CESM1.0.3 tutorial: WACCM and CAM-Chem

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- Transient and static configurations
- WACCM compsets
  - WACCM driven by specified dynamics (SD-WACCM)
  - WACCM with specified chemistry (SC-WACCM)
- CAM-Chem compsets
- Exercise: Change a reaction rate
  - create a case, configure, build and run
- Satellite and aircraft tracking
- Local time history averaging
Transient and static WACCM & CAM-Chem configurations

Specify Dynamics

1850 Control

20th Century

1955-2005

Present Day

RCP8.5

RCP4.5

RCP2.6

RCPs

NCAR

WACCM

Whole Atmosphere Community Climate Model
WACCM full ocean/ice model (B-) compsets

- B_1850_WACCM_CN (B1850WCN): Pre-industrial with carbon-nitrogen cycle in CLM, constant solar, no quasi-biennial oscillation (QBO).
- B_1850-2005_WACCM_CN (B20TRWCN): 20th Century (1850-2005 transient) with carbon-nitrogen cycle in CLM, annually varying solar, prescribed QBO.
- B_1955-2005_WACCM_CN (B55TRWCN): 1955 to 2005 transient, with daily varying solar data, solar proton events (SPEs), prescribed QBO.
- RCP future scenarios: 2005-2100 transient, with daily varying solar data, SPEs, prescribed QBO.
  - B_RCP2.6_WACCM_CN (BRCP26WCN)
  - B_RCP4.5_WACCM_CN (BRCP45WCN)
  - B_RCP8.5_WACCM_CN (BRCP85WCN)
- Resolution: Run B-compsets at 1.9x2.5_gx1v6 (f19_g16).
WACCM prescribed sea ice, data ocean (F-) compsets

- **F_1850_WACCM (F1850W)**: Pre-industrial (perpetual year 1850AD)
- **F_2000_WACCM (FW)**: Present-day (perpetual year 2000AD).
- **F_1955-2005_WACCM_CN (F55WCN)**: 1955 to 2005 transient, with daily solar data and SPEs.
- **F_2000_WACCM_SC (FWSC)**: Specified chemistry, perpetual year 2000
- **F_SD_WACCM (FSDW)**: Specified dynamics
- **Resolution**: Run F-compsets at 1.9x2.5_ 1.9x2.5 (f19_f19).
Specified Chemistry: SC-WACCM

- Significantly faster throughput for dynamical studies.
- Run WACCM using limited chemistry, specified from zonally averaged output of a previous WACCM run: CO$_2$, H, NO, O, O$_2$, O$_3$, QRS_TOT (merged SW heating)
- Namelist variables:
  
  ghg_chem = 'true'
  cam_chempkg = 'waccm_ghg'
  waccm_forcing_datapath = '/path/do/forcing/file'
  waccm_forcing_file = 'ghg_forcing_2000_c110321.nc'

- **F_2000_WACCM_SC** compset repeats year 2000 out of the box. May be modified for transient runs.
- Runs ~2.5 times faster than WACCM with full middle atmosphere chemistry
Specified Dynamics: SD-WACCM

- Reproduce winds and temperatures from specific periods in analyses.
- GEOS5.1 resolution: 0.5°x0.66°, 72 levels (≤80km)
- SD-WACCM resolution: 1.9°x2.5°, 88 levels (≤140km)
- Nudge T, U, V, PS by 1% at every dynamics timestep below ~50 km, fully interactive dynamics aloft.
- Chemistry: standard waccm_mozart middle atmosphere mechanism (57 species, 230 photochemical reactions)
- Ongoing developments for future release:
  - MERRA meteorological fields to cover 1979-2010.
  - MOZART4 troposphere mechanism (122 species, 380 reactions)
CAM-Chem compsets

- **B_2000_TROP_MOZART (BMOZ)**: CAM4 with trop_mozart (103 species) chemistry, full ocean, present day (perpetual year 2000AD)
- **F_2000_TROP_MOZART (FMOZ)**: CAM4 with trop_mozart, data ocean, present day (perpetual year 2000AD)
- **F_SD_CAMCHEM (FSDCHM)**: CAM4 with specified dynamics, trop_mozart, data ocean
- **F_TROP_STRAT_CHEM (FTSC)**: CAM4 with strat_mozart (trop_mozart + about 20 more species and reactions in the stratosphere), data ocean, present day
- **B_2000_CN_CHEM (B2000CNCHM)**: CAM4 with super_fast_llnl chemistry, full ocean, present day
- **B_1850_CN_CHEM (B1850CNCHM)**: CAM4 with super_fast_llnl, full ocean, pre-industrial
- **F_1850_CN_CHEM (F1850CNCHM)**: CAM4 with super_fast_llnl, data ocean, pre-industrial
- **B_1850-2000_CN_CHEM (B20TRCNCHM)**: CAM4 with super_fast_llnl, full ocean, transient 1850-2000
Setting up a simulation

Run the model out of the box (using an existing compset)

- Create a new case called “f1955-2005.2deg.wcm.001”:
  - CESM_ROOT = (/glade/proj3/cseg/collections/cesm1_0_3)
    Go to your model directory CESM_ROOT, then cd scripts and invoke:
    ‣ create_newcase -case ~/f1955-2005.2deg.wcm.001
      -res f19_f19
      -compset F55WCN
      -mach bluefire

A new directory called “f1955-2005.2deg.wcm.001” is created in your home directory

- cd ~/f1955-2005.2deg.wcm.001

- ls

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Changing a reaction rate

- The **chemistry preprocessor**: generates CAM Fortran source code to solve chemistry.
- Input: a simple ASCII file listing chemical reactions and rates.
- The waccm_mozart input file is in `$CCSMROOT/models/atm/cam/src/chemistry/pp_waccm_mozart/chem_mech.in`

### SPECIES

- **Solution**
  - $O_3, O, O_{1D} \rightarrow O, O_2, O_{2_{1S}} \rightarrow O_2, O_{2_{1D}} \rightarrow O_2$
  - End Solution

- **Fixed**
  - $M, N_2$
  - End Fixed
- End SPECIES

### Solution Classes

- **Explicit**
  - $CH_4, N_2O, CO, H_2, CH_3CL, CH_3BR, CFC_{11}, CFC_{12}$
  - End explicit
- **Implicit**
  - $O_3, O, O_{1D}, O_2, O_{2_{1S}}, O_{2_{1D}}$
  - End implicit
- End Solution Classes

### CHEMISTRY

- **Photolysis**
  - $[jo2_a] \ O_2 + hv \rightarrow O + O_{1D}$
  - End Photolysis

- **Reactions**
  - $[cph1,cph] \ O + O_3 \rightarrow 2*O_2$ ; $8e-12, -2060$
  - End Reactions
- END CHEMISTRY
Modifying the chemical preprocessor input file

- **Temperature-independent rates:** \( k \ [\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}] = a_0 \)
  
  \[
  \text{O}_1\text{D} + \text{H}_2\text{O} \rightarrow 2*\text{OH} \quad ; \quad 2.2e-10
  \]

- **Arrhenius type:** \( k = a_0 \times \exp\left(\frac{b_0}{T}\right) \), where \( b_0 = (-E/R) \)
  
  \[
  \text{O} + \text{O}_3 \rightarrow 2*\text{O}_2 \quad ; \quad 8e-12, -2060
  \]

- **Troe rate constant:** \( k = \alpha^x / (1 - \beta^2) \), where:
  
  \[
  \alpha = k_0 * M / k_\infty, \quad \beta = \log_{10}(\alpha), \quad M = \text{air density} \ (\text{molec cm}^{-3}), \quad T = \text{temperature} \ (\text{K})
  \]
  
  \[
  k_0 = a_0 \times (300/T)^{a_1}, \quad k_\infty = b_0 \times (300/T)^{b_1}, \quad x = \text{“exponential factor”}
  \]

- **User-specified reaction rate:**
  
  \[
  \text{[usr11]} \quad \text{CH}_3\text{CO}_3 + \text{NO}_2 + \text{M} \rightarrow \text{PAN} + \text{M} \quad ; \quad 8.5e-29, 6.5, 1.1e-11, 1., .6
  \]

- **Rate defined in routine:** `mo_usrrxt.F90`
Configuring the model with new chemistry

• Copy a sample preprocessor input file to the case directory and edit it:

> cd $CASEROOT

> source Tools/ccsm_getenv

> cp $CCSMROOT/models/atm/cam/src/chemistry/pp_waccm_mozart/
  chem_mech.in my_waccm_mech.in"

> nedit my_waccm_mech.in &

• Modify the temperature-dependence of the reaction $O + O_3 \rightarrow 2*O_2$, changing the exponent term from -2060 to -2050:

[cph1,cph] 0 + O3 -> 2*O2 ; 8e-12, -2050
Configuring the model with new chemistry

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

  ```
  > grep CAM_CONFIG_OPTS env_conf.xml
  <entry id="CAM_CONFIG_OPTS" value="-phys cam4 -chem waccm_mozart" />
  > xmlchange -file env_conf.xml -id CAM_CONFIG_OPTS -val "-phys cam4 -chem waccm_mozart -usr_mech_infile $CASEROOT/my_waccm_mech.in"
  ```

- IF you had previously configured this case, you would need to clean up via:

  ```
  > configure -cleanall
  ```

- Now configure the case:

  ```
  > configure -case
  ```

- These same steps may be used to change chemistry in CAM-Chem compsets as well.
Building and running the model

- Build the model:
  ```
  > ./* .build
  ```

- Edit `env_run.xml` to change the length of the run, number of resubmits, frequency of restart saves, and long-term archiving.

- Edit your `*.run` script to set the maximum wall time, queue, and account number.

- Submit to the batch queue with:
  ```
  > ./* .submit
  ```

- Check submitted batch jobs:
  ```
  > bjobs
  ```
History Column Sampling

- Sample the CAM history buffer along a specified path (satellite, aircraft)
- All history variables can be sampled
- At each timestep, output stream of model columns nearest to specified coordinates for +/- half a timestep in a sequence specified via a tracking file

The corresponding model columns along the flight path are extracted and output in the same sequence as the input tracking file
History Column Sampling

Namelist options:

- `sathist_fincl` = 'PS','Q','T','U','V','O3',...
- `sathist_track_infile` = '.../satellite_profilelist.nc'
- `sathist_mfilt` = 500000
- `sathist_hfilename_spec` = '%c.cam2.sat.%y-%m-%d-%s.nc'

Tracking file:

Required variables:

- `int time(profs)`
  - `time:long_name = "time of day"`
  - `time:units = "s"`
- `int date(profs)`
  - `date:long_name = "date[yyyymmdd]"`
  - `date:units = "yyyymmdd"`
- `float lat(profs)`
  - `lat:long_name = "latitude"`
  - `lat:units = "degrees"`
- `float lon(profs)`
  - `lon:long_name = "longitude"`
  - `lon:units = "degrees"`

Horizontal grid distributed across MPI tasks

Courtesy Francis Vitt
Local time history averaging

Namelist settings:

- `avgflag_pertape` = 'A', 'L'
- `fincl2` = 'Q', 'T', 'PS'
- `lcltod_start` = 0, 0
- `lcltod_stop` = 0, 7200