HEMCO: **H**armonized **Em**issions **Co**mponent as an emissions component for MUSICA/CAM-chem

Haipeng **Lin**

Rev. 2 (20231010) – Now updated for Derecho, HEMCO merged in CESM mainline

https://doi.org/10.5194/gmd-14-5487-2021

HEMCO within CAM-chem/CESM User's Guide

Haipeng **Lin** · @jimmielin · jimmielin.me · hplin@seas.harvard.edu

Can I use HEMCO in CAM-chem/MUSICA today? **Yes**!

- **HEMCO-CESM is now part of CAM as of `cam6_3_118`**
- It works with *any grid** and with recent versions of CAM above 6.3.118**
  - * *tested with 1.9x2.5, 0.9x1.25, ne30np4, ne0np4.KORUS03.ne30x16* but others should work
  - ** *for CESM-2.2, please refer to the older version of these slides*
- Can I mix and match with current offline emissions? *Not directly*
  - You can use HEMCO to read the existing offline emissions on regular grids into the model instead
- An outline of the workflow is included in these slides, but in short:
  - Use the _HCO compsets (e.g., FCnudged_HCO, FCSD_HCO, FCclimo2000_HCO), *or*
  - Enable `use_hemco = .true.` (for existing cases). Sensible defaults are provided.
  - HEMCO **cannot** be mixed and matched with ext_frc_specifier and srf_emis_specifier, to avoid double counting of emissions. If HEMCO is enabled, all file-based emissions go through HEMCO

Setting up: Installing CESM with HEMCO enabled

You can use either CESM master or CESM-2.2 as long as CAM is > `cam6_3_118`

For CESM2.2, please refer to the older version of these slides as changes to CIME and a custom version of CAM is needed.

For CESM master:

- Checkout ESCOMP/CESM at the latest development release (or any version with a recent version of CAM)

```
$ git clone https://github.com/ESCOMP/CESM.git
```

- Checkout externals

```
$ ./manage_externals/checkout_externals
```

Setting up: Installing CESM with HEMCO enabled

HEMCO is configured at runtime. You can either:

- Create case with HEMCO compsets, which will automatically configure HEMCO

  (`FCSD_HCO`, `FCHIST_HCO`, `FCnudged_HCO`, ...)

```
$ cd cime/scripts
$ ./create_newcase --case ~/dev-2211_hemco_compset_test --compset FCSD_HCO --res f09_f09_mg17 --
run-unsupported --project project_id --mach derecho
```

- *Or* use existing chemistry compsets, but disable existing emissions and enable HEMCO in user_nl_cam

```
ext_frc_specifier=''
srf_emis_specifier=''
use_hemco = .true.
```

Setting up: Build and run the case

- Setup and build the case

Now patiently wait for as long as CESM usually takes to compile…

```
$ ./case.setup --reset
$ qcmd -l select=1:ncpus=18 -q share -- ./case.build -v
```

- Run CAM-chem/MUSICA as usual.

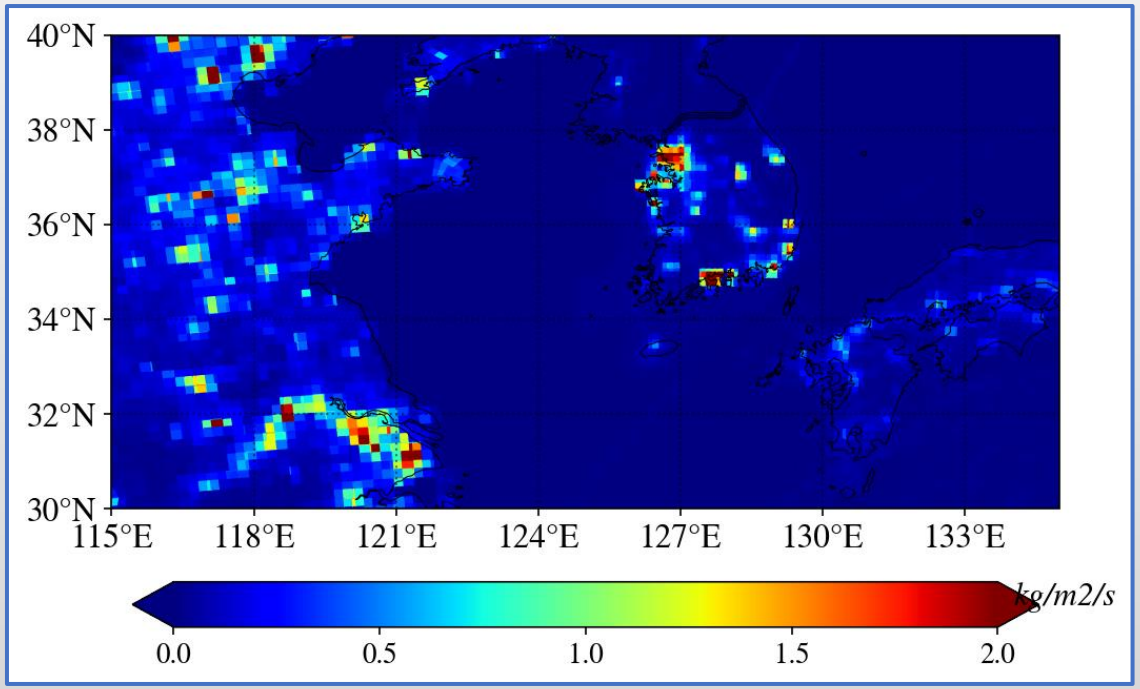
```
$ ./case.submit
```

- Where to look for HEMCO log output:
  - *atm.log*… will show major steps that HEMCO takes. If there is an error in the interface to CESM, it'll error out here.
  - *cesm.log*… and *HEMCO.log* will show HEMCO processing logs, including files read. If HEMCO itself crashes errors will be found here.
- HEMCO emissions are passed to chemistry starting from the **second** model timestep.

Can I see HEMCO output?

- All HEMCO emissions in kg/m2/s are available in the master field list
- HCO_NO, HCO_NO2, etc.
- Available over the entire vertical if emissions are 3-D.

HEMCO-CESM output (HCO_NO)
On MUSICA Korea grid, HEMCO internal res 0.15x0.15deg



Using Vivaldi-a package for Plot_2D
Credit to Duseong Jo for Korea MUSICA Grid

Setting up: Configuring CAM and the HEMCO-CESM interface

(Optional) You can configure HEMCO by modifying `user_nl_cam`

- Change the HEMCO configuration file location

```
hemco_config_file =
'/glade/p/cesmdata/inputdata/atm/cam/geoschem/emis/HEMCO_Config.CC.CEDS_AEIC19.NEx.c230615.rc'
hemco_data_root = '/glade/p/cesmdata/inputdata/atm/cam/geoschem/emis/ExtData/HEMCO'
```

- A default `hemco_config_file` is provided at:
  `/glade/p/cesmdata/inputdata/atm/cam/geoschem/emis/HEMCO_Config.CC.CEDS_AEIC19.NEx.c230615.rc`

  You can copy it and make modifications if necessary and point `hemco_config_file` to it.

- You can change grid parameters (`hemco_grid_xdim`, `hemco_grid_ydim`) to fit model resolution (lower of input data used or model grid resolution)

```
hemco_grid_xdim                 = 288
hemco_grid_ydim                 = 201
```

Setting up: Configuring CAM and the HEMCO-CESM interface

The default HEMCO configuration file includes the following inventories:

Global default inventories from: (can always enable/disable any!)

- CEDSv2 *(Hoesly et al., 2018; McDuffie et al., 2020)*, 0.5x0.5deg
- AEIC 2019 Aircraft Emissions *(Eastham and Fritz)*, 0.5x0.625deg
- GEIA NH_3 *(Bouwman et al., 1997)*, Arctic seabird NH_3 *(Croft et al., 2016)*, Fossil fuel and biofuel C_2H_6 *(Tzompa-Soza et al., 2017)*, C_3H_8 *(Xiao et al., 2008)*, Bromocarbons *(Liang et al., 2010; Ordonez et al., 2012; Sherwen et al., 2016)*.
- GFED4 biomass burning emissions

Setting up: Configuring HEMCO in **HEMCO_Config.rc**

Root data location: paths beginning with $ROOT in the configuration file resolve to `hemco_data_root` in the CAM namelist

You can get most default inventories from $ROOT but you can also use absolute paths for your own data:

```
0 DICE_CARS_CO    $ROOT/DICE_Africa/v2016-10/DICE-Africa-cars-2013-v01-4Oct2016.nc
CO                     2013/1/1/0         C xy    g/m2/yr  CO    26/1008              1   60

0 SOME_INVENTORY  /glade/u/home/hplin/some.nc
NO_agriculture         2000-2017/1-12/1/0 C xy    kg/m2/s  NO    301/306/1009         1/2 56
```

Setting up: Configuring HEMCO in **HEMCO_Config.rc**

Inventory switches:

```
# ----- REGIONAL INVENTORIES ---------------------------------------------
    --> APEI                    :       false    # 1989-2014
    --> NEI2016_MONMEAN         :       false    # 2002-2020
    --> DICE_Africa             :       false    # 2013
# ----- GLOBAL INVENTORIES -----------------------------------------------
    --> CEDSv2                  :       true     # 1750-2019
    --> EDGARv43                :       false    # 1970-2010
    --> HTAP                    :       false    # 2008-2010
…
```

Warning: Inventories were developed for GEOS-Chem species! Non-CEDSv2 inventories may need some work to map species correctly for MOZART-TS1

Notes on inventory support (support = mapping the species correctly!)

This might be trivial:

```
0 CEDS_NO_AGR  NO-em-anthro_CMIP_CEDS_$YYYY.nc NO_agr 1750-2019/1-12/1/0 C xy kg/m2/s NO 25 1 5
```

But this may not be!

```
0 CEDS_SO2_ENE SO2-em-anthro_CMIP_CEDS_$YYYY.nc SO2_ene 1750-2019/1-12/1/0 C xyL=100m:300m kg/m2/s
SO2 - 1 5
0 CEDS_SO4_ENE -                                -       -                  - xyL=100m:300m - so4_a1
8907  1 5

...
# --- CEDS to CAM-Chem scale factors ---
8907 CESM_SO4a1_ENE  0.025    - - - xy 1 1
```

Table S4. MAM4 aerosol parameters for emissions that are specified with emissions files (dust and sea salt are calculated online). Original species refers to labels in emissions inventories.

so4_a1	SO2*0.025 energy, industrial	115	1770	0.261	100-300m

HEMCO is not magic

It's up to you to specify the mapping Between netCDF file and model emiss.!

HEMCO Presentation and Reference Concepts

Emissions are at the heart of atmospheric chemistry modeling

yet have several limitations in current models

Need to preprocess inventories

to model grid

to target chemical scheme

with ad-hoc tools

using time and disk space

Difficult to share data and code

Source of human error

in pre-processing

for different cases/variations

in reproducing past results

Wide range of sources

possible inconsistent treatment

double counting/undercounting

HEMCO is a powerful on-line emissions component that can (mostly) be controlled by a text-based *configuration file*

```
# ----- REGIONAL INVENTORIES -----------------
    --> APEI                  :       false
    --> NEI2011_HOURLY        :       false
    --> NEI2011_MONMEAN       :       false
    --> MIX                   :       false
    --> DICE_Africa           :       false
# ----- GLOBAL INVENTORIES -------------------
    --> CEDS                  :       true
```

HEMCO Emissions Data Library

Gridded global and regional inventories

HEMCO Extensions

State dependent emission algorithms

(Biogenic, Dust, Lightning, …)

& GFED, Volcano, Ship Plumes…

CAM-Chem/MUSICA

CESM-GC

GEOS-Chem 'Classic'

GCHP

WRF-GC

NASA GEOS (GEOS-GC)

Scaling, masking, and adding emissions *from different sources, regions, and species* at runtime *on a user-specified grid* without preprocessing!

Keller et al., 2014

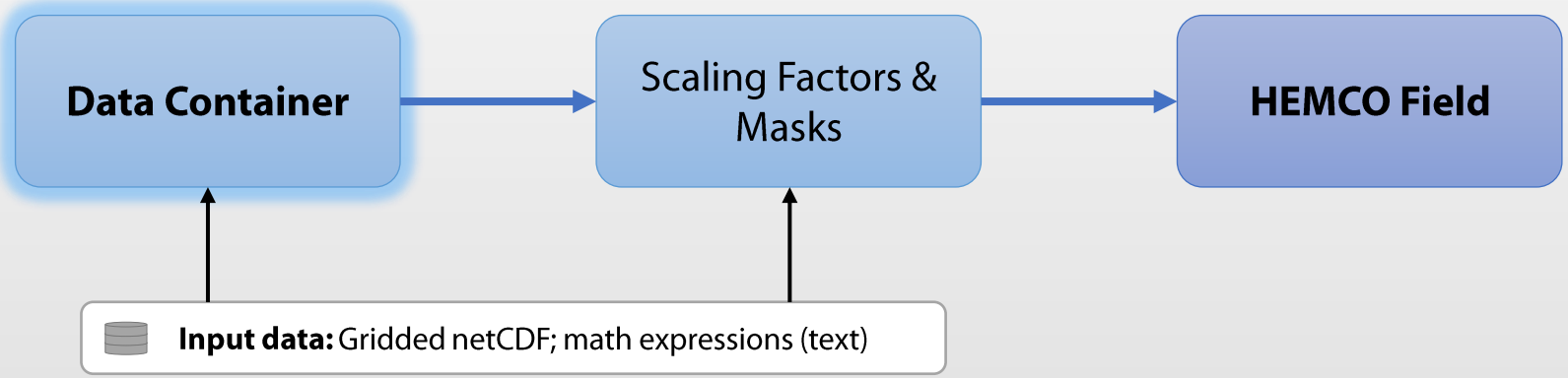
HEMCO is **not magic**, *but it can describe emissions precisely*

- With HEMCO, you still have to
  - Think about the hierarchy between multiple inventories used
  - Specify the speciation (from source file → model emissions)
  - Process emissions data *once* to latitude-longitude input grid, in COARDS-compliant netCDF*
- But you won't have to
  - Re-process emissions input files *every time you change the model configuration*, e.g.
    - Sensitivity experiments (inventories on/off; scale emissions)
    - Apply scaling factors (diurnal; weekly; monthly; gridded time series; vertical)
    - Running for a different year (Interpolate? Use average? Cycle? Nearest time slice?)
  - Re-grid emissions *every time you change the model grid*

** See guides: https://hemco.readthedocs.io/en/latest/geos-chem-shared-docs/supplemental-guides/coards-guide.html and https://hemco.readthedocs.io/en/latest/geos-chem-shared-docs/supplemental-guides/netcdf-guide.html*

How does HEMCO accomplish this?

"**HEMCO Fields**" are the basic building block




```
0 CEDS_NO_AGR   NO-em-total-anthro_CEDS_$YYYY.nc NO_agr 1970-2017/1-12/1/0 C
  Container name  Source netCDF file                 Variable  Date range (Y/M/D/H)  Cycling Opt

xy kg/m2/s NO                  25/1234          1          5
Dim Unit   Model Species Name  Scaling Factors  Category   Hierarchy
```

Example: Emissions data container in HEMCO.

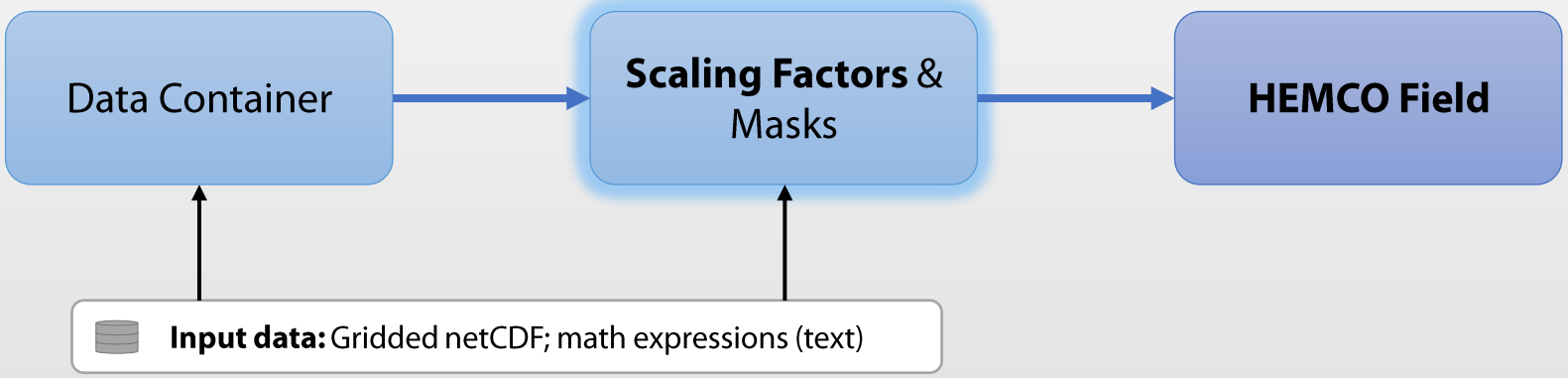
Tokens like $YYYY, $MM, $DD, $HH are automagically replaced into file names

Cycling option: *e.g.,*

- C: cycle closest
- R: only use within range
- RA: range, otherwise avg
- A: average
- I: interpolate nearest two
- E: must be exact match

How does HEMCO accomplish this?

"**HEMCO Fields**" are the basic building block




```
115       NO2toNO   6.521739e-1    -     -     - xy unitless 1
```

Scale factor #, name *Expression* *Dim Unit* *Operation (1 = *, 2 = /, 3 = * scale^2)*

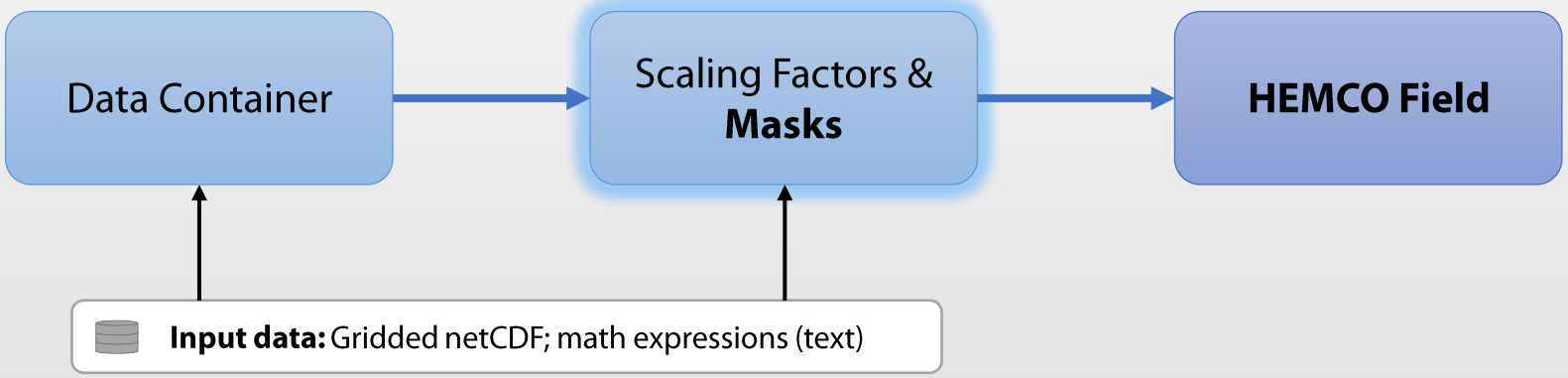
```
22    GEIA_DOW_HC   0.671/1.1102/1.1102/1.1102/1.1102/1.1102/0.768 - - - xy
unitless 1
```

Expression length: 7 = DOW (Sun/Mon/…/Sat); 12 = Jan/Feb/…/Dec; 24 = 00/01/02/…/23 (LT)

Example: Scaling factors in HEMCO.

How does HEMCO accomplish this?

"**HEMCO Fields**" are the basic building block




```
1007 CONUS_MASK   CONUS_Mask.01x01.nc          MASK    2000/1/1/0 C      xy 1 1 -
```

Mask #, name | *netCDF File* | *Variable* | *Time Slice* | *Cycling, Dim, Ignore, Ignore*

```
140/20/-50/60
```

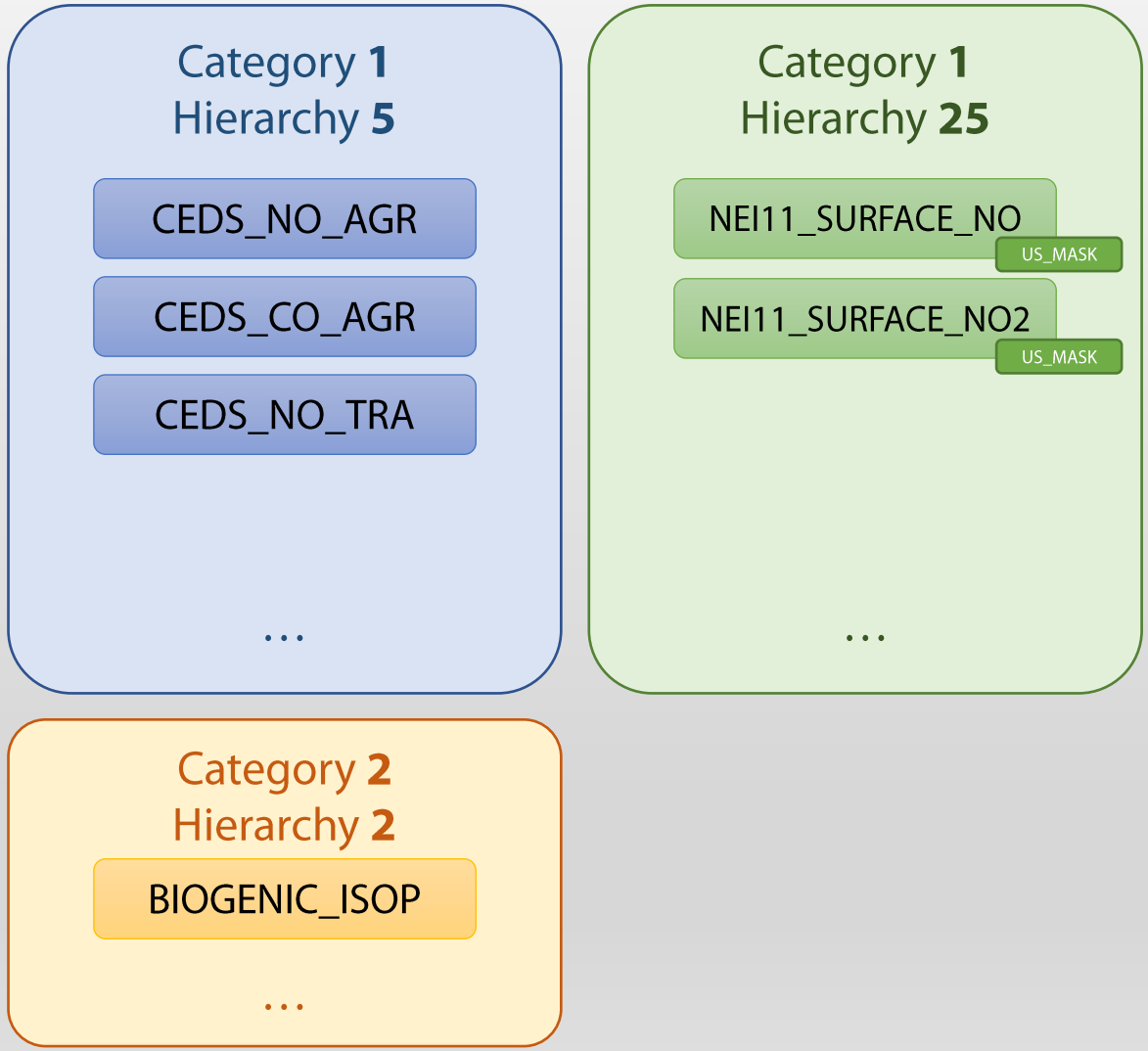
Approximate lat/lon bounds of the mask (to speed up I/O)

Example: Masks in HEMCO. Shown: CONUS mask (masks are binary)

Masks can be regional, 0 is assumed outside the provided region.

How does HEMCO accomplish this?

"**Category**" and "**Hierarchy**" are used to combine emission inventories



CEDS used over global domain
NEI11 used over US_MASK range

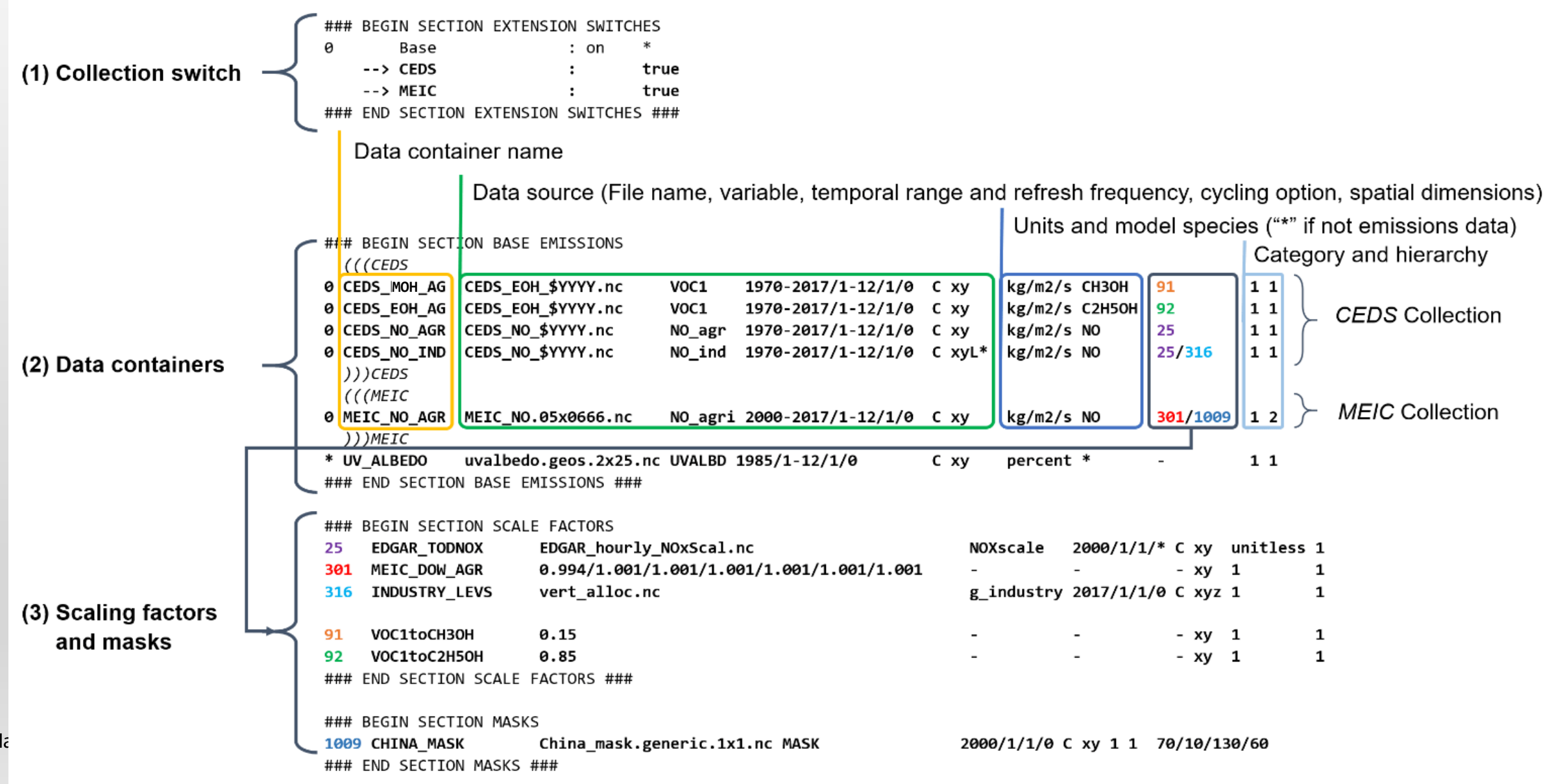
"Category 1 is anthropogenic emissions"

BIOGENIC_ISOP always used over available range

e.g., "Category 2 is biogenic emissions"

Haipeng **Lin** · @jimmielin · jimmielin.me · hplin@seas.harvard.edu

The anatomy of the **HEMCO configuration file**



Case examples / exercises, *easy*

- Problem 1: Scaling up CEDS emissions by 2x
- Problem 2: Scaling up CEDS emissions *every Monday* by 2x

Case examples / exercises, *harder*

- Problem 1: Scaling up CEDS emissions by 2x
- Problem 2: Scaling up CEDS emissions *every Monday* by 2x
- Problem 3: Scaling up CEDS emissions *in China* by 2x

Case examples / exercises, *really?*

- Problem 4: Keeping CEDS emissions normal everywhere, *but use 2010 emissions from CEDS in China*

When you want a feature that cannot be described in text config file…

- **…use HEMCO extensions to describe them in code!**
- HEMCO uses "Extensions" to port-in third-party code, e.g., MEGAN
- Extensions can **read data from HEMCO and the model** and **return processed emissions**.

- e.g., "double the emissions every Tuesday after the first Monday of every month"

HEMCO extensions are used to port-in third party emissions code (e.g. MEGAN)

- Extensions can access meteorology data (e.g., wind speed) from the on-line model and read in datasets from HEMCO

Species*	Extension name and reference
Oceanic DMS, acetone, acetaldehyde, methyl nitrate, ethyl nitrate, methanol	SeaFlux (Johnson, 2010)
Ship plume NO_x, HNO_3, O_3	ParaNO_x (Vinken et al., 2011)
Lightning NO_x	LightNO_x (Murray et al., 2012; Ott et al., 2010)
Soil and fertilizer NO_x	SoilNO_x (Hudman et al., 2012)
Mineral dust aerosols	DEAD (Zender et al., 2003) Ginoux (Ginoux et al., 2001)
Sea salt aerosols	SeaSalt (Chin et al., 2002; Gong, 2003; Jaeglé et al., 2011)
Biogenic VOCs	MEGAN (Guenther et al., 2012)
Biomass burning	GFED (Akagi et al., 2011; Andreae et al., 2001; Giglio et al., 2013; Randerson et al., 2012; van der Werf et al., 2010) FINN (Wiedinmyer et al., 2011)
Volcanic SO_2	Volcano (Carn et al., 2015; Ge et al., 2016)
Inorganic iodine emissions: HOI, I_2	Inorg_Iodine (Carpenter et al., 2013; MacDonald et al., 2014)

HEMCO extensions receive meteorology data through the 'model interface'

```
! USTAR Friction velocity [m/s]
State_CAM_USTAR(I) = cam_in(lchnk)%fv(J) * cam_in(lchnk)%landFrac(J) + cam_in(lchnk)%uStar

! Sea level pressure [Pa] (note difference in units!!)
State_CAM_ps(I) = phys_state(lchnk)%ps(J)

! Dry pressure [hPa] (Pa -> hPa, x0.01)
State_CAM_psdry(I) = phys_state(lchnk)%psdry(J) * 0.01_r8

! Surface temperature [K]
if(ExtState%T2M%DoUse) then
    State_CAM_TS(I) = cam_in(lchnk)%TS(J)
endif
```

```
! Visible surface alb      [1]
if(ExtState%ALBD%DoUse)    en
    call HCO_Grid_CAM2HCO     (State_CAM_ALBD, State_HCO_ALBD)

    call ExtDat_Set(HcoState,    tState%ALBD,   'ALBD_FOR_EMIS', &
                    RC,          F    T,        State_HCO_ALBD)
endif

! Friction velocity
if(ExtState%USTAR%DoUse) then
    call HCO_Grid_CAM2HCO_2D(State_CAM_USTAR, State_HCO_USTAR)

    call ExtDat_Set(HcoState, ExtState%USTAR, 'USTAR_FOR_EMIS', &
                    RC,       FIRST,          State_HCO_USTAR)
endif
```

- Convert model met data to "MERRA2"
- Example in HEMCO-CESM: **hco_cam_convert_state_mod.F90**
- You can look into each extension to find ("%DoUse") which met variables are actually needed. (Not that many!)

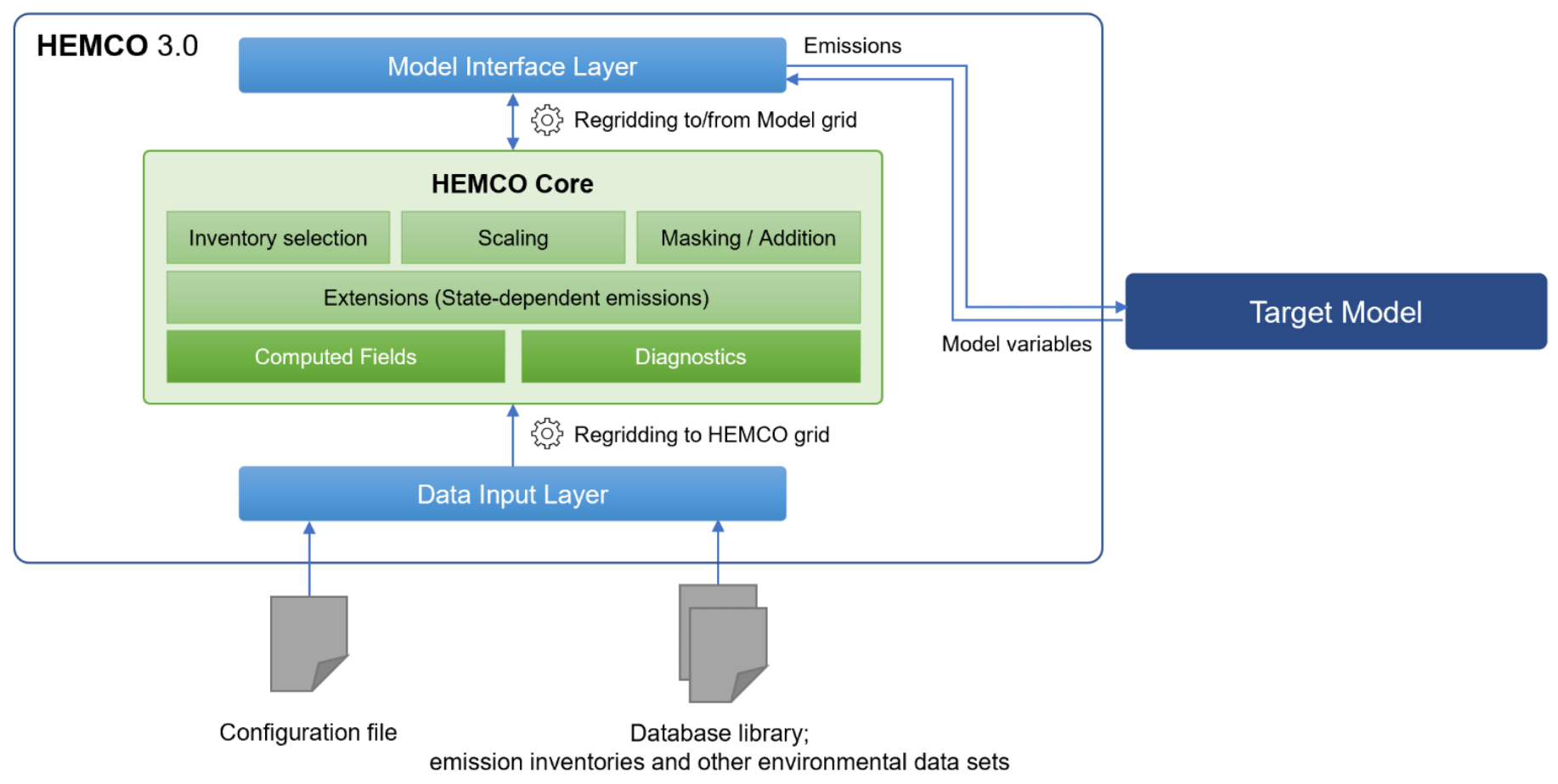
Extensions have built-in scale capabilities (e.g., for sensitivity studies)

- For example, you can scale the output of the GFED Biomass Burning extension

```
111     GFED                        : on
NO/CO/BIGALK/CH3COCH3/MEK/CH3CHO/C3H6/C2H2/C2H4/C3H8/CH2O/C2H6/SO2/NH3/bc_
a4/pom_a4/BENZENE/TOLUENE/XYLENES/C2H5OH/CH3OH
    --> GFED4                   :       true
    --> GFED_daily              :       false
    --> GFED_3hourly            :       false
    --> Scaling_CO              :       1.05
    --> Scaling_bc_a4           :       1.0
    --> Scaling_pom_a4          :       1.4
```

- We scaled the pom_a4 by 1.4* of what GFED extension computes by default

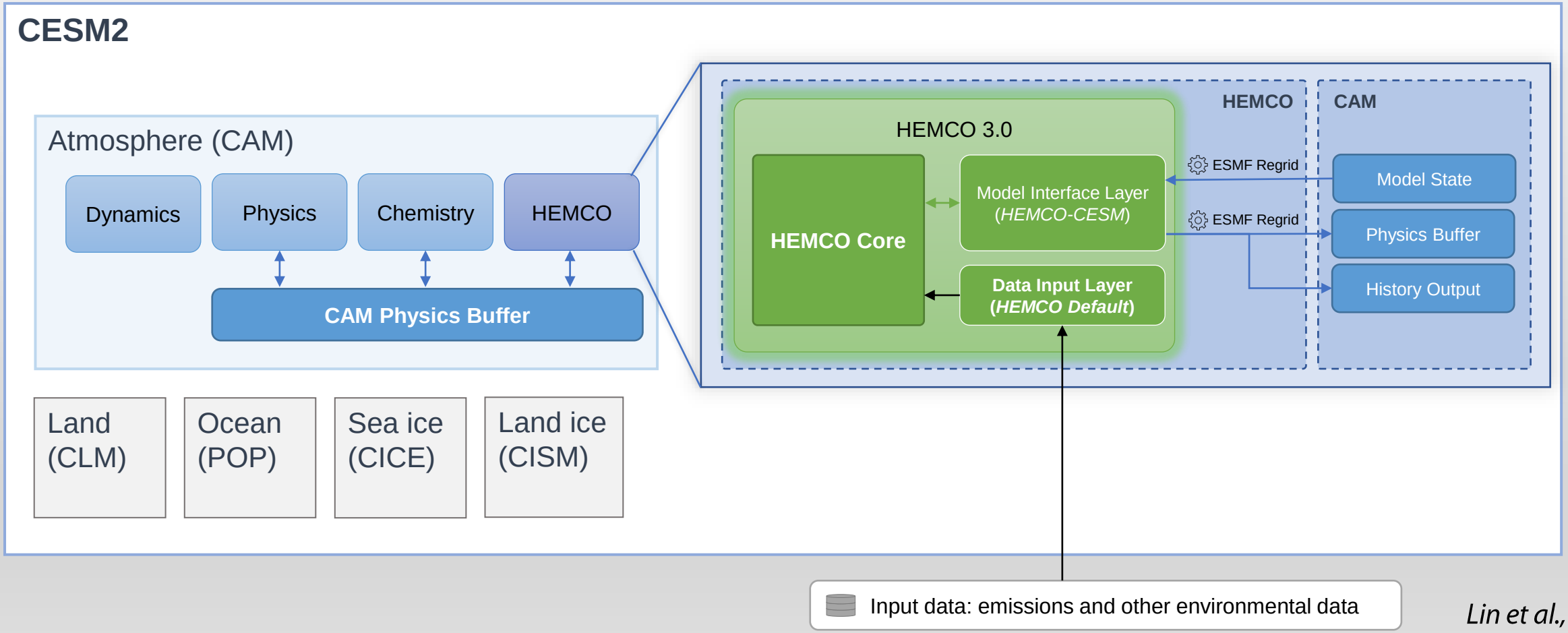
HEMCO restructured as a multi-model data tool



Lin et al., 2021

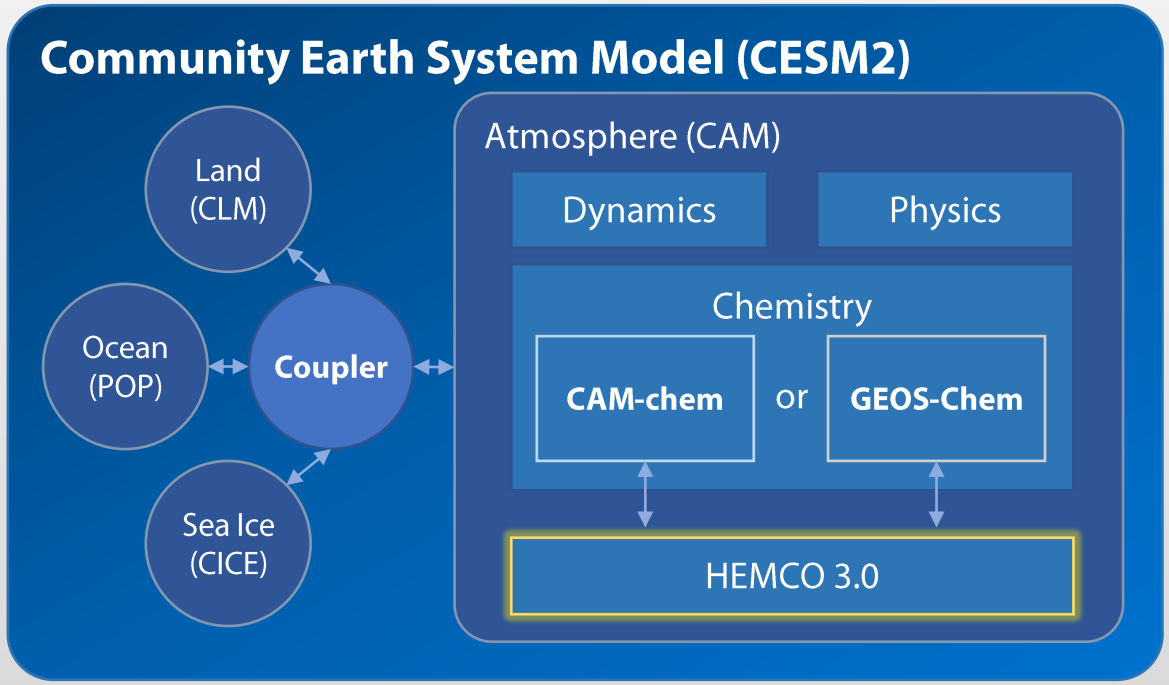
HEMCO implementation within CAM – as a separate component

HEMCO as a separate component in the atmosphere allows serving of data to any atmospheric component, independent of "the outside world"



Lin et al., 2021

HEMCO operates on a separate grid for accuracy and consistency



HEMCO is a separate component in CAM

- Has own grid ("HEMCO grid")
  - Consistent emissions regardless of model resolution
  - Re-grid computed results to model resolution at every time step
- Can serve both CAM-chem or GEOS-Chem chemistry in CESM

Adapted from NSF proposal; GEOS-Chem within CESM2 is Fritz et al., 2022 (in press)

Are there checks and diagnostics available, apart from emission totals?

- Not currently in CESM, but can be implemented in the HEMCO interface (let me know if there is demand!)
- e.g., can be used to get emissions information per sector / extension

```
# Name              Spec    ExtNr   Cat Hier Dim OutUnit   LongName
EmisCO_Total        CO      -1      -1  -1   3   kg/m2/s   CO_emission_flux_from_all_sectors
EmisCO_Aircraft     CO      0       20  -1   3   kg/m2/s   CO_emission_flux_from_aircraft
EmisCO_Anthro       CO      0       1   -1   3   kg/m2/s   CO_emission_flux_from_anthropogenic
EmisCO_BioBurn      CO      111     -1  -1   2   kg/m2/s   CO_emission_flux_from_biomass_burning
EmisCO_Ship         CO      0       10  -1   2   kg/m2/s   CO_emission_flux_from_ships
```

This is available in HEMCO code through a call to `subroutine GetHcoDiagn`, but some work to regrid it to CAM history and output is needed.

What if I want to run HEMCO *outside* of CESM?

https://hemco.readthedocs.io/en/stable/hco-sa-guide/intro.html

- HEMCO has an **off-line version** as well, if you just want to try it out.
- Can reuse all the HEMCO configuration file(s) from other models
- Specify species properties…

```
#ID NAME            MW       K0                  CR        PKA
1   NO              30.00    0.000000E+00        0.00      0.00
2   O3              48.00    0.000000E+00        0.00      0.00
3   PAN            121.00    0.000000E+00        0.00      0.00
4   CO              28.00    0.000000E+00        0.00      0.00
```

- Grid specification…

```
XMIN: -182.5
XMAX:  177.5
YMIN: -90.0
YMAX:  90.0
NX: 72 ...
```

OK, I want to add inventories/features to HEMCO/HEMCO-CESM!

- Thank you! ☺
- Git repositories:
  - **HEMCO** Core code, including Extensions: https://github.com/geoschem/HEMCO/
  - **HEMCO-CESM** interface: https://github.com/ESCOMP/HEMCO_CESM
  - **Configuration files** for CAM-chem/GEOS-Chem within CESM: https://github.com/jimmielin/HEMCO_CESM_configs/
- Please feel free to reach out to me with any questions or bugs!
- Generic HEMCO questions can be asked at the HEMCO GitHub as well (supported by the GEOS-Chem Support Team)

Many useful resources

- HEMCO User's Guide: https://hemco.readthedocs.io
- HEMCO references:
  - HEMCO 3.0 – implementation in several models, including CESM: https://gmd.copernicus.org/articles/14/5487/2021/ (Lin et al., 2021)
  - HEMCO 1.0 – original reference: https://gmd.copernicus.org/articles/7/1409/2014/ (Keller et al., 2014)
- HEMCO in MUSICA:
  - Pull request with setup instructions: https://github.com/ESCOMP/CAM/pull/560
- My email: hplin@seas.harvard.edu

What about point sources?

- HEMCO Core does not support point sources but the *Volcano* extension does:

```
###  LAT (-90,90), LON (-180,180), SULFUR [kg S/s], ELEVATION [m], CLOUD_COLUMN_HEIGHT [m]
### If elevation=cloud_column_height, emit in layer of elevation
### else, emit in top 1/3 of cloud_column_height
volcano::
10.030 -83.770 1.934297e+00 3340 3340
-37.860 -71.160 4.756469e+00 2800 2800
19.420 -155.290 2.736555e+01 1222 1222
3.170 98.390 1.192288e+01 2460 2460
-15.800 -71.860 1.331811e+00 5967 5967
-15.400 167.830 1.786847e+01 1395 1395
..
```