Community Earth System Model

CESM1.2.2 tutorial: WACCM and 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

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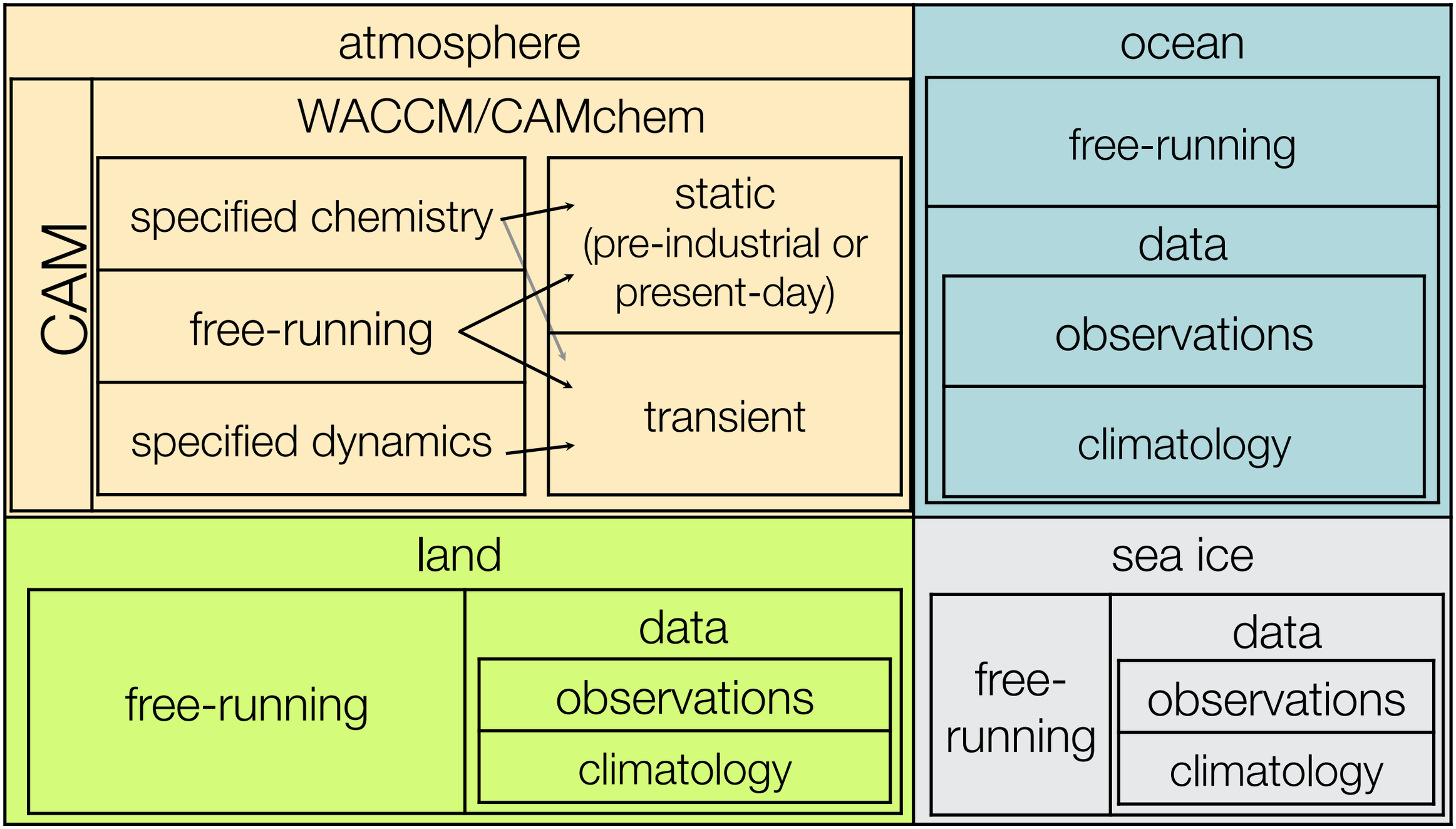
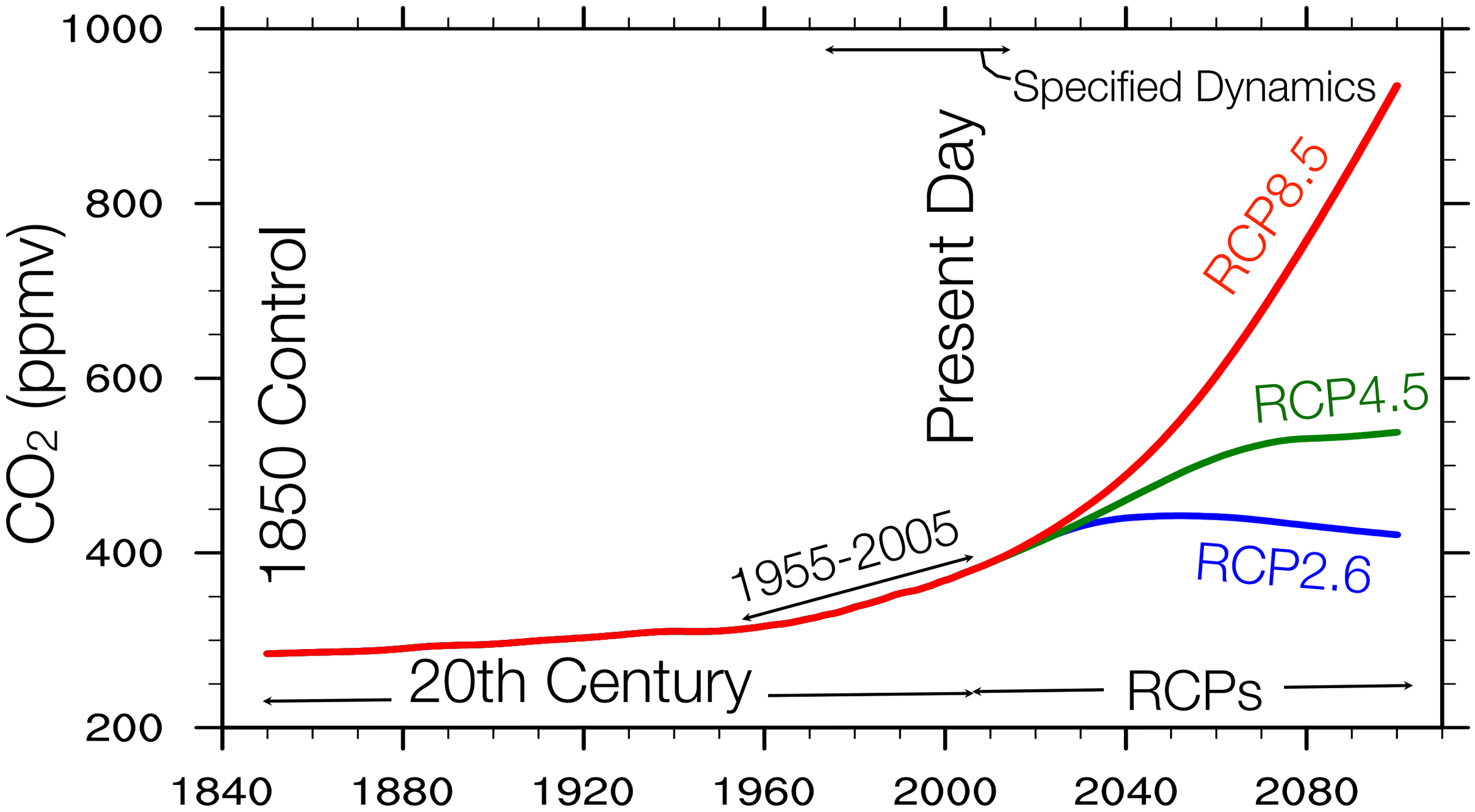
WACCM /CAMChem component configurations



WACCM /CAMChem component configurations



WACCM component configurations

Find scientifically validated compsets here:

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

CESM1.2.2 (WACCM) Compsets	Supported Grids	Components / Meteorology
Full ocean, static: B_1850_WACCM_CN (B1850WCN) B_2000_WACCM_CN (BWCN)	**f19_g16**	**CLM4.0/CN** pre-industrial ← Scientifically validated in CESM1.1.1 present day
Full ocean, transient: B_1850-2005_WACCM_CN (B20TRWCN) B_1955-2005_WACCM_CN (B55TRWCN) B_RCP2.6_WACCM_CN (BRCP26WCN) B_RCP4.5_WACCM_CN (BRCP45WCN) B_RCP8.5_WACCM_CN (BRCP85WCN)	**f19_g16**	**CLM4.0/CN** annual solar variability daily solar variability ← Scientifically validated in CESM1.1.1 daily solar variability daily solar variability daily solar variability
Data ocean, static: F_1850_WACCM (F1850W) F_2000_WACCM (FW) F_2000_WACCM_SC (FWSC) F_2000_WACCMX (FWX) F_1996_WACCMX (FWX1996)	**f19_f19, f45_f45**	**CLM4.0** pre-industrial present day specified chemistry thermosphere extension, solar max thermosphere extension, solar min
Data ocean, transient: F_1955-2005_WACCM_CN (F55WCN) FGEOS_C4WCM_L40CN (FSDW)	**f19_f19, f45_f45**	**CLM4.0/CN, daily solar variability** GEOS5 nudging

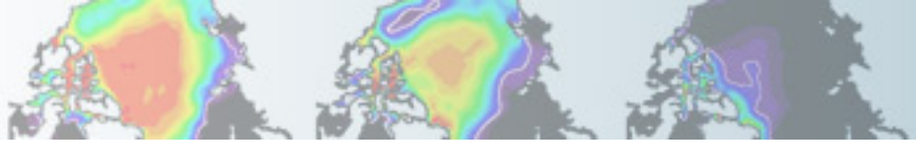
CAMChem component configurations

Find scientifically validated compsets here:

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

Compsets CESM1.2.2. for res: 1.9x2.5	Model (phys)/ radiation	Chemistry	Components / Meteorology
B_2000_TROP_MOZART (BMOZ)	CAM4, active	trop_mozart	All active
B_2000_MOZSOA_CN	f19_g16	+soa chemistry	+ CLM/CN
B_2000_MOZMAM_CN (BMOZMAM)		trop_mozart mam	All active, CLM/CN
F_2000_MOZMAM_CN (FMOZMAM)	CAM4 passive **f19_f19**	trop_mozart	Prescr. ocn/ice, CLM/CN
F_SD_BAM_CN		trop_bam	
B_2000_CN_CHEM (B2000CNCHM)	CAM4, active	super_fast_llnl	MEGAN VOC emis, all active CLM/CN
B_1850_CN_CHEM (B1850CNCHM)			
B_1850-2000_CN_CHEM (B20TRCNCHM)			
F_1850_CN_CHEM (F1850CNCHM)	CAM4, passive		Prescr. ocn/ice, CLM/CN
Data ocean, static/transient:			
F2000_C4SSOA_L40 (FSSOA)	**CAM4, passive f19_f19**	**trop_strat +soa chemistry**	**Prescr. ocn/ice, MEGAN GEOS5 met.**
FGEOS_C4SSOA_L40 (FSDSSOA)			
F2000_STRATMAM3_CN	**CAM5, passive**	**trop_strat mam+soa chemistry**	**Prescr. ocn/ice, CLM/ CN, GEOS5 met.**
FGEOS_STRATMAM3_CN			
F_2000_STRATMAM7_CN	CAM5 passive	trop_strat mam7+soa chemistry	Prescr. ocn/ice, CLM/CN

Scientifically validated in CESM1.2.2



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 compsets:

COMPSET: longname (shortname):

WACCM: F_2000_WACCM (FW)

or

CAM-chem: F_2000_TROP_MOZART (FSSOA)

RESOLUTIONS: name (shortname):

1.9x2.5_1.9x2.5 (f19_f19)

CASENAME: ~/f2000.FW.f19_f19.001 or ~/f2000.FSSOA.f19_f19.001

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

- 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                drv_flds_in      ice_modelio.nml  README           wav_modelio.nml
atm_modelio.nml   docn_in                        drv_in           lnd_in           rof_in
chem_mech.doc     docn_ocn_in                    glc_modelio.nml  lnd_modelio.nml  rof_modelio.nml
chem_mech.in      docn.streams.txt.prescribed    ice_in           ocn_modelio.nml  seq_maps.rc
```

- 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, rename the case to ~/f2000.FW.f19_f19.test1 or ~/f2000.FSSOA.f19_f19.test1
- Look at your chemistry preprocessor file chem_mech.in in CaseDocs and copy it to your case directory

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)

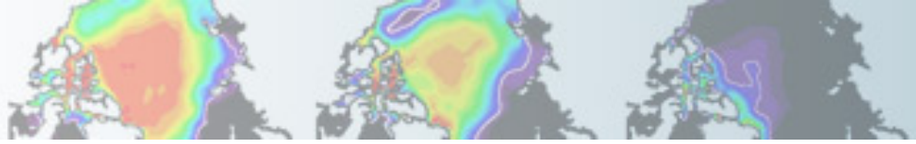
```
 SPECIES
     Solution
O3, O, O1D -> O, O2, O2_1S -> O2, O2_1D -> O2
     End Solution

     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 CAM-chem:

•Change reaction rates (bug in earlier version)

```
      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)

•Check your new mechanism file:

>less CaseDocs/chem_mech.in

•Edit env_build.xml

Exercise 2:
Building the model with new chemistry

For WACCM:

•Change reaction rates (bug in earlier version)

Remove this line (bug in CAMchem)

```
* ------------------------------------------------------
* Odd-Oxygen Reactions (O1D only)
* ------------------------------------------------------
 [cph_O1D_N2,cph] O1D + N2 -> O + N2                    ; 2.15e-11,   110.
 [cph_O1D_O2,cph] O1D + O2 -> O + O2_1S                 ; 3.135e-11,   55.
 [cph_O1D_O2b,cph] O1D + O2 -> O + O2                   ; 1.65e-12,    55.
 O1D + H2O -> 2*OH                                      ; 1.63e-10,    60.
 O1D + N2O -> 2*NO                                      ; 6.70e-11,    20.
 O1D + N2O -> N2 + O2                                   ; 4.70e-11,    20.
```

•Check your new mechanism file:

>less CaseDocs/chem_mech.in

•Edit env_build.xml

Exercise 2:
Building the model with new chemistry

- Edit the file env_build.xml in the case directory to add the CAM configure option - usr_mech_infile pointing to the new preprocessor input file:

```
<!--"CAM configure options, see CAM configure utility for details (char) " -->
<entry id="CAM_CONFIG_OPTS"
 value="-phys cam4 -chem trop_strat_soa –age_of_air_trcs
–usr_mech_infile $CASEROOT/my_chem_mech.in"  />
```

- Re-setup and rebuild your run:
- Check your new mechanism file
- submit the 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/WACCM/

Or install geov on yellowstone:

•Logon to yellowstone (or caldara or geyser):

> ssh -X yellowstone.ucar.edu

•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
>idl geov
```

•View model output on yellowstone:

```
> cd /glade/scratch/$USER/archive/run
> idl geov
```

Post-processing data analysis

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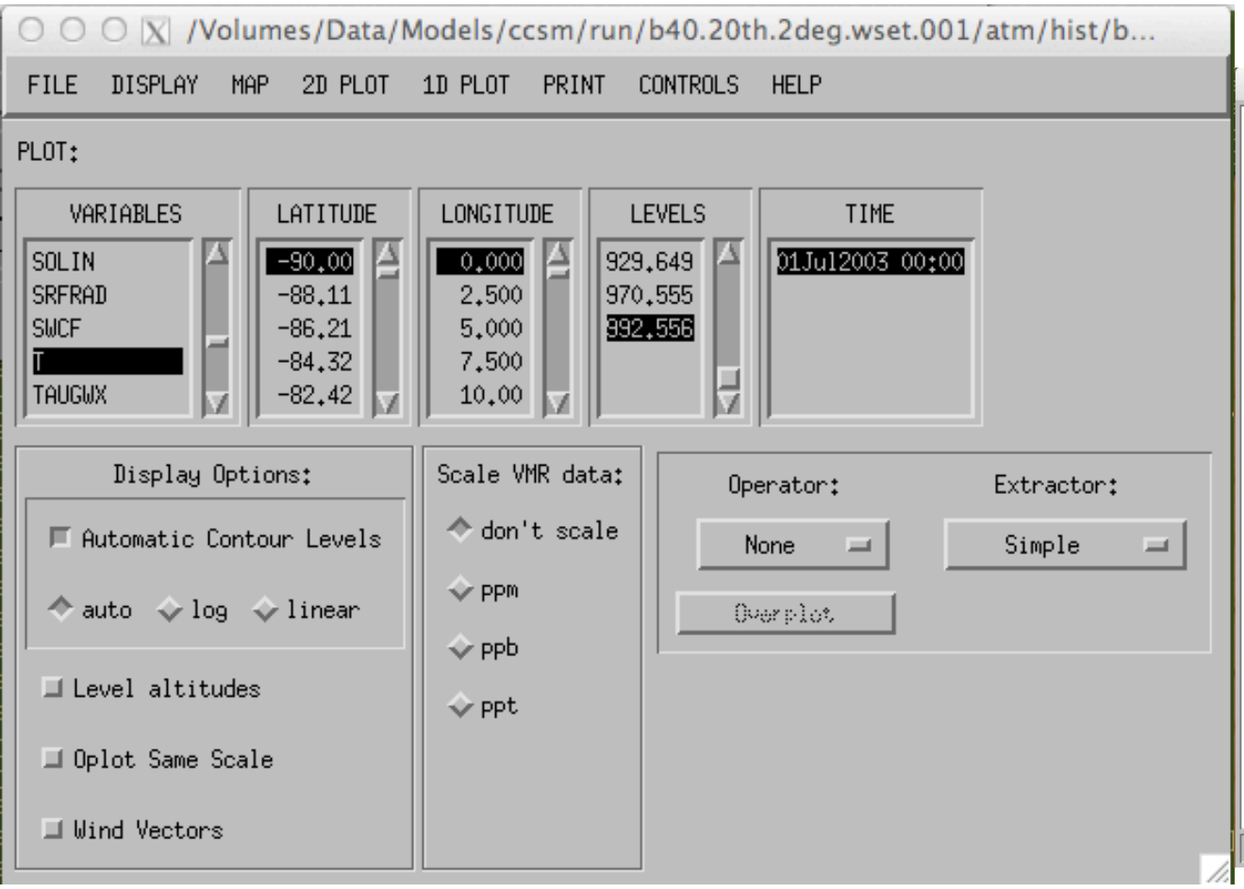

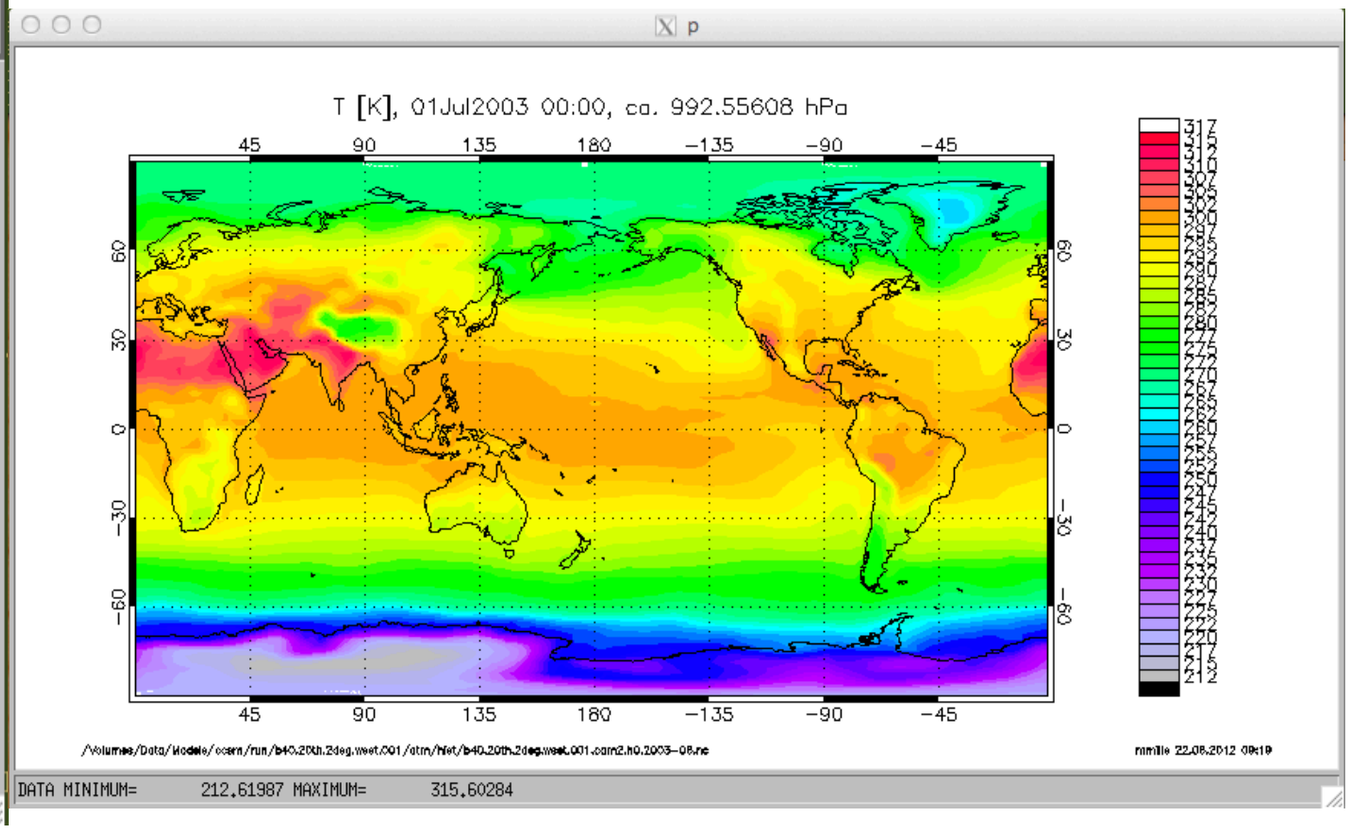

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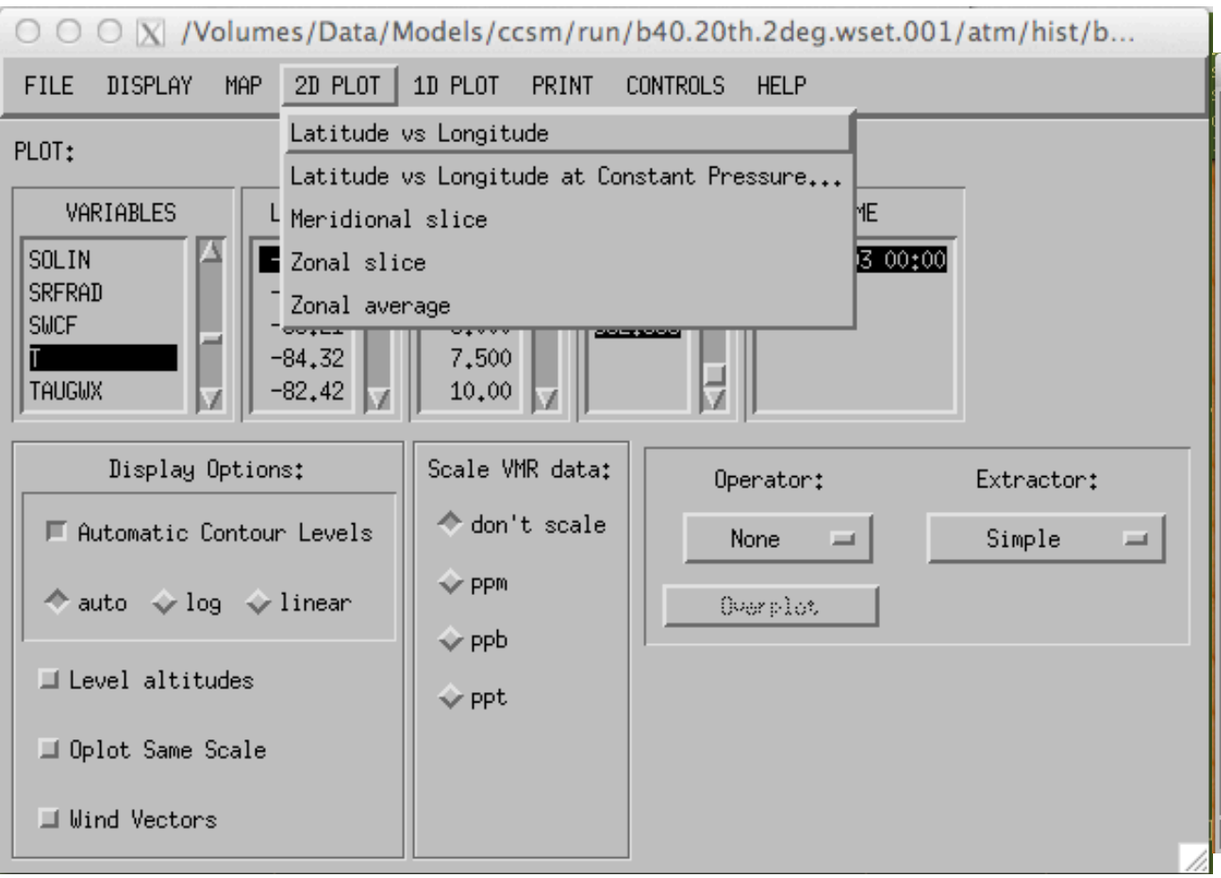
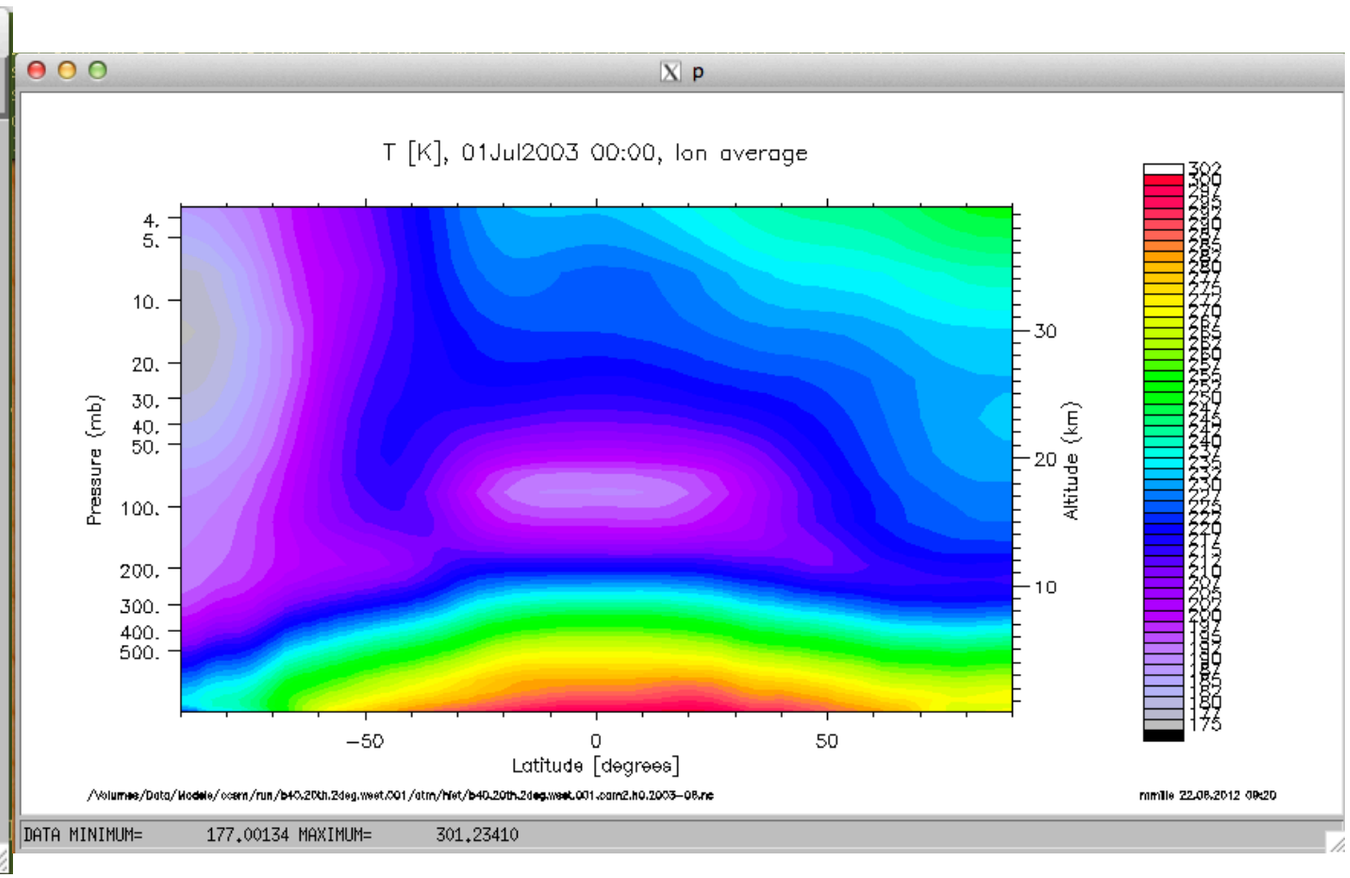
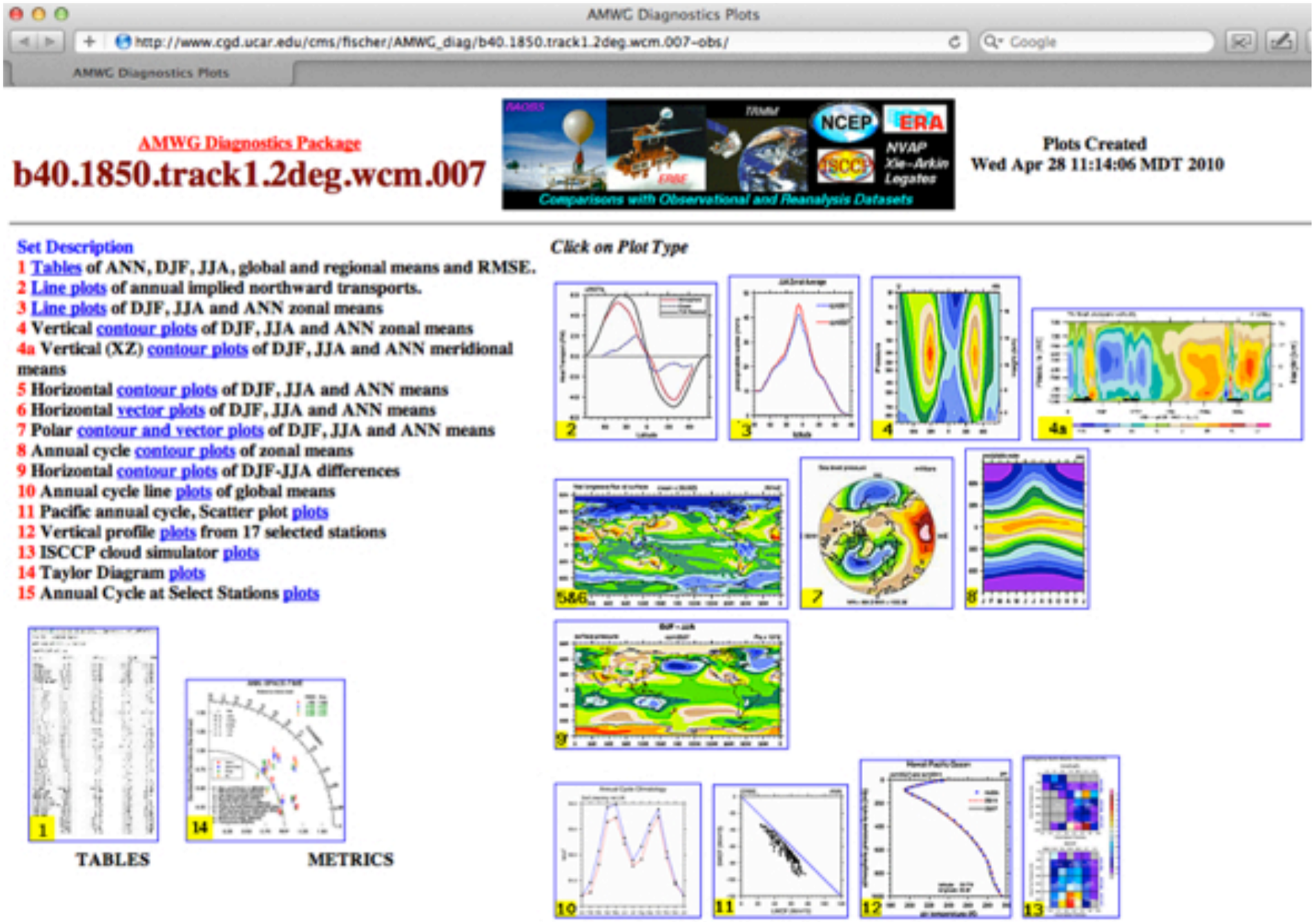




Post-processing data analysis

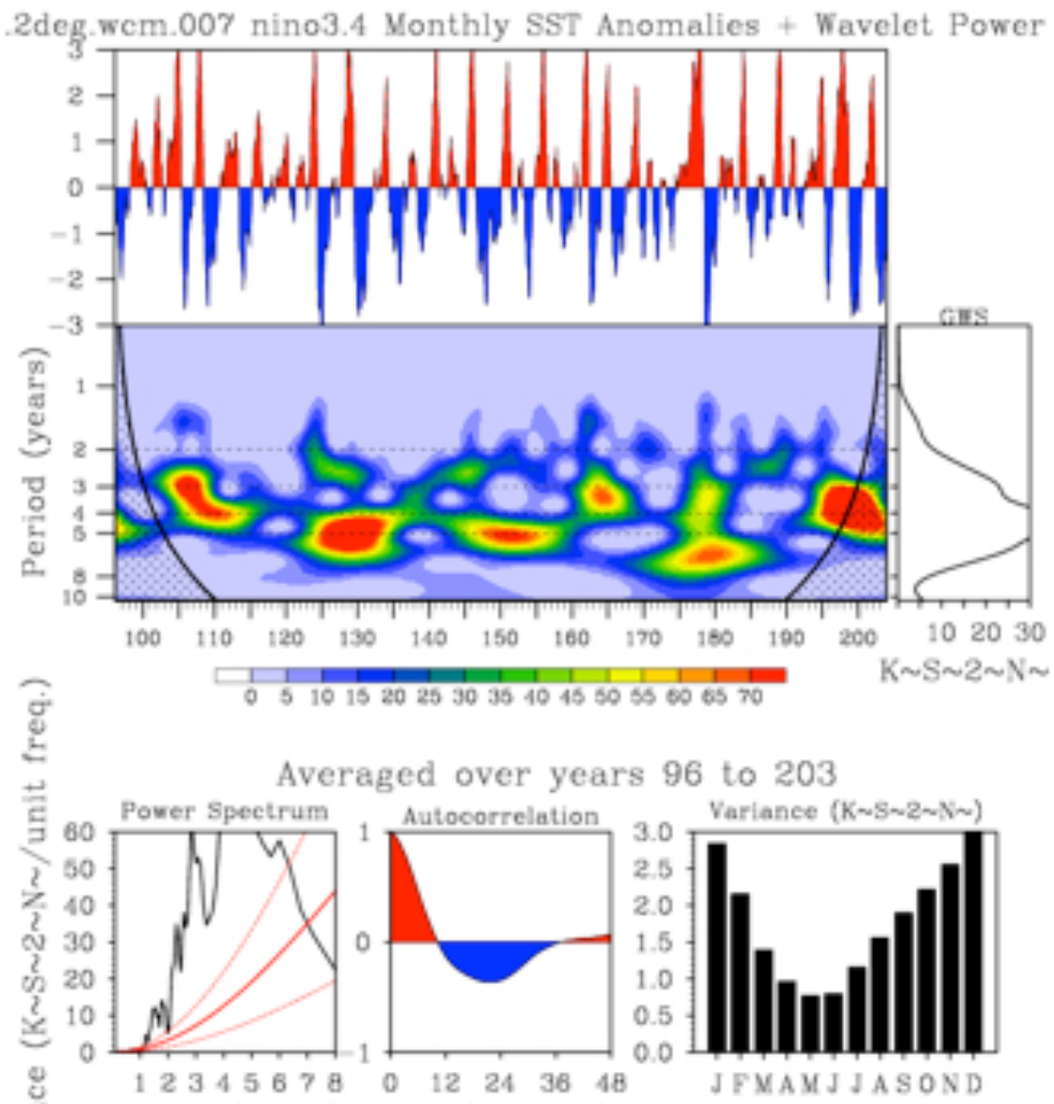
CAM diagnostic packages are described under CAM Post-Processing Utilities on the [CAM documentation page](http://www.cgd.ucar.edu/amp/amwg/diagnostics/) at http://www.cgd.ucar.edu/amp/amwg/diagnostics/.



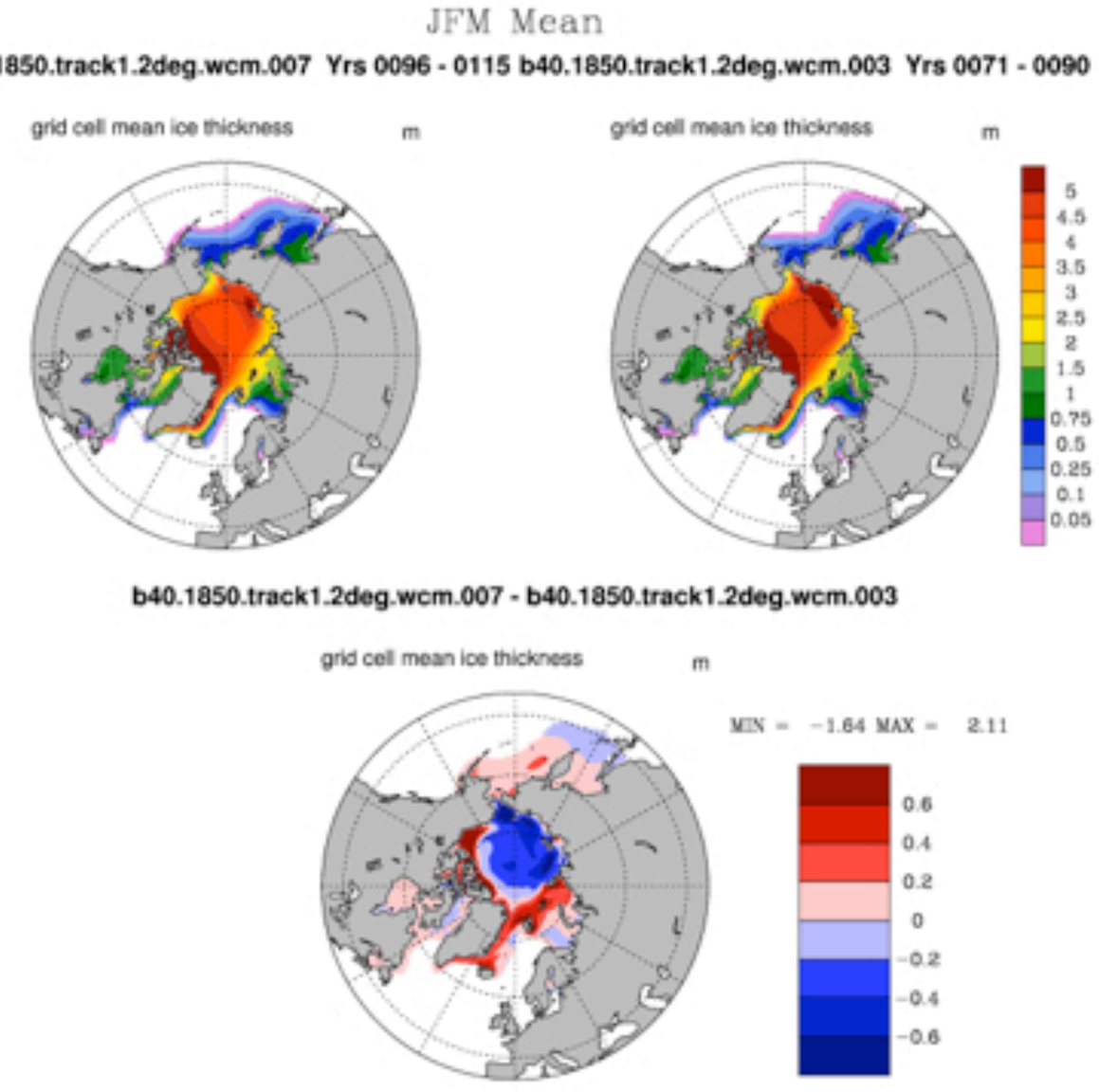
Post-processing data analysis

Diagnostic packages for all model components (atmosphere, land, ice, and ocean) can be found from the component post-processing utilities page (http://www.cesm.ucar.edu/models/cesm1.2/model_diagnostics/).

Ocean ENSO



Sea Ice Thickness



Validating CESM/WACCM

Users may validate their implementation of CESM/WACCM by repeating experiments we have done at NCAR, and using the component post-processing utilities to compare the climate generated to output we have made available publicly on the Earth System Grid (http://www.earthsystemgrid.org).

Please visit our CESM 1.0 experiments and diagnostics page (http://www.cesm.ucar.edu/experiments/cesm1.0/) for an updated list of experiments with links to output data locations.

Output from additional experiments will be made available on a timeline in

CESM1 (WACCM) 2° Pre-Industrial Control **Case Name**: b40.1850.track1.2deg.wcm.007 **Data Availability**: ESG (years 156-185)	156-185 w/observations	Atm	Ice	Land	Ocean	CCR	Ocean Timeseries
CESM1 (WACCM-X) 2° Present Day Control **Case Name**: f.e10.FWX.f19_f19.control.001 **Data Availability**: CESM	2001 w/observations	Atm	Ice	Land	---	---	---

Case Name: b40.1850.track1.2deg.wcm.007
Machine: NCAR:bluefire
CMIP5 ID: ----
Compset: B_1850_WACCM_CN
Resolution: 1.9x2.5_gx1v6
Years: 96-295
Time Frequencies Saved: Monthly, Daily, Subdaily
Initialization: year 156
Start/End Dates: 4/16/10, at year 260 as of 3/1/11
Data Release Date (Full): 11/1/11

Case Name: f.e10.FWX.f19_f19.control.001
Machine: NCAR:bluefire
CMIP5 ID: ----
Compset: F_2000_WACCMX (publicly available 2/21/12)
Resolution: 1.9x2.5_1.9x2.5
Years: 1/2001-2/2002
Time Frequencies Saved: Monthly, Daily, Subdaily
Initialization: startup run type
Start/End Dates: 2/8/12, ongoing
Data Release Date (Full): 2/17/12

WACCM and CAM-Chem Customer Support

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

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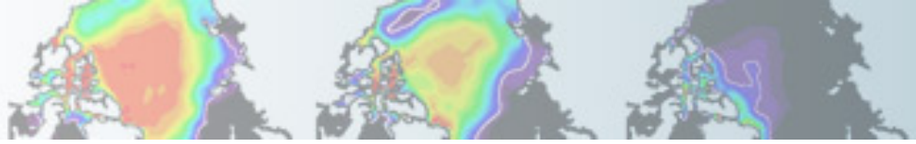

Solution 1:
Run a present-day WACCM/CAMChem compset

- Go to the script directory in your source code

> cd /glade/p/cesm/tutorial/cesm1_2_2.tutorial/scripts

- Run create_newcase command for one of these compsets:

>create_newcase –res f19_f19 –case ~/f2000.FW.f19_f19.001 –compset FW –mach yellowstone

or

>create_newcase –res f19_f19 –case ~/f2000.FSSOA.f19_f19.001 –compset FSSOA –mach yellowstone

- Go to your case directory and setup the run
- Setup the model

>cesm_setup

- Build the model

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

>*build

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

```
! Users should add all user specific namelist changes below in the form of
! namelist_var = new_namelist_value
&cam_inparm
 avgflag_pertape                 = 'A', 'I',
 fincl2          = 'PS', 'Z3', 'T', 'U', 'V','O3'
 mfilt           =  1,    10
 nhtfrq          =  0, -24
/
```

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

  >preview_namelists

- Check your CaseDocs/atm_in

  >less CaseDocs/atm_in (check your atm_in file)

- Resubmit your job

  >*.submit (run the model for 5 days)

Solution 1: Check your model output

- find your model output in your run dir ($run_dir) after finished:
  >ls /glade/scratch/<username>/<casename>/run

```
[tilmes@yslogin1 run]$ ls
atm_in                                                  f2000.FSSOA.f19_f19.001.rtm.rh0.0001-01-06-00000.nc
atm_modelio.nml                                         glc_modelio.nml
cpl_modelio.nml                                         ice_in
docn_in                                                 ice_modelio.nml
docn_ocn_in                                             lnd_in
docn.streams.txt.prescribed                             lnd_modelio.nml
drv_flds_in                                             ocn_modelio.nml
drv_in                                                  rof_in
f2000.FSSOA.f19_f19.001.cam.h1.0001-01-06-00000.nc      rof_modelio.nml
f2000.FSSOA.f19_f19.001.cam.r.0001-01-06-00000.nc       rpointer.atm
f2000.FSSOA.f19_f19.001.cam.rh0.0001-01-06-00000.nc     rpointer.drv
f2000.FSSOA.f19_f19.001.cam.rs.0001-01-06-00000.nc      rpointer.ice
f2000.FSSOA.f19_f19.001.cice.r.0001-01-06-00000.nc      rpointer.lnd
f2000.FSSOA.f19_f19.001.clm2.r.0001-01-06-00000.nc      rpointer.ocn
f2000.FSSOA.f19_f19.001.clm2.rh0.0001-01-06-00000.nc    rpointer.rof
f2000.FSSOA.f19_f19.001.cpl.r.0001-01-06-00000.nc       seq_maps.rc
f2000.FSSOA.f19_f19.001.docn.rs1.0001-01-06-00000.bin   timing
f2000.FSSOA.f19_f19.001.rtm.r.0001-01-06-00000.nc       wav_modelio.nml
```

namelist information

restart information

- find our 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)
- long-time archive your job if needed (do not archive what you don't need for a long time)
- check your cam.h1 file

> ncdump –h f2000.FSSOA.f19_f19.001.cam.h1.0001-01-06-00000.nc

Solution 2:
Building the model with new chemistry

- Setup a new case as done in Exercise 1, rename the case to
~/f2000.FW.f19_f19.test1 or ~/f2000.FSSOA.f19_f19.001
(follow Solution 1, just rename your case)

- Look at your chemistry preprocessor file chem_mech.in in CaseDocs and copy it to your case directory and rename to my_chem_mech.in
- Copy a sample preprocessor input file to the case directory and edit it:
>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

- Edit the file env_build.xml in the case directory to add the CAM configure option - usr_mech_infile pointing to the new preprocessor input file:

```
<!--"CAM configure options, see CAM configure utility for details (char) " -->
<entry id="CAM_CONFIG_OPTS"
 value="-phys cam4 -chem trop_strat_soa –age_of_air_trcs
–usr_mech_infile $CASEROOT/my_chem_mech.in"  />
```

```
<!--"CAM configure options, see CAM configure utility for details (char) " -->
<entry id="CAM_CONFIG_OPTS"   value="-phys cam4 -chem trop_strat_soa -age_of_air_trcs -usr_mech_infile
/glade/u/home/tilmes/f2000.FSSOA.f19_f19.001/my_chem_mech.in"  />
```

- Re-setup and rebuild your run:
  - >cesm_setup –clean
  - >cesm_setup
  - >*.clean_build
  - >*. build
- Check your new mechanism file:
  - >less CaseDocs/chem_mech.in
- submit the new run
  - >*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