Community Earth System Model

CESM2.1 tutorial: CESM2.1(WACCM6) and CESM2.1(CAM6-chem)

Mike Mills
WACCM Liaison
mmills@ucar.edu

Simone Tilmes
CAM-chem Liaison
tilmes@ucar.edu

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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
- WACCM & CAM-chem customer support

NCAR is supported by the
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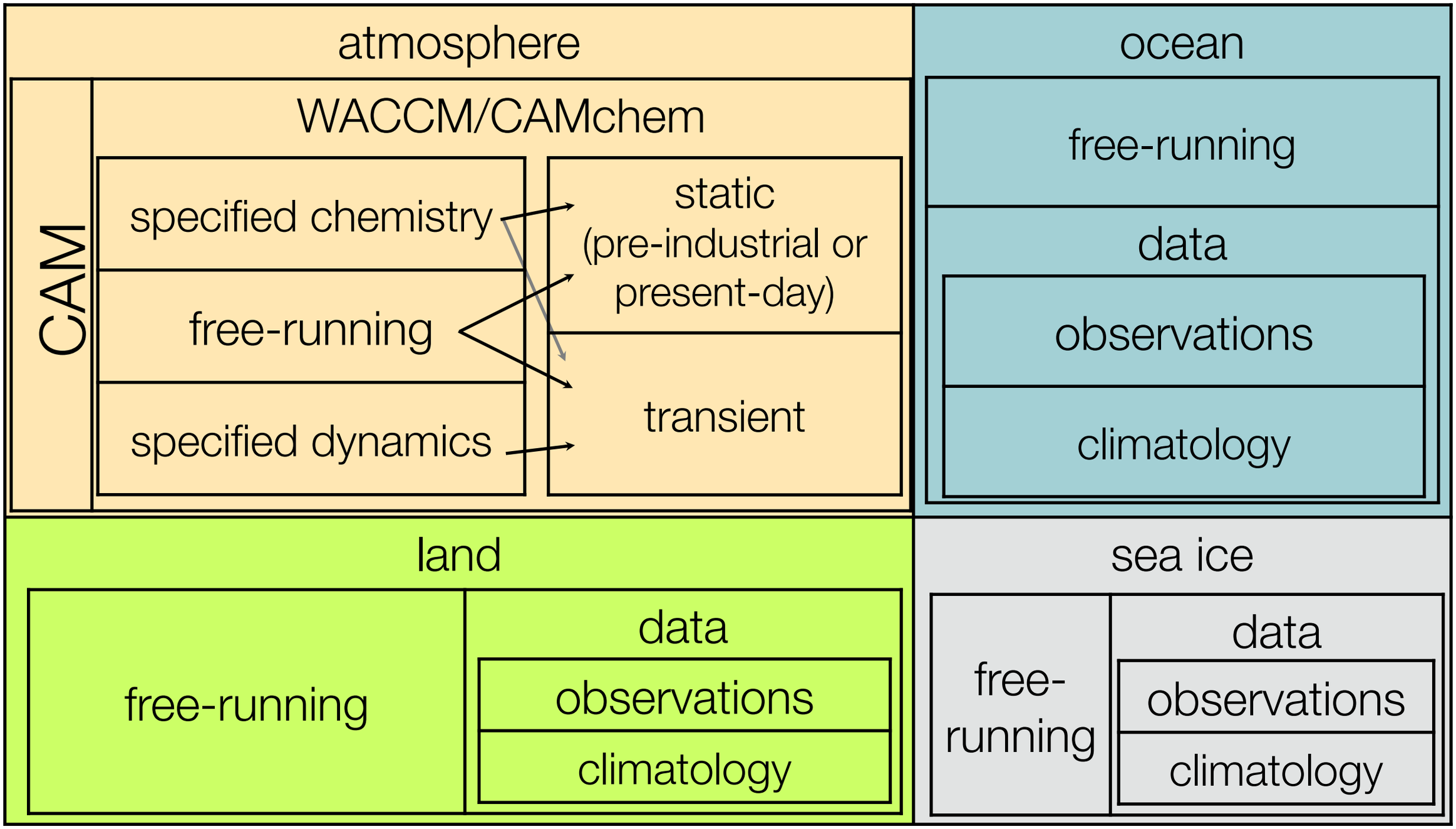
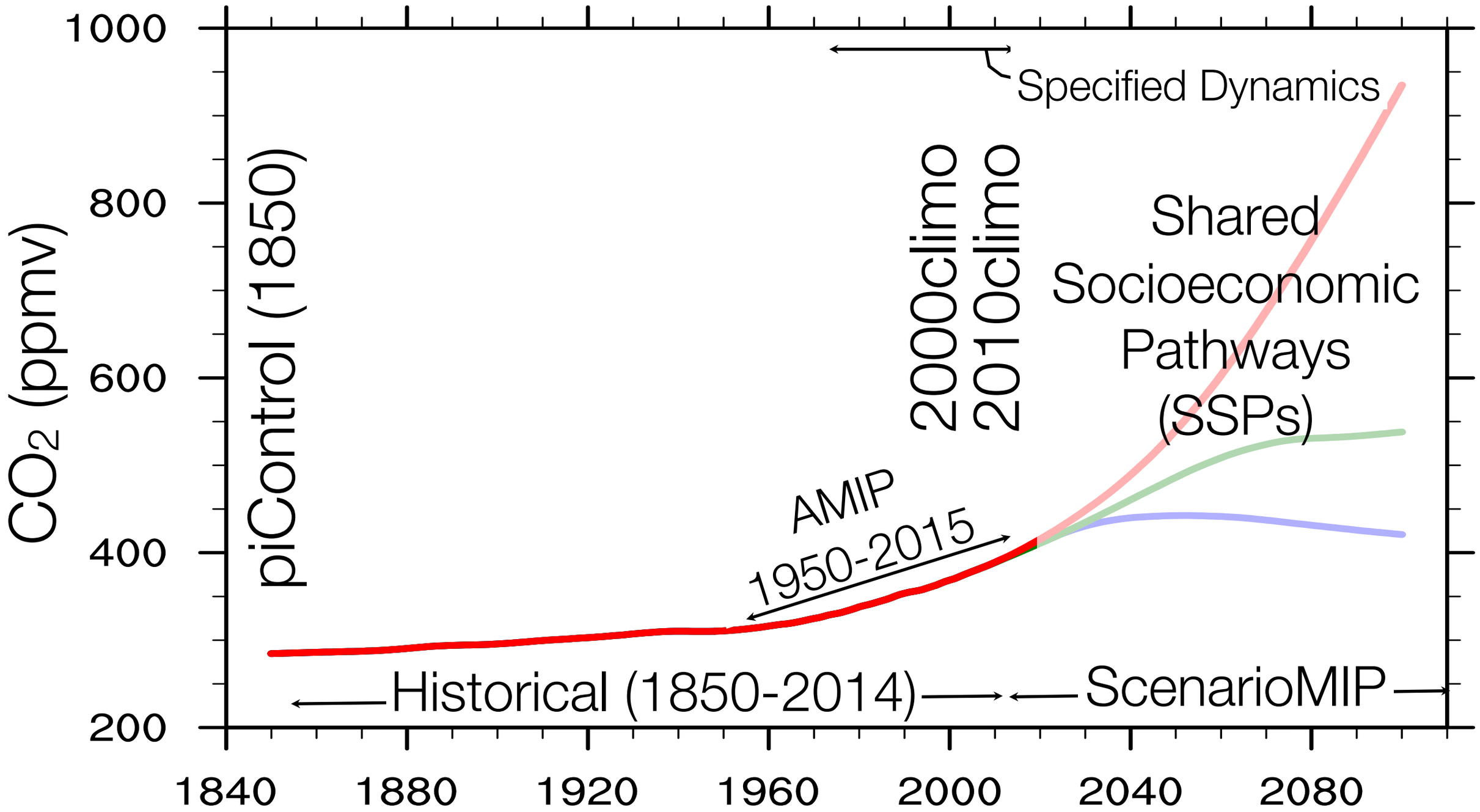
WACCM/CAMChem component configurations



CESM2.1 WACCM6/CAM6-Chem component configurations



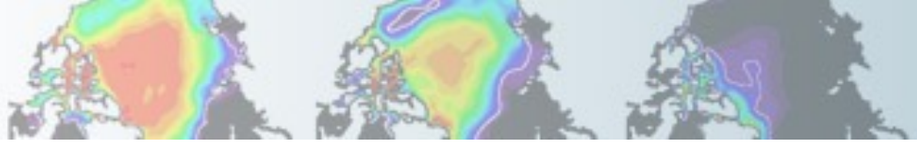
CAM6 User Guide: Chemical mechanisms

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)



CESM2.1 WACCM6 data ocean configurations

Compset	Supported resolutions	Description
FW1850	f09_f09_mg17, f19_f19_mg17	pre-industrial, TSMLT chemistry
FWsc1850	f09_f09_mg17, f19_f19_mg17	pre-industrial, specified chemistry
FW2000climo	f09_f09_mg17, f19_f19_mg17	1995-2005 average, TSMLT chemistry
FWsc2000climo	f09_f09_mg17, f19_f19_mg17	1995-2005 average, specified chemistry
FW2010climo	f09_f09_mg17, f19_f19_mg17	2006-2014 average, TSMLT chemistry
FWsc2010climo	f09_f09_mg17, f19_f19_mg17	2006-2014 average, specified chemistry
FWHIST	f09_f09_mg17, f19_f19_mg17	1850-2014, TSMLT chemistry
FWHIST_BGC	f09_f09_mg17, f19_f19_mg17	1850-2014, TSMLT chemistry, BGC in CLM
FWmaHIST_BGC	f09_f09_mg17, f19_f19_mg17	1850-2014, MA chemistry, BGC in CLM
FWmadHIST	f09_f09_mg17, f19_f19_mg17	1850-2014, MA + D-region chemistry
FWSD	f09_f09_mg17	MERRA2 nudging, TSMLT chemistry
FWmaSD	f09_f09_mg17	MERRA2 nudging, MA chemistry
FWmadSD	f09_f09_mg17	MERRA2 nudging, MA + D-region chemistry
FWscSD	f09_f09_mg17	MERRA2 nudging, specified chemistry

```
$SRCROOT/cime/scripts/query_config --compsets | grep %W
```

CESM2.1 WACCM6 coupled ocean configurations

Compset	Supported resolutions	CMIP6 experiment	Description
BW1850	f09_g17	*piControl*	TSMLT chemistry
BW1850cmip6	f09_g17	*piControl*	TSMLT chemistry, CMIP6 output
BWma1850	f19_g17, f09_g17	*piControl*	MA chemistry
BWsc1850	f09_g17	*piControl*	specified chemistry
BWCO2x4cmip6	f09_g17	*abrupt4xCO2*	TSMLT chemistry, CMIP6 output
BWmaCO2x4cmip6	f19_g17, f09_g17	*abrupt4xCO2*	MA chemistry, CMIP6 output
BW1PCTcmip6	f09_g17	*1pctCO2*	TSMLT chemistry, CMIP6 output
BWma1PCTcmip6	f19_g17	*1pctCO2*	MA chemistry, CMIP6 output
BWHIST	f09_g17	*historical*	TSMLT chemistry
BWHISTcmip6	f09_g17	*historical*	TSMLT chemistry, CMIP6 output
BWmaHIST	f19_g17, f09_g17	*historical*	MA chemistry
BWscHIST	f09_g17	*historical*	specified chemistry
BWSSP126	f09_g17	*SSP1-2.6*	TSMLT chemistry
BWSSP245	f09_g17	*SSP2-4.5*	TSMLT chemistry
BWSSP370	f09_g17	*SSP3-7.0*	TSMLT chemistry
BWSSP585	f09_g17	*SSP5-8.5*	TSMLT chemistry
BWSSP534os	f09_g17	*SSP5-3.4os*	TSMLT chemistry
BWSSP126cmip6	f09_g17	*SSP1-2.6*	TSMLT chemistry, CMIP6 output
BWSSP245cmip6	f09_g17	*SSP2-4.5*	TSMLT chemistry, CMIP6 output
BWSSP370cmip6	f09_g17	*SSP3-7.0*	TSMLT chemistry, CMIP6 output
BWSSP585cmip6	f09_g17	*SSP5-8.5*	TSMLT chemistry, CMIP6 output
BWSSP534oscmip6	f09_g17	*SSP5-3.4os*	TSMLT chemistry, CMIP6 output

```
$SRCROOT/cime/scripts/query_config --compsets | grep %W
```

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.

Planned WACCM-X update to CAM6 physics to come later (estimated end of 2019).

CAM6 User Guide: CAM-chem compsets

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

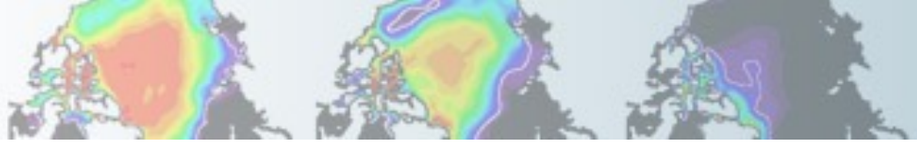
4.4. CAM-chem tested compsets

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 compset

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

WACCM: --compset FW2000climo --res f09_f09_mg17

CAM-chem: --compset FC2000climo --res f09_f09_mg17

WACCM-X: --compset FX2000 --res f19_f19_mg16

CASENAME: ~/f.e21.$compset.$res.tutorial.test1

i.e. for **CAM-chem:** f.e21.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

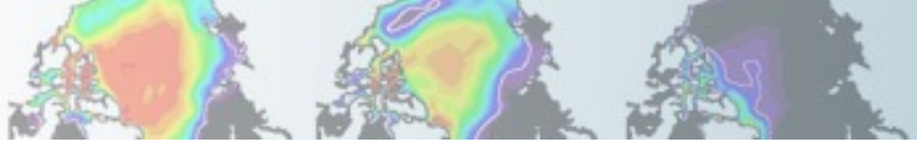
Exercise 1: Run a present-day WACCM/CAMChem compset

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.e21.$compset.$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 $SRCROOT/components/cam/src/chemistry/pp_* (i.e. pp_waccm_tsmlt_mam4)

```
 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
```

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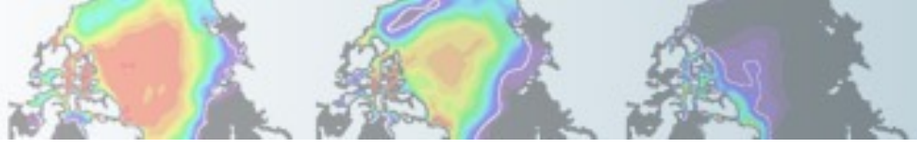


Reaction rate types in the chempp input file

- 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)

```
*********************************
*** odd-oxygen
*********************************
[ag1]                    O2_1D  -> O2                          ; 0.000258
[ag2]                    O2_1S  -> O2                          ; 0.085
[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_O2,cph=32.91]       O1D + O2  -> O + O2_1S                ; 2.64e-11, 55
[O1D_O2b,cph=189.81]     O1D + O2  -> O + O2                   ; 6.6e-12, 55
[O1D_O3]                 O1D + O3  -> O2 + O2                  ; 1.2e-10
[O2_1D_N2,cph=94.3]      O2_1D + N2  -> O2 + N2                ; 1e-20
[O2_1D_O,cph=94.3]       O2_1D + O  -> O2 + O                  ; 1.3e-16
[O2_1D_O2,cph=94.3]      O2_1D + O2  -> 2*O2                   ; 3.6e-18, -220
[O2_1S_CO2]              O2_1S + CO2  -> O2_1D + CO2           ; 4.2e-13
```

Change to 1.65e-12

- 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
```

- Use xmlchange to append a pointer to your user mechanism:

➢
```
"--usr_mech_infile `pwd`/my_chem_mech.in"
```

- When you query the updated CAM configure options, it should be appended:

➢
```
./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:

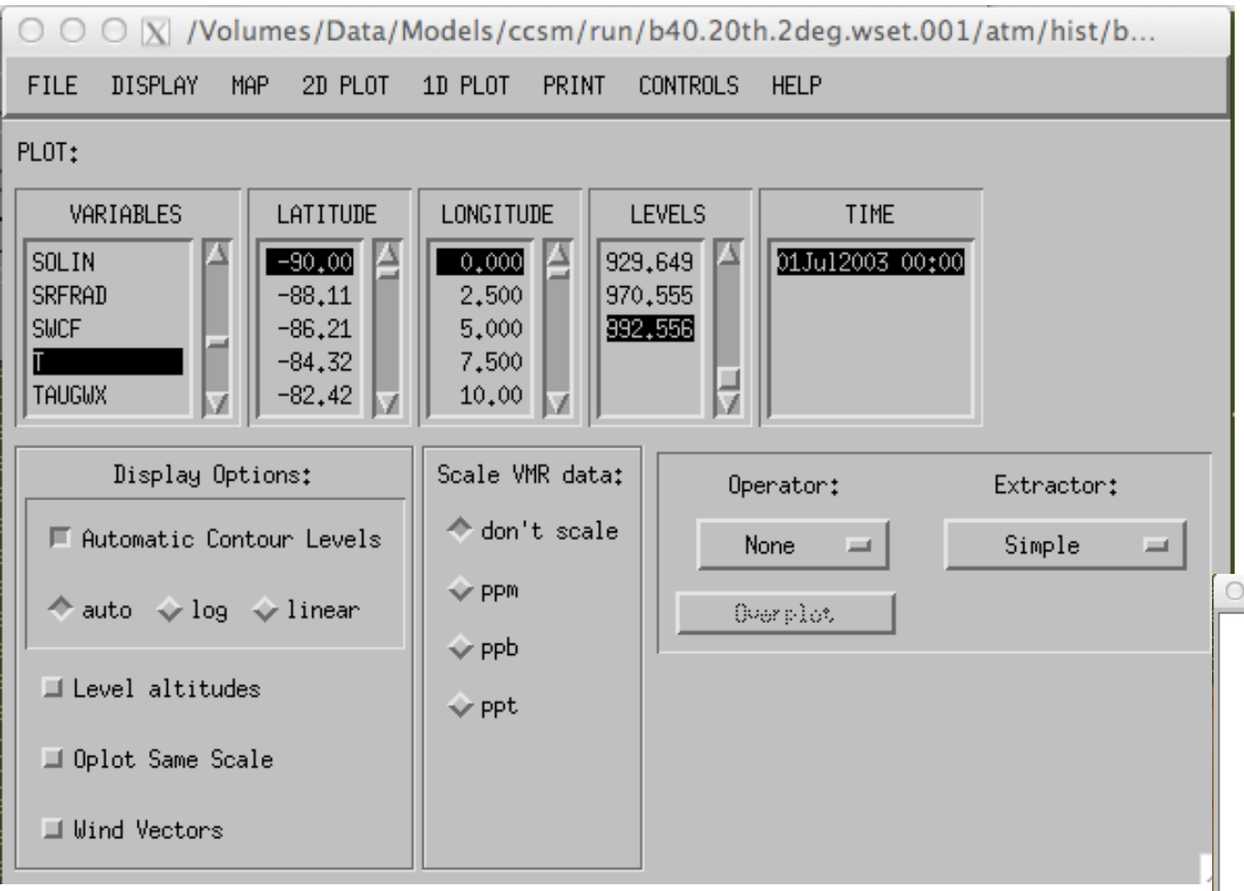
```
setenv IDL_STARTUP ~fvitt/idl_startup
```

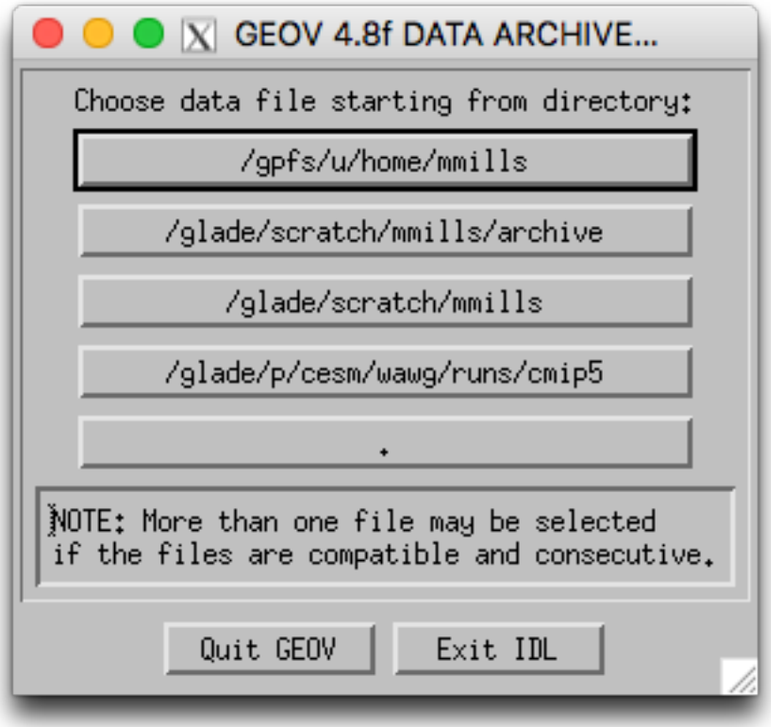
- ~fvitt/idl_startup sets the idl path to include GEOV:

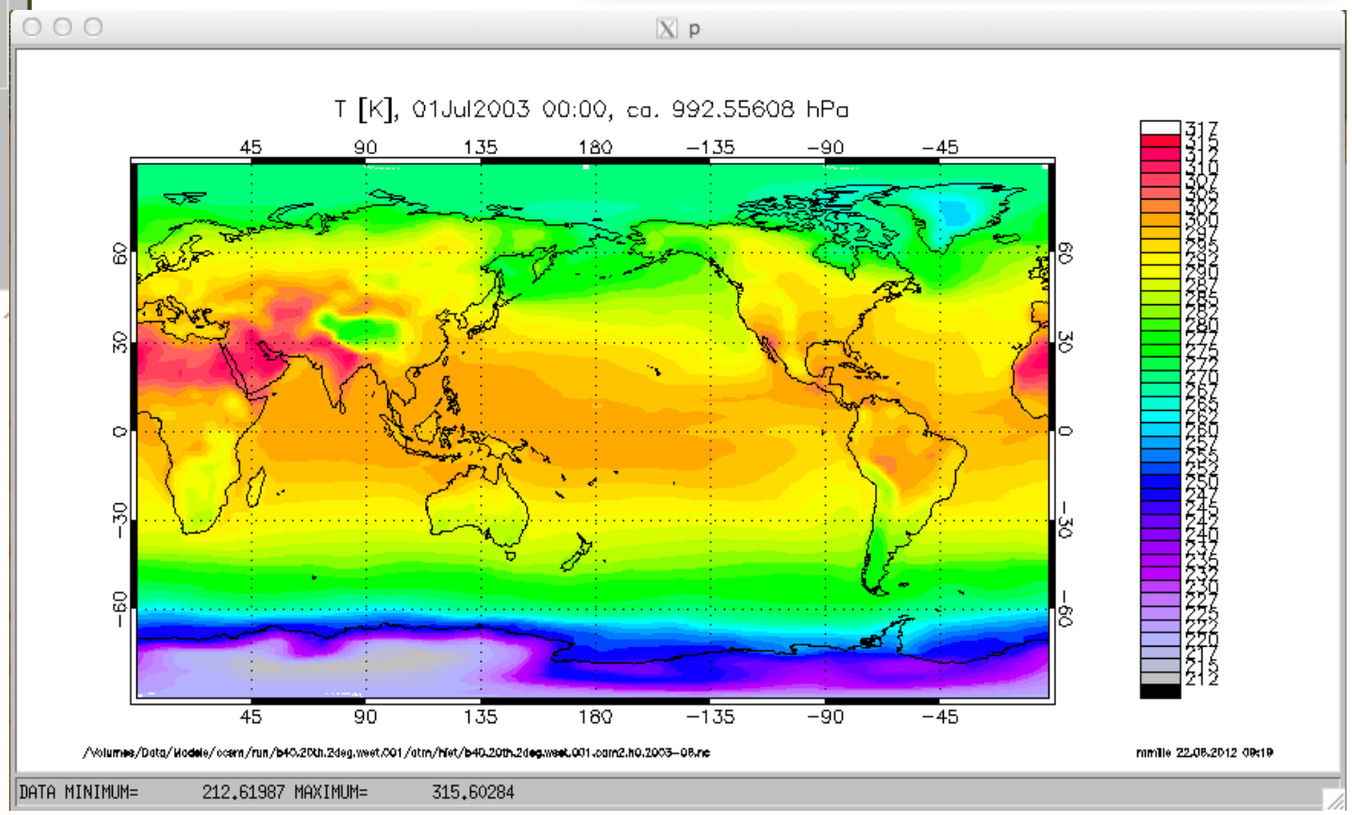
```
idl_path = expand_path('+~fvitt/geov')
!path=!path+':'+idl_path
```

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

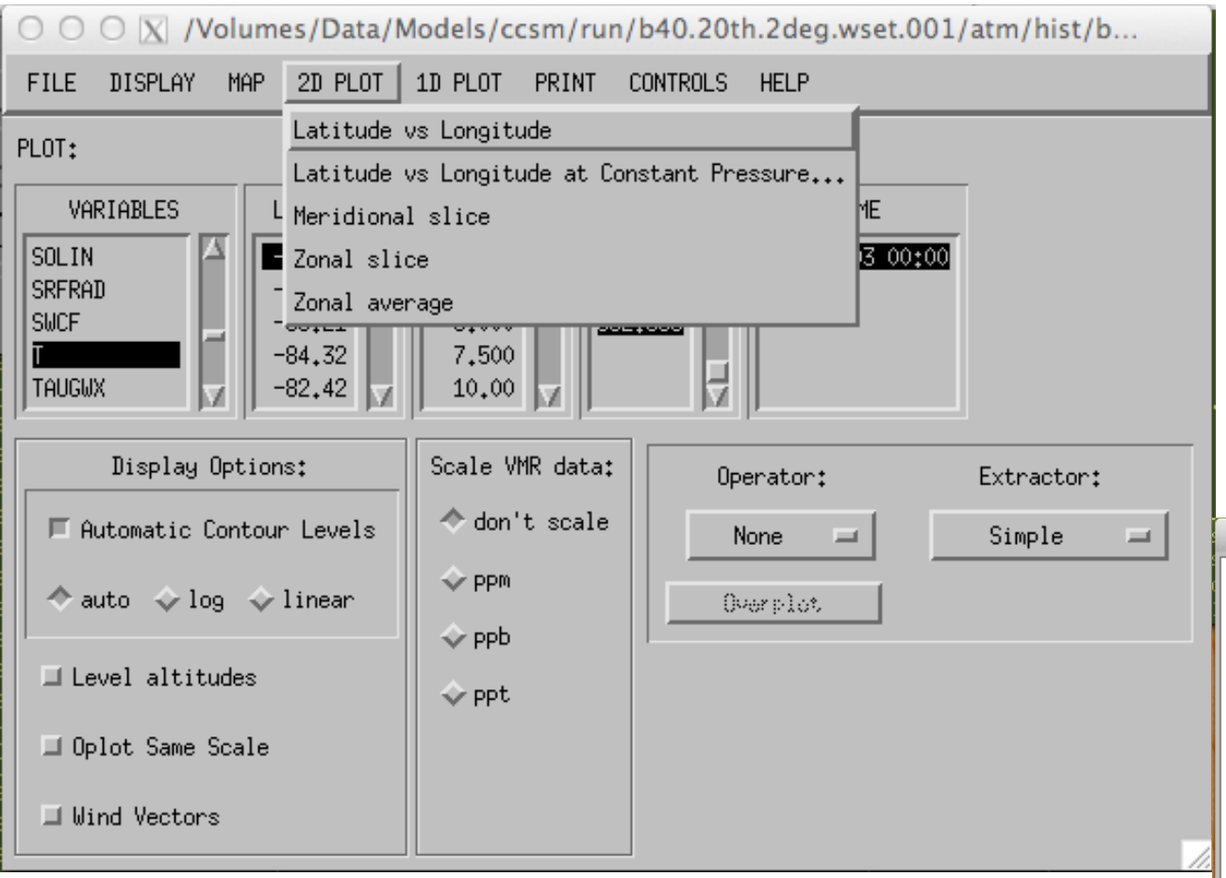
GEOV graphical user interface

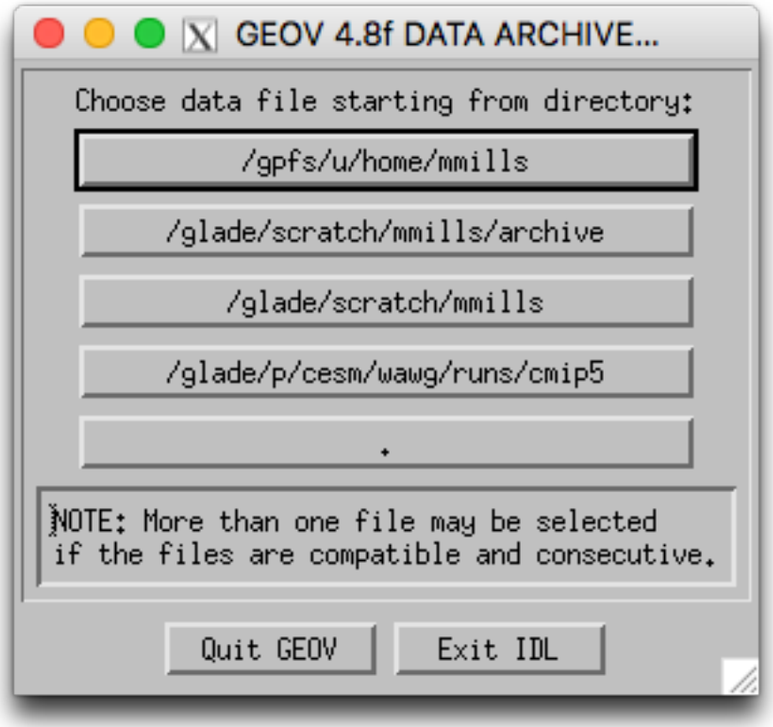


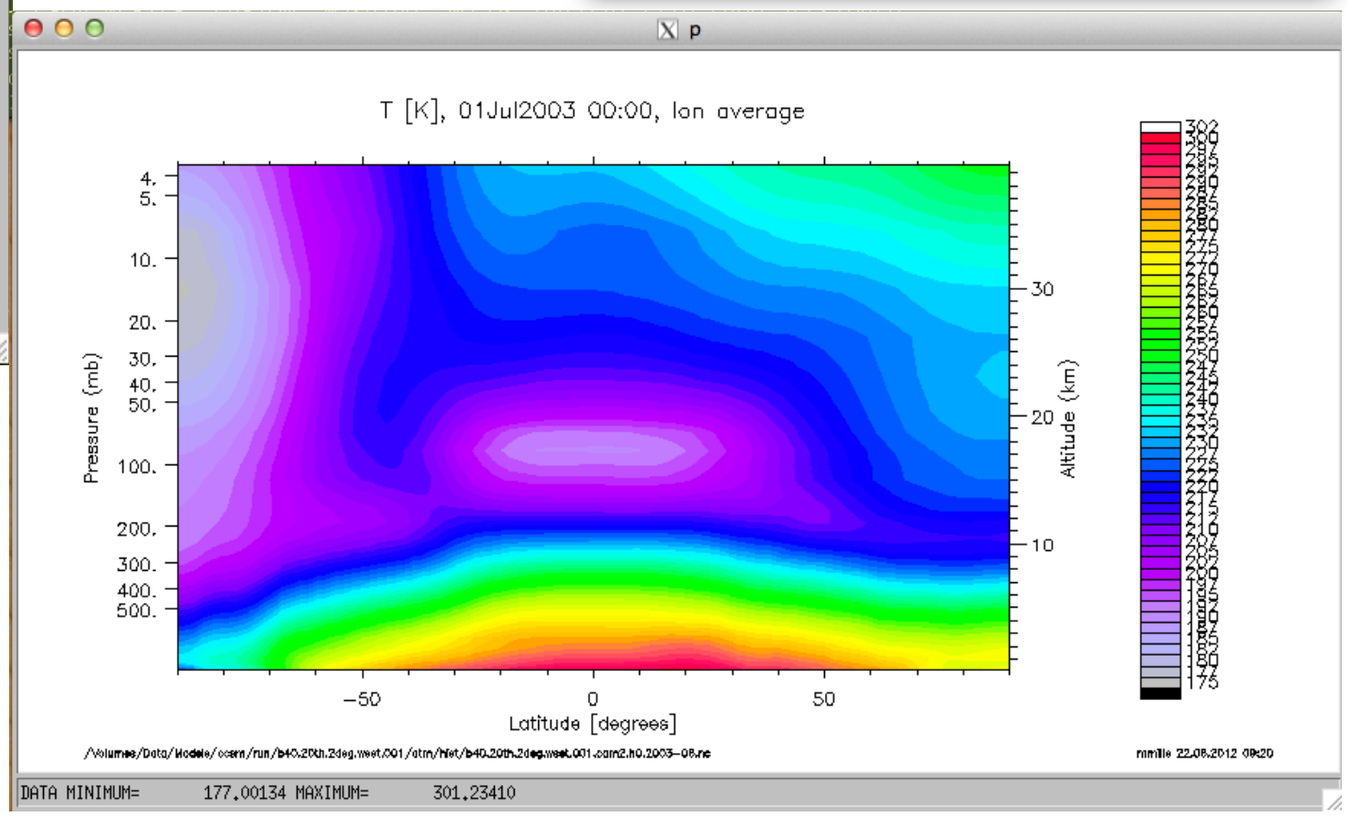




GEOV graphical user interface







WACCM and CAM-Chem Customer Support

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

Mike Mills
WACCM Liaison
mmills@ucar.edu
(303) 497-1425

Simone Tilmes
CAM-chem Liaison
tilmes@ucar.edu
(303) 497-1445

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

- Go to the script directory in your source code

```
> cd /glade/p/cesm/tutorial/cesm2.1_tutorial2022/cime/scripts
```

- Run create_newcase command for one of these compsets:

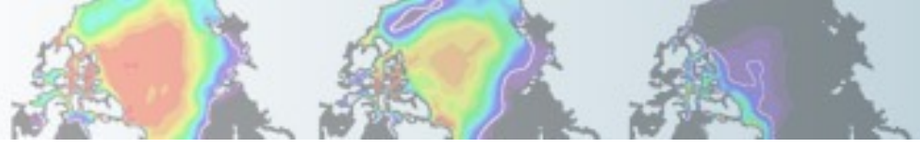
CAM-chem:
```
> ./create_newcase --compset FC2000climo --res f09_f09_mg17
  --case ~/f.e21.FC2000climo.f09_f09_mg17.tutorial.test1
```

WACCM:
```
> ./create_newcase --compset FW2000climo --res f09_f09_mg17
  --case ~/f.e21.FW2000climo.f09_f09_mg17.tutorial.test1
```

WACCM-X:
```
> ./create_newcase --compset FX2000 --res f19_f19_mg16
  --case ~/f.e21.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
f.e20.FC2000climo.f09_f09.tutorial.test1.cam.rh0.0001-01-06-00000.nc
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.e21.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/cesm2.1_tutorial2022/cime/scripts`

WACCM:

- `./create_newcase --compset FW2000climo --res f09_f09_mg17 --case ~/f.e21.FW2000climo.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"`
- Reset your case and re-rebuild your run:
  - `./case.setup --reset`
  - `./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