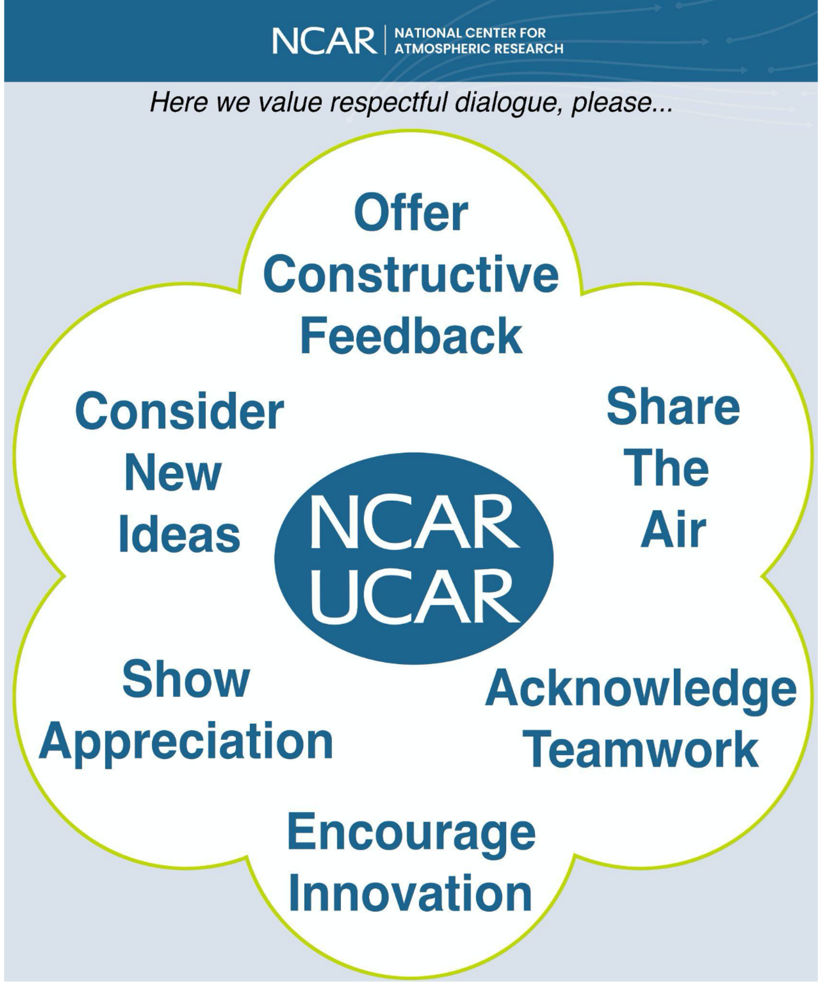
MUSICA Tutorial Series 2021-2022: 1. How to use MUSICAv0 output

MUSICA: MUlti-Scale Infrastructure for Chemistry and Aerosols

12 November 2021

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.


NCAR | NATIONAL CENTER FOR ATMOSPHERIC RESEARCH
Here we value respectful dialogue, please...
Offer Constructive Feedback
Share The Air
Acknowledge Teamwork
Encourage Innovation
Show Appreciation
Consider New Ideas
NCAR UCAR

Overview of Tutorial Series

Overall goal is to introduce various components of MUSICA:

Variable resolution global modeling (MUSICAv0)

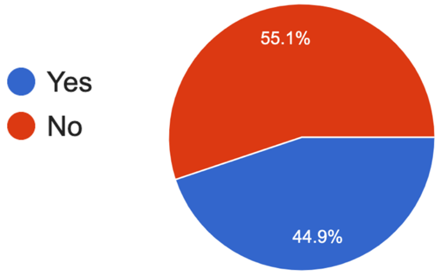
Box modeling (MusicBox)

Model evaluation (MELODIES)

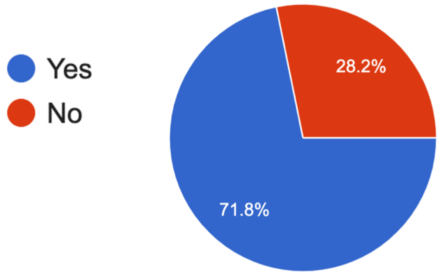
- November 12: How to use MUSICAv0 output (unstructured grids)
  November 19: Office hours
- December 10: How to run MUSICAv0 (CAM-chem with CONUS grid)
- January 14: How to create your own variable resolution grid
- February 11: How to run MusicBox
- March 11: How to use MELODIES
- April 8: Additional topics, user requests

You are a group with diverse interests and experience

Have you run CESM?
78 responses



Are you familiar with python and jupyter notebooks?
78 responses



Topics: Air quality, smoke transport, data assimilation, PM2.5 trends, aerosols, aerosol-cloud interactions, SOA, stratospheric aerosol injections, aviation NOx, volcanoes, dust storm and biogenic forecast, impact on health & crop yield, Asian monsoon, water vapor isotopes

Regions: Brazil, Latin America & Caribbean, Mexico, southern Africa, Himalayan region, Asia, Europe, Michigan, Thailand and SE Asia, UTLS

Career stage: Grad students, postdocs, professors, research scientists, ...

We hope to make this accessible and interesting for all!

Agenda for Today

- Introduction and overview of MUSICA (Louisa Emmons)
- Overview of unstructured grids (Louisa Emmons)
- Description of the Community CONUS grid simulation, format and contents of output files (Louisa Emmons)
- Demonstration of plotting and analysis tools (Duseong Jo)
- Hands-on exercises (everyone)

Goal for the Day:

- Introduce the format of MUSICAv0 output - for users of Community simulation, those who want to run MUSICAv0
- Introduce some python plotting notebooks to handle unstructured grids

MUSICA

Multiscale Infrastructure for Chemistry and Aerosols

Introduction and Overview of MUSICA

MUSICA
Multiscale Infrastructure for Chemistry and Aerosols

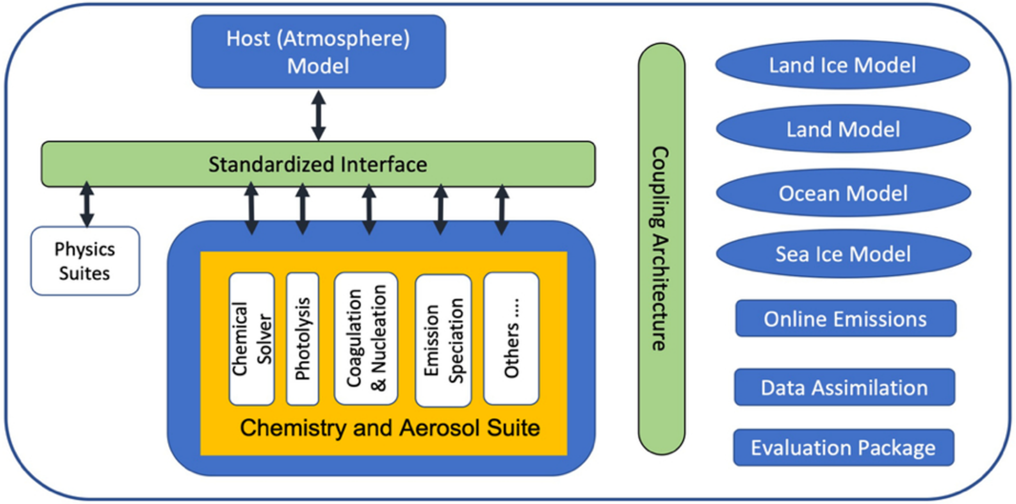
MUSICA: MUlti-Scale Infrastructure for Chemistry & Aerosols

A new model-independent infrastructure, which will enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion

Will **facilitate use of a variety** of chemistry schemes, physics parameterizations and atmospheric models

Coupled to other **earth system** component models (land, ocean, sea ice, etc.)

Whole atmosphere framework: troposphere to thermosphere



https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

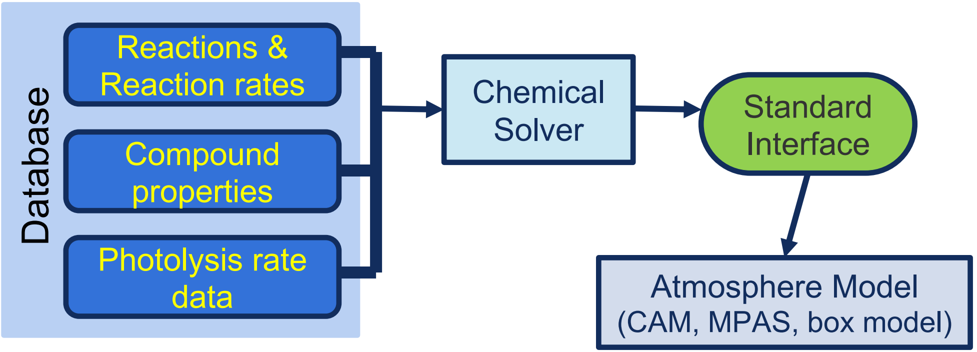
MUSICA Vision paper published in BAMS (Pfister et al., 2020: https://doi.org/10.1175/BAMS-D-19-0331.1)

Model-Independent Chemistry Module (MICM)

Database of chemical mechanisms and data needed for solving chemistry

Allows easily changing the chemical mechanism

Will allow use of the same chemistry in different atmosphere models and



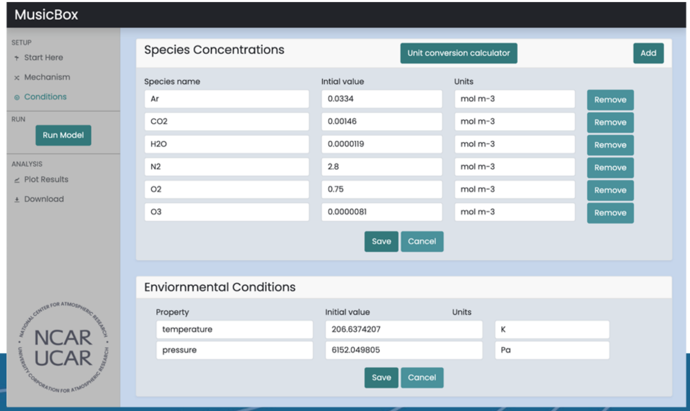
MusicBox: MICM in a box model: https://github.com/NCAR/music-box

Available with command-line control or browser interface

Allows for easy:

- Modification of chemical mechanism
- Specification of initial and time-varying environment

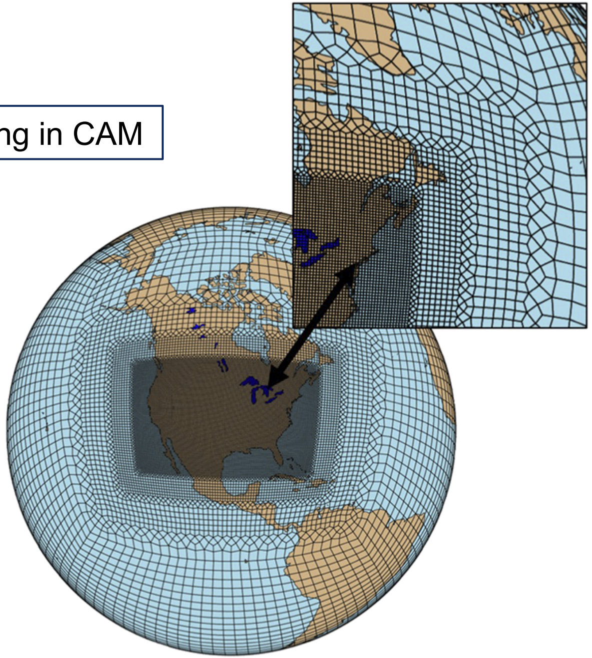
Browser interface plots results, allows comparison of 2 mechanisms



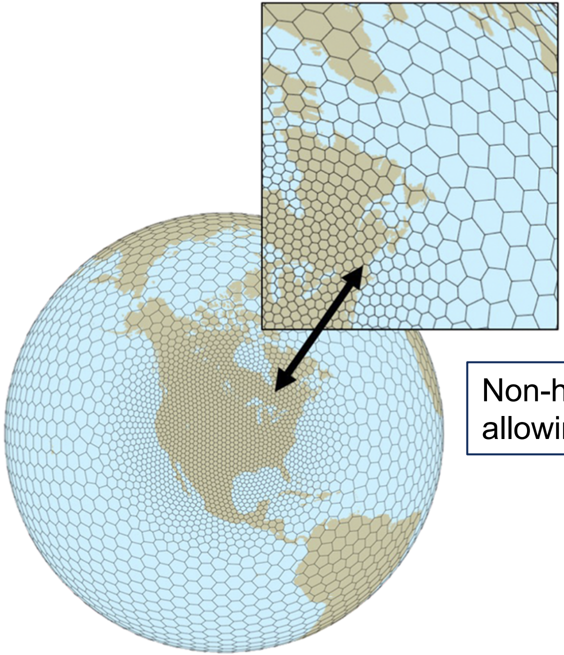
Choices for variable resolution atmosphere models

Spectral Element
(SE - cubed sphere)

Currently running in CAM

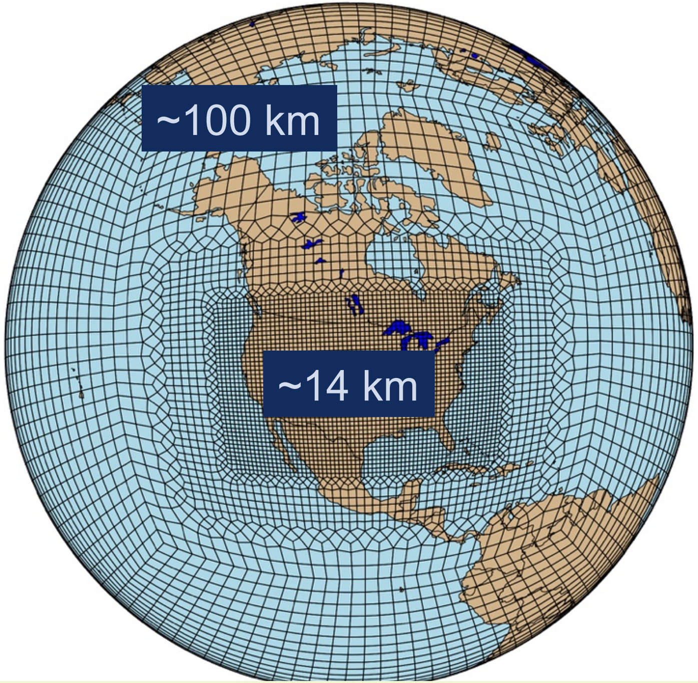


Model for Prediction Across Scales
(MPAS - hexagonal mesh)



Non-hydrostatic
allowing for finer scales

MUSICAv0 - released in CESM2.2



Users can create their own grids

MUSICAv0 is a configuration of the Community Earth System Model (**CESM**):

CAM-chem (Community Atmosphere Model with Chemistry)

With Spectral Element (SE) dynamical core and Regional Refinement (RR) [CAM-chem-SE-RR]

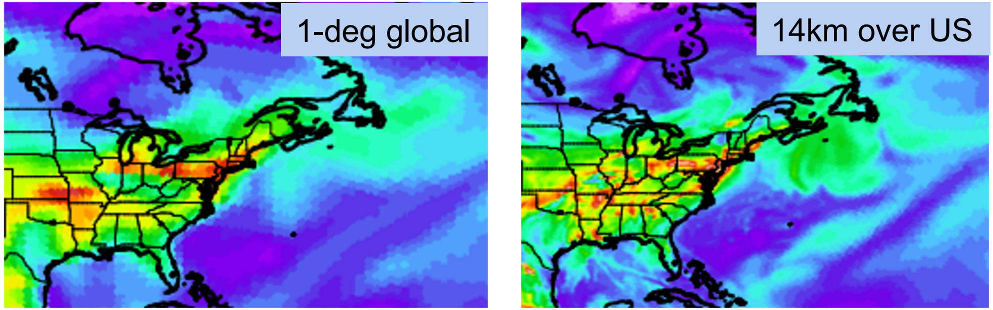
- At finer resolution, emissions and chemistry are more accurately represented
- Simulated pollutants on human exposure-relevant scales
- Global feedbacks are directly included
- Most of the grid points are in refined region, so no additional cost to simulate the whole globe

MUSICAv0 – Results

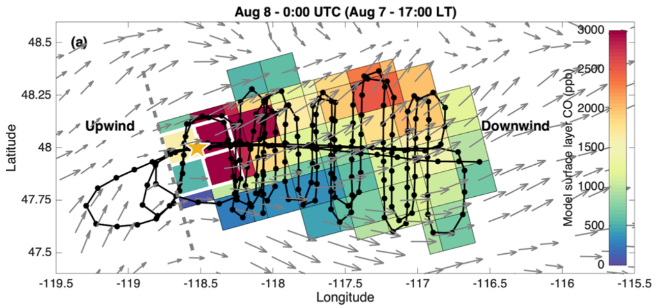
Impact of higher resolution on chemistry versus increased chemical complexity

Becky Schwantes (NOAA),
Forrest Lacey (NCAR/ACOM+RAL)
Papers in prep.

Surface Ozone – Aug 9, 2013 18Z



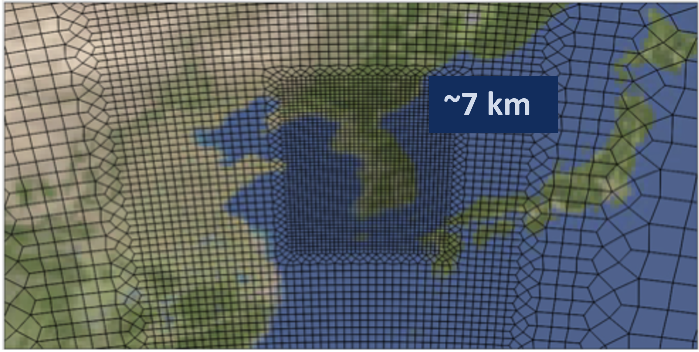
MUSICAv0 Surface CO with DC-8 flight



Wenfu Tang, NCAR/ACOM+ASP

Improving representation of fire emissions

Analysis of Korea air quality and impact of model resolution



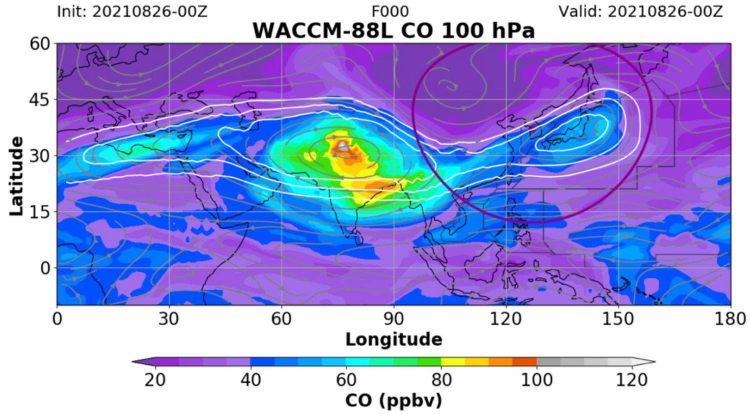
Duseong Jo, NCAR/ACOM+ASP

Simulations in support of ACCLIP

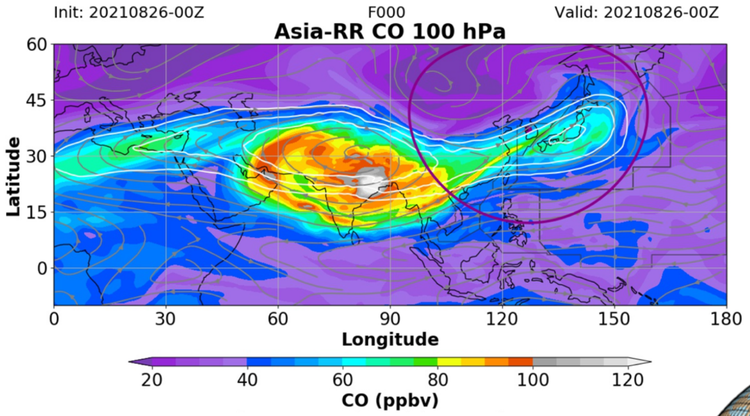
Asian Summer Monsoon Chemical and Climate Impact Project

100 hPa

WACCM

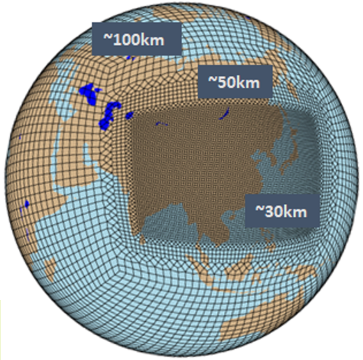


MUSICA



The regionally-refined MUSICAv0 Asia grid enhances the convective transport of pollutants by the Asian monsoon into the UTLS when compared to WACCM

Sampling these air masses is a key objective of the ACCLIP field phase in summer 2022

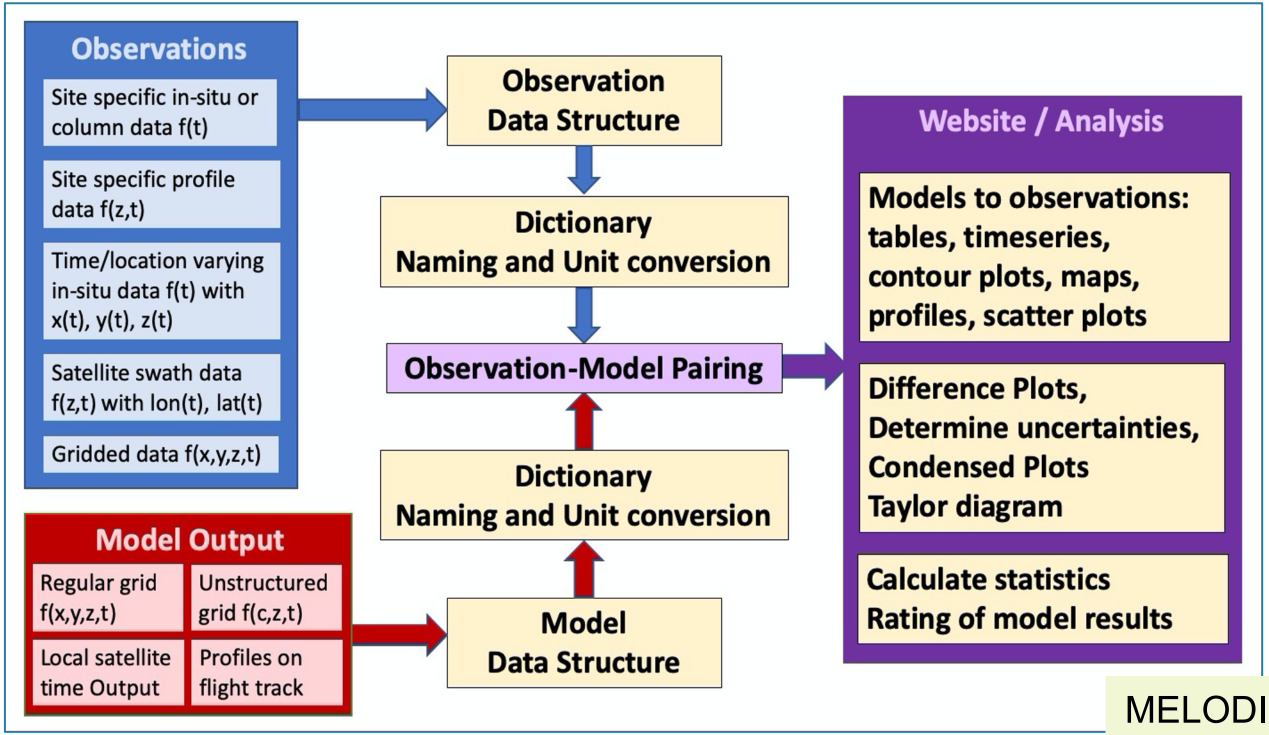


Ren Smith, NCAR/ACOM

MELODIES for MUSICA: A modular framework to compare model results and observations of atmospheric chemistry

MELODIES: Model EvaLuation using Observations, DIagnostics and Experiments Software

EarthCube



- Modular framework
- User-friendly interface
- User Guides will be produced
- Tutorial for community, targeting students and postdocs

MELODIES is being built on MONET
https://github.com/noaa-oar-arl/monet

MUSICA Goals

- To be developed collaboratively with university and government researchers
- To become the next-generation community infrastructure for atmospheric chemistry & aerosol research
- To deepen existing, and establish new, working relations of the research community with a variety of users ranging from the research community to stakeholders
- To contribute to both advancing the science and to providing relevant and actionable information for the development of mitigation policies or warning systems

MUSICA
Multiscale Infrastructure for Chemistry and Aerosols

Community Involvement Welcome

We invite the community to participate in development, evaluation and application of MUSICA:
https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

Working groups:

- Model Architecture
- Emissions and Deposition
- Chemical Schemes
- Aerosols
- Physics, Transport, sub-scale Processes
- Whole Atmosphere
- Evaluation and Data Assimilation

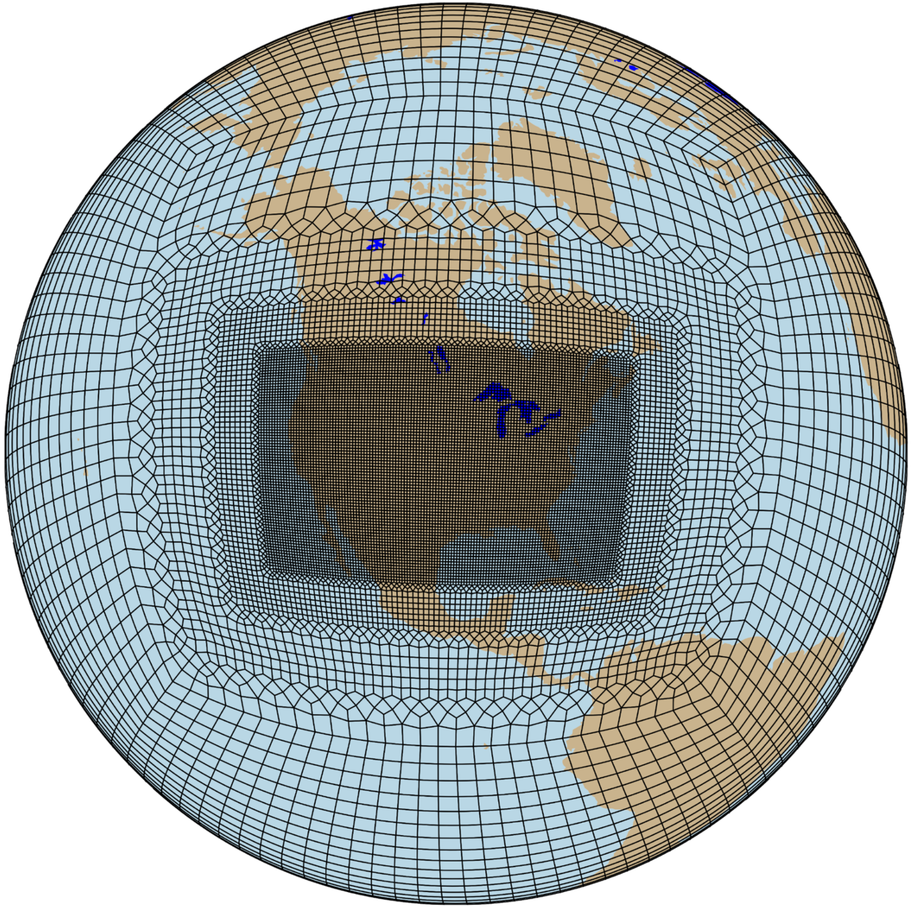
Visit MUSICA website to join working groups

Implementation plans are being developed

Also:

- **Join email list to receive MUSICA Newsletters and updates**
- **Access existing MUSICAv0 simulations**
- **Contribute to python library**
- **Contribute to MELODIES**

Overview of unstructured grids

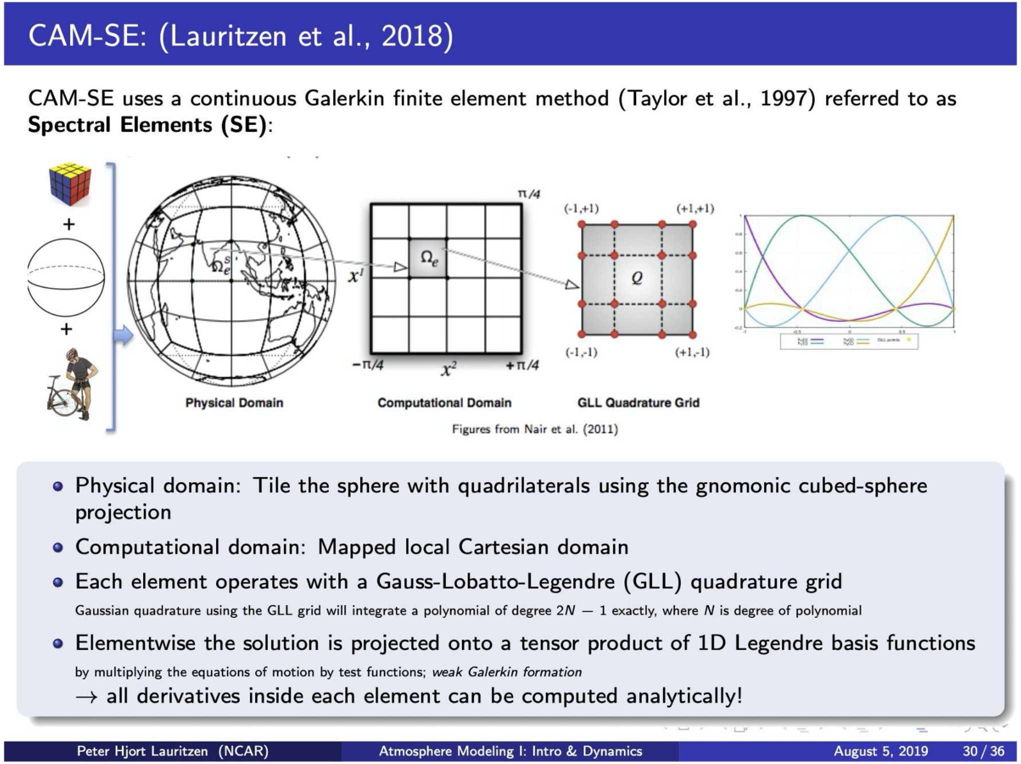


Description of Spectral Element in CAM

Lauritzen, P. H., et al.,
NCAR release of CAM-SE in CESM2.0: A reformulation of the spectral-element dynamical core in dry-mass vertical coordinates with comprehensive treatment of condensates and energy,

J. Adv. Model. Earth Syst., 2018.

https://doi.org/10.1029/2017MS001257

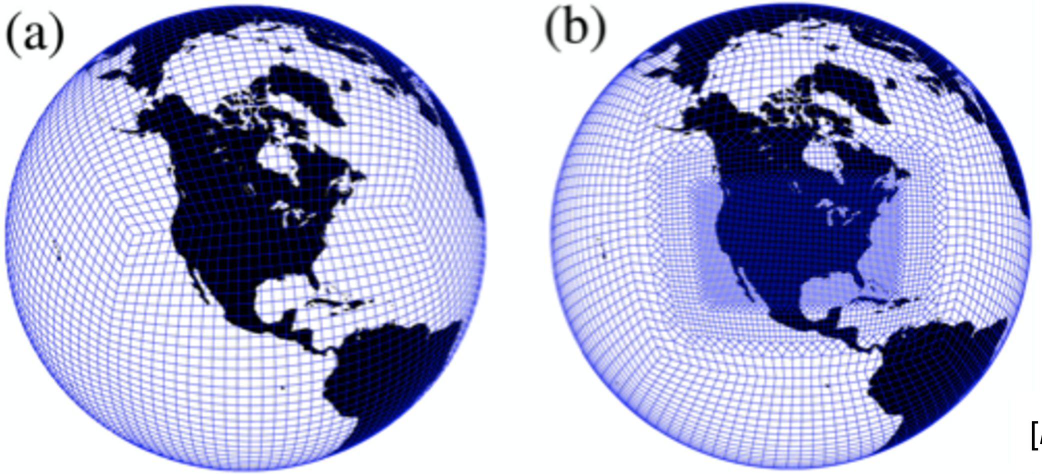


CESM Tutorial: https://www.cesm.ucar.edu/events/tutorials/2019/files/Lecture2-lauritzen.pdf

ACOM Fundamentals of Modeling workshop: https://www.acom.ucar.edu/webt/fundamentals/2018/Lecture3_lauritzen2.pdf

CESM Spectral Element

- The spectral element (SE) method has been considered as a numerical method for the fluid flow solver in global weather/climate models
- The main motivations were the SE methods' near-perfect scalability, GPU acceleration, high-order accuracy for smooth problems, and mesh refinement capabilities
- For some time CESM has supported a SE dynamical core option in CAM discretized on a cubed-sphere grid



[*Laurizen et al., 2018; Fig 1*]

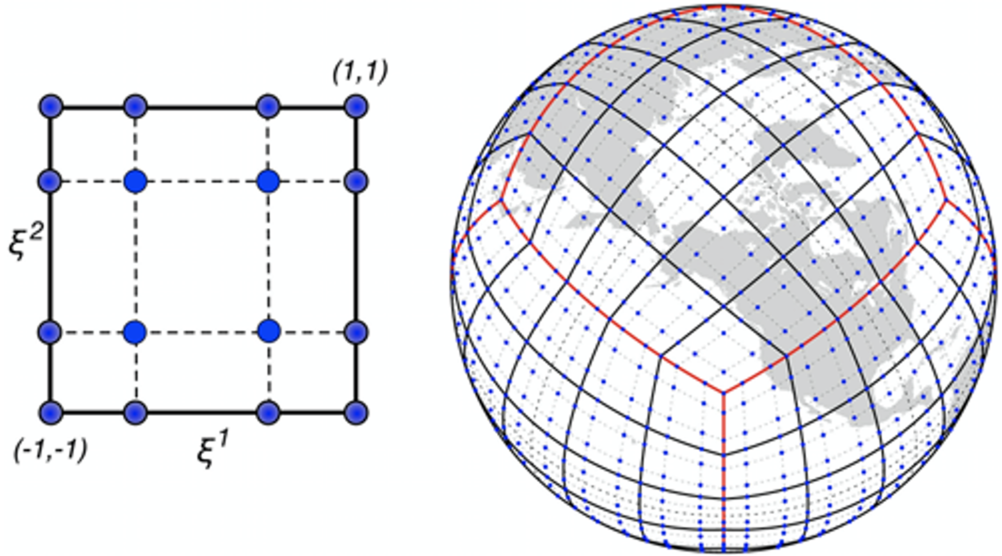
CESM-SE output

The Spectral Element model output is on unstructured grids

Model output provides the lat, lon of the center of each model grid, but the edges and vertices are not

This information is available in “SCRIP” files for each grid

The SCRIP files are read in the plotting examples to allow plotting maps to show the native grid



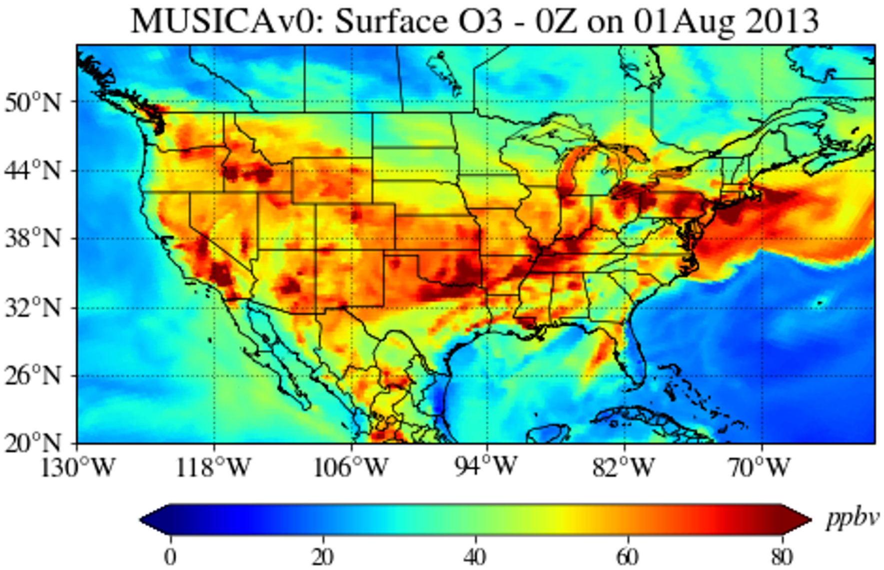
The left panel shows the Gauss-Lobatto-Legendre (GLL) grid with Np×Np quadrature points defined on a standard element [−1,1]2, where Np=4. The right panel shows the cubed-sphere ( ) grid system tiled with spectral elements Ωe, where Ne is the number of elements in each coordinate direction on a panel (in this case Ne=5). Each element Ωe on has the GLL grid structure.
[*Laurizen et al., 2018; Fig 2*]

Pause to start JupyterHub

To be ready for the hands-on portion, start your JupyterHub server now - it may be slow if everyone connects at once…

https://www2.acom.ucar.edu/sites/default/files/workshop/MUSICA_Tutorial_2021-11-12_jupyterhub.pdf

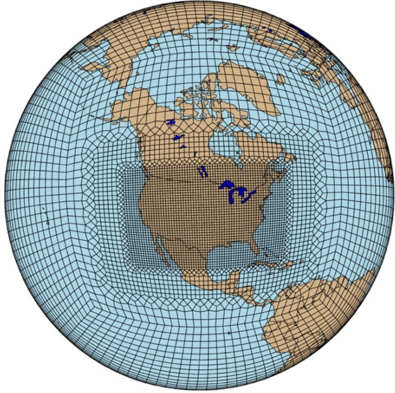
Just first 3 steps (slides 2, 3, 4)



Description of the Community CONUS grid simulation

Format and contents of output files

Description of the Community MUSICAv0 simulation



CESM2.2 CAM-chem with Spectral Element,
Regional Refinement (⅛ degree) over CONUS

Chemistry: MOZART-TS1 (standard trop-strat scheme in CESM2)

Meteorology: nudged to MERRA2 reanalyses

Simulated years: 2012-2013 (so far)

Emissions:

- Anthropogenic: CAMS-v5.1
- Fires: QFED (FINN EFs applied to QFED CO_2)
- Biogenic: MEGANv2.1 in CLM
- Ocean: OASISS for DMS

CO tags: anthropogenic for various regions (CO01 - CO12),
biomass burning (CO13)

Community MUSICAv0 Simulation Output

Output available on NCAR DASH Repository: https://doi.org/10.5065/tgbj-yv18

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.

DASH Repository

Files available for direct download individually or with scripts to get all files (very large)

UCAR NCAR Closu

NCAR UCAR | DASH Digital Asset Services Hub

NCA
National Sc

Home Search How to Submit Data Contact FAQs About

Nov 8, 2021

Community MUSICAv0 CONUS Simulations

Version: 1.0

The Community MUSICAv0 CONUS simulations have been produced using the Community
Version 2.2.0 with comprehensive tropospheric and stratospheric TS1 chemistry, using the s
dynamical core, with regional refinement over the contiguous U.S., having a grid mesh with
horizontal grid spacing over most of the globe that refines to 1/8 degree (~14 km) over the U
simulation without the regional refinement for comparison, link to follow.

The file names are as follows:
.cam.h0.nc files are monthly mean output fields on the 0.9x1.25 degrees regular horizonta
.cam.h1.nc files are monthly mean output fields on the native grid;
.cam.h2.nc files are daily mean output fields on the native grid.

DOI
https://doi.org/10.5065/tgbj-yv18

Download Data and Documentation (2658 Files, 193.87 GB Total)

- Individual Files - View, select and download individual files from this Dataset.
- Zip File - Download a ZIP file containing all files.
- Wget shell script - Download all files using Wget, preferred for Linux.
- Curl shell script - Download all files via Curl, preferred for MacOS.

Temporal Resolution
1.0 month
1.0 day
6.0 hour

Spatial Resolution
1.0 degreesLatitude
1.0 degreesLongitude
0.125 degreesLatitude
0.125 degreesLongitude

Related Links
MUSICA

DASH Repository: Download page

Download Files

Community MUSICAv0 CONUS Simulations

Use search box to refine list to a manageable size

Select one or more files and then choose which type of download script you wish to use for downloading the files.

Download Curl Script

Download the selected files via Curl, preferred for MacOS.

Download Wget Script

Download the selected files using Wget, preferred for Linux.

Download ZIP File

Download a ZIP file containing the selected files.

Showing 1 to 2 of 2 entries (filtered from 2,658 total entries)

Search: .h0.O3.

	File Name	Size	Date Modified	Type	Media Type
☐	f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.h0.O3.201201-201212.nc md5:8da7ce1ca45b225e8089a218fc193e5e	50.94 MB	2021-11-04 09:24:03Z	Data	application/x-hdf
☐	f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.h0.O3.201301-201312.nc md5:ec14933d6907294867cb3cbdbbd2970a	51.06 MB	2021-11-04 09:13:37Z	Data	application/x-hdf

Showing 1 to 2 of 2 entries (filtered from 2,658 total entries)

Dimensions and grids

Standard CESM (finite volume) regular grids:
dimensions:

lat = 192 ;
lon = 288 ;
time = UNLIMITED ; // (1 currently)
lev = 32

lat(lat)
lon(lon)
lev(lev)

O_3(time, lev, lat, lon)

Finite Volume (FV)
[regular lat-lon]

Spectral element output:
dimensions:

ncol = 174098 ;
time = UNLIMITED ; // (1 currently)
lev = 32 ;

lat(ncol)
lon(ncol)
lev(lev)
area(ncol)

O_3(time, lev, ncol)

Spectral Element (SE)
[cubed-sphere]

Additional grid information files

The CESM output files do not currently contain all the information about unstructured grids.

SCRIP file: contains centers ***and corners*** of each grid cell

Vertical dimension

The dimension **lev** indexes the model layers:

index 0 = top of the model

index 31 = surface layer (if number of lev = 32) [in python can use index = -1]

The variable **lev** is the global mean pressure for each model layer (mid-level), units = hPa

The variable **PMID** is the pressure for each grid box:

```
PMID(time, lev, ncol) ;
        PMID:units = "Pa" ;
        PMID:long_name = "Pressure at layer midpoints" ;
```

Z3(time, lev, ncol) - Geopotential Height (above sea level) of each grid box; units = "m"

PS(time, ncol) - surface pressure; units = "Pa"

PDELDRY(time, lev, ncol) - layer thickness; units = "Pa"

Output variables available

Chemical species: find explanations of the chemistry and the species in
Emmons et al., JAMES, 2020: https://doi.org/10.1029/2019MS001882

Meteorological & dynamics variables, for example:

- T: temperature (K); U,V: wind speeds (m/s); PRECC, PRECL: precipitation
- CLOUD, CLDTOT: cloud fraction, integrated column cloud fraction
- PBLH: boundary layer height (m)

Emissions diagnostics:

- Total surface emissions: SF{species}
- Biogenic emissions: MEG_{species}
- integrated column of vertical emissions: {species}_CLXF
- Lightning emissions: LNO_COL_PROD (2D), LNO_PROD (3D)

Deposition:

- Dry deposition velocity, flux: DV_{species}, DF_{gas-species}, {aerosol}DDF
- Wet dep, integrated flux: WD_{species}

https://ncar.github.io/CAM/doc/build/html/CAM6.0_users_guide/model-output.html

https://www.cesm.ucar.edu/models/cesm2/atmosphere/docs/ug6/hist_flds_f2000.html

Various output streams available

Use the 'ncdump' command on any file from the UNIX command line to get a list of the variables, their dimensions, long names, and units

/glade/campaign/acom/acom-climate/tilmes/CO_CONUS/
f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01/atm/

$casename = f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01

./hist/ **{many variables for small number of timesteps in each file}**
$casename.cam.h0.YYYY-MM.nc : Monthly mean files, interpolated to 0.9x1.25 regular grid
$casename.cam.h1.YYYY-MM.nc : Monthly means, on native grid
$casename.cam.h2.YYYY-MM-DD-00000.nc : Daily averages, on native grid
$casename.cam.h3.YYYY-MM-DD-00000.nc : 6-hr output, interpolated to 0.9x1.25 regular grid
$casename.cam.h4.YYYY-MM-DD-00000.nc : 1-hr output, on native grid

./proc/tseries/month_1/ **{one variable for long time series in each file}**
$casename.cam.h0.{species}.YYYY01-YYYY12.nc
$casename.cam.h1.{species}.YYYY01-YYYY12.nc
./proc/tseries/day_1/
$casename.cam.h2.{species}.YYYYMM01-YYYYMM31 : one species, daily averages for 1 month

Community Simulation: h0 files

f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.**h0.**YYYY-MM.nc

- Monthly mean files interpolated to 0.9°x1.25° (lat x lon) regular grid
- Many variables, but they are **interpolated (not conservatively regridded)** to the regular grid, so not suitable for budgets (e.g., emissions totals, etc.)
- Helpful for quick looks using tools you have for regular grids

Community Simulation: h1 files

f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam**.h1.**YYYY-MM.nc

- Monthly means on SE variable resolution grid *(fewer variables than h0 because of file size)*
- Gas-phase Species: CH4, CO, H2O, O3, O3S {stratospheric ozone}, OH
- Aerosols: PM25_SRF (PM2.5 at surface only), bc_a1, bc_a4, dst*, ncl* num*, pom*, so4*, soa*, CCN3
- Total surface emissions: SFCO, SFDMS, SFNO, SFSO2, OCN_FLUX_DMS
- Biogenic emissions from MEGAN: MEG_ISOP, MEG_MTERP
- Lightning NO emissions: LNO_COL_PROD(time, ncol)
- Meteorology: T, U, V, Q, CLOUD(time, lev, ncol), CLDTOT(time, ncol), PRECC, PRECL, PBLH, PS {surface pressure}, CAPE

Community Simulation: h2, h3, h4 files

f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.**h2**.YYYY-MM-DD-00000.nc

- Daily averages on native grid

f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.**h3**.YYYY-MM-DD-00000.nc

- Interpolated to 0.9x1.25 regular grid, 6-hr output
- Many species suitable for regional model boundary conditions

f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.**h4**.YYYY-MM-DD-00000.nc

- On native grid, hourly output
- Some species only available for surface layer: {species}_SRF

Community Simulation: Timeseries files

Directory:
/glade/campaign/acom/acom-climate/tilmes/CO_CONUS/
f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01/**atm/proc/tseries/**

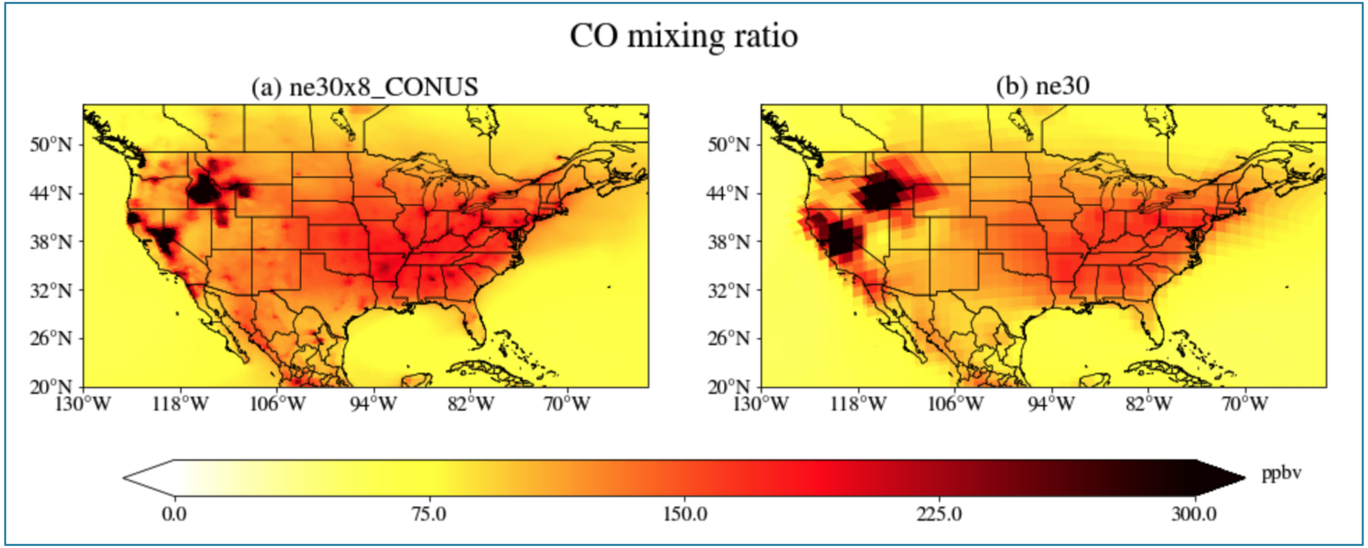
- Each file has 1 variable for a month (hourly output) or a year (monthly averages)

./month_1/

- $casename.cam.h0.{species}.YYYY01-YYYY12.nc (interpolated to regular grid)
- $casename.cam.h1.{species}.YYYY01-YYYY12.nc (on native grid)

./day_1/

- $casename.cam.h2.{species}.YYYYMM01-YYYYMM31 : one species, daily averages for 1 month



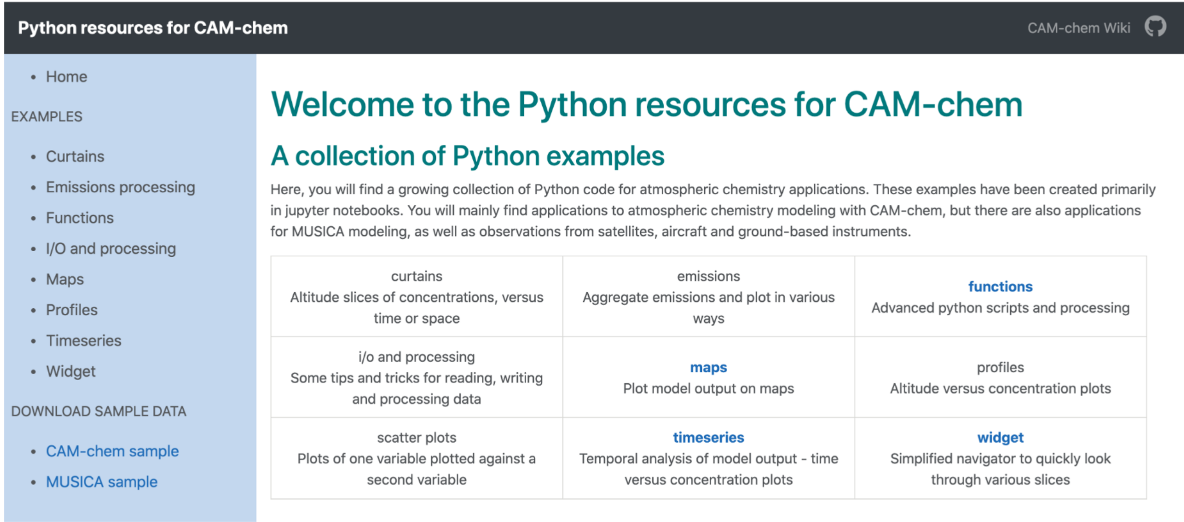
Demonstration of python plotting examples

Python Plotting Examples

Tutorial example notebooks: https://github.com/NCAR/musica-tutorial

Examples of a variety of plots:
https://ncar.github.io/CAM-chem/index.html

Contributions welcome!


Python resources for CAM-chem
CAM-chem Wiki

- Home

EXAMPLES

- Curtains
- Emissions processing
- Functions
- I/O and processing
- Maps
- Profiles
- Timeseries
- Widget

DOWNLOAD SAMPLE DATA

- CAM-chem sample
- MUSICA sample

Welcome to the Python resources for CAM-chem

A collection of Python examples

Here, you will find a growing collection of Python code for atmospheric chemistry applications. These examples have been created primarily in jupyter notebooks. You will mainly find applications to atmospheric chemistry modeling with CAM-chem, but there are also applications for MUSICA modeling, as well as observations from satellites, aircraft and ground-based instruments.

curtains Altitude slices of concentrations, versus time or space	emissions Aggregate emissions and plot in various ways	**functions** Advanced python scripts and processing
i/o and processing Some tips and tricks for reading, writing and processing data	**maps** Plot model output on maps	profiles Altitude versus concentration plots
scatter plots Plots of one variable plotted against a second variable	**timeseries** Temporal analysis of model output - time versus concentration plots	**widget** Simplified navigator to quickly look through various slices

We are going to learn

- *Read MUSICAv0 output file(s)*
- *View file structure*
- *Basic array manipulation*
- *Various 2D map applications with an unstructured grid output (global, regional, custom colorbar, overlaying observations, log-scale plot, multi-panel, gridlines)*
- *Calculate global/regional emission total*
- *Calculate and plot vertical profile*
- *Simple regridding and cross section calculation*
- *Find an index of a specific location on the unstructured MUSICAv0 grid*
- *Timeseries plot*
- *Regrid unstructured grid data to structured grid data and save as a new NetCDF file*