Community Earth System Model

CESM2 tutorial:
CESM2 (WACCM) and CESM2(CAM-chem)

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- CESM-WACCM and CAM-chem component configurations
- Quickstart guide for present-day chemistry compsets
- Exercise 1: Run WACCM or CAM-chem with new daily output
- Exercise 2: Change reaction rate in the chemical mechanism
- Post-processing data analysis using goev
- Validating CESM/WACCM
- WACCM & CAM-chem customer support

NCAR is supported by the
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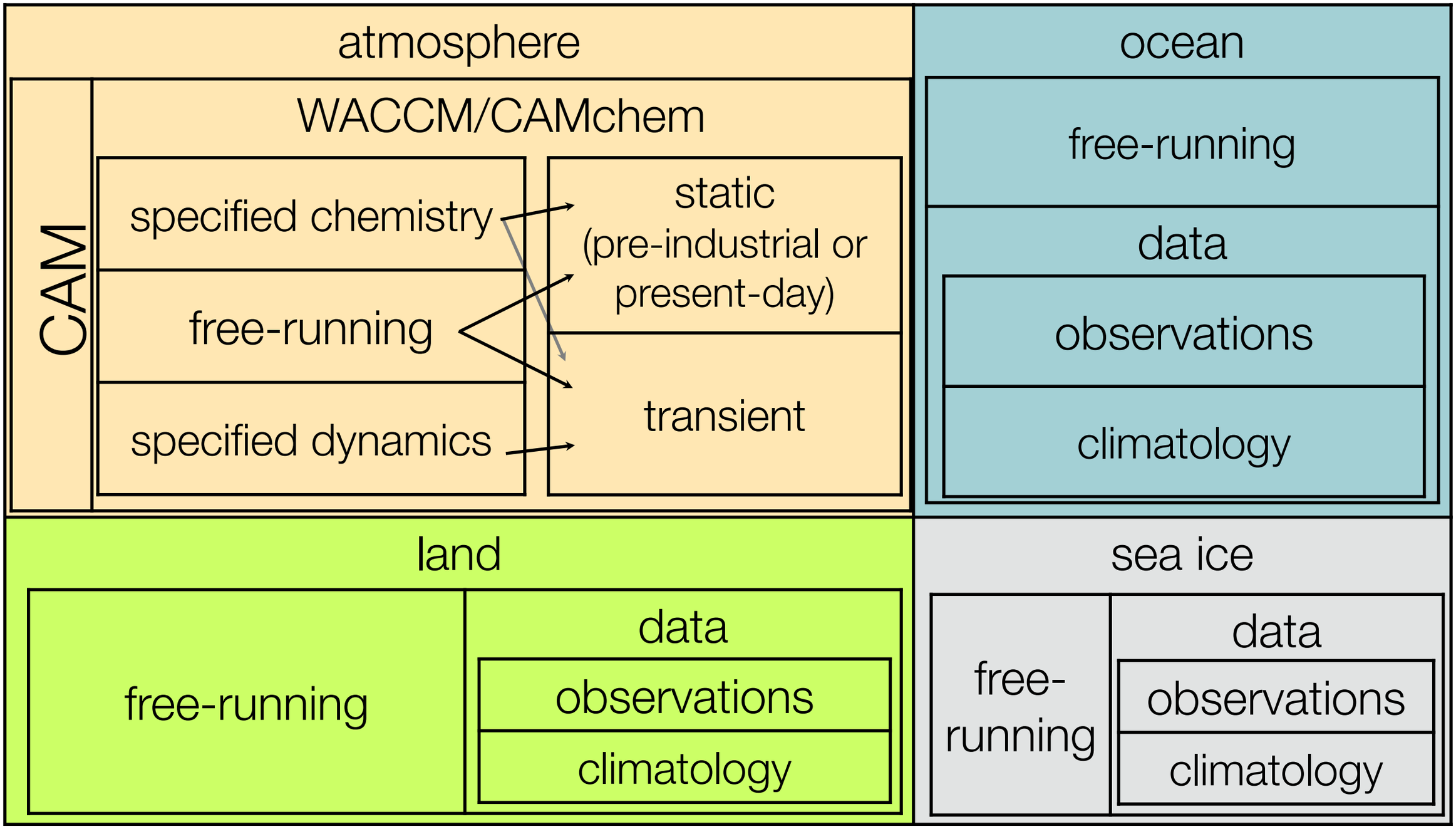
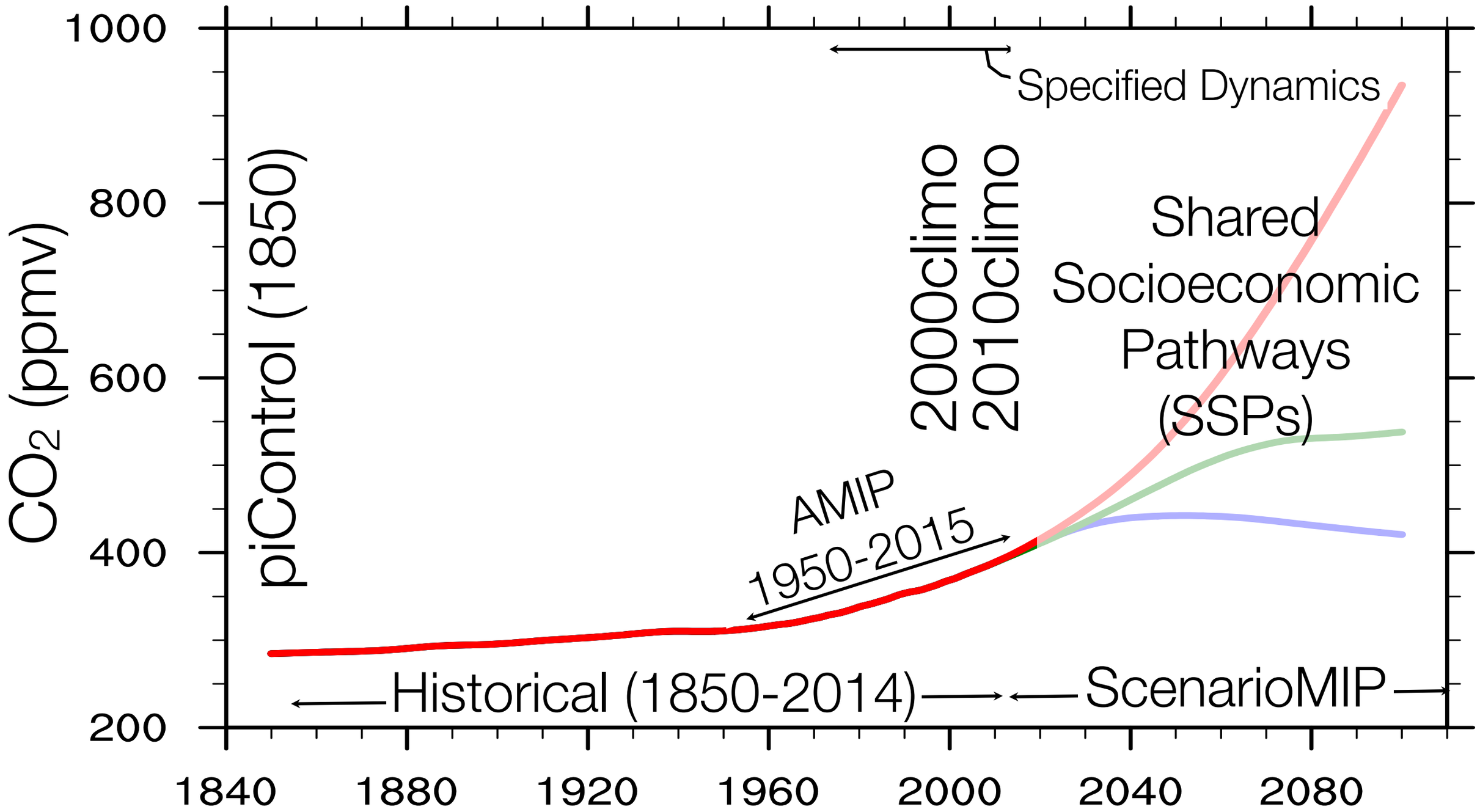
WACCM /CAMChem component configurations



CESM2 WACCM /CAMChem component configurations



CAM-6.0 (CESM2.0) User Guide

https://ncar.github.io/CAM/doc/build/html/users_guide/CAM-chem-specifics.html#chemical-mechanisms

9.1. Chemical mechanisms

CESM2.0 supports 6 chemical mechanism (as listed in the Table). The CESM chemical mechanism is a set used to calculate chemical reactions using the chemical preprocessor (http://www.cesm.ucar.edu/working_groups/Chemistry/chemistry.preprocessor.pdf). For existing compsets the preprocessor has been used to compile fortran routines required to run the model: under $CCSMROOT/components/cam/src/chemistry/.

Mechanism (pre-processor code)	Model: Chemistry Description	#Species	#Reactions
TSMLT1 (pp_waccm_tsmlt_mam4)	WACCM: Troposphere, stratosphere, mesosphere, and lower thermosphere	231 solution, 2 invariant	583 (433 kinetic, 150 photolysis)
TS1 (pp_trop_strat_mam4_vbs)	CAM-chem: Troposphere and stratosphere	221 solution, 3 invariant	528 (405 kinetic, 123 photolysis)
MA (pp_waccm_ma_mam4)	WACCM: Middle atmosphere (stratosphere, mesosphere, and lower thermosphere)	98 solution, 2 invariant	298 (207 kinetic, 91 photolysis)
MAD (pp_waccm_mad_mam4)	WACCM: Middle atmosphere plus D-region ion chemistry	135 solution, 2 invariant	593 (489 kinetic, 104 photolysis)
SC (pp_waccm_sc_mam4)	WACCM: Specified chemistry	29 solution, 8 invariant	12 (11 kinetic, 1 photolysis)
CAM	CAM: Aerosol chemistry	25 solution, 7 invariant	7 (6 kinetic, 1 photolysis)

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CAM-6.0 (CESM2.0) User Guide

https://ncar.github.io/CAM/doc/build/html/users_guide/atmospheric-configurations.html#waccm-compsets

CAM6 user guide does not include compsets with interactive ocean and sea ice components (B compsets)

Find scientifically validated configurations here:

http://www2.cesm.ucar.edu/models/scientifically-supported

4.5. WACCM compsets

4.5.1. Scientifically supported WACCM atmosphere compsets

Scientifically supported WACCM atmosphere configurations for CESM2.0 use TSMLT1 chemistry (see chemical mechanisms) and 0.95° latitude x 1.25° longitude horizontal resolution (f09_f09_mg17). Additional scientifically validated configurations will be available in CESM2.1.

Compset	Resolution	Description	Period
FW1850	f09_f09_mg17	Pre-industrial control WACCM6 using 1-degree FV dycore, TSMLT1, CMIP6 piControl emissions, year 1850 SSTs, coupled to interactive land and MEGAN2.1	1850
FWHIST	f09_f09_mg17	Historical WACCM6 using 1-degree FV dycore, TSMLT1, CMIP6 emissions, historical SSTs, coupled to interactive land and MEGAN2.1	1974 to 2015
FW2000	f09_f09_mg17	Year 2000 WACCM6 1deg compset using 1-degree FV dycore, TSMLT1, year 2000 CMIP6 emissions, year 2000 SSTs, coupled to interactive land and MEGAN2.1	2000
FWSD	f09_f09_mg17	Historical SD-WACCM6 using GEOS5 analysis with a 50-hour relaxation, TSMLT1, CMIP6 emissions, historical SSTs, coupled to interactive land and MEGAN2.1	2005 to 2015
FWscHIST	f09_f09_mg17	Historical SC-WACCM6 using 1-degree FV dycore, specified chemistry, historical SSTs	1976 to 2015

4.5.2. Tested WACCM atmosphere compsets

Tested WACCM atmosphere configurations for CESM2.0 use middle atmosphere (MA) and middle atmosphere plus D-region (MAD) chemistry (see chemical mechanisms) and 0.95° latitude x 1.25° longitude horizontal resolution (f09_f09_mg17).

Compset	Resolution	Description	Period
FWmaHIST	f09_f09_mg17	Historical WACCM6 using 1-degree FV dycore, MA chemistry, CMIP6 emissions, historical SSTs, coupled to interactive land and MEGAN2.1	1974 to 2015
FWmadHIST	f09_f09_mg17	Historical WACCM6 using 1-degree FV dycore, MAD chemistry, CMIP6 emissions, historical SSTs, coupled to interactive land and MEGAN2.1	1974 to 2015
FWmaSD	f09_f09_mg17	Historical SD-WACCM6 using GEOS5 analysis with a 50-hour relaxation, MA chemistry, CMIP6 emissions, historical SSTs, coupled to interactive land and MEGAN2.1	2005 to 2015
FWmadSD	f09_f09_mg17	Historical SD-WACCM6 using GEOS5 analysis with a 50-hour relaxation, MAD chemistry, CMIP6 emissions, historical SSTs, coupled to interactive land and MEGAN2.1	2005 to 2015

CAM6 User Guide: WACCM-X compsets

https://ncar.github.io/CAM/doc/build/html/users_guide/atmospheric-configurations.html#waccm-x-compsets

4.6. WACCM-X compsets

WACCM-X has three compsets/resolutions which are supported scientifically. These compsets are detailed in the following table. A specific compset may be listed below, but unless the resolution is also listed, that compset/resolution combination is not scientifically supported. Different resolutions exhibit different behavior and as a result require different tunings. The scientifically supported designation is limited to the specific compset/resolution pairs listed in the following table.

Scientifically supported WACCM-X compsets

Compset Name	Supported Resolution	Description	Period
FXHIST	f19_f19_mg16	Historical WACCM-X based on CAM4 using 2 degree FV dycore, MA chemistry, CCMI emissions, historical SSTs, coupled to land, prescribed ice, river	2000 to 2015
FX2000	f19_f19_mg16	Year 2000 WACCM-X based on CAM4 2 degree FV dycore, using MA chemistry, year 2000 CCMI emissions and SSTs, coupled to interactive land, prescribed ice, river	2000
FXSD	f19_f19_mg16	Historical SD-WACCM-X based on CAM4 using 2 degree FV dycore, MERRA1 with a 50-hour relaxation, MA chemistry, CCMI emissions, historical SSTs, coupled to interactive land, prescribed ice, river	2000 to 2015

It should be noted that these WACCM-X compsets are based on the previous version 4 of CAM/WACCM and therefore are not derivatives of the version 6 CAM/WACCM compsets described above.

WACCM-X compsets will be updated with new functionality and bug fixes in CESM2.1.
Planned WACCM-X update to CAM6 physics will come later (estimated end of 2019).

Additional and upcoming CESM2 WACCM configurations

Compsets (Release)	Supported Grids	Components / Meteorology
Full ocean, static:		**CAM6/CLM5.0/BGC, CICE5, POP5**
BW1850 (CESM2.0)	f09_g17	pre-industrial, TSMLT chemistry
BWma1850 (CESM2.0)	f09_g17, f19_g17	pre-industrial, MA chemistry
Full ocean, transient:		
BWHIST (CESM2.1)	f09_g17	historical, TSMLT chemistry
Data ocean, static:		**CAM6/CLM5.0/BGC**
FW2000climo (CESM2.1)	f09_f09_mg17	present day (1995-2005 average), TSMLT
FW2010climo (CESM2.1)		present day (2006-2014 average), TSMLT
Data ocean, transient:		**CAM6, CLM5.0/BGC**
FWSD (CESM2.1 update)	f09_f09_mg17	MERRA2 nudging, TSMLT chemistry
FWmaSD (CESM2.1 update)	f09_f09_mg17	MERRA2 nudging, MA chemistry
FWmadSD (CESM2.1 update)	f09_f09_mg17	MERRA2 nudging, MAD chemistry

CESM2.1 updates:

- SD-WACCM will use MERRA2 instead of GEOS5.
- Additional new compsets will be added/updated (i.e. SC-WACCM).

ScenarioMIP compsets (SSPs) will come later (CESM2.2).

CAM6 User Guide: CAM-chem compsets

https://ncar.github.io/CAM/doc/build/html/users_guide/atmospheric-configurations.html#cam-chem-tested-compsets

4.4. CAM-chem tested compsets

CAM-chem tested compsets in CESM2.0 (CAM-chem scientifically supported compsets will be available in CESM2.1)

CAM-chem has a number of compsets/resolutions which are tested in CESM2.0, see Table. All available compsets use observed SSTs and sea-ice values and CMIP6 emissions until 2015. Specified dynamics compsets are nudged to winds, temperature and surface fluxes and run on 56 levels, aligned with the MERRA2 vertical levels. Additional SD configurations are tested to run with 32 levels that are not availble at this point. Half-degree SD compsets use 1-degree emissions. Users have to change to half-degree emissions if desired.

Compset Name	tested resolution	Description	Period
FCHIST	f09_f09_mg17	Historical CAM6-chem using 1 degree FV dycore, using CMIP6 emissions, coupled to interactive land and MEGAN2.1	1979 to 2015
FCSD	f09_f09_mg17	Historical CAM6-chem 1deg compset using MERRA2 analsysis with a 50-hour relaxation. See details in the text	1980 to 2015
FCSD	f05_f05_mg17	Historical CAM6-chem half deg compset using MERRA2 analysis	1980 to 2015
FC2000climo	f09_f09_mg17	Climatological CAM6-chem using 1 degree FV dycore, averaged SSTs, emissions, and lower boundary conditions (1995-2005)	1995-2005 average climo
FC2010climo	f09_f09_mg17	Climatological CAM6-chem using 1 degree FV dycore, averaged SSTs, emissions, and lower boundary conditions (2006-2014)	2006-2014 average climo

Additional compsets will be released later

Exercise 1:
Run a present-day WACCM/CAMChem compset

- Go to the script directory in your source code
- Run create_newcase command for one of these configurations:

WACCM: --compset FW2000 --res f09_f09_mg17
CAM-chem: --compset FC2000climo --res f09_f09_mg17
WACCM-X: --compset FX2000 --res f19_f19_mg16

CASENAME: ~/f.e20.$compset.$res.tutorial.test1
i.e. for CAM-chem: f.e20.FC2000climo.f09_f09_mg17.tutorial.test1

- Go to your case directory and setup and build the model
- Add or modify history stream 2 (fincl2) to output daily instantaneous values of: 'PS','Z3','T','U','V','O3'

Change user_nl_cam: fincl2, avgflag_pertape, mfilt, nhtfrq

- Run the model for 5 days
- Check your model output in your run directory

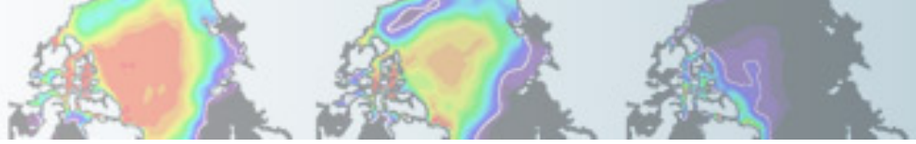
Exercise 1: Run a present-day WACCM/CAMChem compset

Important! Check the newly generated namelist prior run

- `ls CaseDocs/*`

```
atm_in              cpl_modelio.nml                  glc_modelio.nml  ocn_modelio.nml
atm_modelio.nml     docn_in                          ice_in           rof_modelio.nml
chem_mech.doc       docn.streams.txt.prescribed      ice_modelio.nml  seq_maps.rc
chem_mech.in        drv_flds_in                      lnd_in           wav_modelio.nml
cism.config         drv_in                           lnd_modelio.nml
cism_in             esp_modelio.nml                  mosart_in
```

- **atm_in: atmospheric namelist varliables**
- **chem_mech.in: chemical mechanism file**
- **drv_flds_in: dry deposition variables, MEGAN variables (if used)**
- **lnd_in: land namelist variables**
- **…**



Exercise 2:
Building the model with new chemistry

- Setup a new case as done in Exercise 1, with case name
~/f.e20.$compset.$res.tutorial.test2

- Look at your chemistry preprocessor file chem_mech.in in CaseDocs and copy it to your case directory

```
➢ less CaseDocs/chem_mech.in
➢ cp CaseDocs/chem_mech.in my_chem_mech.in
```

The chemical preprocessor and the mechanism file

The **chemistry preprocessor**: generates CAM Fortran source code to solve chemistry.

Input: a simple ASCII file listing chemical reactions and rates.

The chemistry preprocessor input file used in your previous run is in your $CASEROOT/CaseDocs/chem_mech.in

Additional input files for default chemical mechanisms are in each source code subdirectory for mechanisms under $CCSMROOT/models/atm/cam/src/chemistry/pp_* (i.e. pp_waccm_mozart)

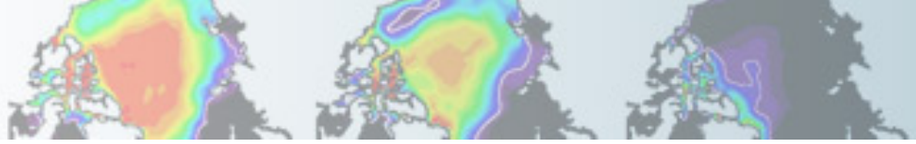
```
 SPECIES
     Solution
O3, O, O1D -> O, O2, O2_1S -> O2, O2_1D -> O2
     End Solution

     Fixed
M, N2
     End Fixed
 End SPECIES

 Solution Classes
     Explicit
      CH4, N2O, CO, H2, CH3CL, CH3BR, CFC11, CFC12
     End explicit
     Implicit
      O3, O, O1D, O2, O2_1S, O2_1D
     End implicit
  End Solution Classes

  CHEMISTRY
     Photolysis
 [jo2_a] O2 + hv -> O + O1D
     End Photolysis

     Reactions
  [cph1,cph] O + O3 -> 2*O2      ; 8e-12, -2060
     End Reactions
END CHEMISTRY
```



Reaction rate types in the chempp input file

- Temperature-independent rates: k [cm^3 $molec^{-1}$ s^{-1}]= a_0

```
O1D + H2O -> 2*OH                                   ; 2.2e-10
```

- Arrhenius type: k = a_0 * exp(b_0/T), where b_0 = (-E/R)

a_0, b_0

```
O + O3 -> 2*O2                                      ; 8e-12, -2060
```

- Troe rate constant: k = α^x / (1 - β^2), where:

$\alpha = k_0 * M / k_\infty$, $\beta = \log_{10}(\alpha)$, M= air density (molec cm^{-3}), T = temperature (K)

$k_0 = a_0 * (300/T)^{**} a_1$, $k_\infty = b_0 * (300/T)^{**} b_1$, x= “exponential factor”

```
[usr11] CH3CO3 + NO2 + M -> PAN + M ; 8.5e-29, 6.5, 1.1e-11, 1., .6
```

a_0, a_1, b_0, b_1, x

- User-specified reaction rate:

```
[usr1] O + O2 + M -> O3 + M
```

rate defined in routine `mo_usrrxt.F90`

Exercise 2:
Building the model with new chemistry

For WACCM / CAM-chem:

- Change reaction rates (bug in earlier version)

```
      Reactions
************************************
*** odd-oxygen
************************************
[O1D_H2]                 O1D + H2   -> H + OH                    ; 1.2e-10
[O1D_H2O]                O1D + H2O  -> 2*OH                      ; 1.63e-10, 60
[O1D_N2,cph=189.81]      O1D + N2   -> O + N2                    ; 2.15e-11, 110
[O1D_O2ab]               O1D + O2   -> O + O2                    ; 3.3e-11, 55
[O1D_O3]                 O1D + O3   -> O2 + O2                   ; 1.2e-10
[O_O3,cph=392.19]        O + O3   -> 2*O2                        ; 8e-12, -2060
[usr_O_O,cph=493.58]     O + O + M  -> O2 + M
[usr_O_O2,cph=101.39]    O + O2 + M  -> O3 + M
```

Change to 1.65e-12 (bug in earlier version)

- Edit your new mechanism file:
  - `nedit my_chem_mech.in`

Exercise 2:
Building the model with new chemistry

- Query the default CAM configure options:

➢
```
./xmlquery CAM_CONFIG_OPTS
CAM_CONFIG_OPTS: -phys cam6 -chem trop_strat_mam4_vbs -age_of_air_trcs
```

- Append a pointer to your user mechanism:

➢
```
xmlchange --append CAM_CONFIG_OPTS="--usr_mech_infile `pwd`/my_chem_mech.in"
```

- Query the updated CAM configure options:

➢
```
./xmlquery CAM_CONFIG_OPTS
CAM_CONFIG_OPTS: -phys cam6 -chem trop_strat_mam4_vbs -age_of_air_trcs
--usr_mech_infile
/gpfs/u/home/<username>/f.e20.FC2000climo.f09_f09_mg17.tutorial.test2/
my_chem_mech.in
```

- Reset your case setup, and build again
- Submit a new run
- Check output and compare 5th day output to earlier run using geov

Post-processing data analysis: GEOV

CESM history files are in standard netCDF format, and may be analyzed with standard analysis tools, including Matlab, IDL, NCL, and NCO.

GEOV is an IDL-based viewer for geophysical history files created by NCAR's CAM, WACCM and MOZART models.

GEOV can be downloaded from the WACCM webpage
http://www.cesm.ucar.edu/working_groups/Whole-Atmosphere/code-release.html

Or install geov on cheyenne:

- Add idl module:
  - `module load idl`
- Edit .cshrc file. Add line:

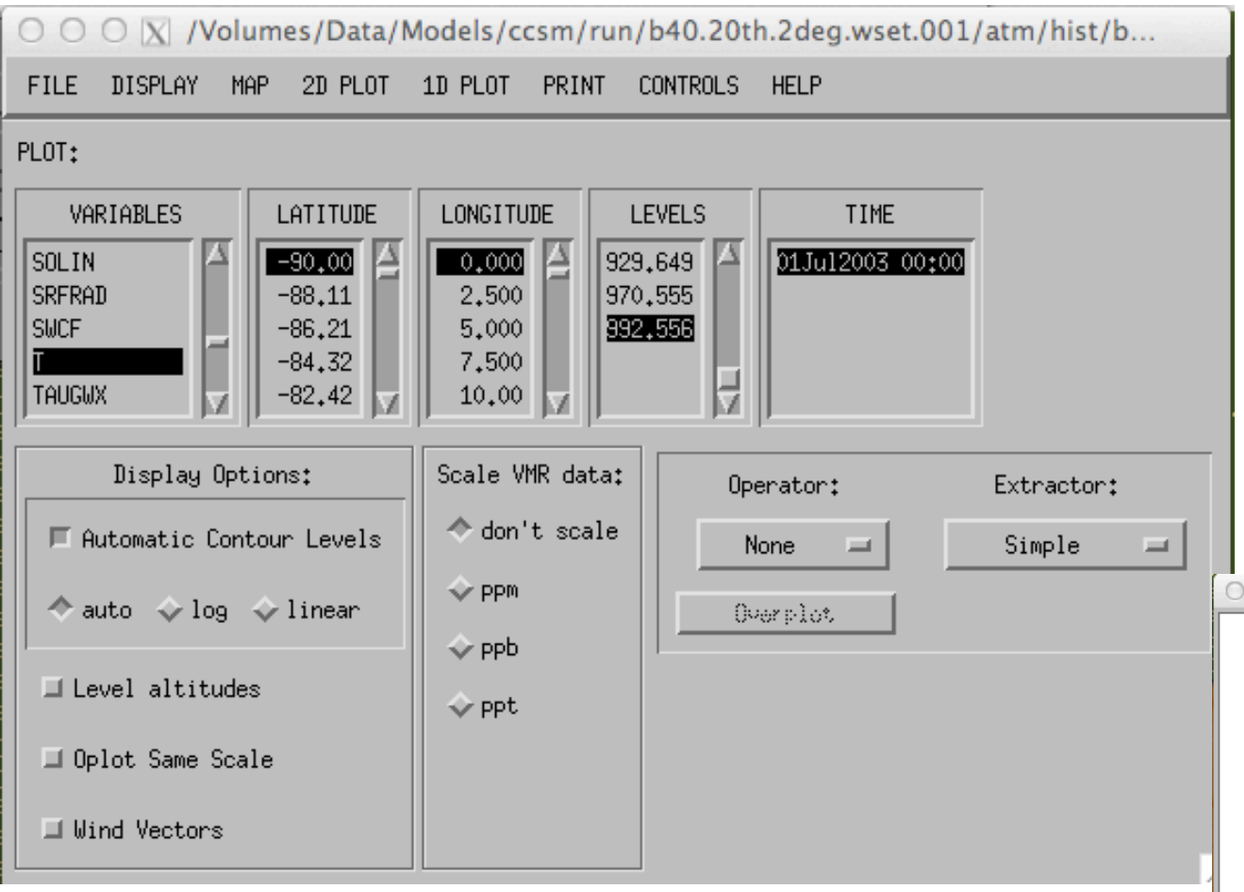
```
setenv IDL_STARTUP ~fvitt/idl_startup
```

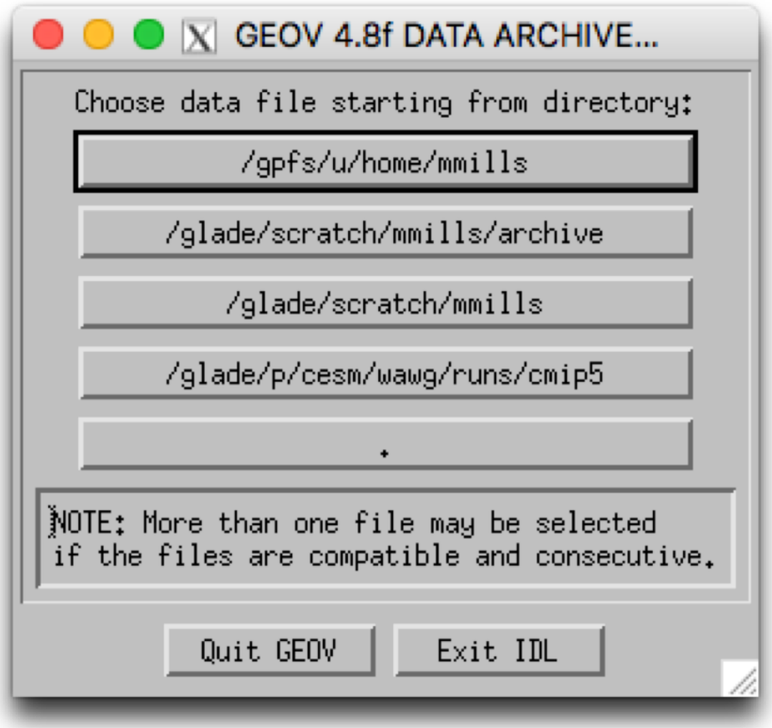
- ~fvitt/idl_startup sets the idl path to include GEOV:

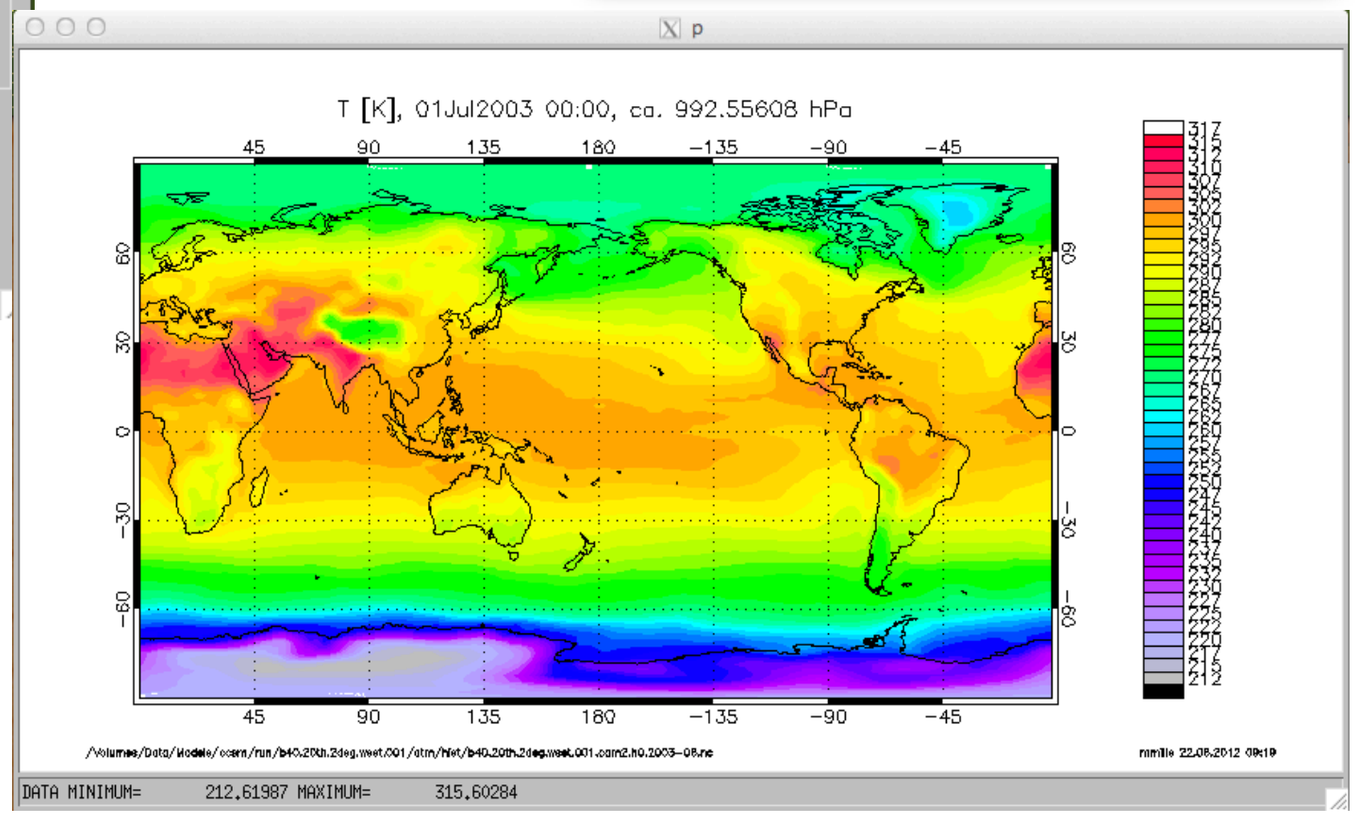
```
idl_path = expand_path('+~fvitt/geov')
!path=!path+':'+idl_path
```

  - `source .cshrc`
  - `cd /glade/u/home/fvitt/geov4.8e`
  - `idl geov`

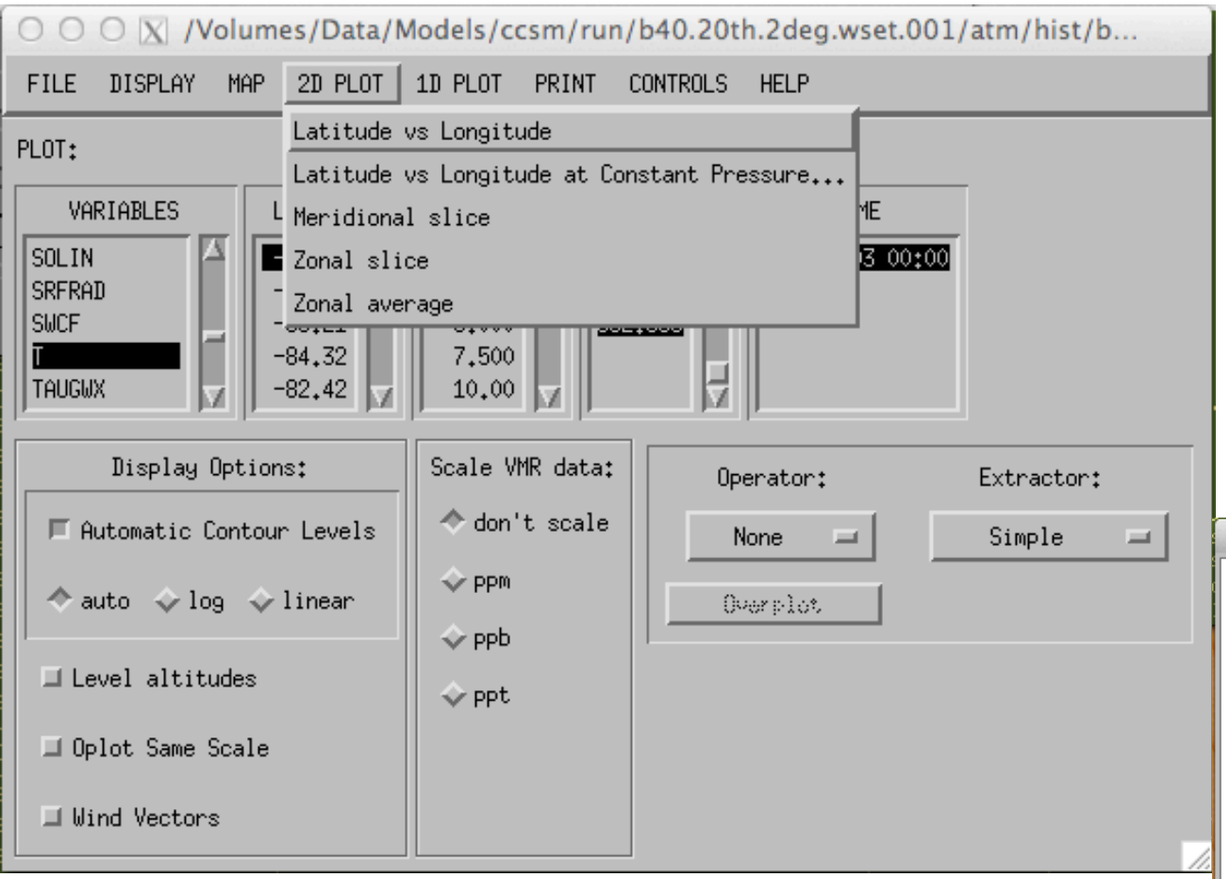
GEOV graphical user interface

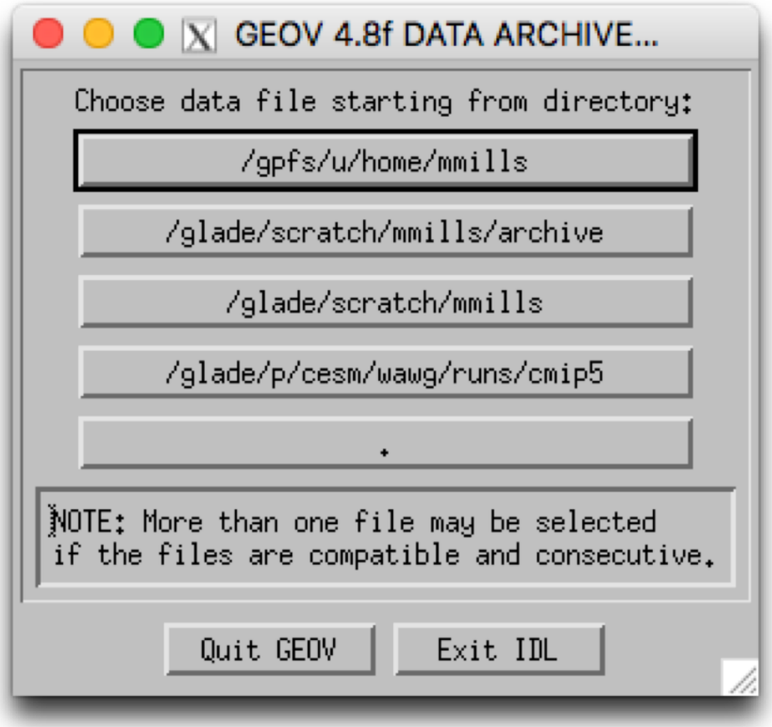


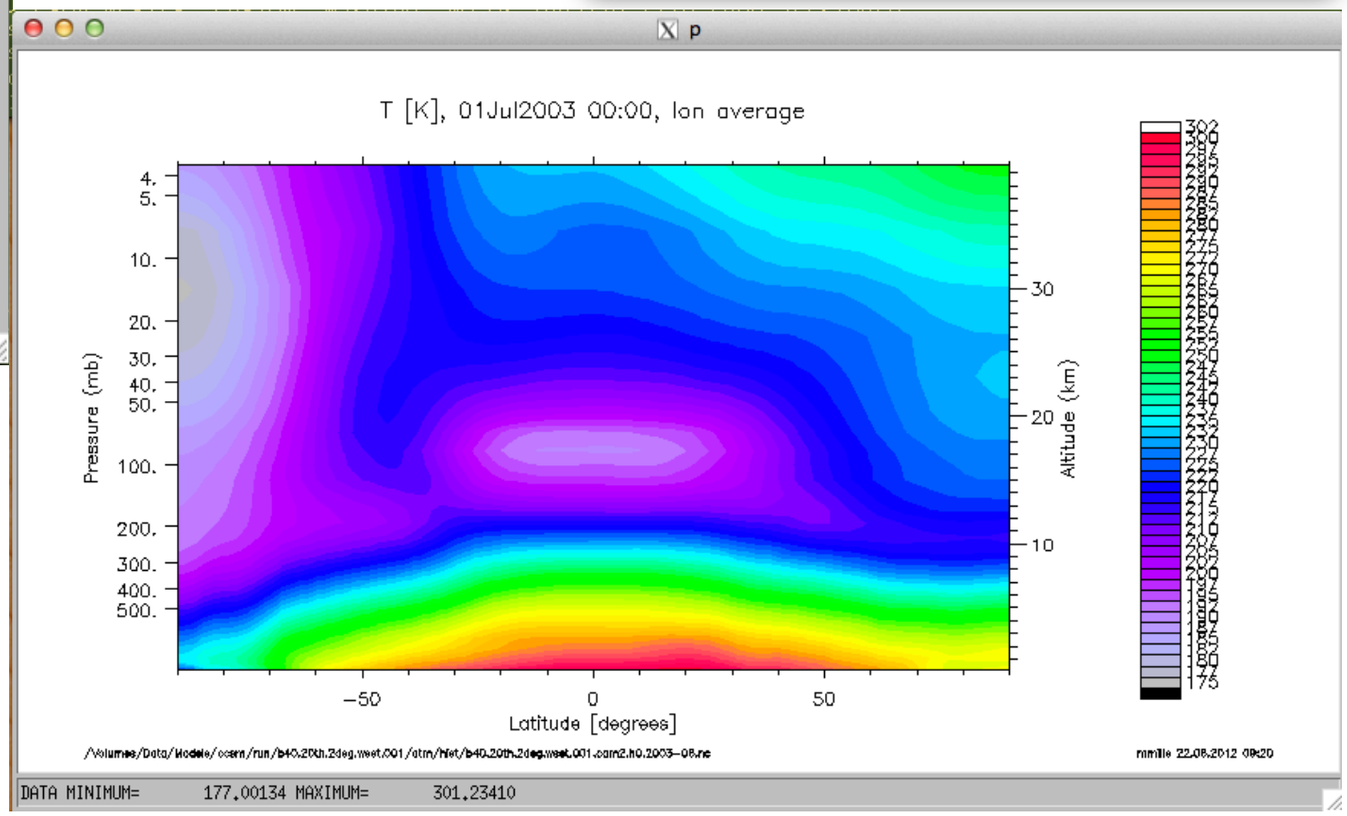




GEOV graphical user interface







WACCM and CAM-Chem Customer Support

CGD Forum: http://bb.cgd.ucar.edu/

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Solution 1:
Run a present-day WACCM/CAMChem compset

- Go to the script directory in your source code

```
> cd /glade/p/cesm/tutorial/cesm2.0.0_tutorial/cime/scripts
```

- Run create_newcase command for one of these compsets:

CAM-chem:
```
> ./create_newcase --compset FC2000climo --res f09_f09_mg17
  --case ~/f.e20.FC2000climo.f09_f09_mg17.tutorial.test1
```

WACCM:
```
> ./create_newcase --compset FW2000 --res f09_f09_mg17
  --case ~/f.e20.FW2000.f09_f09_mg17.tutorial.test1
```

WACCM-X:
```
> ./create_newcase --compset FX2000 --res f19_f19_mg16
  --case ~/f.e20.FX2000.f19_f19_mg16.tutorial.test1
```

- Go to your case directory and setup the run
- Setup the model `>./case.setup`
- Build the model: `> qcmd -- ./case.build`

namelists (atm_in, ice_in, lnd_in, docn_in) will appear in the CaseDocs subdirectory, as well as in your $rundir

Solution 1: How do I change model output?

- Update the user_nl_cam file in your $casedir and add/change the fincl2 output

```
> nedit user_nl_cam
```

- Paste avgflag_pertap, mfilt, nhtfrq from CaseDocs/atm_in, i.e. for WACCM:

```
avgflag_pertape = 'A', 'A', 'A', 'A', 'A', 'A', 'A', 'A', 'I'
mfilt           = 1,   30, 120, 240, 240, 480, 365,  73,  30
nhtfrq          = 0,  -24,  -6,  -3,  -1,   1, -24,-120,-240
```

- Make changes:

```
avgflag_pertape = 'A', 'I', 'A', 'A', 'A', 'A', 'A', 'A', 'I'
mfilt           = 1,   30, 120, 240, 240, 480, 365,  73,  30
nhtfrq          = 0,  -24,  -6,  -3,  -1,   1, -24,-120,-240
fincl2          = 'PS','Z3','T','U','V','O3'
```

- Preview namelists and make sure changes are in your CaseDocs/atm_in file

```
> ./preview_namelists
```

- Check your CaseDocs/atm_in

```
> less CaseDocs/atm_in
```

- Resubmit your job (run the model for 5 days)

```
> ./case.submit
```

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Solution 1: Check your model output

- **find your model output in your run dir ($run_dir) after finished:**

```
> ls /glade/scratch/<username>/<casename>/run
```

```
f.e20.FC2000climo.f09_f09.tutorial.test1/run> ls
atm_in
atm_modelio.nml
CASEROOT
cism.config
cism_in
cpl_modelio.nml
docn_in
docn.streams.txt.prescribed
drv_flds_in
drv_in
esp_modelio.nml
f.e20.FC2000climo.f09_f09.tutorial.test1.cam.h1.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.cam.r.0001-01-06-00000.nc
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f.e20.FC2000climo.f09_f09.tutorial.test1.cam.rs.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.cice.r.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.cism.r.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.clm2.r.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.clm2.rh0.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.cpl.r.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.docn.rs1.0001-01-06-00000.bin
f.e20.FC2000climo.f09_f09.tutorial.test1/run>
```

```
f.e20.FC2000climo.f09_f09.tutorial.test1.mosart.r.0001-01-06-00000.nc
f.e20.FC2000climo.f09_f09.tutorial.test1.mosart.rh0.0001-01-06-00000.nc
finidat_interp_dest.nc
glc_modelio.nml
ice_in
ice_modelio.nml
lnd_in
lnd_modelio.nml
mosart_in
ocn_modelio.nml
rof_modelio.nml
rpointer.atm
rpointer.drv
rpointer.glc
rpointer.ice
rpointer.lnd
rpointer.ocn
rpointer.rof
seq_maps.rc
timing
wav_modelio.nml
```

namelist information

restart information

- **find your model output in the short-time archive**

```
> ls /glade/scratch/<username>/archive/<casename>/…
```

(note: there will be no monthly values available if you just run for 5 days)

- **check your cam.h1 file**

```
> ncdump –h f.e20.FC2000climo.f09_f09_mg17.tutorial.test1.cam.h1.0001-01-06-00000.nc
```

Solution 2:
Building the model with new chemistry

- Go to the script directory in your source code
  - `cd /glade/p/cesm/tutorial/cesm2.0.0_tutorial/cime/scripts`

WACCM:

- `./create_newcase --compset FW2000 --res f09_f09_mg17 --case ~/f.e20.FW2000.f09_f09_mg17.tutorial.test2`
- `cd $CASEROOT`
- `cp CaseDocs/chem_mech.in my_chem_mech.in`
- `nedit my_chem_mech.in &` (use any editor to edit your script)

```
      Reactions
* ------------------------------------------------------------
* Odd-Oxygen Reactions
* ------------------------------------------------------------
 [usr_O_O2]          O + O2 + M -> O3 + M
 [O_O3]              O + O3 -> 2*O2                          ; 8.00e-12, -2060.
 [usr_O_O]           O + O + M -> O2 + M

* ------------------------------------------------------------
* Odd-Oxygen Reactions (O1D only)
* ------------------------------------------------------------
 [O1D_N2]            O1D + N2 -> O + N2                      ; 2.15e-11,   110.
 [O1D_O2b]           O1D + O2 -> O + O2                      ; 3.30e-11,    55.
 [ox_l1]             O1D + H2O -> 2*OH                       ; 1.63e-10,    60.
 [O1D_N2Oa]          O1D + N2O -> 2*NO                       ; 7.25e-11,    20.
 [O1D_N2Ob]          O1D + N2O -> N2 + O2                    ; 4.63e-11,    20.
```

Change to 1.65e-12 (bug in earlier version)

Solution 2:
Building the model with new chemistry

- Append pointer to user mechanism:
  - `xmlchange --append CAM_CONFIG_OPTS="--usr_mech_infile `pwd`/my_chem_mech.in"`
- Re-rebuild your run:
  - `./case.build --clean`
  - `./case. build`
- submit the new run
  - `./case.submit`
- Check output after the run
  - `ls /glade/scratch/<username>/archive/<casename>/…`

Solution 2: Building the model with new chemistry

- Compare your output with the other run, using geov