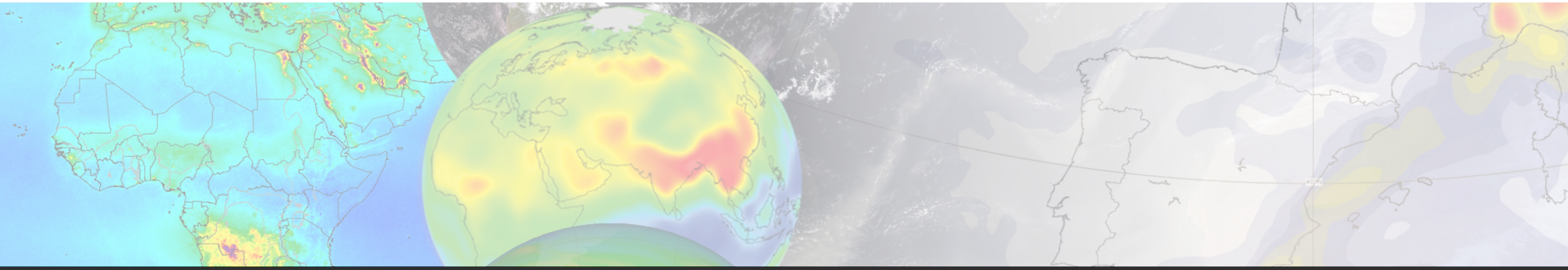


Introduction to CESM, CAM-chem, and MUSICAv0

Louisa Emmons, Wenfu Tang, Jun Zhang

Atmospheric Chemistry Observations and Modeling Laboratory

National Center for Atmospheric Research

CESM & MUSICA Tutorial at Nanjing University
September 2024

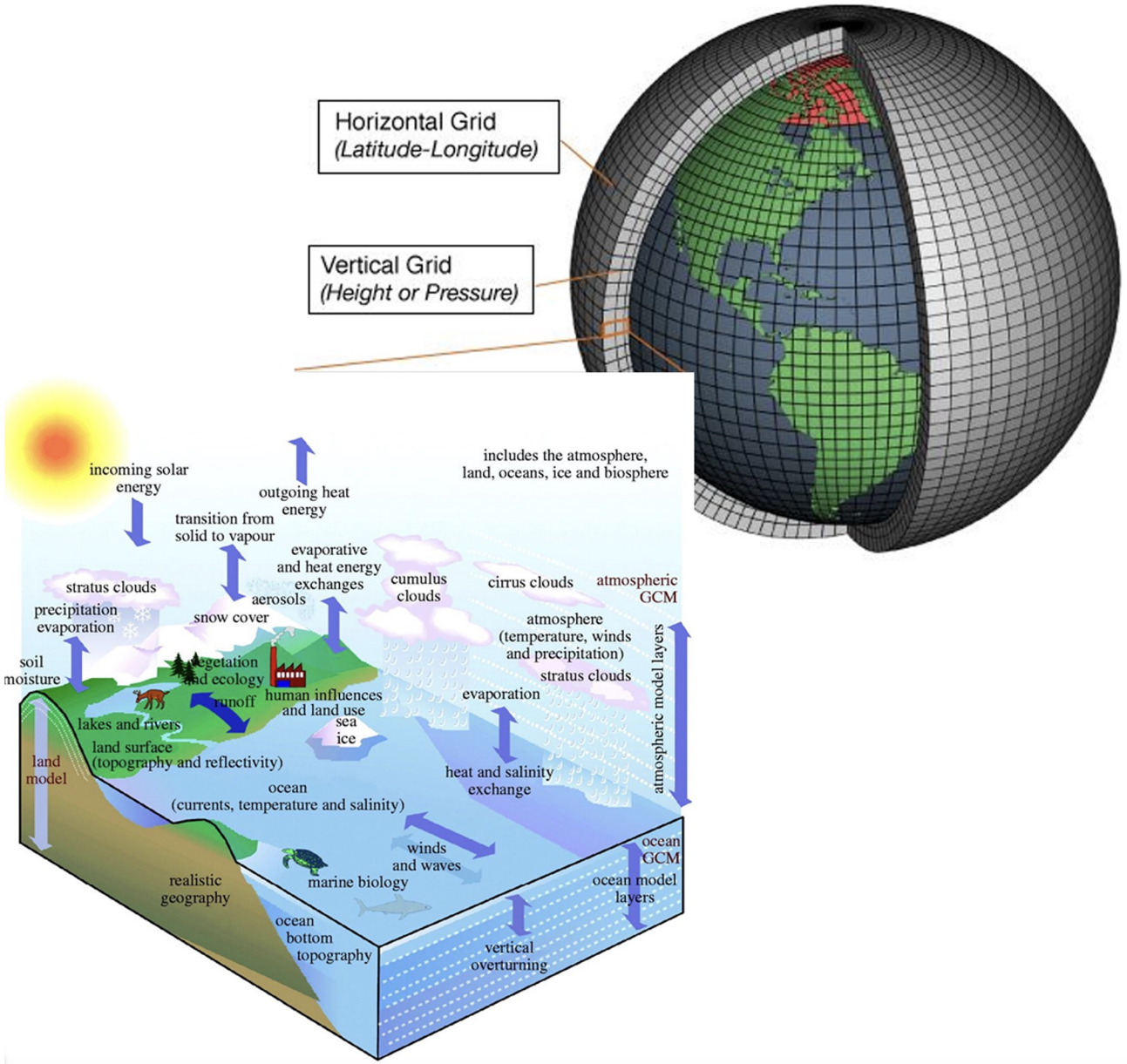
This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.

Global Earth System Models

The models use physical equations to simulate key fields and processes in the atmosphere, ocean, land, sea-ice, land-ice, etc.

Processes that remain below the grid resolution need to be parameterized.

Models build on our understanding of processes from observations and highly-detailed models (e.g., process models, large eddy simulations).

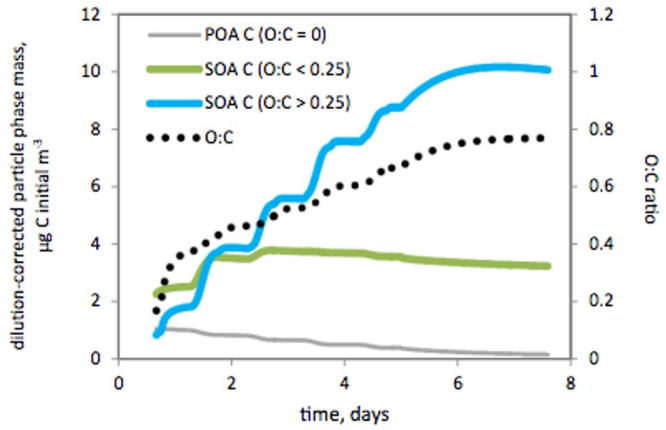


Current Atmospheric Chemistry Modeling Ecosystem

Understanding Air Quality and Chemistry in Detail

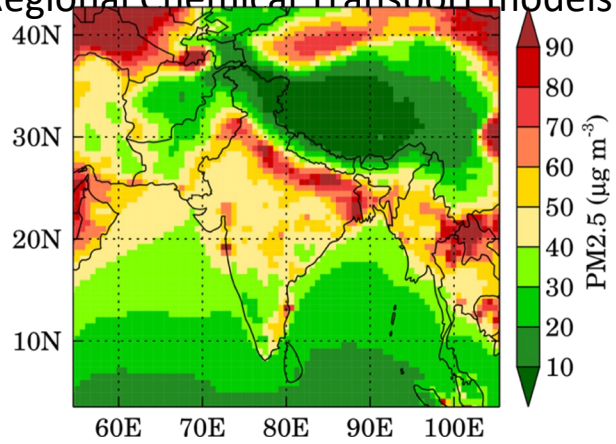
Chemical Box Models
Column Models
LES and CFD models , etc.

Radiative Transfer models
Biogenic & Canopy models
Hyper-explicit chemical models, etc.



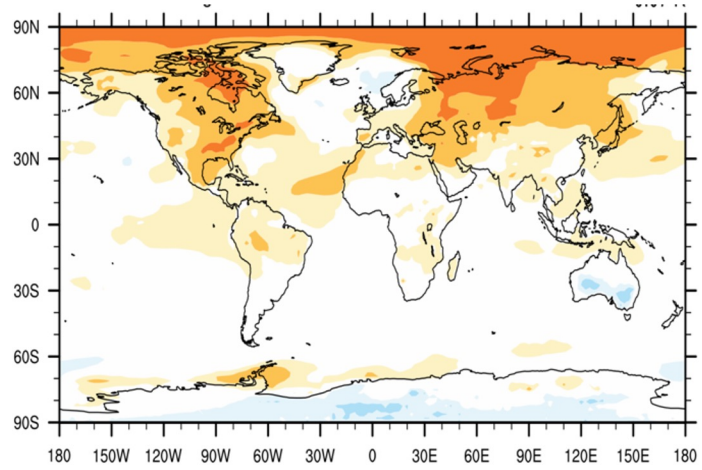
Examining the Urban/Cloud Resolving to Regional Scales

Regional Chemical Transport models



Global Scale Impacts of Atmospheric Chemistry

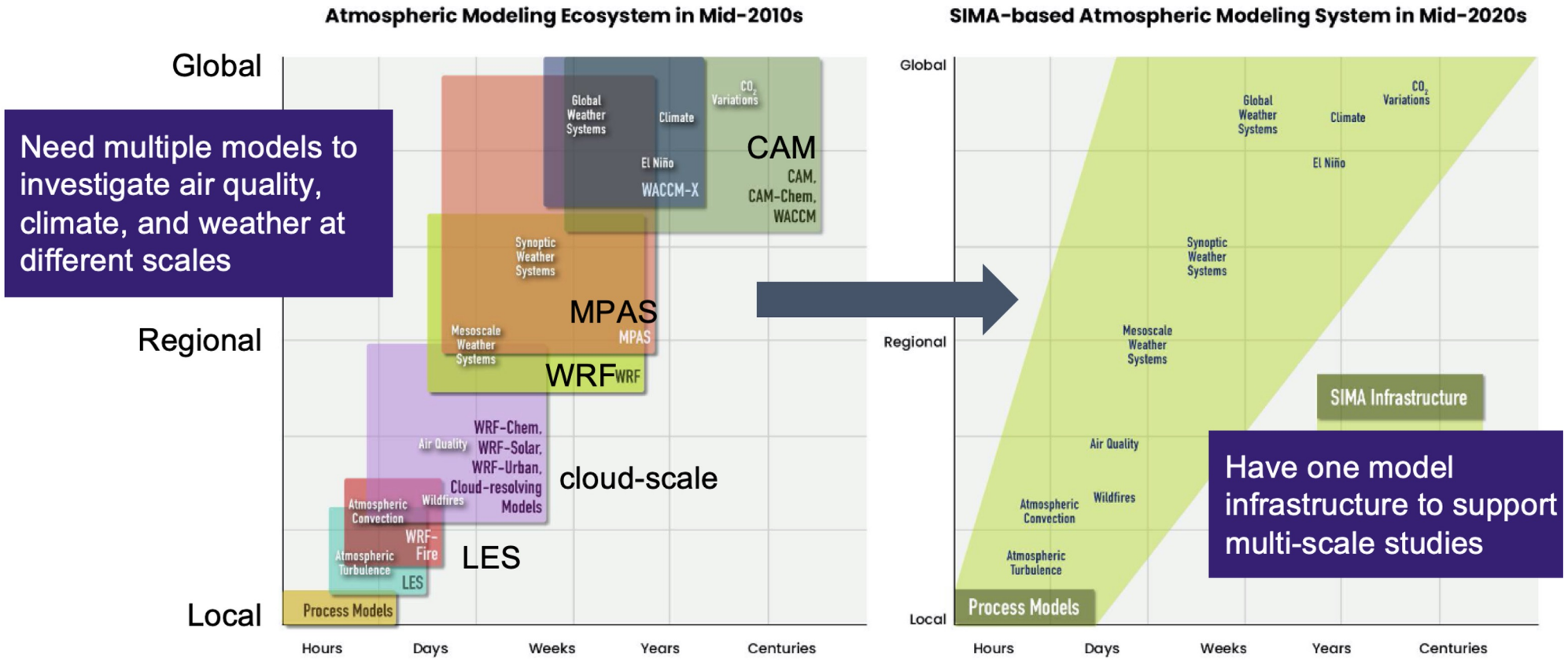
Global Chemical Transport Models
Earth System Models



Shift in modeling ecosystem towards unified scale-aware frameworks

The atmosphere is inextricably connected to the physics, chemistry and biology of the Earth system including ocean, ice, land and solar influence - and humans.

Next-gen models need to seamlessly cover the local emission scale all the way up to the global forcing scale within a single framework, and connect the Earth System components.



Unified models:

- Enable scientific research at the intersection between standard disciplines
- Improve integration of observing and modeling systems
- Accelerate progress by communities jointly developing models and tools

MUSICA – MUlti-Scale Infrastructure for Chemistry & Aerosols

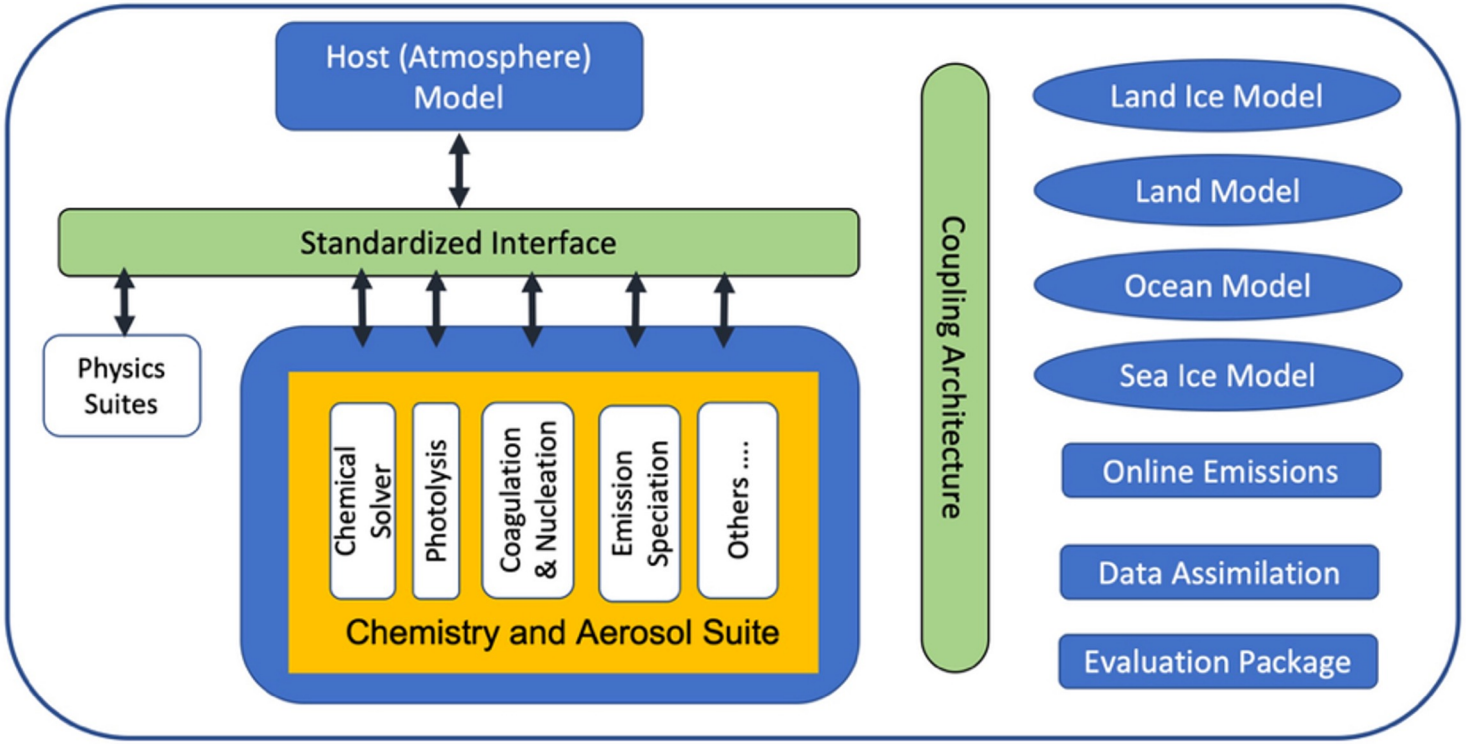
A new model-independent infrastructure, which will enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion

MUSICA
Multiscale Infrastructure for Chemistry and Aerosols

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

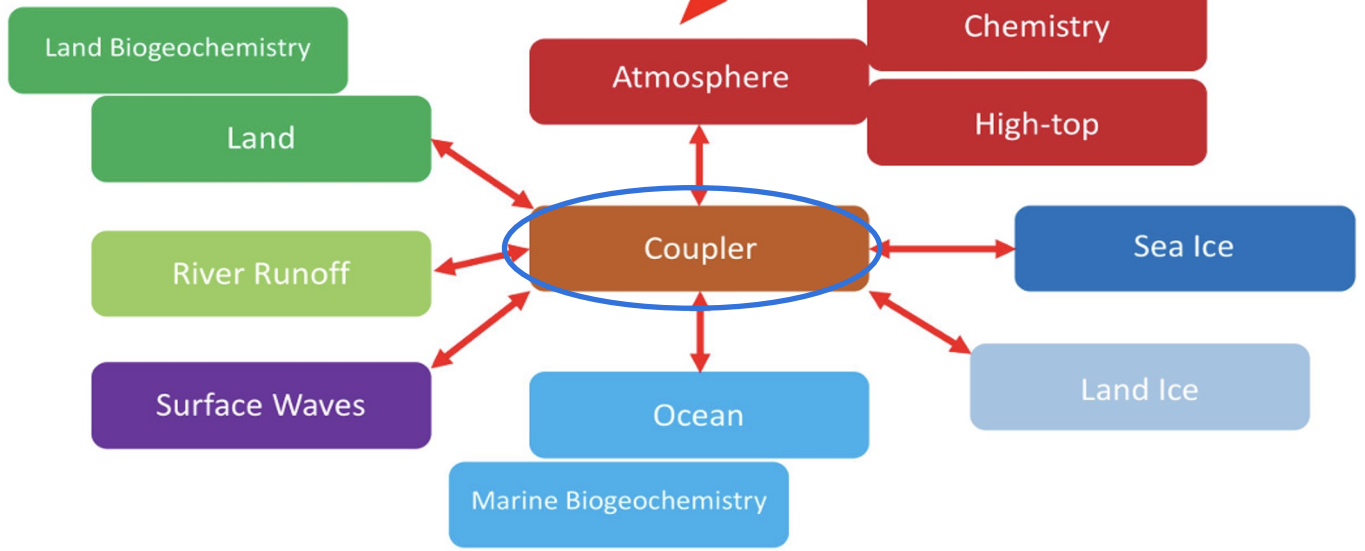


https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

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

CESM

Community Earth System Model is an open-source community model available via GitHub.

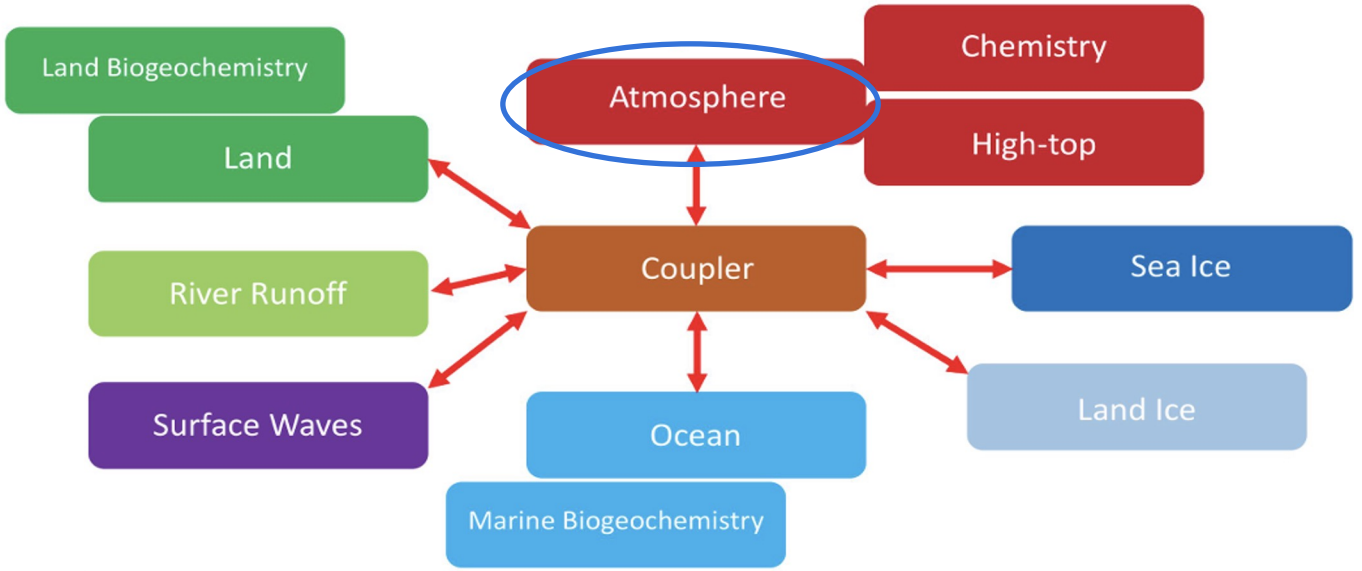


CESM has multiple different earth components coupled with a coupler.

https://github.com/ESCOMP/CESM

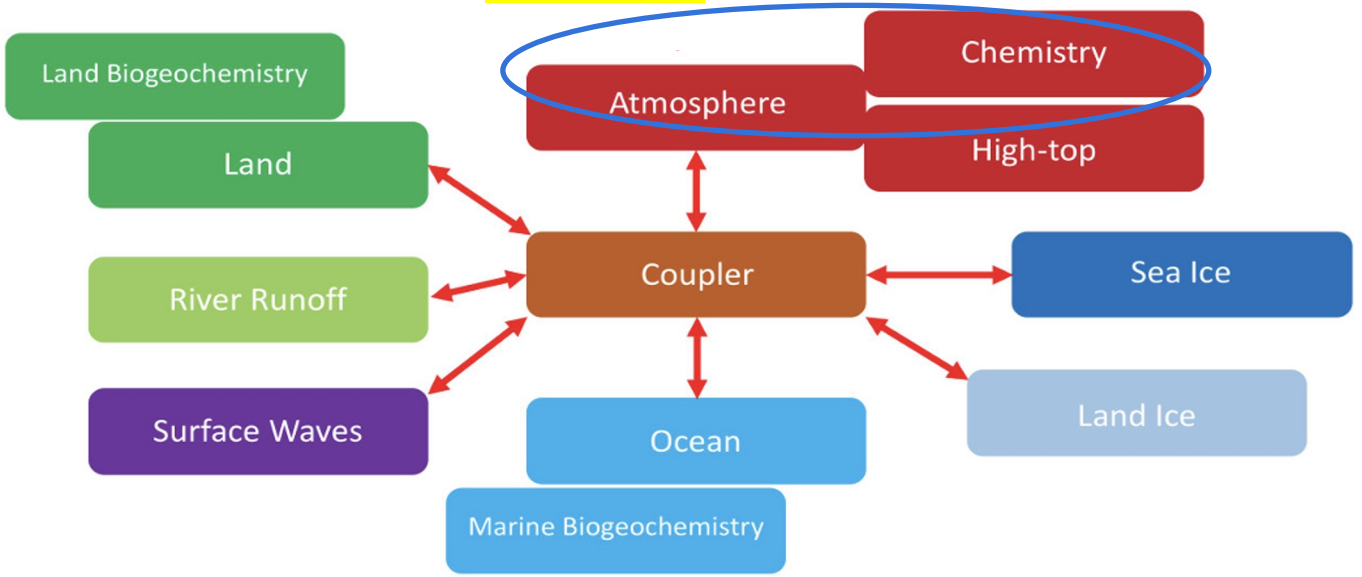
CAM

The atmosphere model in CESM is called **CAM** (Community Atmosphere Model)



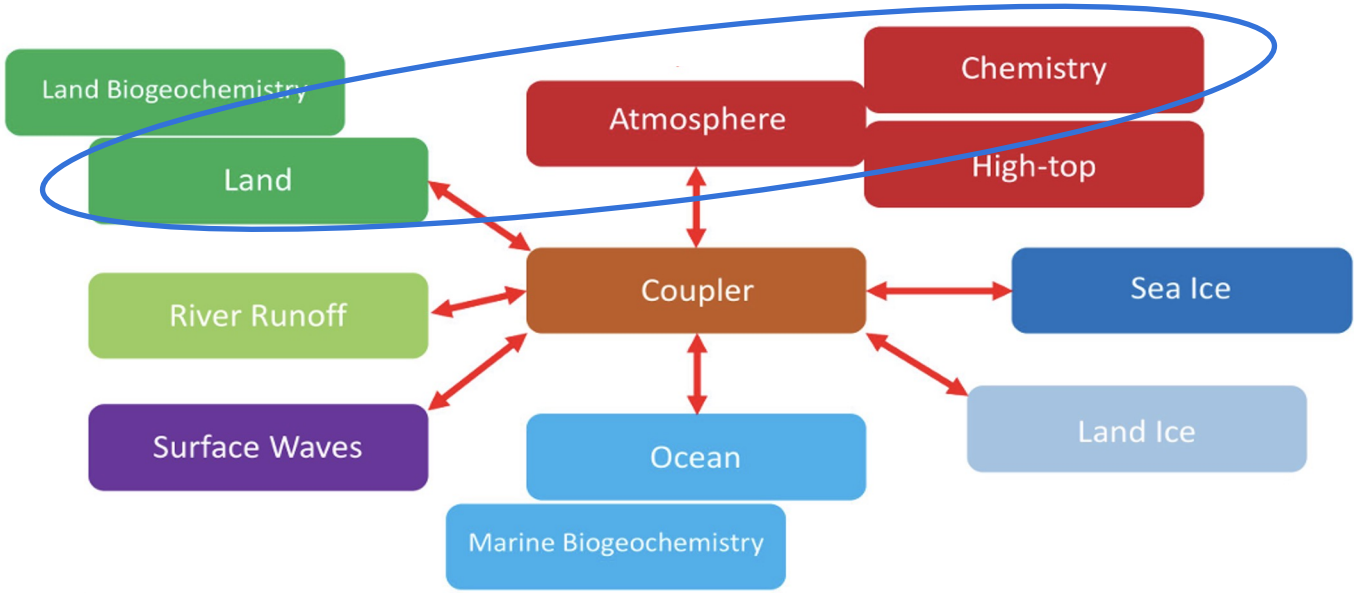
CAM-chem

The Community Atmosphere Model with Chemistry (**CAM-chem**) is a component of CESM.



CAM-chem

When running CAM-chem, the land component is on by default. The other components can be on or off by different settings.



CESM3 Chemistry Options

There are multiple chemistry options in CAM-chem and CESM.

WACCM

T1MA
234 tracers

Middle Atmosphere (MA)
100 tracers

Specified Chemistry (SO Chemistry)
31 tracers

Provides Upper Boundary Conditions

oxidants, ozone, strat. aerosol

Air Quality Chemistry

T1S: 231 tracers

T3S: 278 tracers

SLH chemistry: 277 tracers

MOSAIC/CARMA

Climate Chemistry

T4S: 141 tracers
30% cheaper than T1S

As T1S but cheaper tropospheric chemistry for climate

SO Chemistry

31 tracers
prescribed ozone, oxidants, aerosol (stratosphere) interactive GHGs and aerosols in the troposphere

140 km

WACCM (High Top Model) 132L

80 km

"Workhorse" (Mid Top) Model 93L

40 km

Low Top Model 58L

Emissions in CESM

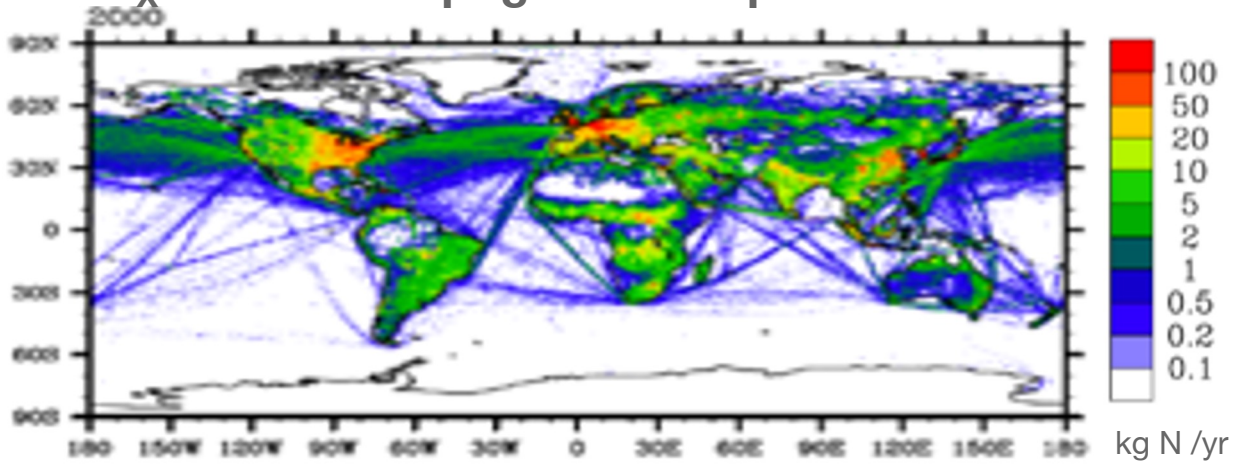
Emissions

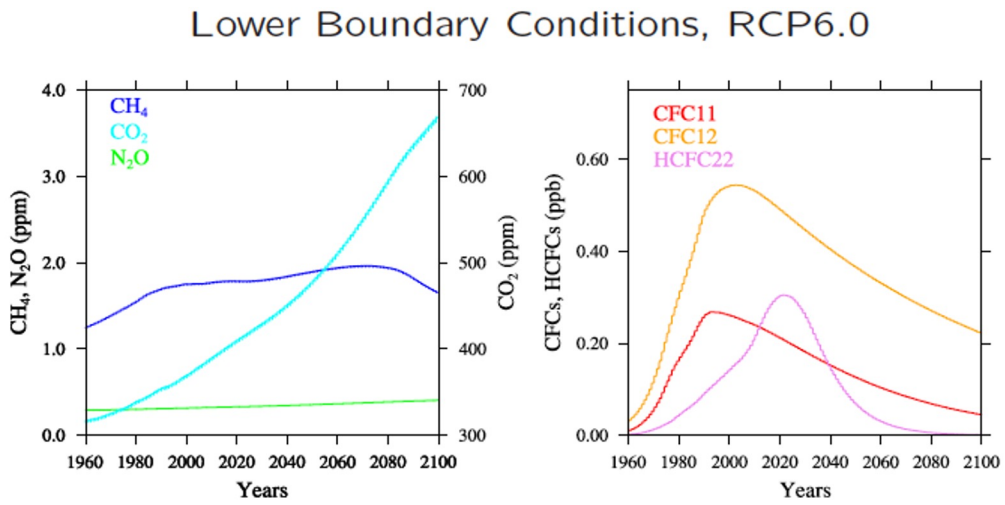
- Surface emissions: anthropogenic, biogenic, biomass burning (fire), ocean, soil
- Vertical emissions: (external forcings): aircraft, volcanoes, power plants, (fire optional)
- Interactive: Dust, biogenic, ocean DMS, (fire optional/experimental)

Surface concentrations

- Lower boundary conditions (greenhouse gases CO_2, CH_4, N_2O and, long-lived gases CFCs). Can vary latitudinally.

NO_X from anthropogenic + ship + fire sources





Anthropogenic Emissions

Anthropogenic emissions are specified in offline emissions files

Various inventories are available in CESM format:

- CMIP6 (CEDS)
- CAMS (Copernicus Atmosphere Monitoring Service)

HEMCO (Harmonized Emissions Component) is available in CESM3(beta), allowing for:

- easy combination of regional inventories (NEI, etc.) with global inventories
- application of diurnal variation
- application of vertical distribution (power plant heights)

Biomass Burning Emissions

Biomass burning emissions are generally specified with offline emissions files.

Available in CESM:

- CMIP6 (1750-2015)
- GFED
- QFED (near-real-time and historical)
- FINNv2.5 (2002-2023, and near-real-time)
- GFAS (in progress)

CLM contains an online fire model which can provide emissions to the atmosphere, but they are not realistic for present-day.

“Other” offline emissions

Climatological inventories are used for soil and ocean emissions:

- Ocean CO and hydrocarbons
- Soil NO
- Soil NH3

Interactive emissions: Dust

$F_{dustemis} = F_{dustemis}(u_*, w)$ becomes $F_{dustemis} = F_{dustemis}(u_*, w, z_{0,rock}, \mathrm{LAI}, \sigma_{\tilde{u}})$

(CESM default)

horizontal wind/friction

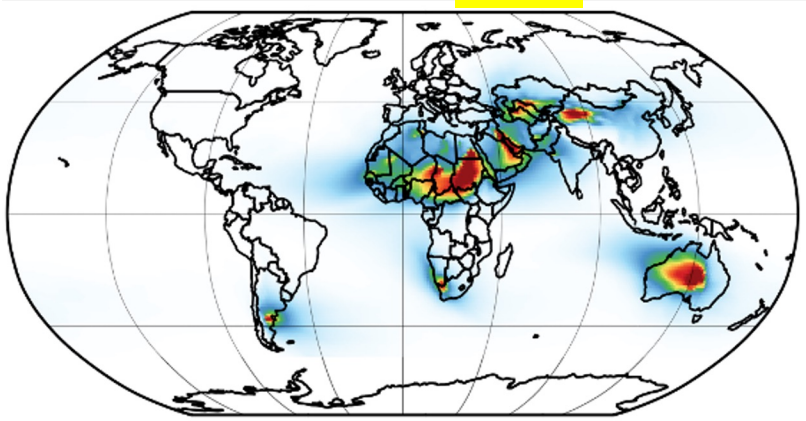
soil moisture

(Leung 2023)

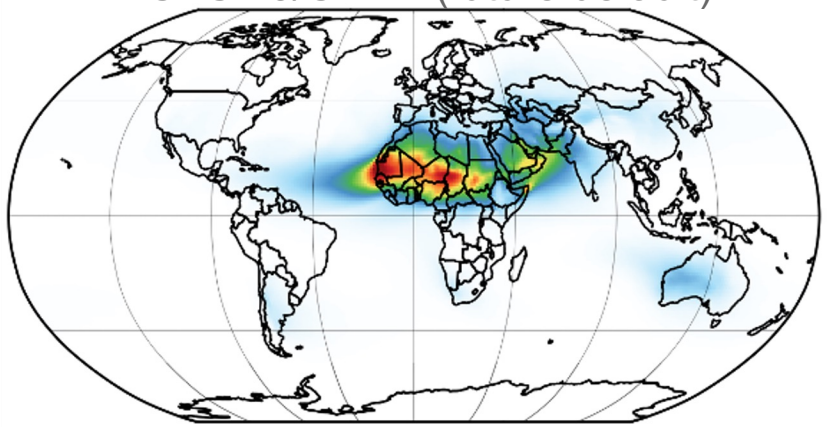
Drag partition due to surface roughness

Subtimestep wind following the similarity theory

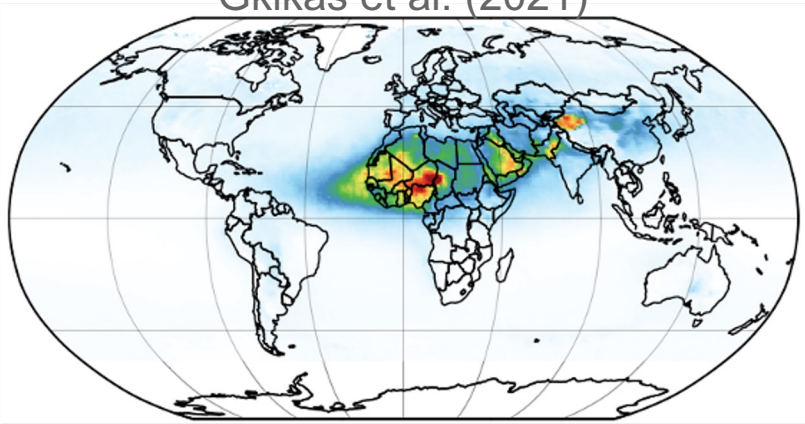
Charlie Zender et al. (2003; DEAD)
CESM2/CAM6 default



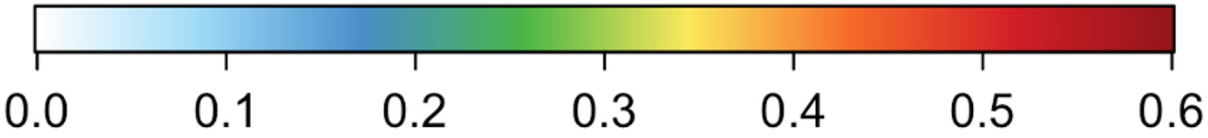
Danny Leung et al. (2023; L23)
CESM3/CAM7 (future default)



MIDAS (MODIS/Aqua) dust
Gkikas et al. (2021)



AOD from dust



Slide: Danny Leung

Interactive emissions: Biogenic

MEGAN: Model of Emissions of Gases and Aerosols from Nature

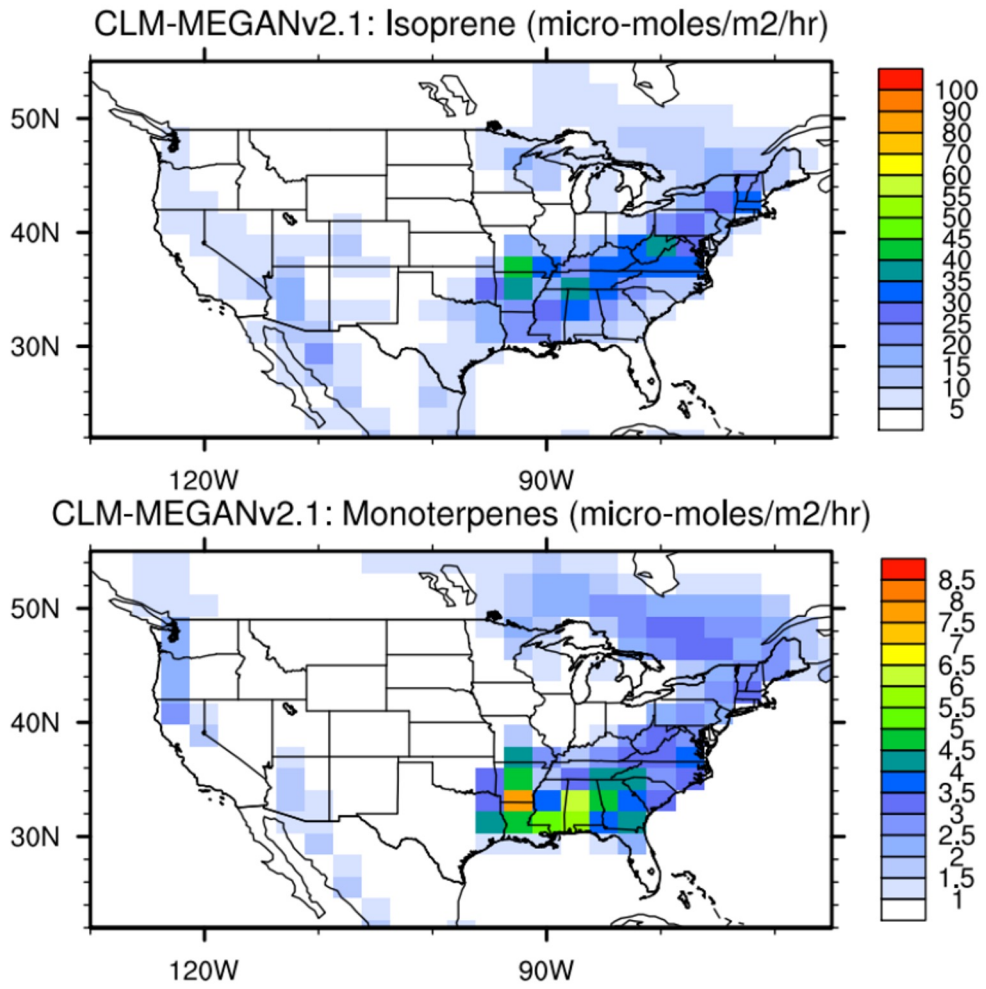
MEGAN is a modeling system for estimating the emission of gases and aerosols from terrestrial ecosystems into the atmosphere (Guenther et al., GMD, 2012; https://gmd.copernicus.org/articles/5/1471/2012/)

The MEGANv2.1 algorithm is included in CESM within the Community Land Model (CLM) to use the model vegetation and meteorology. Emissions are calculated by the equation:

$$F_i = \gamma_i \, \Sigma \, \varepsilon_{i,j} \, \chi_j$$

where

- γ_i : emission activity factor, depends on **leaf area index (LAI)**, **meteorology** (T, solar radiation), **leaf age**, with separate light-dependent and light-independent factors
- $\varepsilon_{i,j}$: emission factor at standard conditions for vegetation type (PFT) j
- χ_j : fractional area of **PFT** j



Interactive emissions: Ocean DMS

DMS emissions from ocean are calculated online based on the Online Air-Sea Interface for Soluble Species (OASISS) module:

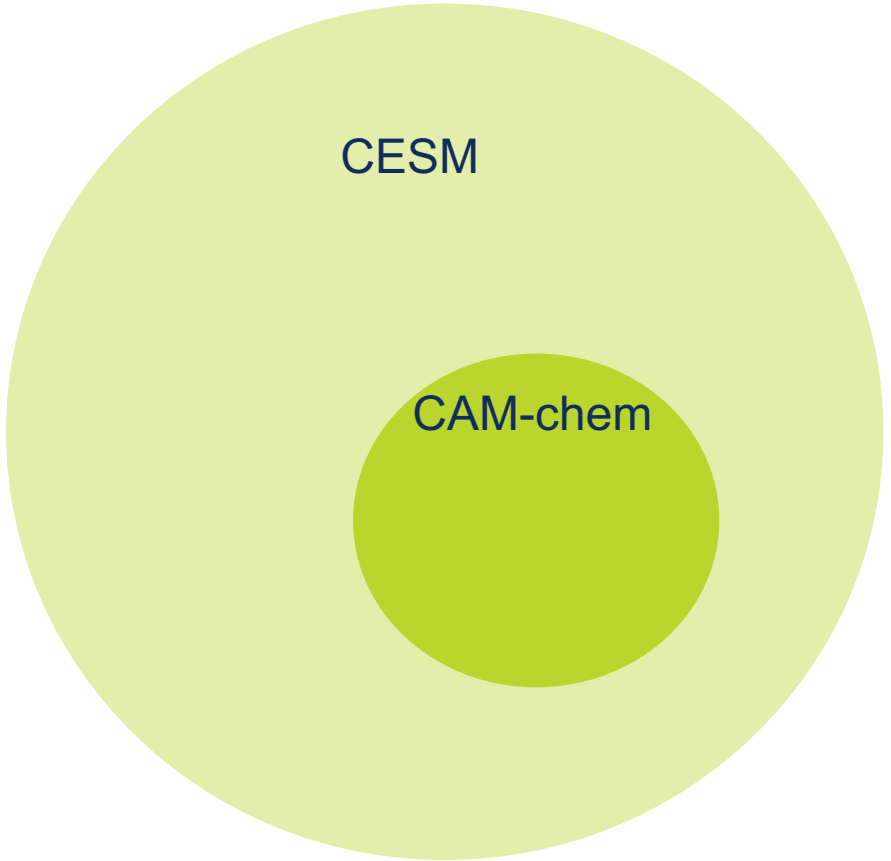
https://wiki.ucar.edu/pages/viewpage.action?pageId=358319521

Seawater concentrations are specified and the emissions flux is calculated each timestep based on the model winds, etc.

Wang, S., Apel, E. C., Schwantes, R. H., Bates, K. H., Jacob, D. J., Fischer, E. V., et al. (2020). Global Atmospheric Budget of Acetone: Air-Sea Exchange and the Contribution to Hydroxyl Radicals. *Journal of Geophysical Research: Atmospheres*, 125, e2020JD032553. https://doi.org/10.1029/2020JD032553

Summary

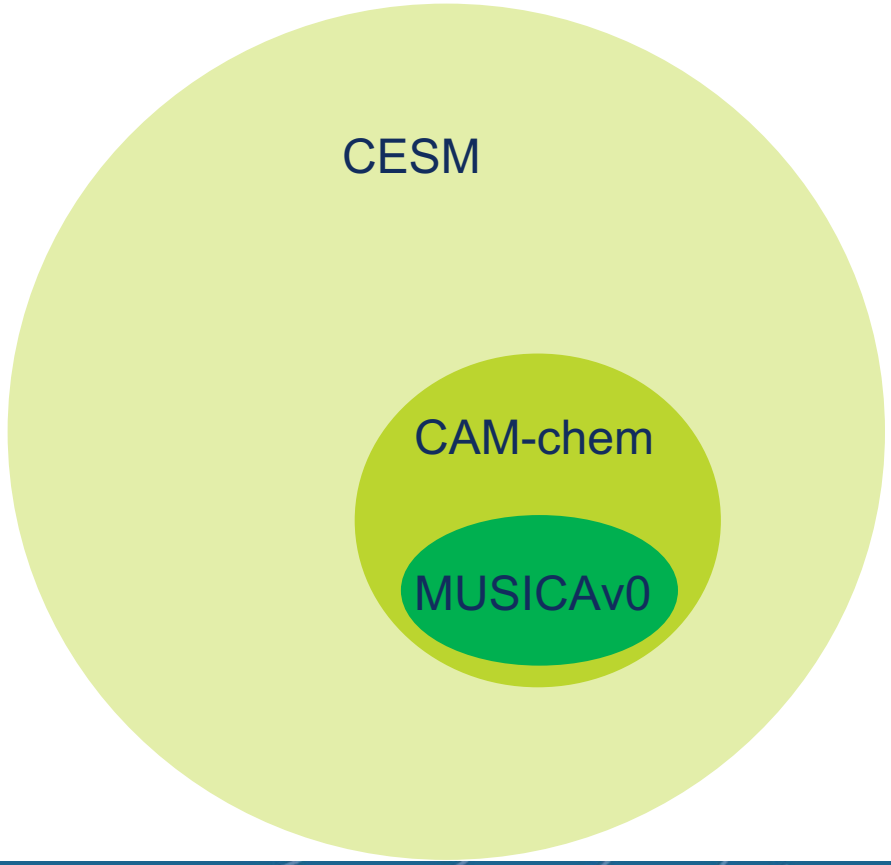
CAM-chem is a component of CESM.



MUSICA version 0 (MUSICAv0)

MUSICAv0 = CAM-chem-SE-RR

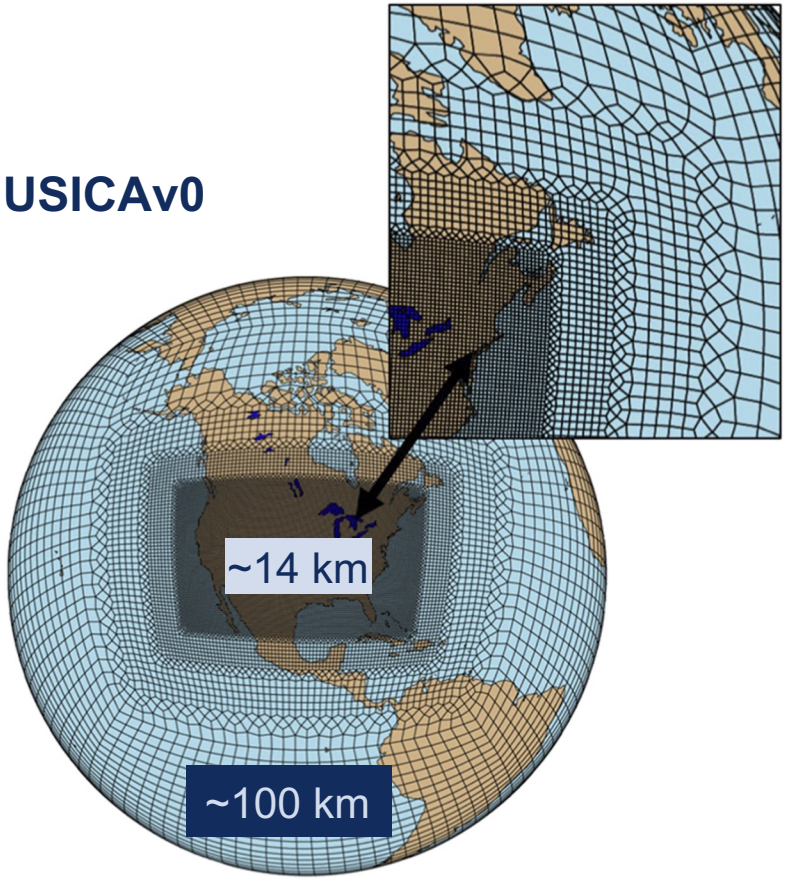
MUSICAv0 is **CAM-chem**
With Spectral Element (SE) dynamical core and
Regional Refinement (RR)
→ **CAM-chem-SE-RR**



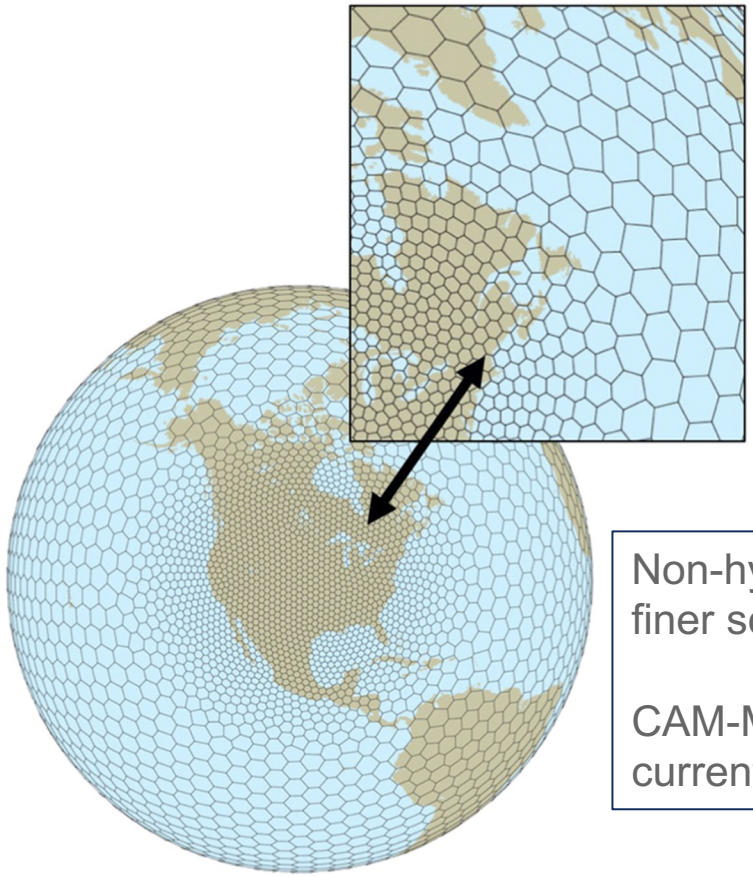
Choices for variable resolution atmosphere models

Spectral Element
(SE - cubed sphere)

MUSICAv0



Model for Prediction Across Scales
(MPAS - hexagonal mesh)



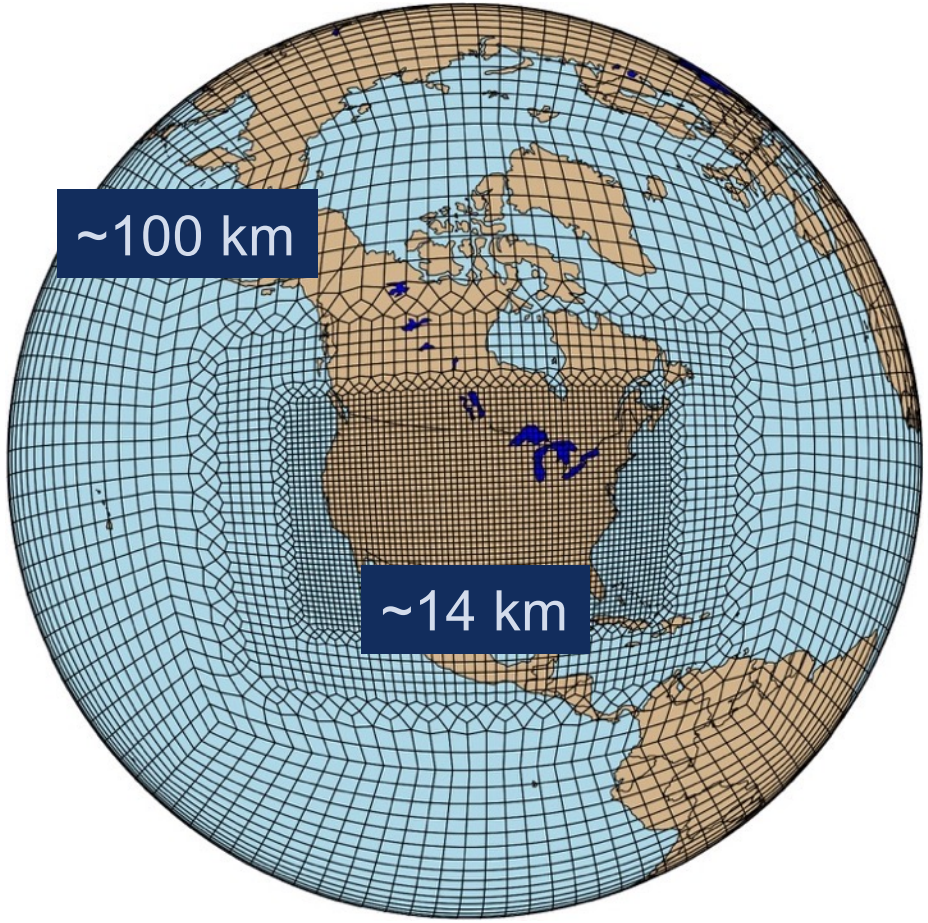
MUSICAv1
(in development)

Non-hydrostatic allowing for finer scales (< 1km)

CAM-MPAS, CAM-MPAS-chem currently being tested

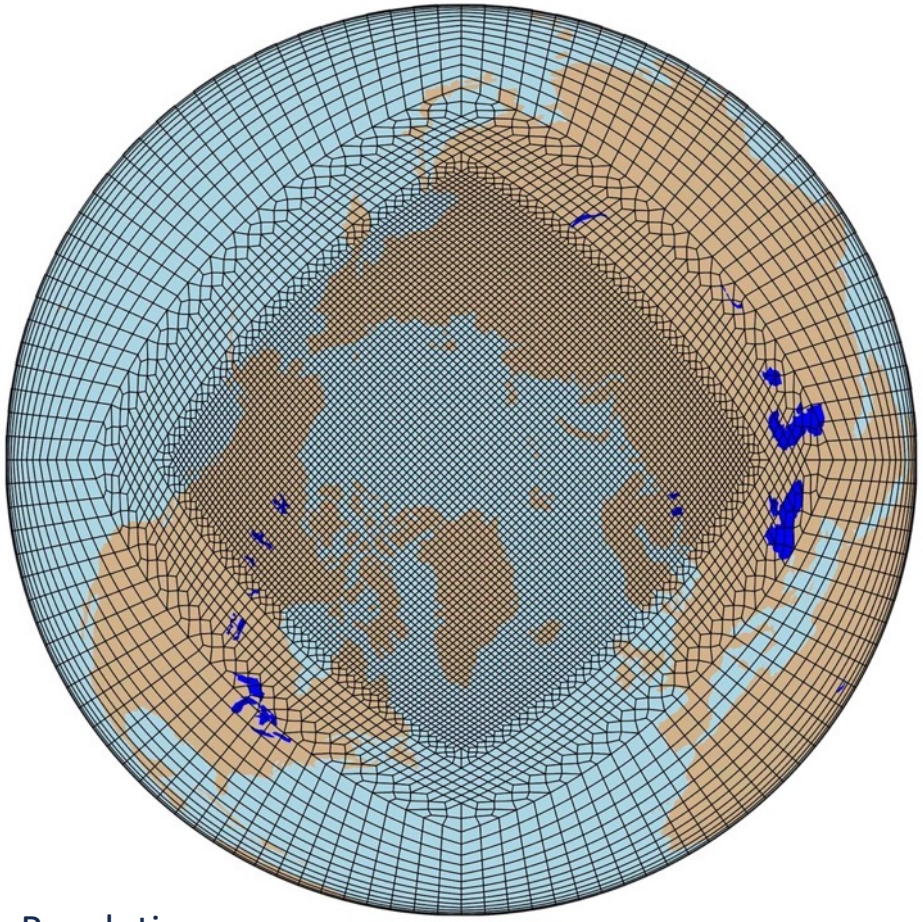
Grids Available in CESM (v2.2 and later)

CONUS



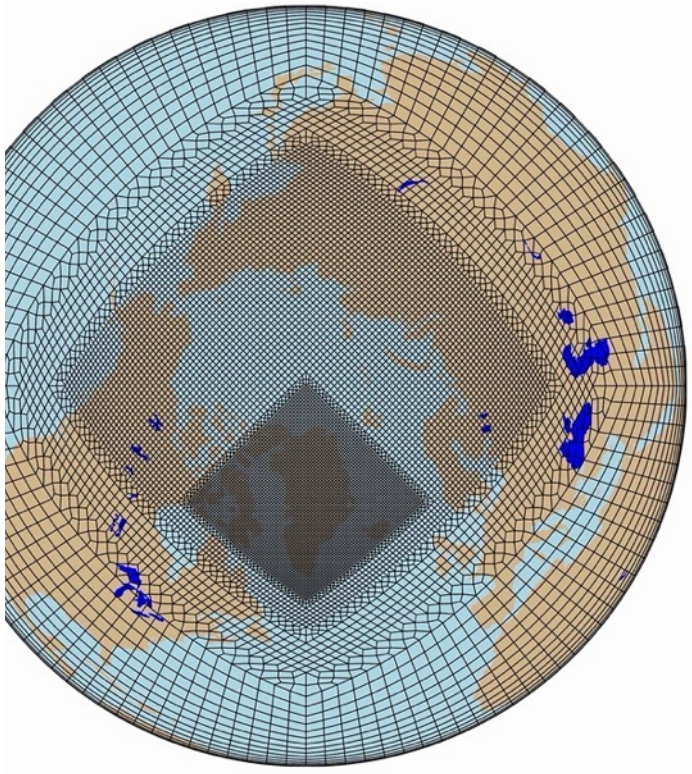
Resolution:
ne0CONUSne30x8_ne0CONUSne30x8_mt12

ARCTIC



Resolution:
ne0ARCTICne30x4_ne0ARCTICne30x4_mt12

ARCTICGRIS
(Greenland Ice Sheet)



Resolution:
ne0ARCTICGRISne30x8_ne0ARCTICGRISne30x8_mt12

Refined Grids Available for Many Regions

https://wiki.ucar.edu/display/MUSICA/Available+Grids

Pages / MUSICA Home

Available Grids

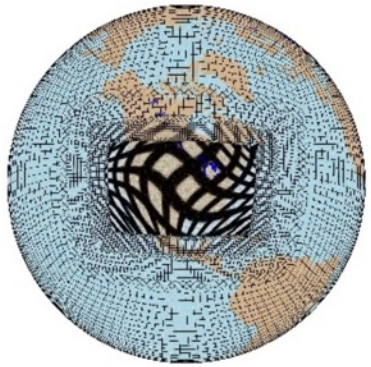
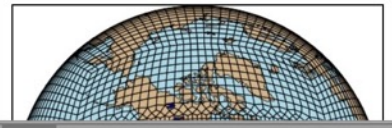
Created by Louisa Emmons, last modified on Nov 16, 2023

A number of grids have been created by various users for use in MUSICAv0 which we list here to demonstrate the diverse capability of MUSICAv0. The CONUS ne30x8 and ARCTIC grids are available resolutions in CESM2.2, but the other grids have been developed for various science applications which have not yet been published. In the future we plan to have a public repository of grids, or may provide some grids in future model results.

Protocol: Please contact the developer of the grid if you are interested it in using it and include them as co-author of any work using that grid.

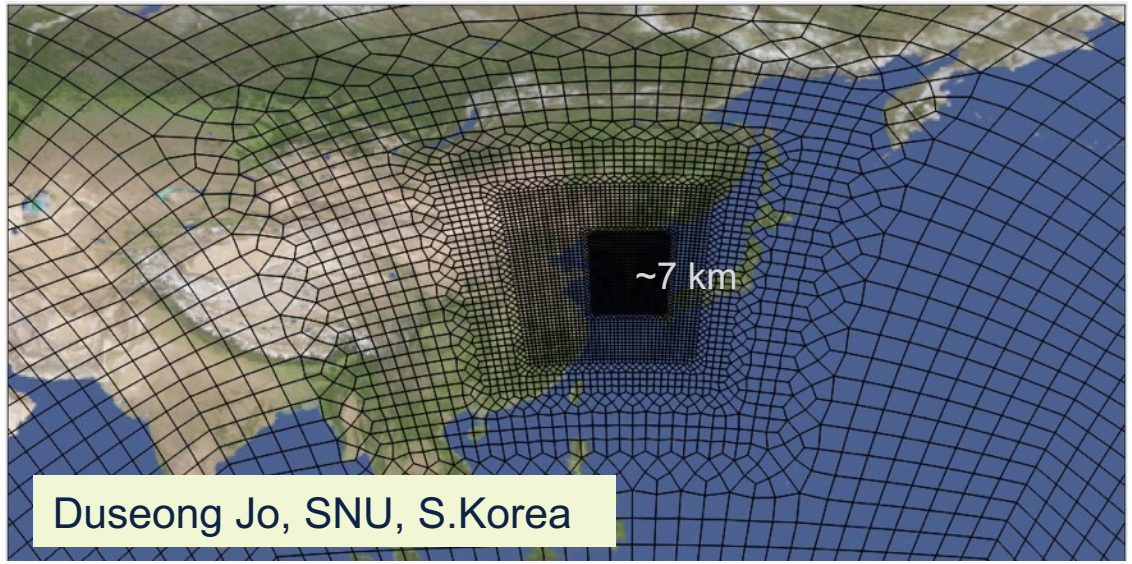
Emissions may be available for sharing for these grids - contact the grid developers. We will develop a public repository for those as well.

The grid resolutions (e.g., ne30x{N}) are defined at the bottom of this page.

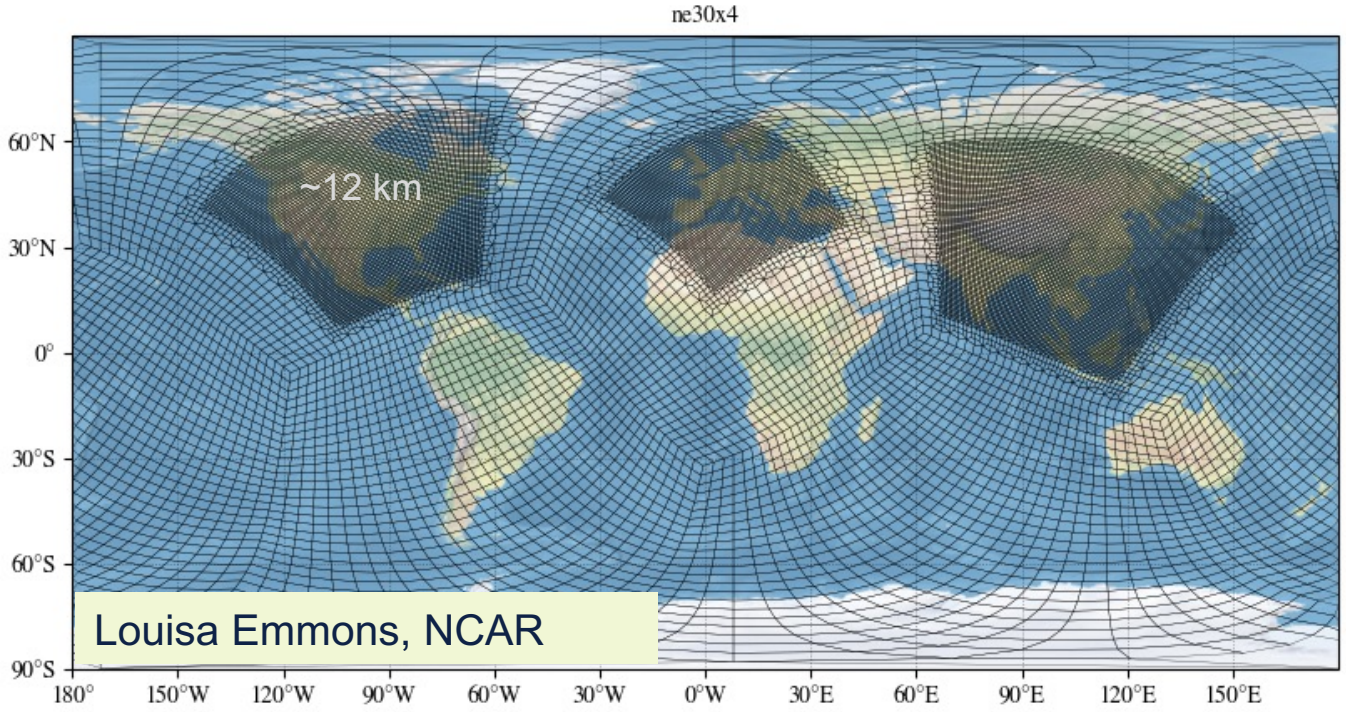
Refined region	Resolution, Repository, Contact	Image (click for full size)
CONUS 1/8 degree (14 km)	Resolution: ne0CONUSne30x8_ne0CONUSne30x8_mt12 Repository: part of CESM2.2 (CAM User's Guide) Output from community simulation - DOI: https://doi.org/10.5065/tgbj-yv18 Publications: • Schwantes, R. et al., JAMES, in press. • Tang, Wenfu, et al., JGR-Atmospheres, in review.	
CONUS 1/4 degree (28 km)	Resolution: ne0np4.CONUS.ne30x4_mt12 Repository: /glade/campaign/acom/acom-weather/MUSICA/musica_repo/ne0np4.CONUS.ne30x4 Contact: Louisa Emmons, NCAR/ACOM	

Screenshot

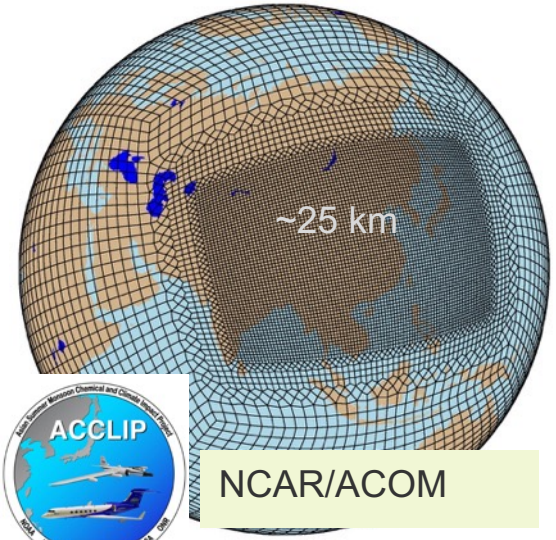
Custom Grids



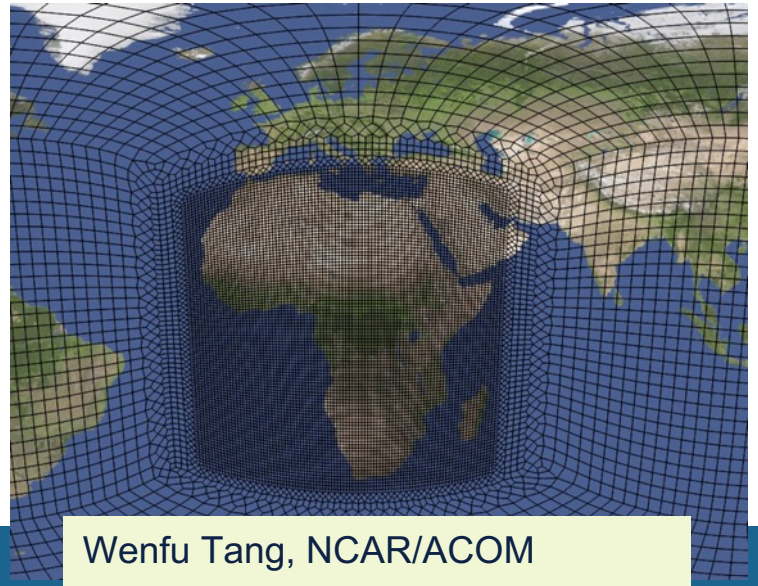
Duseong Jo, SNU, S.Korea



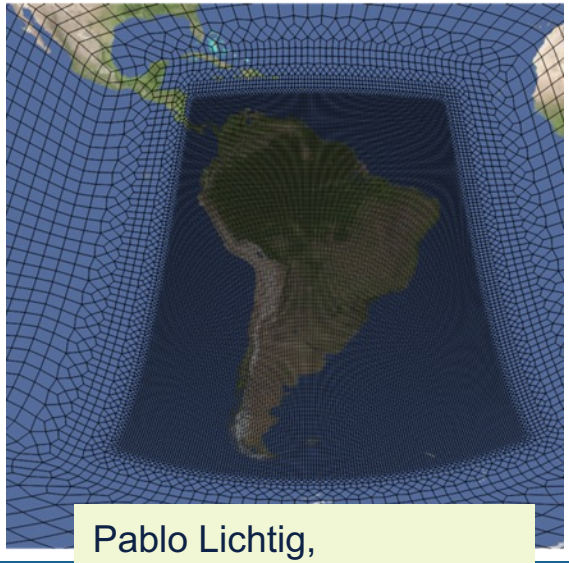
Louisa Emmons, NCAR



NCAR/ACOM



Wenfu Tang, NCAR/ACOM

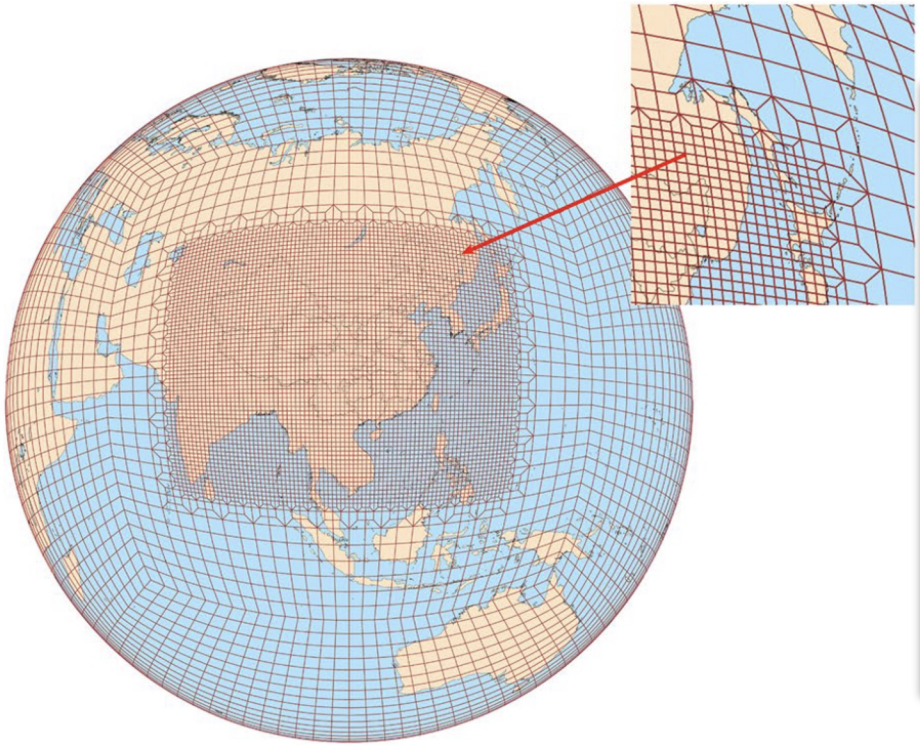


Pablo Lichtig,
CNEA, Argentina

Rebecca Buchholz,
NCAR/ACOM

NCAR
UCAR

Example of MUSICAv0 application



AGU ADVANCING EARTH AND SPACE SCIENCES

JGR Atmospheres

RESEARCH ARTICLE
10.1029/2023JD039130

Key Points:

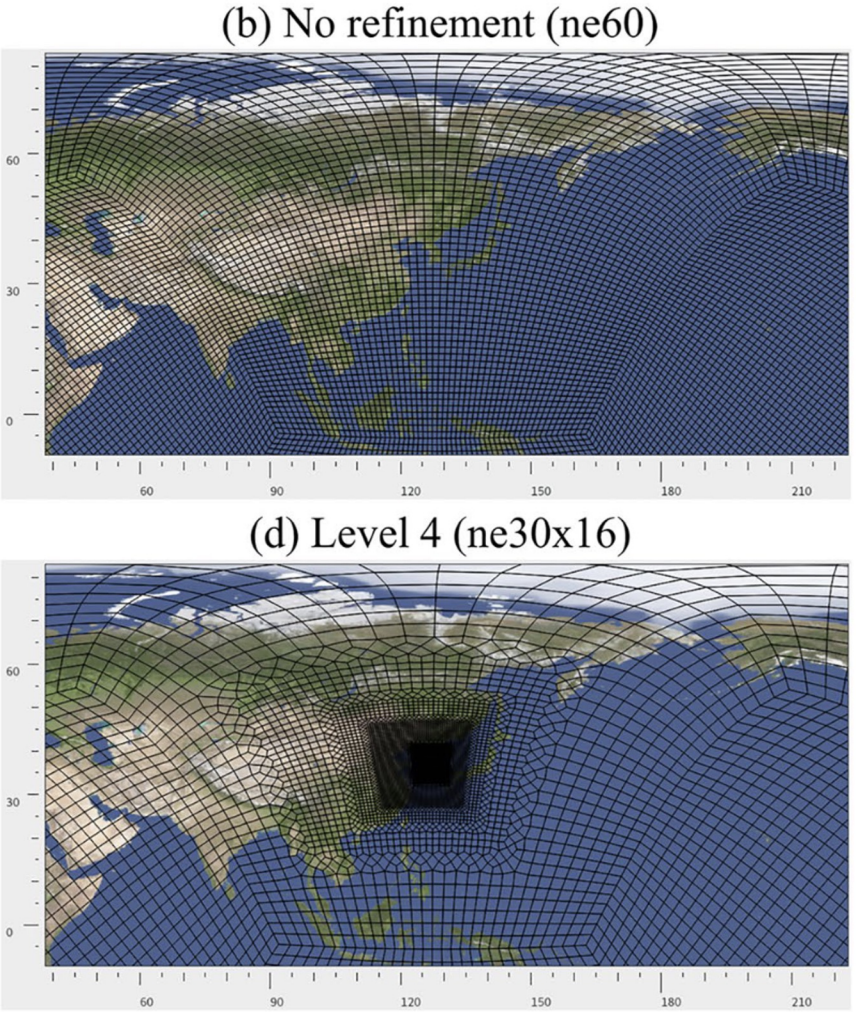
- The MUSICAv0 model with regional refinement over East Asia improves haze event simulations, especially in complex terrain areas
- Finer grids can resolve a greater range of NO_x and volatile organic compounds (VOC) chemical regimes, significantly reducing the ozone overestimation in coarser grids

Modeling the Air Pollution and Aerosol-PBL Interactions Over China Using a Variable-Resolution Global Model

Man Yue[1,2], Xinyi Dong[1], Minghuai Wang[1], Louisa K. Emmons[3], Yuan Liang[1], Dan Tong[4], Yawen Liu[1], and Yaman Liu[1]

[1]School of Atmospheric Sciences, Nanjing University, Nanjing, China, [2]Zhejiang Institute of Meteorological Sciences, Hangzhou, China, [3]Atmospheric Chemistry Observations & Modeling Laboratory, National Center for Atmospheric Research, Boulder, CO, USA, [4]Department of Earth System Science, Ministry of Education Key Laboratory for Earth System Modeling, Institute for Global Change Studies, Tsinghua University, Beijing, China

Example of MUSICAv0 application



AGU ADVANCING EARTH AND SPACE SCIENCE

JAMES | Journal of Advances in Modeling Earth Systems

RESEARCH ARTICLE
10.1029/2022MS003458

Key Points:

- The dependence of simulated chemical species on model resolution is quantified in a single modeling framework
- Model evaluations can be substantially affected by grid resolution, especially for urban surface and aircraft measurements at low altitudes
- Grid resolution strongly impacts the oxidation of volatile organic compounds through differences in diurnal variation of oxidants

Supporting Information:

Supporting Information may be found in the online version of this article.

Correspondence to:

D. S. Jo,
cdswk@ucar.edu

Comparison of Urban Air Quality Simulations During the KORUS-AQ Campaign With Regionally Refined Versus Global Uniform Grids in the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) Version 0

Duseong S. Jo[1,2], Louisa K. Emmons[1], Patrick Callaghan[3], Simone Tilmes[1], Jung-Hun Woo[4], Younha Kim[5], Jinseok Kim[4], Claire Granier[6,7], Antonin Soulié[6], Thierno Doumbia[6], Sabine Darras[8], Rebecca R. Buchholz[1], Isobel J. Simpson[9], Donald R. Blake[9], Armin Wisthaler[10,11], Jason R. Schroeder[12,13], Alan Fried[14], and Yugo Kanaya[15]

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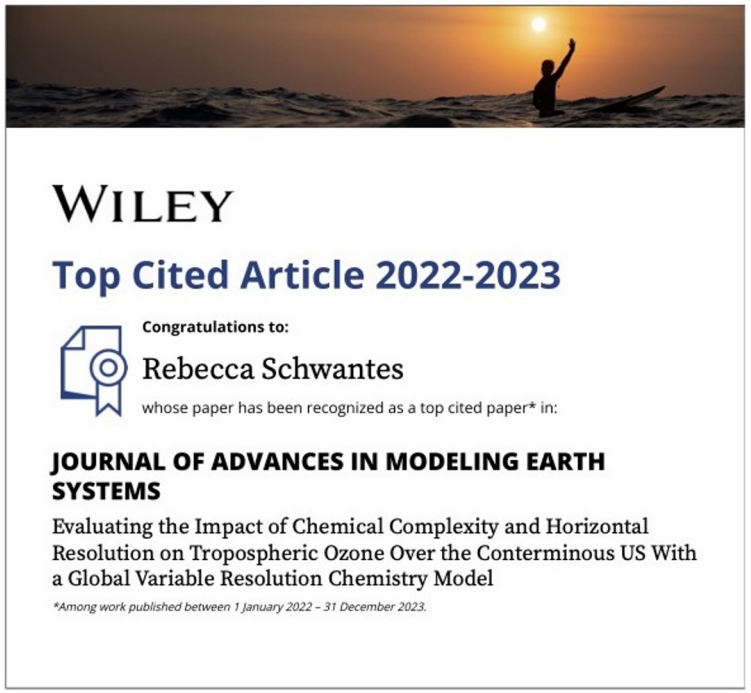
MUSICAv0 Publications

https://www2.acom.ucar.edu/sections/musica-publications



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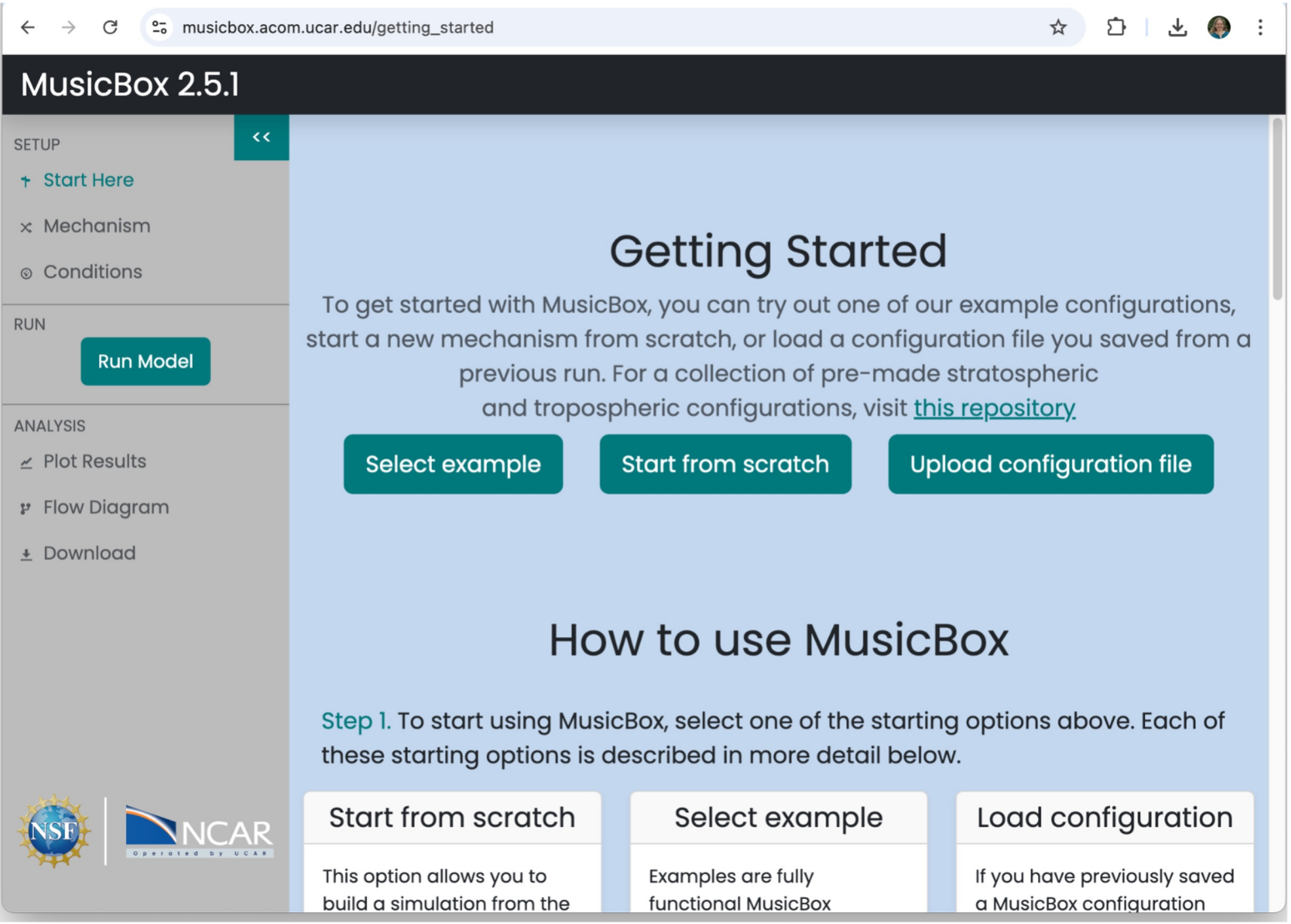
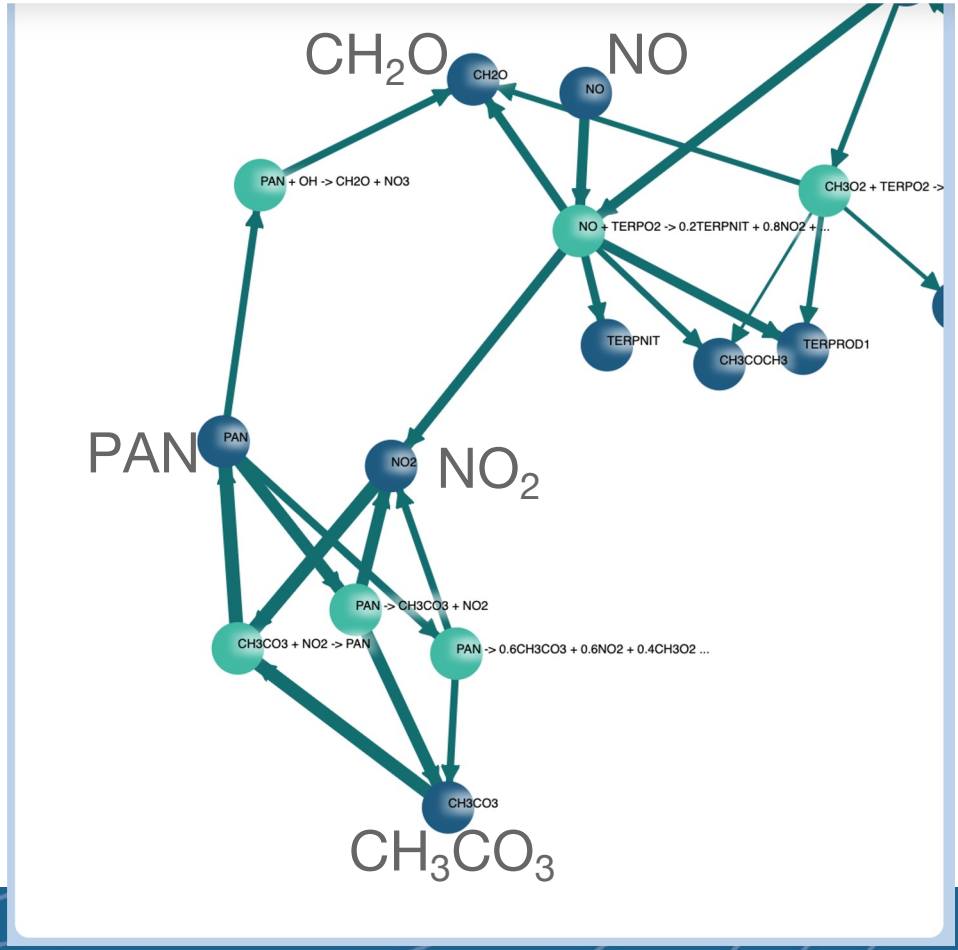
MusicBox: https://musicbox.acom.ucar.edu/





MELODIES MONET: https://melodies-monet.readthedocs.io/

A python model evaluation framework for comparing observations & model results

MELODIES-MONET
Configuration file
- Define comparisons and analysis
- Call driver script
- Python notebook workflow
- Development scripts

YAML configuration file

MONET I/O
Model Object Preparation
- Reads global attributes, grid and variables
- Converts time, latitudes and longitudes

Read model

MONET I/O
Measurement Object preparation
- Retrieves data if necessary and possible (url, OpenDap, Amazon cloud)
- Converts to netCDF if necessary
- Reads and

Read obs

MONET
Pairing and Processing Objects
- Pairs observations and mode
- Methods for visualization and

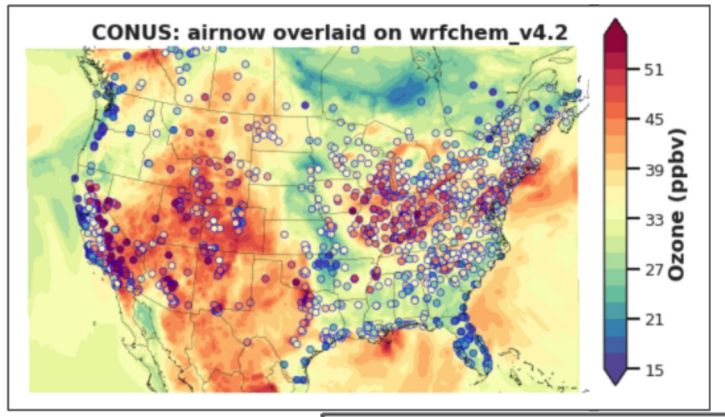
Match model to obs

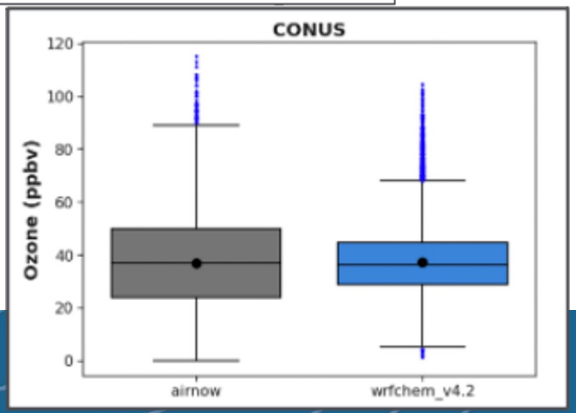
Goal: Output that can be browsed in a html page format

Plots, statistics

Python (Xarray, NumPy, SciPy, Pandas, …)

Obs:
surface, aircraft, satellite, …
Models:
MUSICAv0, WRF-Chem, CMAQ, …





Tutorial Schedule

Friday afternoon:

- Lecture: How to run CESM & MUSICAv0
- Hands-on: Running CESM
- Hands-on: Plotting CESM output (unstructured grids)

Saturday morning:

- Lecture: How to create your own grid
- Hands-on: Creating a grid

Saturday afternoon:

- Creating input files for new grid
- Continue creating a grid and plotting output