MUSICA Tutorial Series 2021-2022: 2. Running MUSICAv0

MUSICA: MUlti-Scale Infrastructure for Chemistry and Aerosols

**10 December 2021**

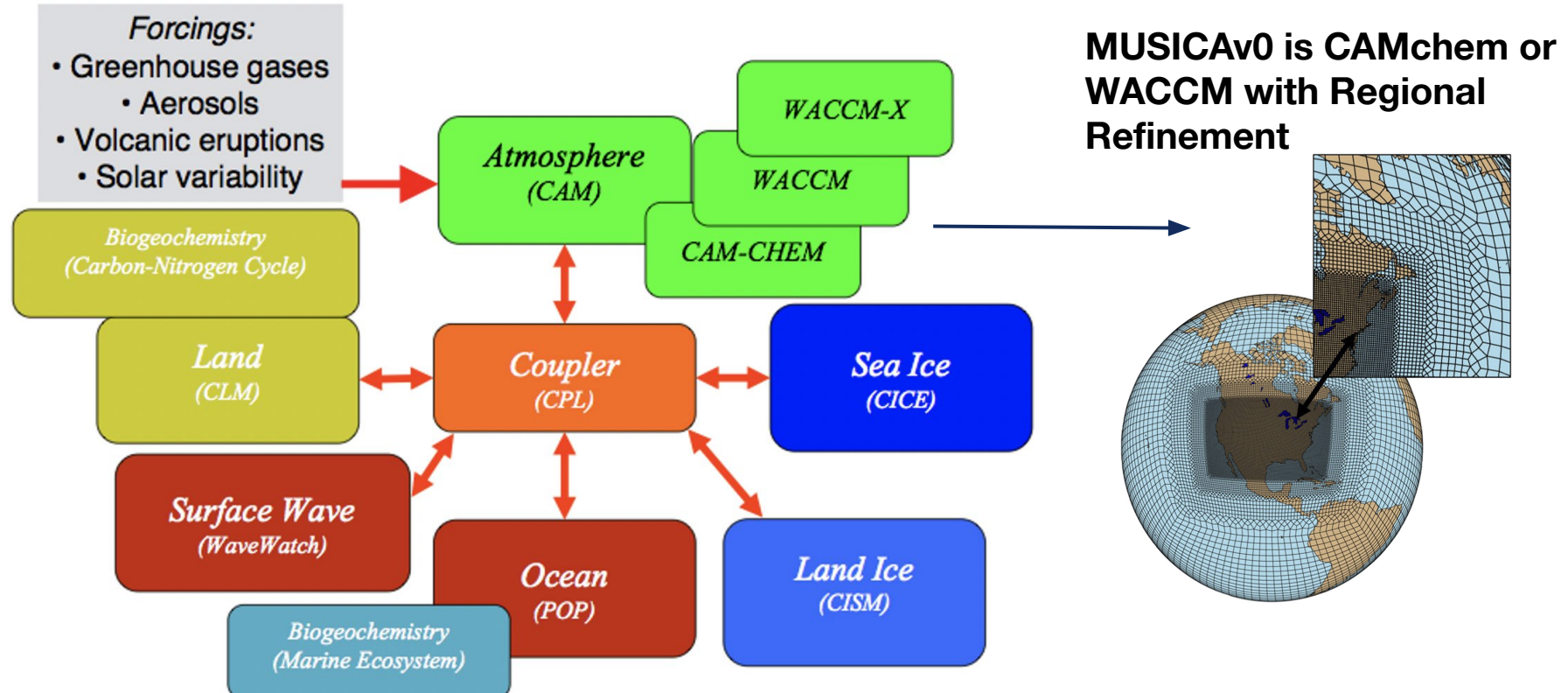# MUSICAv0 CONUS Community Simulations

- Production runs between 2012 and 2013 with regional refinement over the contiguous U.S.

- New component set and data sets have been developed for easy reproduction, extension and modification of the model simulations by the users

- Output of the existing simulations have been published for easy access for analysis
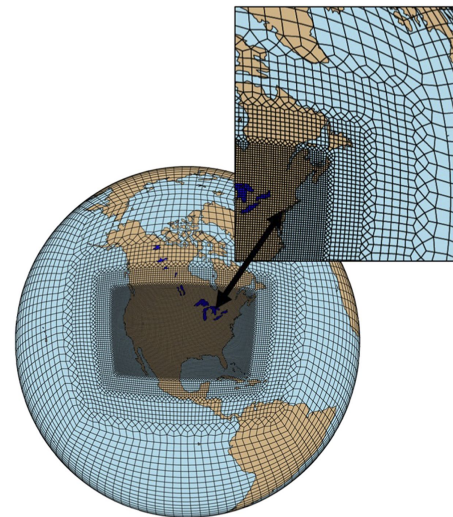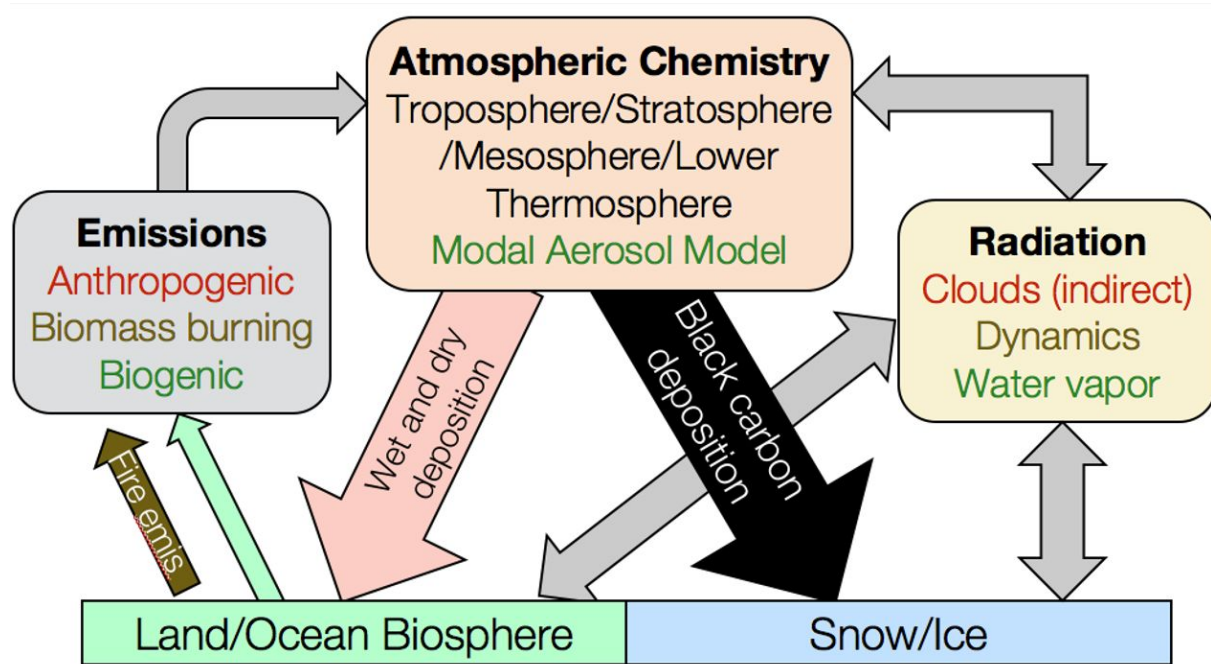
Overview

- Introduction into the MUSICAv0 CONUS Community Simulations including updates to the CESM2 CAMchem release version
  - Model configuration updates
  - Default setting

- Setting up the "out of the box" MUSICAv0 CONUS run

- Modifying model start date (year, month)
  - Updating initial conditions for land and atmosphere

- Modifying the output and emissions of the run

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CESM components and MUSICAv0

Forcings:
- Greenhouse gases
- Aerosols
- Volcanic eruptions
- Solar variability

Biogeochemistry (Carbon-Nitrogen Cycle)

Land (CLM)

Surface Wave (WaveWatch)

Biogeochemistry (Marine Ecosystem)

Atmosphere (CAM)

WACCM-X

WACCM

CAM-CHEM

Coupler (CPL)

Ocean (POP)

Sea Ice (CICE)

Land Ice (CISM)

MUSICAv0 is CAMchem or WACCM with Regional Refinement

CESM components and MUSICAv0

- WACCM and CAMChem are comprehensive Earth-System Models, including various processes and coupling.

- Component sets (compsets) have been produced for the community to easily perform simulations that are scientifically validated.

- Default MUSICAv0 configuration uses meteorological analysis to nudge winds and temperature.

Compsets available for MUSICAv0 CONUS

Two options:

1. Use compset "**FCcotagsNudged**" that has been created for the MUSICAv0 CONUS community runs (using CAMchem) based on cesm2.2.0 plus modifications (described in the next slide). Requires an account on cheyenne and reproduces the results from the community runs, and *does not require you to download your own source code!*

2. Use the release compset "**FCnudged**" (cesm2.2.0 and later, using CAMchem). This may not reproduce exactly the results from the community runs. You can get your own Source code as described here: https://escomp.github.io/CESM/release-cesm2/downloading_cesm.html

MUSICAv0 CONUS Community Runs

The compset "**FCcotagsNudged**" includes the following settings (to be included in next release), available only in a code tag on cheyenne (not in released github version)

- Code base: cesm2.2.0 release
- Chemistry TS1 mechanism for troposphere and stratosphere plus changes: Added CO tags, and bug fixes (as described on the CAMchem wiki page)
- Code fix in the land model to allow specific output (needed for surface ozone adjustment calculation)
  (this is not in the current compset and would need to be added by hand)
- Updated lightning and dust tuning
- Lower boundary conditions (greenhouse gas concentrations and CFCs) using SSP5-8.5 after 2014
- Updated nudging values (10% nudging as suggested by Davis et al., 2021)
- Anthropogenic Emissions: CAMS V5.1 for years 2000-2021 available
- Biomass Burning Emissions: QFED (2010-2020)
- Online Air-Sea Interface for Soluble Species OASISS Ocean emissions (DMS emissions from machine learning implementation)
- Updated sea-surface temperature file until 2021

MUSICAv0 CONUS Community Runs

Default settings for FCcotagsNudged in development code

- Start date: **2012-01-01**
- Initial conditions based on a spinup using a Spectral Element ne30 (1deg) configuration starting in 2010
- Output variables: currently monthly averages, daily averages, 6-hourly, hourly

```
Monthly fields:$CASENAME.cam.h0.YYYY-MM.nc (interpolated to a regular 0.9x1.25 grid)
                $CASENAME.cam.h1.YYYY-MM.nc (native SE CONUS grid)
Daily fields:   $CASENAME.cam.h2.YYYY-MM.nc (native SE CONUS grid)
6-hourly fields: $CASENAME.cam.h3.YYYY-MM.nc (interpolated to a regular 0.9x1.25 grid)  (WRF boundary)
1-hourly fields: $CASENAME.cam.h4.YYYY-MM.nc (native SE CONUS grid)
```

Nudging to meteorological reanalysis

- Winds (U, V) and Temperature are nudged towards MERRA2 meteorological analysis. MERRA2 data have been interpolated to the CAMchem model grid (32 levels) in the vertical and the CONUS regional refined horizontal grid using (using 10% nudging) for the years 2012 - 2021(August)
- Nudging can be changed to only be applied outside the CONUS region. More information can be found here: https://wiki.ucar.edu/display/MUSICA/Regridding+meteorological+data

Setup your "out of the box" CONUS run (1/2)

1.   Create your new case in your case directory: case_dir

Go to the $CESM_ROOT directory. In our case we use the available sandbox:

```
>cd  /glade/work/fvitt/cesm/cesm2.2.0_cotags/cime/scripts
>./create_newcase --compset FCcotagsNudged
--res ne0CONUSne30x8_ne0CONUSne30x8_mt12
--project <$PROJECT_NUMBER> --case <your_path/$CASENAME> --run-unsupported
```

2.   Commands to set up, build and submit your run

```
>cd <your_path/$CASENAME>
>./case.setup
>qcmd -A $PROJECT_NUMBER  -- ./case.build
>./case.submit
```

3.   Check your model run

```
>qstat -u <username>  -> status of your run
>qdel  <run_number>  -> delete a run
```

Setup your "out of the box" CONUS run (2/2)

4. Check your model output and other files in your run directory

```
>cd  /glade/scratch/<username>/run
```

Note: the default setup will produce a 5-day model run.

5. After your run finished: check your archive (/glade/scratch/<username>/archive/<casename>)

Output:

```
> ls /glade/scratch/<username>/archive/<casename>/atm/hist
```

Restart and log files:

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

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

See https://wiki.ucar.edu/display/camchem/Run+CAM-Chem+on+Cheyenne for more information

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Modifying model start date (year, month) - 1

MUSICAv0 CONUS community runs are available from Jan 2012- Dec 2013. If you want to run a different year, you have to do the following:

1. Change your start date (and length of your run)

2. Update your initial condition (IC) file for the atmosphere and land (available for 2010-2020)
- Requires interpolating the atmospheric ne30 IC file to the CONUS model grid
- A land file for the CONUS grid exists for different months

3. Checking your run:
- Make sure your nudging variables and emissions and lower boundary conditions cover the desired time period
- Make sure your sea-surface temperature files cover the desired time period
  (currently till 2021)

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Modifying model start date (year, month) - 2

1. Change your start date (in your case directory)

*xml files (those help you to modify the details of your run, setup, etc.)

- **env_run.xml:** change start date, duration of the run, and restart files (see below)
- **env_workflow.xml**: change "`JOB_QUEUE`" (`premium, regular, economy`)

<div align="center">

"`JOB_WALLCLOCK_TIME`" (`maximum "12:00:00"`)

</div>

To change your start date: after a successful run of 5 days, you can also start a longer run

```
>./xmlchange RUN_STARTDATE=$run_start
>./xmlchange STOP_OPTION=$stop_option
>./xmlchange STOP_N=$stop_n
>./xmlchange CONTINUE_RUN=TRUE  (continue run where you stopped if you have restart files)

    RUN_STARTDATE has format YYYY-MM-DD.
    STOP_OPTION has many options including ndays, nmonths, or nyears (see env_run.xml for more
    options).
    STOP_N will stop after the specified number of STOP_OPTION increments. For example the
    default values will stop simulations after 5 days.
```

Also consider changing the restart file frequency

```
>./xmlchange REST_OPTION=$stop_n
>./xmlchange REST_N=$stop_n
```

Modifying model start date (year, month) - 3

2. Update your initial condition (IC) file for the atmosphere and land

2.1. Interpolate IC files for the atmosphere (in your home directory):

```
>cd
>git clone https://github.com/NCAR/IPT
>cd Initial_conditions and modify regrid_all_spectral_data_conus.ncl
```

- modify your destination directory and file name where your regrid file will be written to

```
    regrid_dir   = "<your_VRM_Files>/<your_grid>/inic/"  (e.g., /glade/scratch/$USER/inic/)
    regrid_fname = regrid_dir + src_fname+"_<your_grid>.nc"   (your_grid: ne0CONUSne30x8)
```

- modify the date of the initial condition file you want to regrid (change YYYY-MM)

```
    ; USER CHANGES
    ; Change to the starting date you need.
    src_dir   = "/glade/p/acom/MUSICA/init/ne30_ne30/"
    src_fname =
"f.e22.FCnudged.ne30_ne30_mg17.release-cesm2.2.0_spinup.2010_2020.001.cam.i.<restart_date>-01-00000.nc"
```

To run with CESM, the file has to be then converted to a cdf5 format

```
>nccopy -k cdf5 oldfile newfile
```

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Modifying model start date (year, month) - 4

2. Update your initial condition (IC) file for the atmosphere and land

Initial condition files are changed in the user_nl_cam and user_nl_clm files

2.2. Add the new atmospheric IC file to the user_nl_cam namelist

edit **user_nl_cam** and add your new initial conditions file:

```
! Users should add all user specific namelist changes below in the form of
! namelist_var = new_namelist_value
!add nc_data file
ncdata          = 'regrid_dir + src_fname+"_<your_grid>.cdf5.nc'
```

Note: If you run a case that starts between 2012 and Jan 2014, you can also use initial condition files from the existing output: /glade/p/acom/MUSICA/init/ne0CONUSne30x8/atm

Modifying model start date (year, month) - 5

2. Update your initial condition (IC) file for the atmosphere and land

Initial condition files are changed in the user_nl_cam and user_nl_clm files

2.3. Add land IC file to the user_nl_cam namelist

edit **user_nl_clm** and add your new initial conditions file:

```
finidat  = '/glade/p/acom/MUSICA/init/ne0CONUSne30x8/lnd/<land_ic_file>.nc'
use_init_interp = .true.
```

Find land restart files for different months (2012 and 2013) here:
```
/glade/p/acom/MUSICA/init/ne0CONUSne30x8/lnd/
```

Note: Land IC files don't have to match **the specific year but should match the month you want to run**. If you want to simulate a different year where no restart files exist, in that case you have to add: use_init_interp = .true.

Specifying output, emissions etc

3. Check / modify your setup

Check your namelist settings after changing your user_nl_cam, user_nl_clm files and modify if needed

Paste and modify changes into your user_nl_cam file

```
>./preview_namelists
>view CaseDocs/atm_in
```

- ncdata: Initiation Condition file
- flbc_file: lower boundary conditions (greenhouse gases and CFCs) (check date range)

 Nudging variables (make sure they cover the period you want to run)

- nudge_beg_day, nudge_beg_month, nudge_beg_year
- nudge_end_day, nudge_end_month, nudge_end_year
- nudge_tcoef   = 0.25, nudge_ucoef   = 0.25, nudge_vcoef   = 0.25

 Emissions:

- srf_emis_specifier, ext_frc_specifier

 Output:

- fincl1,   fincl2 etc… includes desired output variables
- mfilt   = 1,1,1,4,24
- nhtfrq   = 0,0,-24,-6,-1
- interpolate_output   = .true.,.false.,.false.,.true.,.false.

mfilt: number of time stamps in output file; nhfrq: time stamp (0: monthly; -X: X hours; X: X time steps

Also avgflag_pertape = 'A' or 'I' - average or instantaneous for each file.

Run a branch run from available restart files

MUSICAv0 CONUS community runs are available from Jan 2012- Dec 2013. You can run a branch from monthly restart files between 2012 and 2013 and compare your results with the existing output (e.g, for 2015-01-01)

1. **Create your new case in your case directory (see Slide 8)**
2. **Modify your case to become a branch run in your case directory (change env_run.xml)**

```
>./xmlchange RUN_TYPE=branch
>./xmlchange RUN_REFCASE=f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01
>./xmlchange RUN_REFDATE=$branch_start
>./xmlchange RUN_STARTDATE=$branch_start
```

3. **Set up your case first**

```
>./case.setup
```

4. **Copy restart files to your run directory**

```
>cd /glade/scratch/<username>/run
>cp
/glade/p/acom/MUSICA/restart/ne0CONUSne30x8/f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01/
/YYYY-MM-DD/* .
```

5. **Build and start your run (as described on Slide 8)**

Meteorological Data and Emissions

- **MERRA2 meteorological analysis have been interpolated to the CONUS grid for the 32-level CAM-chem model between the years 2012-2020**

  `/glade/p/acom/MUSICA/met_data/MERRA2_ne0CONUS30x8_L32/`

  If you need to process other years, please find more information here:

  https://wiki.ucar.edu/display/MUSICA/Regridding+meteorological+data

- **Different Emissions are available and may need to be interpolated to the CONUS grid.**

  https://wiki.ucar.edu/display/MUSICA/Available+Input+Datasets

  More details on emission inventories can be found at

  https://wiki.ucar.edu/display/camchem/Emission+Inventories

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Plotting and Postprocessing

After the successful model run you want to look at the output.

Please see previous tutorial on
How to use MUSICAv0 output, 12 November 2021
https://www2.acom.ucar.edu/workshop/musica-tutorial-2021

Producing timeseries after you run (if desired), see:
https://wiki.ucar.edu/display/camchem/CAM-chem+automated+diagnostics

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Community MUSICAv0 Simulation Output

Output available on NCAR DASH Repository: https://doi.org/10.5065/tgbj-yv18
(now called GDEX: Geoscience Data EXchange)

Output:

- Each file has a single variable (e.g., T, O3, etc.) for a timeseries
- Monthly averages are grouped by year
  - Available on native variable resolution grid and interpolated to 0.9x1.25 regular grid
- Daily averages are grouped by month (on variable resolution grid)
- Hourly averages will be available soon

A comparable simulation at uniform ne30 (1-degree) resolution for 2010-2020 is also available. This provides monthly initial conditions files that can be regridded for variable resolution simulations.

Resources

MUSICA wiki page: https://wiki.ucar.edu/display/MUSICA/MUSICA+Home

CAM-chem wiki page: https://wiki.ucar.edu/display/camchem/Home

CESM2 website: https://www.cesm.ucar.edu/models/cesm2/

CESM Tutorial: http://www.cesm.ucar.edu/events/tutorials/2019/

CESM Forum: https://bb.cgd.ucar.edu/cesm/forums/cam-chem.154/

CESM for Containers and Cloud platforms:

　　　https://bb.cgd.ucar.edu/cesm/forums/containers-cloud-platforms.162/

Upcoming Events

January 14: MUSICA Tutorial: How to create your own variable resolution grid

February 7-11: CESM Winter Working Group Meeting for Atmosphere, Chemistry-Climate and Whole Atmosphere

February 11: MUSICA Tutorial: How to run MELODIES (model evaluation package)

Download MUSICAv0 source code

MUSICAv0 is a configuration of CESM available in CESM2.2. If you will be running MUSICAv0 on your own computer, please check the hardware, OS and software requirements in the CESM2 documentation: https://escomp.github.io/CESM/release-cesm2/introduction.html

If you are working on cheyenne, or another computer, first get your own copy of the source code (also see CESM2 download instructions https://escomp.github.io/CESM/release-cesm2/downloading_cesm.html):

```
> git clone -b release-cesm2.2.0 https://github.com/ESCOMP/CESM.git my_cesm_sandbox
> cd my_cesm_sandbox
> ./manage_externals/checkout_externals
```

"my_cesm_sandbox" should be a directory in your home or work directory (not scratch). This directory is referred to as $CESM_ROOT.