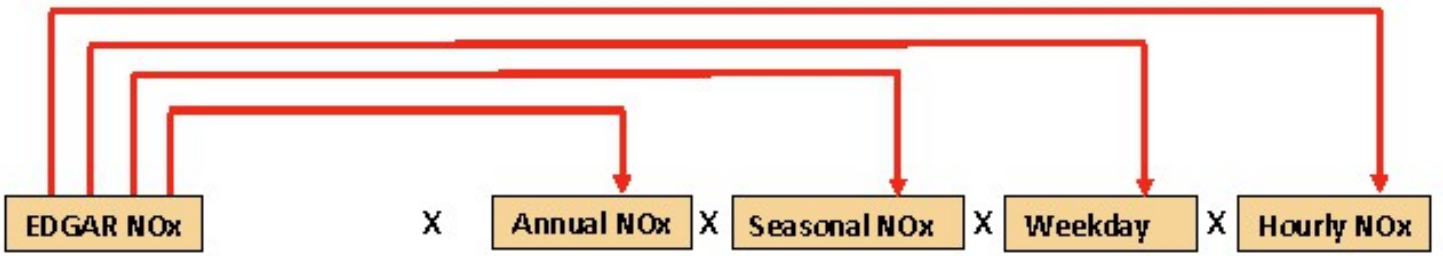
The 2 x 2.5 plot looks similar.

Applying the scale factors: Pointers!



In this example, HEMCO finds the **EDGAR base emissions,** in the linked list, then multiplies it only by the **scale factors** that are relevant. (You specify scale factors for each inventory in the configuration file.)

EDGAR NOx for given time step:



Courtesy of Christoph Keller

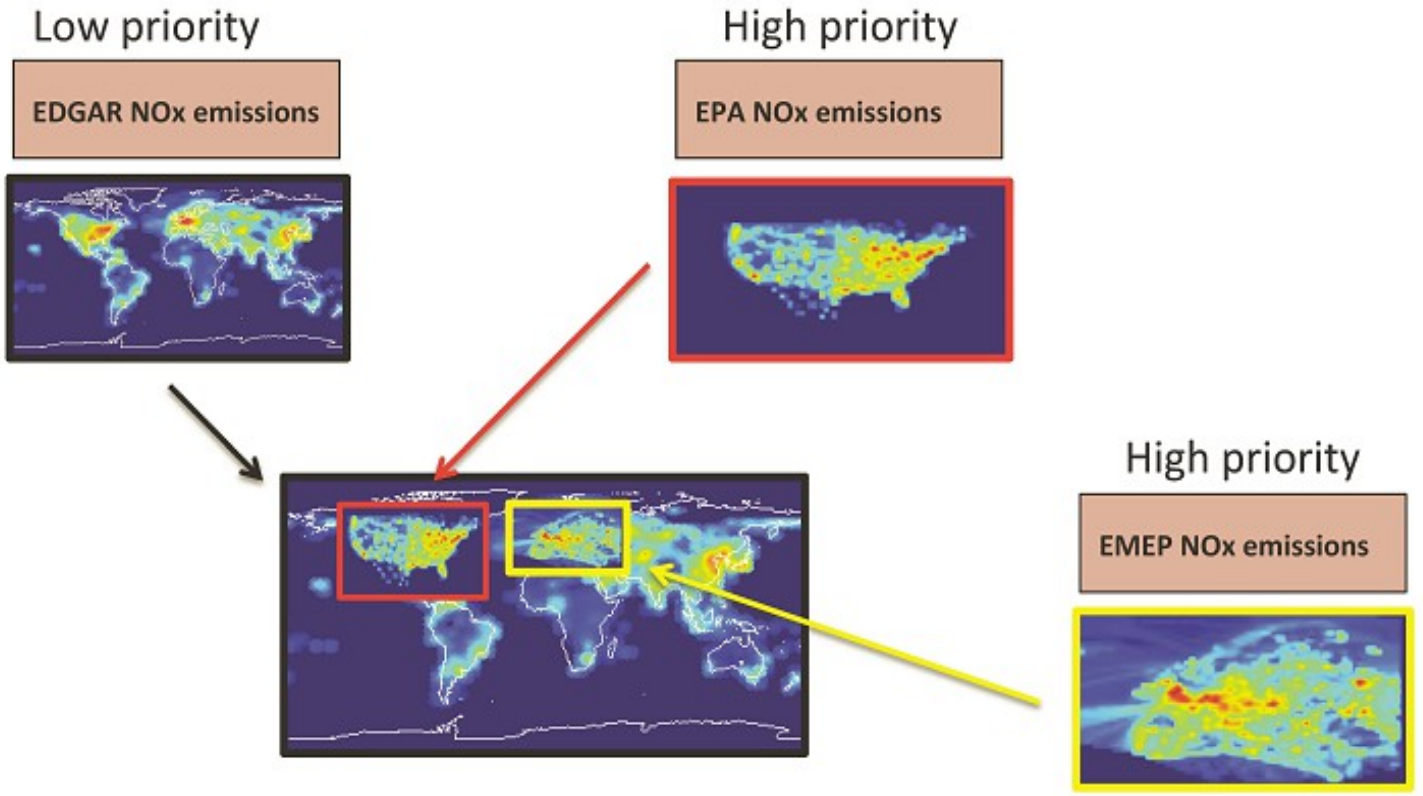
Field priorities

- Hierarchy of emissions defined through field priorities
- High-priority emissions overwrite low-priority emissions

In the HEMCO configuration file, you can specify the **priorities** for each species in each inventory.

Emissions of different ***categories*** are added together (e.g. anthro + biomass NO).

Emissions in the same category (e.g. anthro NO) may be assigned a ***hierarchy*** (higher values overwrite lower values).



Courtesy of Christoph Keller

The HEMCO Configuration file

1) Settings
2) Base Emission Switches
3) Base Emissions Data
4) Extensions Switches
5) Extensions Data
6) Scale Factors
7) Masks
8) Non-Emissions Data

HEMCO configuration file: *Settings*

```
###############################################################################
### BEGIN SECTION SETTINGS
###############################################################################

ROOT:                           /n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid/data/ExtData/HEMCO
Logfile:                        HEMCO.log
DiagnFile:                      HEMCO_Diagnostics.rc
DiagnPrefix:                    HEMCO_diagnostics
DiagnFreq:                      End
Wildcard:                       *
Separator:                      /
Unit tolerance:                 1
Negative values:                0
Only unitless scale factors:    false
Verbose:                        0
Warnings:                       1

### END SECTION SETTINGS ###
```

The HEMCO configuration file (usually named HEMCO_Config.rc) is where you specify emissions settings. You can specify general information for HEMCO in the **SETTINGS** area at the top of the file.

- **ROOT** is the path to the HEMCO data directories (this will vary on each system, above is shown for Odyssey)
- **Logfile** specifies the name of the log file where errors, warnings, and verbose output will be sent.
- **DiagnFile** is optional. It is a file where you list which quantities you would like HEMCO to archive to netCDF files.
- **DiagnPrefix** and **DiagnFreq** specify the file template and frequency for saving HEMCO diagnostics to netCDF files.
- **Unit Tolerance** controls the amount of tolerance **(1=recommended)** if netCDF file units differ from the listed units.
- **Verbose** and **Warnings** control the amount of output that will be sent to the log file (3=most, 0=least).

HEMCO configuration file: *Base Emissions Switches*

```
# ExtNr ExtName             on/off  Species
0       Base                : on    *
    --> HEMCO_RESTART       :       true
    --> AEIC                :       true
    --> BIOFUEL             :       true
    --> BOND                :       true
    --> BRAVO               :       true
    --> CAC                 :       true
    --> XIAO                :       true
    --> C2H6                :       true
    --> EDGAR               :       true
    --> HTAP                :       false
    --> EMEP                :       true
    --> EMEP_SHIP           :       true
    --> GEIA                :       true
    --> LIANG_BROMOCARB     :       true
    --> NEI2005             :       false
    --> NEI2011             :       true
    --> RETRO               :       true
    --> SHIP                :       true
    --> NEI2011_SHIP        :       false
    --> MIX                 :       true
    --> STREETS             :       false
    --> VOLCANO             :       true
    --> RCP_3PD             :       false
    --> RCP_45              :       false
    --> RCP_60              :       false
    --> RCP_85              :       false
    --> QFED2               :       false
```

HEMCO computes emissions in two ways:

Base Emissions are emissions that can just be read from disk. Most emission inventories fall into this category.

Some emissions are implemented as **HEMCO Extensions**. In this case HEMCO has to compute these emissions using meteorological inputs (P, T, RH, U, V, etc.). More on these in the next few slides.

The list at left shows the various input options in the **Base Emissions**. This list appears at the top of the ***Base Emissions Switches*** section in the HEMCO_Config.rc file. You can toggle individual emission inventories on or off.

For example, if you wanted to turn off the **AEIC aircraft inventory,** you would change its setting under the Species column from true to false.

HEMCO configuration file: *Base Emissions Data*

```
#==============================================================================
# --- AEIC aircraft emissions ---
#
# ==> Now emit aircraft BC and OC into hydrophilic tracers BCPI and OCPI.
#==============================================================================
(((AEIC
0 AEIC_NO   $ROOT/AEIC/v2014-10/aeic_2005.geos.1x1.47L.nc  NO       2005/1-12/1/0 C xyz kg/m2/s NO   110/115 20 1
0 AEIC_CO   $ROOT/AEIC/v2014-10/aeic_2005.geos.1x1.47L.nc  CO       2005/1-12/1/0 C xyz kg/m2/s CO   110     20 1
0 AEIC_SO2  $ROOT/AEIC/v2014-10/aeic_2005.geos.1x1.47L.nc  FUELBURN 2005/1-12/1/0 C xyz kg/m2/s SO2  111     20 1
0 AEIC_SO4  -                                              -        -             - -   -       SO4  112     20 1
0 AEIC_BCPI -                                              -        -             - -   -       BCPI 113     20 1
0 AEIC_OCPI -                                              -        -             - -   -       OCPI 113     20 1
0 AEIC_ACET $ROOT/AEIC/v2014-10/aeic_2005.geos.1x1.47L.nc  HC       2005/1-12/1/0 C xyz kg/m2/s ACET 114/101 20 1
0 AEIC_ALD2 -                                              -        -             - -   -       ALD2 114/102 20 1
0 AEIC_ALK4 -                                              -        -             - -   -       ALK4 114/103 20 1
0 AEIC_C2H6 -                                              -        -             - -   -       C2H6 114/104 20 1
0 AEIC_C3H8 -                                              -        -             - -   -       C3H8 114/105 20 1
0 AEIC_CH2O -                                              -        -             - -   -       CH2O 114/106 20 1
0 AEIC_PRPE -                                              -        -             - -   -       PRPE 114/107 20 1
0 AEIC_MACR -                                              -        -             - -   -       MACR 114/108 20 1
0 AEIC_RCHO -                                              -        -             - -   -       RCHO 114/109 20 1
)))AEIC
```

Further down in the HEMCO_Config.rc file (in the ***Base Emissions Data*** section), you will find the entry for the AEIC aircraft emissions. Each of these lines indicates that you want HEMCO to read a specific species from the AEIC inventory. For each species, you list **the container name**, **the data file** to be read, the **name of the variable** in the file, the **time range**, the **units**, the **G-C species to which these emissions will be added**, any **scale factors** you wish to apply, and the **category and hierarchy** of the data.

All of the entries between the brackets **(((AEIC** and **)))AEIC** will be ignored if you turned off AEIC emissions in the ***Base Emissions Switches*** section shown on the previous slide.

HEMCO configuration file: *Base Emissions Data*

Specifying time information:

```
0 AEIC_NO   $ROOT/AEIC/v2014-10/aeic_2005.geos.1x1.47L.nc  NO  2005/1-12/1/0 C  ...
```

For each file, you can tell HEMCO when it should read data from disk.
Specify requested data times in **YEAR(S)/MONTH(S)/DAY(S)/HOUR(S)** format.

Periodicity options:
C = cycling: Use the first data year for simulation dates preceding the start of the data; or the last data year for simulation dates that occur after the end of the data.
R = Range: Only read data during the specified time range.
E = Exact: Only read data if the file timestamp exactly matches the simulation date/time.

Examples:

`2000/1/1/0 C`
Read data for date 2000/01/01 @ 00:GMT and apply it to all simulation times (cycling)

`1980-2007/1-12/1-31/0-23 R`
Read hourly for each day of the years 1980-2007. Do not read data outside of this time range.

For more information, please see:
http://wiki.geos-chem.org/The_HEMCO_User's_Guide#HEMCO_settings

HEMCO configuration file: *Extension Switches*

```
# ------------------------------------------------------------------------------
100     Custom              : off   -
101     SeaFlux             : on    DMS/ACET
102     ParaNOx             : on    NO/NO2/O3/HNO3
    --> LUT data format     :       nc
    --> LUT source dir      :       $ROOT/PARANOX/v2015-02

       . . . etc skipping some lines . . .

111     GFED                : on    NO/CO/ALK4/ACET/MEK/ALD2/PRPE/C3H8/CH2O/C2H6/SO2/NH3/BCPO/BCPI/OCPO/OCPI/POA1/NAP
    --> GFED3               :       false
    --> GFED4               :       true
    --> GFED_daily          :       false
    --> GFED_3hourly        :       false
    --> Scaling_CO          :       1.05
    --> Scaling_POG1        :       1.27
    --> Scaling POG2        :       1.27
    --> Scaling NAP         :       2.75e-4
    --> hydrophilic BC      :       0.2
    --> hydrophilic OC      :       0.5
    --> fraction POG1       :       0.49
 114 FINN                   : off   NO/CO/ALK4/ACET/MEK/ALD2/PRPE/C3H8/CH2O/C2H6/SO2/NH3/BCPI/BCPO/OCPI/OCPO/GLYC/HAC
    --> FINN_daily          :       false
    --> Scaling_CO          :       1.0
    --> hydrophilic BC      :       0.2
    --> hydrophilic OC      :       0.5
```

The ***Extension Switches Section*** (back up near the top of the HEMCO_Config.rc file) lets you select options for the various HEMCO Extensions. You specify the **extension number and name**, whether you want to **turn an extension on or off**, which **species to use with that extension**, and other **options used by the extension.**

HEMCO configuration file: *Extension data*

```
#==============================================================================
# --- GFED biomass burning emissions (Extension 111)
# NOTE: These are the base emissions in kgDM/m2/s.
#==============================================================================
111 GFED_HUMTROP    $ROOT/GFED3/v2014-10/GFED3_humtropmap.nc              humtrop           2000/1/1/0             C xy 1          * - 1 1

(((GFED3
111 GFED_WDL        $ROOT/GFED3/v2014-10/GFED3_gen.1x1.$YYYY.nc           GFED3_BB__WDL_DM  1997-2011/1-12/01/0    C xy kgDM/m2/s * - 1 1
111 GFED_AGW        $ROOT/GFED3/v2014-10/GFED3_gen.1x1.$YYYY.nc           GFED3_BB__AGW_DM  1997-2011/1-12/01/0    C xy kgDM/m2/s * - 1 1
111 GFED_DEF        $ROOT/GFED3/v2014-10/GFED3_gen.1x1.$YYYY.nc           GFED3_BB__DEF_DM  1997-2011/1-12/01/0    C xy kgDM/m2/s * - 1 1
111 GFED_FOR        $ROOT/GFED3/v2014-10/GFED3_gen.1x1.$YYYY.nc           GFED3_BB__FOR_DM  1997-2011/1-12/01/0    C xy kgDM/m2/s * - 1 1
111 GFED_PET        $ROOT/GFED3/v2014-10/GFED3_gen.1x1.$YYYY.nc           GFED3_BB__PET_DM  1997-2011/1-12/01/0    C xy kgDM/m2/s * - 1 1
111 GFED_SAV        $ROOT/GFED3/v2014-10/GFED3_gen.1x1.$YYYY.nc           GFED3_BB__SAV_DM  1997-2011/1-12/01/0    C xy kgDM/m2/s * - 1 1
)))GFED3

(((GFED4
111 GFED_WDL        $ROOT/GFED4/v2015-03/GFED4_gen.025x025.$YYYY.nc       WDL_DM            2000-2013/1-12/01/0    C xy kg/m2/s   * - 1 1
111 GFED_AGW        $ROOT/GFED4/v2015-03/GFED4_gen.025x025.$YYYY.nc       AGW_DM            2000-2013/1-12/01/0    C xy kg/m2/s   * - 1 1
111 GFED_DEF        $ROOT/GFED4/v2015-03/GFED4_gen.025x025.$YYYY.nc       DEF_DM            2000-2013/1-12/01/0    C xy kg/m2/s   * - 1 1
111 GFED_FOR        $ROOT/GFED4/v2015-03/GFED4_gen.025x025.$YYYY.nc       FOR_DM            2000-2013/1-12/01/0    C xy kg/m2/s   * - 1 1
111 GFED_PET        $ROOT/GFED4/v2015-03/GFED4_gen.025x025.$YYYY.nc       PET_DM            2000-2013/1-12/01/0    C xy kg/m2/s   * - 1 1
111 GFED_SAV        $ROOT/GFED4/v2015-03/GFED4_gen.025x025.$YYYY.nc       SAV_DM            2000-2013/1-12/01/0    C xy kg/m2/s   * - 1 1
)))GFED4

(((GFED_daily
111 GFED_FRAC_DAY   $ROOT/GFED3/v2014-10/GFED3_dailyfrac_gen.1x1.$YYYY.nc GFED3_BB__DAYFRAC 2002-2011/1-12/1-31/0  C xy 1          * - 1 1
)))GFED_daily

(((GFED_3hourly
111 GFED_FRAC_3HOUR $ROOT/GFED3/v2014-10/GFED3_3hrfrac_gen.1x1.$YYYY.nc   GFED3_BB__HRFRAC  2002-2011/1-12/01/0-23 C xy 1          * - 1 1
)))GFED_3hourly
```

Further down in the HEMCO_Config.rc file, there is an ***Extension Data Section***. In this section you list entries for data files that pertain to each of the HEMCO extensions. (You use the same syntax as for the ***Base Emissions Data*** section.).

Here the GFED extension data is shown (GFED4 is highlighted). The brackets (((GFED4 and)))GFED4 are used to turn the GFED4 emissions on or off (depending on the settings in ***Extension Switches***). Note that the number at the start of the line now is 111 and not 0, this corresponds to the GFED extension number.

HEMCO configuration file: *Scale Factors*

```
#==============================================================================
# --- temporary scale factors for comparisons
#==============================================================================
919 NO_ratio $ROOT/AnnualScalar/v2014-07/NO_ratio_2005_2002.nc NOXscalar 2005/1/1/0 C xy 1 1
918 CO_ratio $ROOT/AnnualScalar/v2014-07/CO_ratio_2005_1985.nc COscalar  2005/1/1/0 C xy 1 1

#==============================================================================
# --- day-of-week scale factors ---
# ==> data is Sun/Mon/.../Sat
#==============================================================================
20 GEIA_DOW_NOX 0.784/1.0706/1.0706/1.0706/1.0706/1.0706/0.863 - - - xy 1 1
21 GEIA_DOW_CO  0.683/1.1076/1.0706/1.0706/1.0706/1.0706/0.779 - - - xy 1 1
22 GEIA_DOW_HC  0.671/1.1102/1.1102/1.1102/1.1102/1.1102/0.768 - - - xy 1 1

#==============================================================================
# --- diurnal scale factors ---
#==============================================================================
25 EDGAR_TODNOX $ROOT/EDGARv42/v2015-02/NO/EDGAR_hourly_NOxScal.nc NOXscale 2000/1/1/HH C xy 1 1
26 GEIA_TOD_FOSSIL
0.45/0.45/0.6/0.6/0.6/0.6/1.45/1.45/1.45/1.45/1.4/1.4/1.4/1.4/1.45/1.45/1.45/1.45/0.65/0.65/0.65/0.65/0.45
/0.45 - - - xy 1 1
```

In the ***Scale Factors*** section of the HEMCO_Config.rc file, you may specify the scale factors that will be applied to the various emissions inventories listed in the ***Base Emissions Data*** and ***Extensions Data*** sections.

Scale factors can be:

- Gridded lon-lat data (read from a netCDF file), follows mostly same format as Base Emissions Data
- A list of values (i.e. global values for a sequence of years, months, or days)
- A single value

In the **units** column, "1" means the same as **"unitless"**
Scale factors also let you specify an **operation (1=multiplication, -1=division, 2=square)**

HEMCO configuration file: *Masks*

```
#==============================================================================
# Country/region masks
#==============================================================================
1000 EMEP_MASK    $ROOT/MASKS/v2014-07/EMEP_mask.geos.1x1.nc             MASK     2000/1/1/0 C xy 1 1 -30/30/45/70
1001 MEXICO_MASK  $ROOT/MASKS/v2014-07/BRAVO.MexicoMask.generic.1x1.nc  MASK     2000/1/1/0 C xy 1 1 -118/17/-95/33
1002 CANADA_MASK  $ROOT/MASKS/v2014-07/Canada_mask.geos.1x1.nc          MASK     2000/1/1/0 C xy 1 1 -141/40/-52/85
1003 SEASIA_MASK  $ROOT/MASKS/v2014-07/SE_Asia_mask.generic.1x1.nc      MASK     2000/1/1/0 C xy 1 1  60/-12/153/55
1004 NA_MASK      $ROOT/MASKS/v2014-07/NA_mask.geos.1x1.nc              MASK     2000/1/1/0 C xy 1 1 -165/10/-40/90
1005 USA_MASK     $ROOT/MASKS/v2014-07/usa.mask.nei2005.geos.1x1.nc     MASK     2000/1/1/0 C xy 1 1 -165/10/-40/90
1006 ASIA_MASK    $ROOT/MASKS/v2014-07/MIX_Asia_mask.generic.025x025.nc MASK     2000/1/1/0 C xy 1 1  46/-12/180/82
1007 NEI11_MASK   $ROOT/MASKS/v2014-07/USA_LANDMASK_NEI2011_0.1x0.1.nc  LANDMASK 2000/1/1/0 C xy 1 1 -140/20/-50/60
1008 USA_BOX      -129/25/-63/49                                         MASK     2000/1/1/0 C xy 1 1 -129/25/-63/49
```

In the ***Masks*** section, (near the end of the HEMCO_Config.rc file), you can define geographical (lon-lat) masks that are used with the regional emissions inventories. A mask is usually set to 1 where a regional inventory is used, and 0 where it is not used. Fractional values can also be specified (in v11-01 and higher).

To specify a mask for a rectangular region, you can **simply give the lon and lat of at the lower left and upper right corners**. For irregularly-shaped regions, it is better to create a netCDF file for the mask.

For each mask, you specify the following:

- **A number and container name for the mask**
- **The file where the mask resides (optional)**
- **The name of the variable in the file**
- **The time range**
- **The units ("1" = "unitless")**
- **The operation you want to do: 1=multiplication (most common), -1=division, 3=invert mask**
- **The longitude and latitude range of the mask (only used for MPI environments)**

HEMCO configuration file: *Non-Emissions Data*

```
# --- Time zones (offset to UTC) ---
* TIMEZONES $ROOT/TIMEZONES/v2015-02/timezones_1x1.nc UTC_OFFSET 2000/1/1/0 C xy count * - 1 1

# --- UV albedo, for photolysis (cf Hermann & Celarier, 1997) ---
(((+UValbedo+
* UV_ALBEDO $ROOT/UVALBEDO/v2015-03/uvalbedo.geos.2x25.nc UVALBD 1985/1-12/1/0 C xy 1 * - 1 1
)))+UValbedo+

# --- TOMS/SBUV overhead ozone colums, for photolysis ---
(((+TOMS_SBUV_O3+
* TOMS_O3_COL   $ROOT/TOMS_SBUV/v2015-03/TOMS_O3col_$YYYY.geos.1x1.nc TOMS   1971-2010/1-12/1/0 C xy dobsons     * - 1 1
* DTOMS1_O3_COL -                                                     DTOMS1 -                   - -  dobsons/day * - 1 1
* DTOMS2_O3_COL -                                                     DTOMS2 -                   - -  dobsons/day * - 1 1
)))+TOMS_SBUV_O3+

# --- Linear stratospheric chemistry fields ---
# These fields will only be read if the +LinStratChem+ toggle is activated.

(((+LinStratChem+

# --- Stratospheric Bry data from the CCM model  ---
* GEOSCCM_Br_DAY      $ROOT/STRAT/v2015-01/Bry/GEOSCCM_Bry.2007$MM.day.nc   BR     2007/$MM/1/0 C xyz pptv * - 60 1
* GEOSCCM_Br_NIGHT    $ROOT/STRAT/v2015-01/Bry/GEOSCCM_Bry.2007$MM.night.nc BR     2007/$MM/1/0 C xyz pptv * - 60 1
... etc...


#--- GMI chemistry: prod/loss rates (for strato-/mesosphere) ---
* GMI_LOSS_A3O2       $ROOT/GMI/v2015-02/gmi.clim.A3O2.geos5.2x25.nc        loss    2000/$MM/1/0 C xyz s-1   A3O2     - 1  1
* GMI_PROD_A3O2       $ROOT/GMI/v2015-02/gmi.clim.A3O2.geos5.2x25.nc        prod    2000/$MM/1/0 C xyz v/v/s A3O2     - 1  1
... etc ...
)))+LinStratChem+
```

The ***Non-Emissions Data*** section is similar to ***Base Emissions Data*** section, with a couple of differences:

- The switches +UValbedo+ and +TOMS_SBUV_O3+ will be automatically set if FAST-JX is turned on.
- The switch +LinStratChem+ will be automatically set if stratospheric chemistry is turned on.

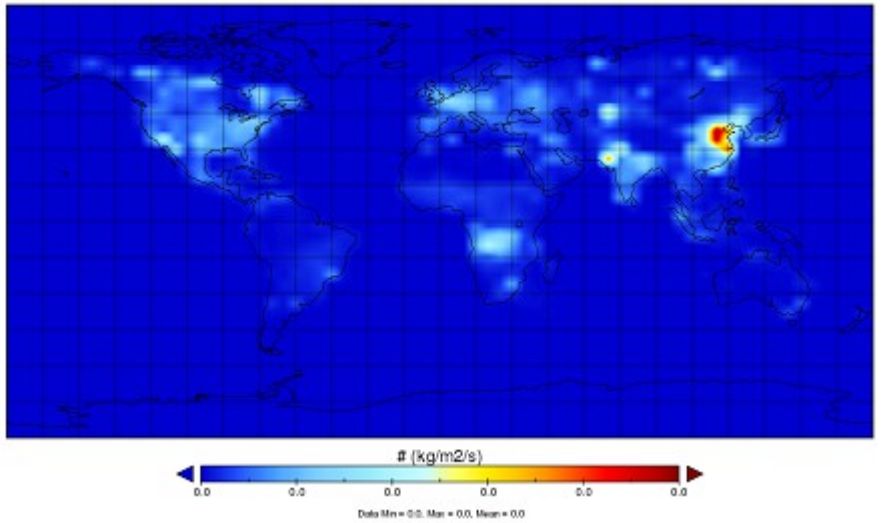
This prevents errors caused by inconsistent input between `input.geos` and `HEMCO_Config.rc`.

You must manually retrieve non-emissions data into your GEOS-Chem routine with a call to `HCO_GetPtr.`

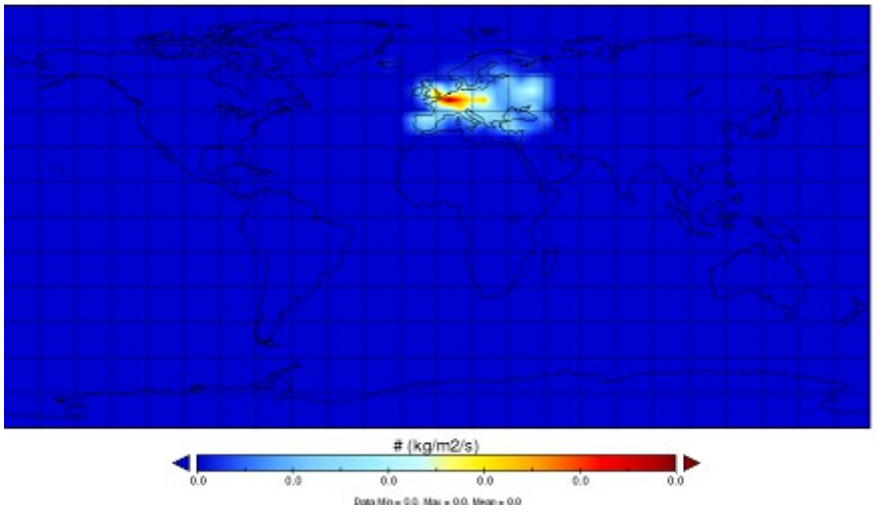
```
# Sample HEMCO_diagnostics.rc file
#
# This is the file specified in the “DiagnFile” slot of HEMCO_Config.rc.
# It specifies which HEMCO quantities you would like to archive to netCDF files.
#
# The netCDF file names begin with “DiagnPrefix” (from HEMCO_Config.rc),
# and will be archived at frequency “DiagnFreq” (also from HEMCO_Config.rc).
#
# NOTE: Category 1/2 means to put all of the emissions into category #1
# (which is anthropogenic) and zero category #2 (which is biomass).
# This is needed for those inventories that lump anthro + biomass together.
#
# Name        Spec ExtNr Cat Hier Dim Unit

TOTAL_NO      NO    -1    -1  -1   2   kg/m2/s   # NO from all sources

EMEP_NO       NO     0   1/2  10   2   kg/m2/s   # NO just from EMEP

GFED_CO       CO   111     5  -1   2   kg/m2/s   # CO from GFED biomass burning

# If you want to just diagnose regional emissions, then you need to set the
# diagnostics extension number, category and hierarchy accordingly:
#
NEI2011_CO    CO     0     1  50   2   kg/m2/s   # CO just from NEI2011
```

Output from the HEMCO_Diagnostic_201307020000.nc file

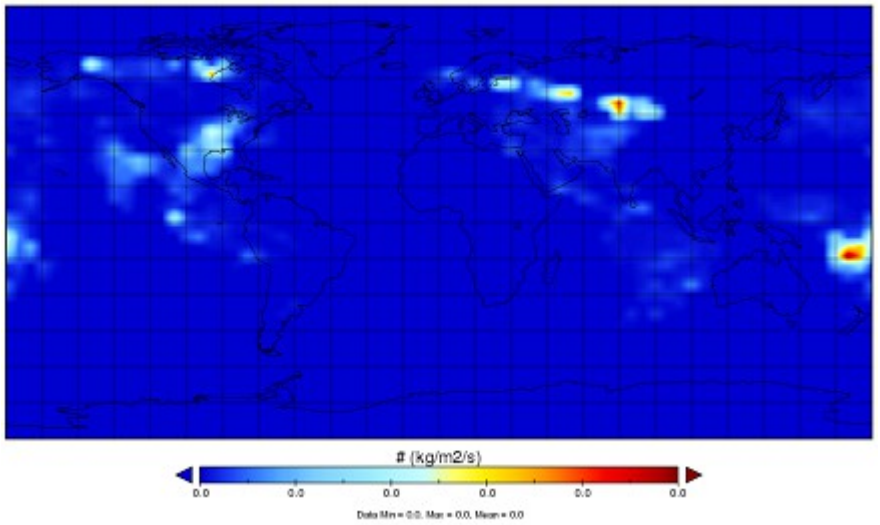
TOTAL_NO



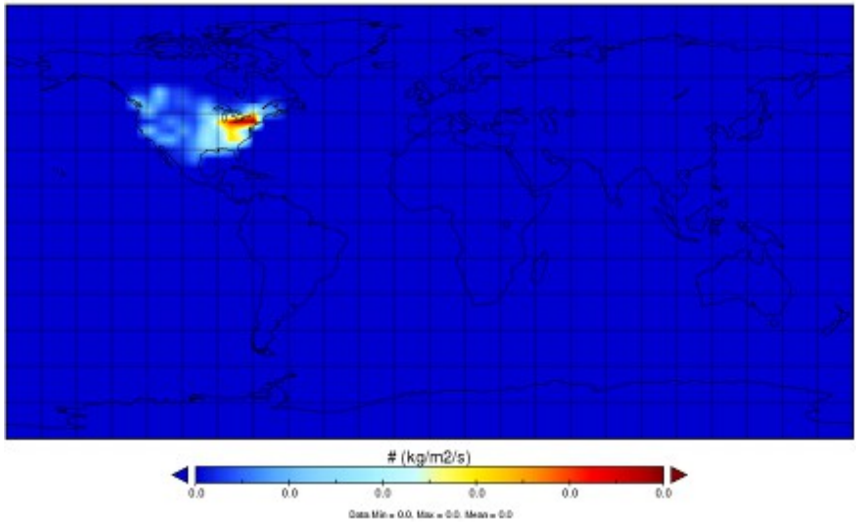
EMEP_NO



GFED_CO



NEI2011_CO



HEMCO standalone mode

- When you compile GEOS-Chem, it creates the HEMCO standalone executable in folder:
  - `bin/hemco_standalone.x`
- You can use the HEMCO standalone to test new emissions inventories without having to run them in GEOS-Chem
- For more information:
  - **wiki.geos-chem.org/The_HEMCO_User's_Guide#Stand-alone_interface**

FlexChem overview

- FlexChem completely removed SMVGEAR and all related code (i.e. no more CSPEC, JLOP, etc).
- Based on the KPP (Kinetic Pre-Processor) code by Adrian Sandu et al
- In the future we may be able to upgrade to Kppa (KPP-Accelerated) by ParaTools (John Linford)
- For more information:
  - **wiki.geos-chem.org/FlexChem**

Updating a FlexChem mechanism

- You must modify 3 input files for the KPP solver:
  - `gckpp.kpp`
    - Defines integrator, P/L families, and inlined rate functions
  - `globchem.spc`
    - Defines the list of variable and fixed species
  - `globchem.eqn`
    - Defines each of the reactions in the mechanism
    - Specifies the rate function corresponding to each reaction
      - Gas-phase rates are defined in **`gckpp.kpp`**
      - Hetchem rates are defined instead in **`gckpp_HetRates.F90`**

```
#INTEGRATOR rosenbrock
#LANGUAGE Fortran90
#DRIVER none
#HESSIAN off
#MEX off
#STOICMAT off

#INCLUDE globchem.spc
#INCLUDE globchem.eqn

#FAMILIES
POx : O3 + NO2 + 2NO3 + PAN + PMN + PPN + HNO4 + 3N2O5 + HNO3 + BrO + HOBr
+ BrNO2 + 2BrNO3 + MPN + ETHLN + ISN1 + ISOPNB + ISOPND + MACRN + MVKN +
PROPNN + R4N2 + INPN + ISNP + INO2 + ISNOOA + ISNOOB + ISNOHOO + MAN2 +
PRN1 + PRPN + R4N1 + PMNN + MACRNO2 + ClO + HOCl + ClNO2 + 2ClNO3 + 2Cl2O2
+ 2OClO + O + O1D;
LOx : O3 + NO2 + 2NO3 + PAN + PMN + PPN + HNO4 + 3N2O5 + HNO3 + BrO + HOBr
+ BrNO2 + 2BrNO3 + MPN + ETHLN + ISN1 + ISOPNB + ISOPND + MACRN + MVKN +
PROPNN + R4N2 + INPN + ISNP + INO2 + ISNOOA + ISNOOB + ISNOHOO + MAN2 +
PRN1 + PRPN + R4N1 + PMNN + MACRNO2 + ClO + HOCl + ClNO2 + 2ClNO3 + 2Cl2O2
+ 2OClO + O + O1D;
PCO : CO;
LCO : CO;
PSO4 : SO4;

#INLINE F90_RATES
  REAL(kind=dp) FUNCTION OH_O1D (J, H2O, TEMP, NUMDEN)
  ... etc ...
```

gckpp.kpp: Defines the following quantities:

- Integrator (e.g. Rosenbrock, Runge-Kutta, etc.)
- Language (this is always “Fortran90”)
- Prod/Loss families for GC diagnostics.
- Inlined Fortran functions to compute rate constants for reactions

```
#include atoms

#DEFVAR

      A3O2            =         IGNORE;
      ACET            =         IGNORE;
      ALD2            =         IGNORE;
      ALK4            =         IGNORE;
      ATO2            =         IGNORE;
      B3O2            =         IGNORE;
      BENZ            =         IGNORE;
      C2H6            =         IGNORE;
      C3H8            =         IGNORE;
      CH2O            =         IGNORE;
      CH4             =         IGNORE;
       ... etc ...

#DEFFIX

      ACTA            =         IGNORE;
      EMISSION        =         IGNORE;
      EOH             =         IGNORE;
      H2              =         IGNORE;
      HCOOH           =         IGNORE;
      MNO3            =         IGNORE;
      MOH             =         IGNORE;
      N2              =         IGNORE;
      NH2             =         IGNORE;
      NH3             =         IGNORE;
      O2              =         IGNORE;
      RCOOH           =         IGNORE;
```

globchem.spc

Variable (aka active) species go under the #DEFVAR heading.

Fixed (aka inactive) species go under the #DEFFIX heading.

globchem.eqn
Reactions are listed along with the Fortran functions that compute their rates.
Gas-phase rate functions are in **gckpp.kpp** and hetchem functions in **gckpp_HetRates.F90**.
Comments are contained between {} characters. Equation numbers removed from v11-02.

```
#Equations
{1} O3 + NO = NO2 + O2 :                          GCARR(3.00E-12, 0.0E+00, -1500.0);
{2} O3 + OH = HO2 + O2 :                          GCARR(1.70E-12, 0.0E+00, -940.0);
{3} O3 + HO2 = OH + O2 + O2 :                     GCARR(1.00E-14, 0.0E+00, -490.0);
{4} O3 + NO2 = O2 + NO3 :                         GCARR(1.20E-13, 0.0E+00, -2450.0);
{5} O3 + MO2 = CH2O + HO2 + O2 :                  GCARR(2.90E-16, 0.0E+00, -1000.0);
{6} OH + OH = H2O + O :                           GCARR(1.80E-12, 0.0E+00, 0.0);
{7} OH + OH {+M} = H2O2 :                         GCJPLPR(6.90E-31, 1.0E+00, 0.0, ...
{8} OH + HO2 = H2O + O2 :                         GCARR(4.80E-11, 0.0E+00, 250.0);
{9} OH + H2O2 = H2O + HO2 :                       GCARR(1.80E-12, 0.0E+00, 0.0);
{10} HO2 + NO = OH + NO2 :                        GCARR(3.30E-12, 0.0E+00, 270.0);
{11} HO2 + HO2 = H2O2 + O2 :                      GC_HO2NO3(3.00E-13, 0.0E+00, ...
{12} CO + OH = HO2 + CO2 :                        GC_OHCO(1.50E-13, 0.0E+00, 0.0);
{13} OH + CH4 = MO2 + H2O :                       GCARR(2.45E-12, 0.0E+00, -1775.0);
{14} MO2 + NO = CH2O + HO2 + NO2 :                GCARR(2.80E-12, 0.0E+00, 300.0);
{15} MO2 + HO2 = MP + O2 :                        GCARR(4.10E-13, 0.0E+00, 750.0);
{16} MO2 + MO2 = MOH + CH2O + O2 :                GC_TBRANCH(9.50E-14, 0.0E+00, ...
{17} MO2 + MO2 = 2.000CH2O + 2.000HO2 :           GC_TBRANCH(9.50E-14, 0.0E+00, ...
{18} MP + OH = MO2 + H2O :                        GCARR(2.66E-12, 0.0E+00, 200.0);
{19} MP + OH = CH2O + OH + H2O :                  GCARR(1.14E-12, 0.0E+00, 200.0);
{20} ATOOH + OH = ATO2 + H2O :                    GCARR(2.66E-12, 0.0E+00, 200.0);
{21} ATOOH + OH = MGLY + OH + H2O :               GCARR(1.14E-12, 0.0E+00, 200.0);
{22} CH2O + OH = CO + HO2 + H2O :                 GCARR(5.50E-12, 0.0E+00, 125.0);
{23} NO2 + OH {+M} = HNO3 {+M} :                  GCJPLPR(1.80E-30, 3.0E+00, 0.0, ...
... etc ...
```

Updating FlexChem mechanisms

- Thankfully, Melissa has added very detailed information to the FlexChem wiki page
- Follow these instructions:
  - **wiki.geos-chem.org/FlexChem#Adding_chemical_mechanisms_in_FlexChem**

GEOS-Chem Species Database: A one-stop shop for species physical properties

Introduced in v11-01

GEOS-Chem Species Database

- The species database is a vector of derived-type objects stored within `State_Chm`
- Each element in the vector is an object of type `SPECIES` (defined in `species_mod.F90`)
- Each `SPECIES` object contains information about a single GEOS-Chem species:
  - Indices and inquiry variables (i.e. is it advected?)
  - Molecular weights and Henry's law constants
  - Wetdep, drydep, aerosol, & other relevant parameters

The **species database** is implemented as a sub-field of the **`State_Chm`** object.

`State_Chm` also carries several **counters** and **mapping arrays** that are used in conjunction with the **species database**.

```
!=========================================================================
! Derived type for Chemistry State
!=========================================================================
TYPE, PUBLIC :: ChmState

   ! Number of species
   INTEGER                   :: nSpecies            ! # of species
   INTEGER                   :: nAdvect             ! # of advected species
   INTEGER                   :: nDrydep             ! # of drydep species
   INTEGER                   :: nKppSpc             ! # of KPP chem species
   INTEGER                   :: nWetDep             ! # of wetdep species

   ! Mapping vectors to subset types of species
   INTEGER,          POINTER :: Map_Advect (:     ) ! Advected species ID's
   INTEGER,          POINTER :: Map_DryDep (:     ) ! Drydep species ID's
   INTEGER,          POINTER :: Map_KppSpc (:     ) ! KPP chem species ID's
   INTEGER,          POINTER :: Map_WetDep (:     ) ! Wetdep species IDs'

   ! Physical properties about tracers & species
   TYPE(SpcPtr),     POINTER :: SpcData(:)          ! Species database

   ... etc ...

END TYPE ChmState
```

Obtaining information from the species database [edit]

To get the physical properties for a given species from the species database, you can use code such as:

```
      DO N = 1, State_Chm%nSpecies

         ! Get Henry's law parameters
         K0  = State_Chm%SpcData(N)%Info%Henry_K0
         CR  = State_Chm%SpcData(N)%Info%Henry_CR
         pKA = State_Chm%SpcData(N)%Info%Henry_pKa

      ENDDO
```

To simplify the coding, you can create an object of type `Species` to point to each entry in the species database. For example this code

```
      USE Species_Mod, ONLY : Species

      TYPE(Species), POINTER :: ThisSpc

      DO N = 1, State_Chm%nSpecies

         ThisSpc => State_Chm%SpcData(N)%Info

         ! Get Henry's law parameters
         K0  =  ThisSpc%Henry_K0
         CR  =  ThisSpc%Henry_CR
         pKA =  ThisSpc%Henry_pKa

         ThisSpc => NULL()

      ENDDO
```

is much less wordy and easier to read.

Adding species to the GC Species DB

To add a new species, add the relevant information into GEOS-Chem module `Headers/species_database_mod.F90`

Example 2: Add a gas-phase species that is advected, dry-deposited, and wet-deposited [edit]

Hydrogen peroxide is an example of a GEOS-Chem species that is advected, dry-deposited, and wet-deposited. It is defined with the following settings:

```
CASE( 'H2O2' )
   CALL Spc_Create( am_I_Root     = am_I_Root,                &
                    ThisSpc       = SpcData(N)%Info,          &
                    ModelID       = N,                        &
                    Name          = NameAllCaps,              &
                    FullName      = 'Hydrogen peroxide',      &
                    MW_g          = 34.0_fp,                  &
                    Is_Advected   = T,                        &
                    Is_Gas        = T,                        &
                    Is_Drydep     = T,                        &
                    Is_Wetdep     = T,                        &
                    DD_F0         = 1.0_fp,                   &
                    DD_Hstar_old  = 1e+5_fp,                  &
                    Henry_K0      = 8.30e+4_f8,               &
                    Henry_CR      = 7400.0_f8,                &
                    WD_RetFactor  = 5e-2_fp,                  &
                    WD_LiqAndGas  = T,                        &
                    WD_ConvFacI2G = 4.36564e-1_fp,            &
                    RC            = RC )
```

For more information about the properties that can be stored in the Species Database, see:
http://wiki.geos-chem.org/GEOS-Chem_species_database
http://wiki.geos-chem.org/Physical_properties_of_GEOS-Chem_species

Adding species to the GC Species DB

There are several options you can specify when you add a new species:
Gas or aerosol? Is it advected? Is it dry-deposited? Is it wet-deposited?
Is it carried in moles of carbon?

Example 4: Add a hydrocarbon species carried as equivalent carbon atoms [edit]

Several GEOS-Chem hydrocarbon species (e.g. acetone, isoprene, etc.) are emitted and transported as equivalent carbon atoms instead of a single molecule.

```
CASE( 'ACET' )
   CALL Spc_Create( am_I_Root     = am_I_Root,                &
                    ThisSpc       = SpcData(N)%Info,          &
                    ModelID       = N,                        &
                    Name          = NameAllCaps,              &
                    FullName      = 'Acetone',                &
                    MW_g          = 58.08_fp,                 &
                    EmMW_g        = 12.00_fp,                 &
                    MolecRatio    = 3.0_fp,                   &
                    Is_Advected   = T,                        &
                    Is_Gas        = T,                        &
                    Is_Drydep     = T,                        &
                    Is_Wetdep     = F,                        &
                    DD_F0         = 1.0_fp,                   &
                    DD_Hstar_Old  = 1e5_fp,                   &
                    Henry_K0      = 2.7e+1_f8,                &
                    Henry_CR      = 5300.0_f8,                &
                    RC            = RC )
```

```
SUBROUTINE MySub( ..., State_Chm, ... )

     !%%% Example of the new indexing scheme %%%

     ! Uses
     USE State_Chm_Mod, ONLY : Ind_

     ! Local variables
     INTEGER  :: id_O3, id_Br2, id_CO

     ! Find species indices with the Ind_() function
     id_O3  = Ind_( 'O3'  )
     id_Br2 = Ind_( 'Br2' )
     id_CO  = Ind_( 'CO'  )

     ! Print concentrations
     ! NOTE: Should test to see if indices are valid, omitted here!!
     print*, 'O3  at (23,34,1) : ', State_Chm%Species(23,34,1,id_O3 )
     print*, 'Br2 at (23,34,1) : ', State_Chm%Species(23,34,1,id_Br2)
     print*, 'CO  at (23,34,1) : ', State_Chm%Species(23,34,1,id_CO )

     ! Print the molecular weight of O3
     ! obtained from the Species Database
     print*, 'Mol wt of O3 [g]: ', State_Chm%SpcData(id_O3)%Info%MW_g

  END SUBROUTINE MySub
```

New method: function `Ind_()`

This function returns the species index that is consistent with the ordering in the GEOS-Chem species database.

This is also consistent with the chemical species ordering for FlexChem.

New method: function `Ind_()`, continued

By default, **`Ind_()`** returns the overall species index.

You can supply optional arguments to **`Ind_()`** to return other species indices, as shown below:

```
! Position of HNO3 in the list of advected species
AdvectId = Ind( 'HNO3', 'A' )

! Position of HNO3 in the list of dry deposited species
DryDepId = Ind( 'HNO3', 'D' )

! Position of HNO3 in the list of wet deposited species
WetDepId = Ind( 'HNO3', 'W' )

! Position of HNO3 in the list of fixed KPP species
KppFixId = Ind( 'HNO3', 'F' )

! Position of HNO3 in the list of variable KPP species
KppVarId = Ind( 'HNO3', 'V' )
```