Multi-scale modeling of air quality and mechanism comparison with MUSICA

MUSICA: the MUlti-Scale Infrastructure for Chemistry and Aerosols

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Motivation for a new modeling infrastructure

- To aid decision-makers, atmospheric chemistry models need to:
  - Couple with other Earth system components
  - Cover scales from urban/local to regional to global
  - Extend from surface to top of atmosphere
  - Predict on time scales from hours – weeks – seasonal – decadal
  - Connect atmospheric composition with weather and climate

- Future modeling systems will need the ability to:
  - Change spatial scales in a consistent manner
  - Resolve multiple spatial scales in a single simulation
  - Couple model components that represent different Earth system processes
  - Easily mix and match model components for specific applications

Past and Current Approach	Future Approach including MUSICA
Impacts of the Asian monsoon on weather and climate	
Hemispheric to global impacts without resolving convection or surface air quality over the monsoon region.	More realistic predictions by resolving local air quality and convection in monsoon region consistently with global impacts.
Exploiting the future constellation of geostationary satellites for atmospheric composition	
Global analysis at resolutions coarser than that of observations or regional analysis without considering	Matching measurement resolution over the key regions together with global feedbacks results in more seamless
troposphere–lower stratosphere or regional models dependent on boundary conditions.	fold regions will allow better representation of frontal passages and the filaments associated with intrusions.
Global models providing bounda regional models only consider on are inconsistent in nature.	
Coarse vertical and spatial resolu numerical diffusion prevents simu structure of the troposphere.	
Aerosols seeding extreme events (e.g., hurricanes)	
High resolution over impact regions but coarse resolution over aerosol source regions and/or from lateral boundary conditions leads to poor aerosol prediction and affects feedback on extreme event predictions.	High resolution enabled over impacts and aerosol source regions in a consistent framework with fully enabled feedback of meteorology, chemistry, and dynamics and between ocean and atmosphere.
Feedback loop of climate change on trace gas and aerosol gas concentrations	
Global simulations with coarse resolution over high-emissions regions impact the accuracy of simulated pollutant life cycles and land–sea–atmosphere exchange.	Global feedbacks with increased spatial resolution over high-emission regions better represent the life cycles of short-lived pollutants and land–sea–atmosphere exchange.

Effect of megacities on global atmospheric composition and climate

Disconnected spatial and temporal scales, separate models for local/regional and global impacts.

A fully coupled system accounts for detailed chemistry/ emissions over megacities, and enables quantifying their impacts on remote regions (e.g., Arctic) and the global atmosphere.

Air quality (AQ) under a changing climate

Use downscaling methods to provide meteorological and chemical initial and boundary conditions to a regional AQ model.

Conduct an ensemble of simulations under various future scenarios with a single self-consistent model with sufficient resolution to simulate key AQ metrics.

Gravity wave processes impacting stratosphere and mesosphere temperature and mixing	
Global simulations with general circulation, chemistry, and climate dependent on parameterized wave sources, characteristics, and transport; or costly high-resolution "nature runs."	Better resolution of the gravity wave spectrum within the refined region and a more internally consistent gravity wave parameterization on the global grid.
Effect of megacities on global atmospheric composition and climate	
	system accounts for detailed chemistry/ megacities, and enables quantifying their ote regions (e.g., Arctic) and the global
	valuation
	-developed as integral part of MUSICA tive of updating concentrations and inputs s) efficiently. Commonalities between DA will be addressed in parallel.
Air quality (AQ) under a changing climate	
Top-down emission estimates	
Either coarse resolution or inconsistency in modeling and emissions when constraining sources and sinks of long-lived species.	Improved accuracy and consistency by simulating transport and chemistry of long-lived species consistently across all scales.
Land surface coupling	
Coarser-resolution climate models are limited in their representation of land–atmosphere couplings, such as biogenic emissions and dry deposition of atmospheric constituents. Many regional models lack full coupling between land and atmosphere processes.	Land–atmosphere coupling and regionally finer resolution improves representation of meteorology, biogenic emissions and wet and dry deposition (e.g., simulating effect of acid rain on vegetation).

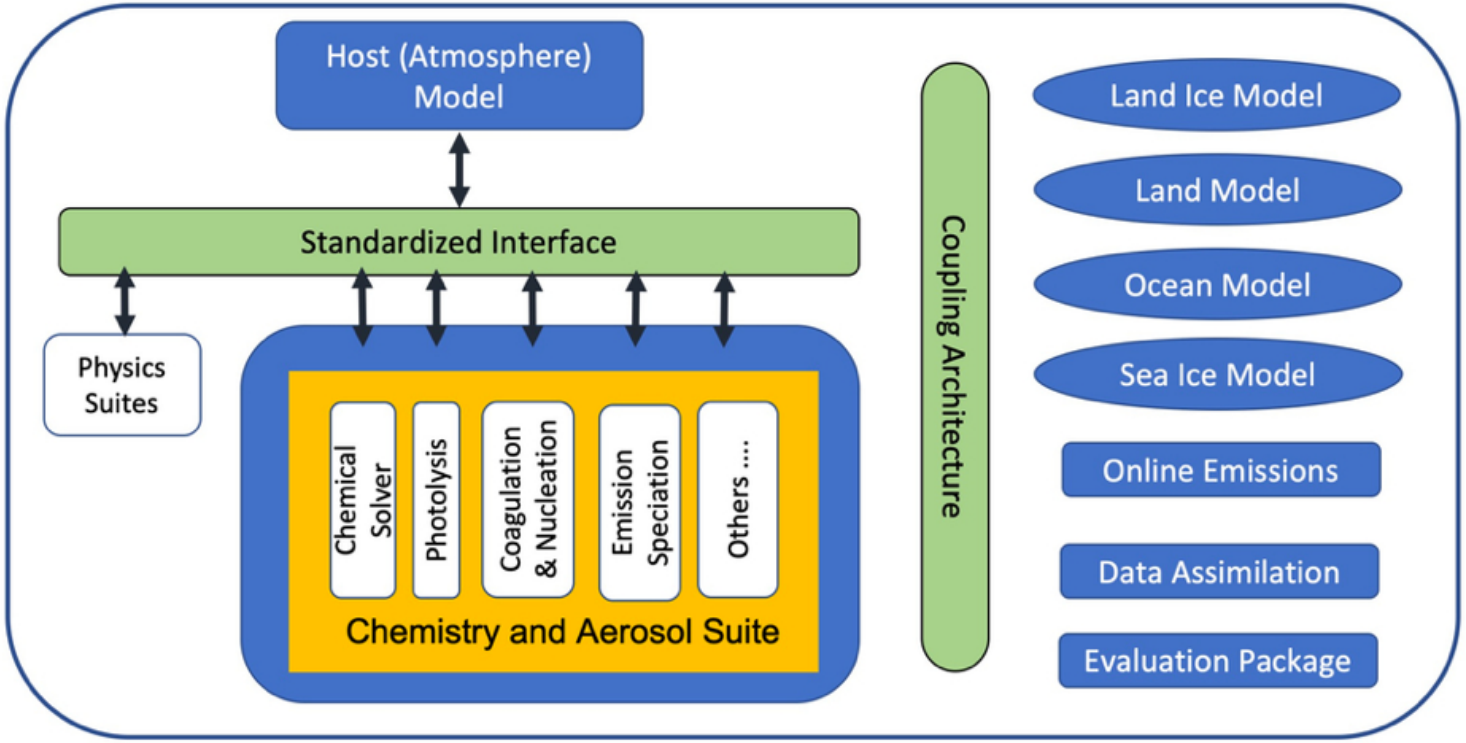
Pfister et al., BAMS, 2020

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



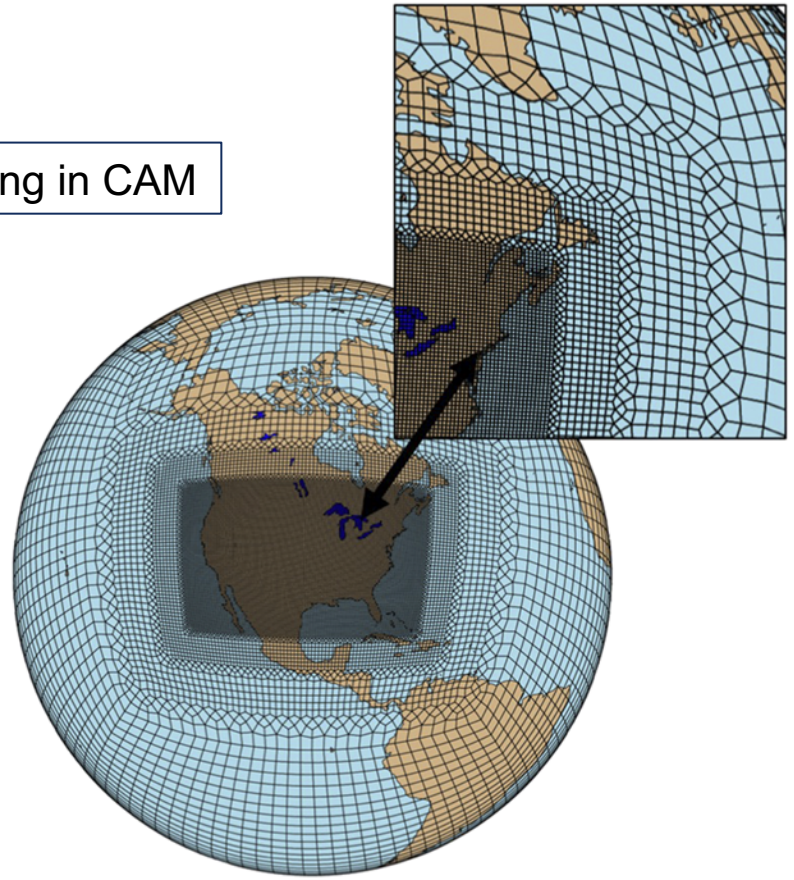
https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica

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

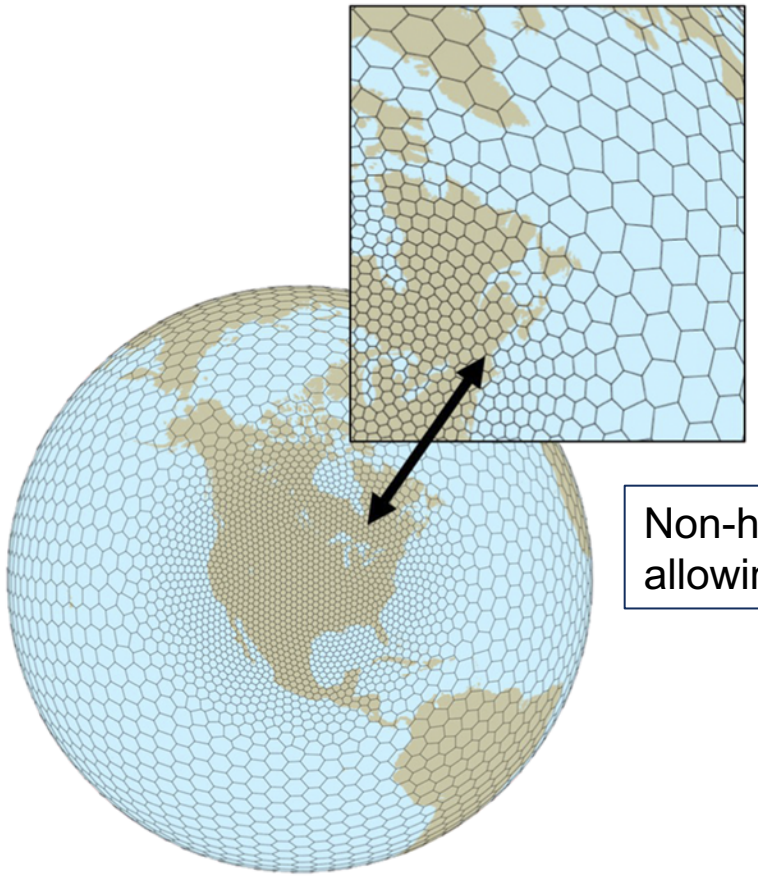
Choices for variable resolution atmosphere models

Spectral Element
(cubed sphere)

Currently running in CAM



MPAS
(hexagonal mesh)



Non-hydrostatic
allowing for finer scales

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

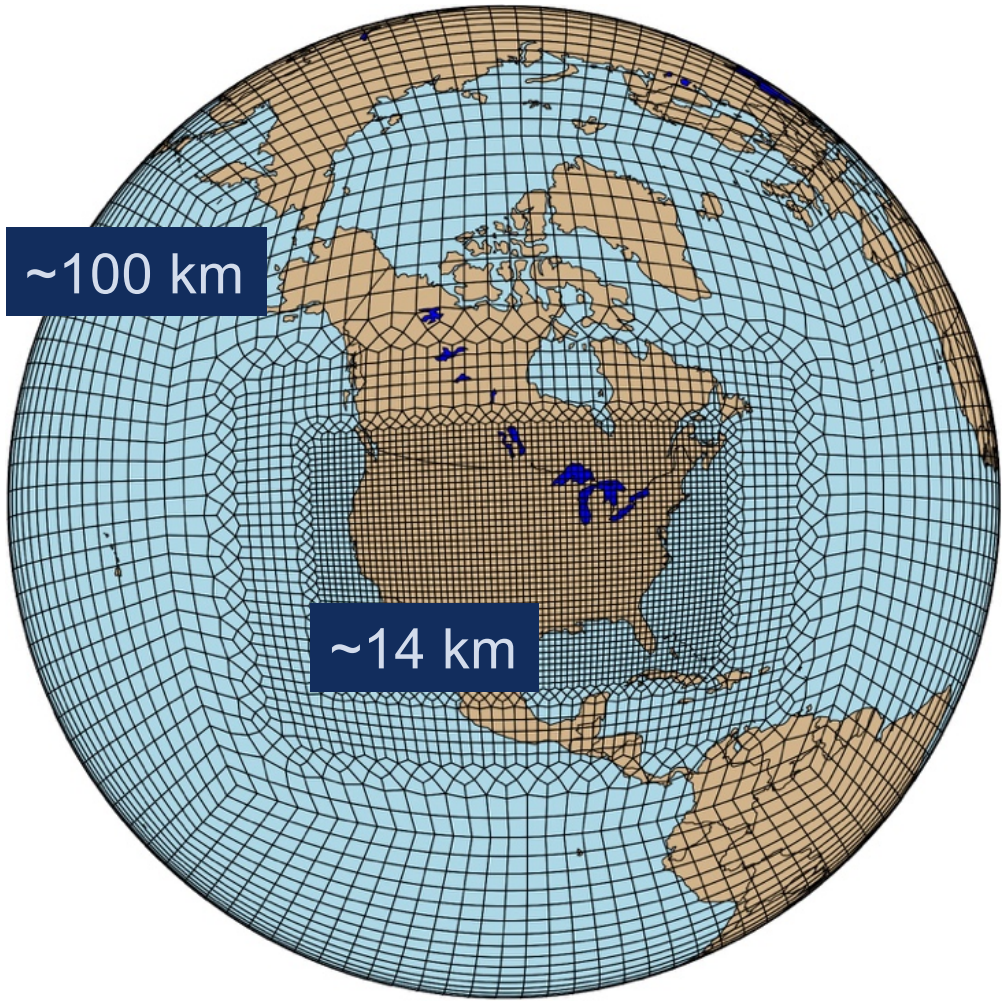
Working groups:

- 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

MUSICA-V0 - released in CESM2.2



MUSICA-V0 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

Pollutants are simulated on human exposure-relevant scales

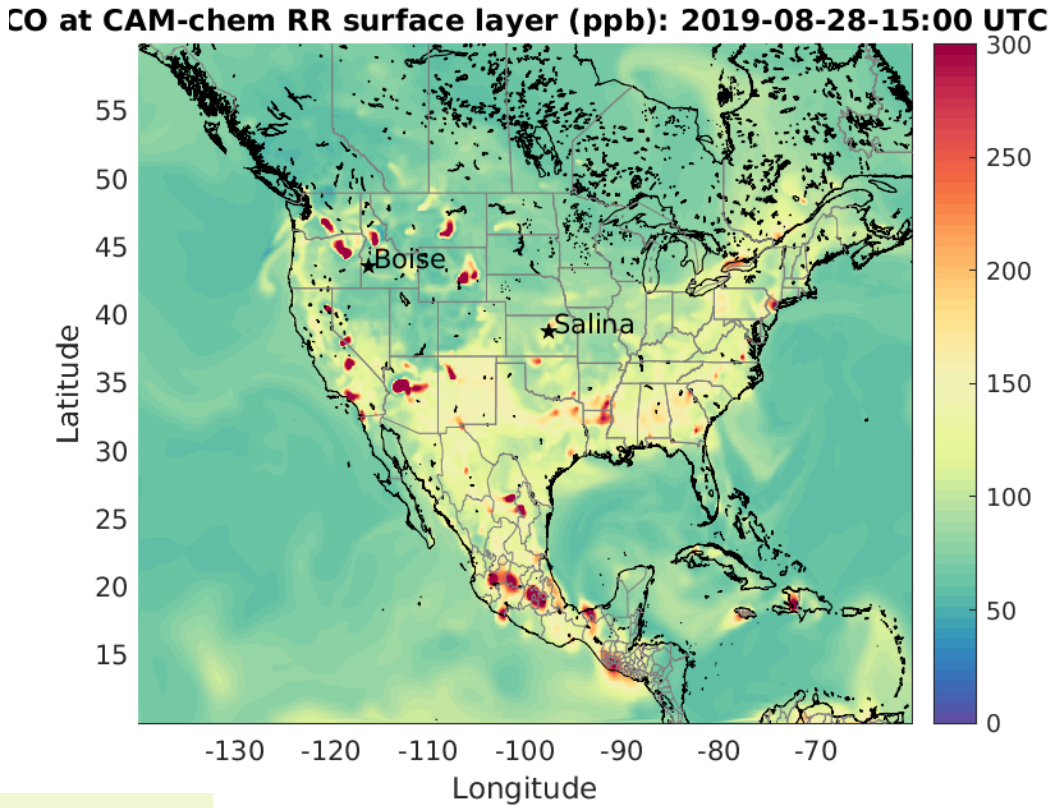
Global feedbacks are directly included

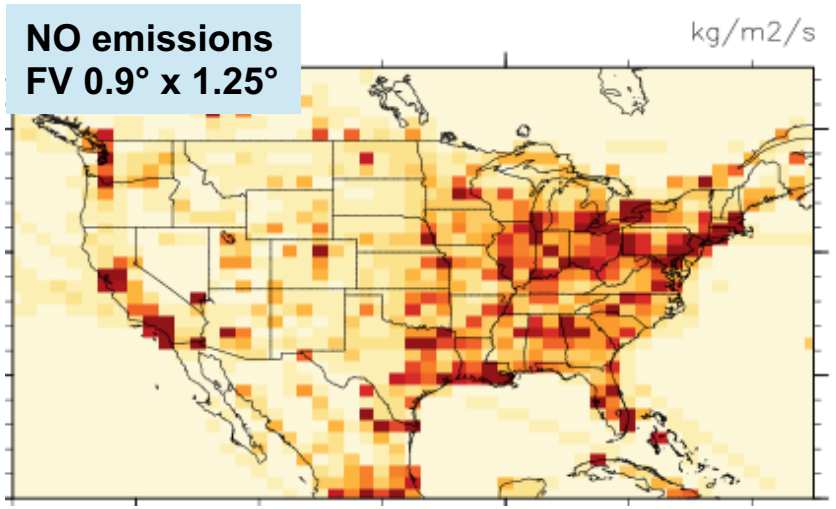
Most of the grid points are in refined region, so no additional cost to simulate the whole globe

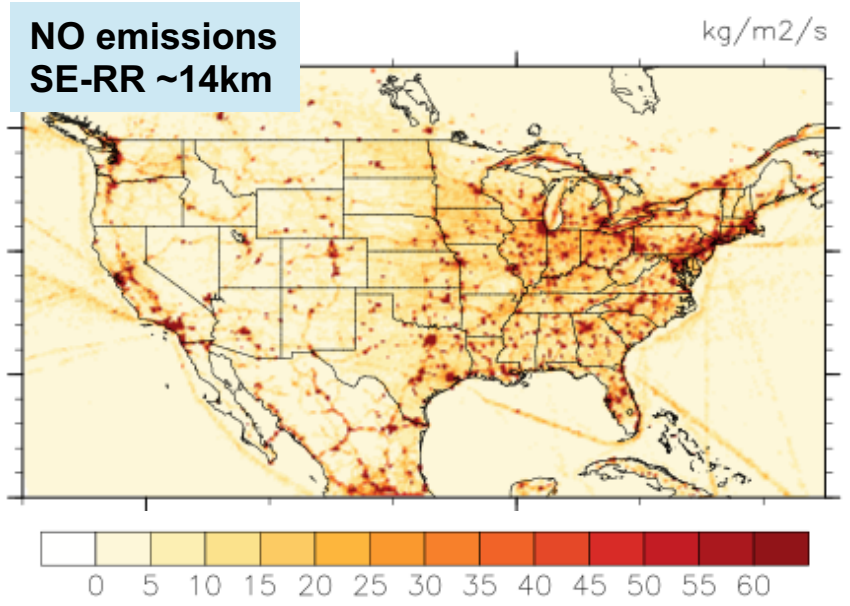
MUSICAv0

Air quality simulations are improved with emissions on more realistic scale

- Segregates urban and rural emissions
- Represents fire plumes







Wenfu Tang, NCAR/ASP

Impact of resolution on chemistry

1/8-degree (~14 km) compared to 1-degree (~100 km) over continental US:

Hourly output of surface ozone – Aug 9, 2013 18Z

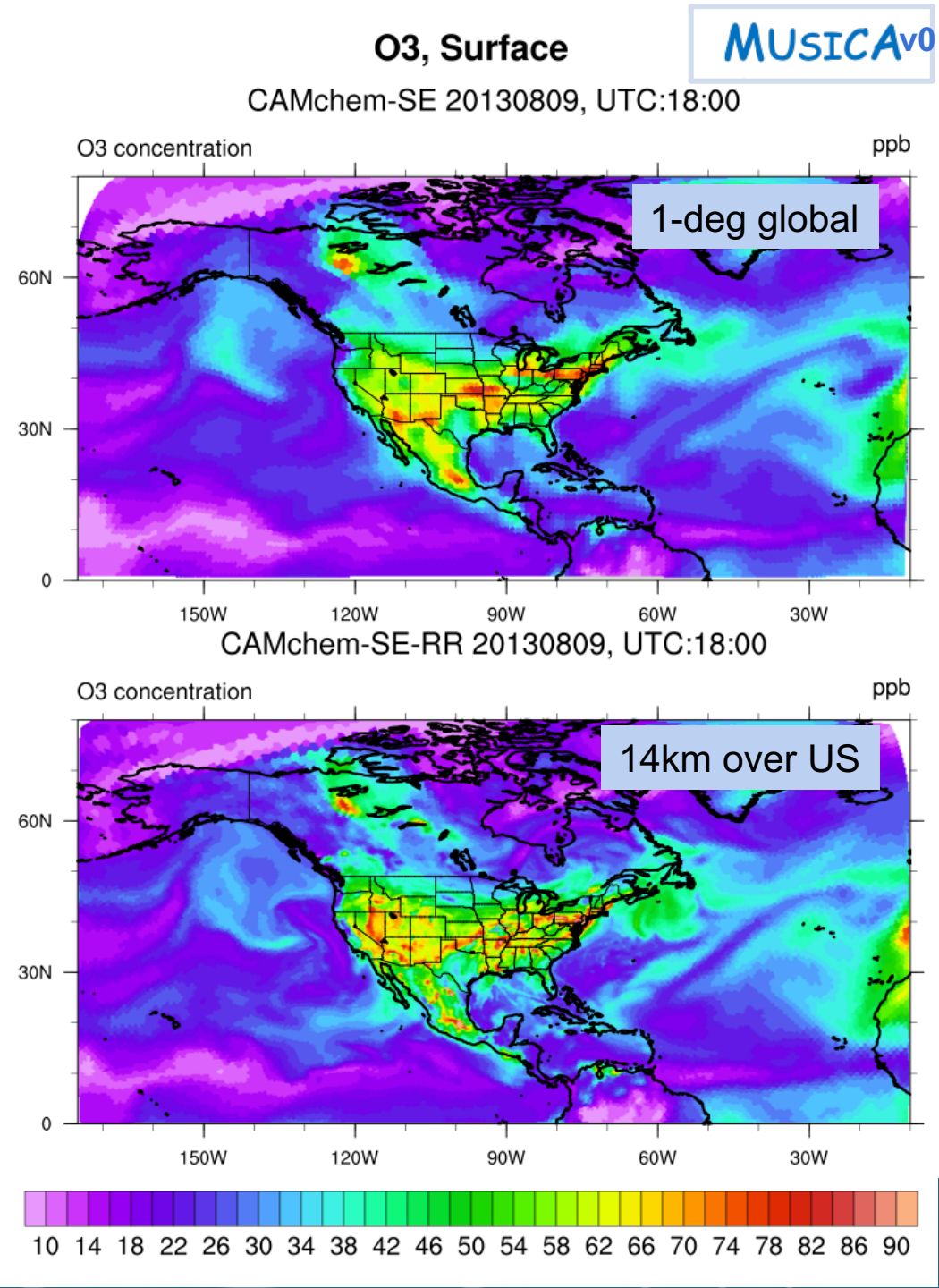
- General features of distribution the same in RR as 1-deg
- Urban pollution more resolved, with lower ozone in rural regions
- Higher ozone mixing ratios in continental outflow (over Atlantic, Gulf of Mexico, Baja California)

This configuration is available in CESM2.2

Model description and evaluation papers in prep. by Becky Schwantes and Forrest Lacey

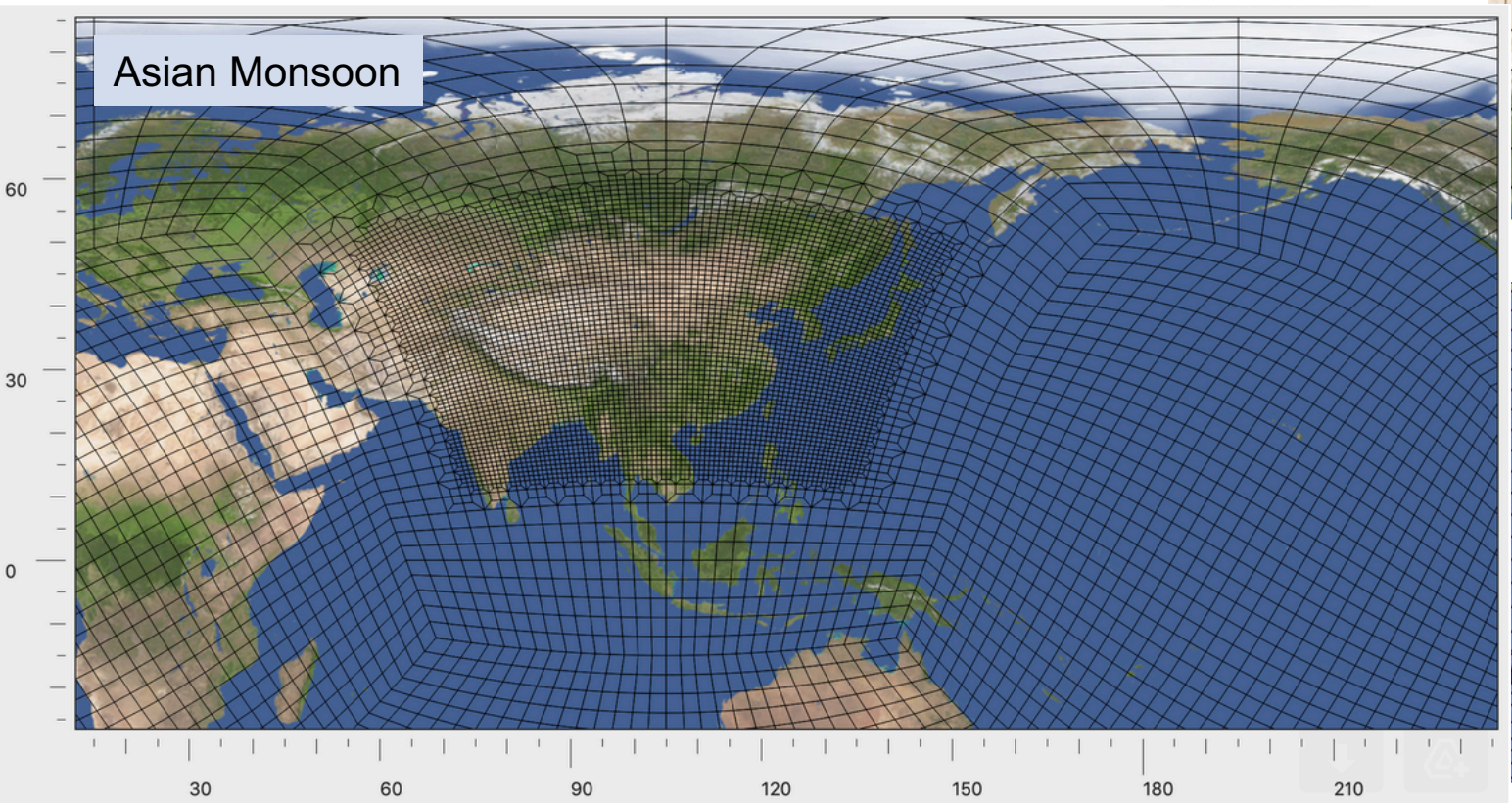
Online tutorial is being developed:

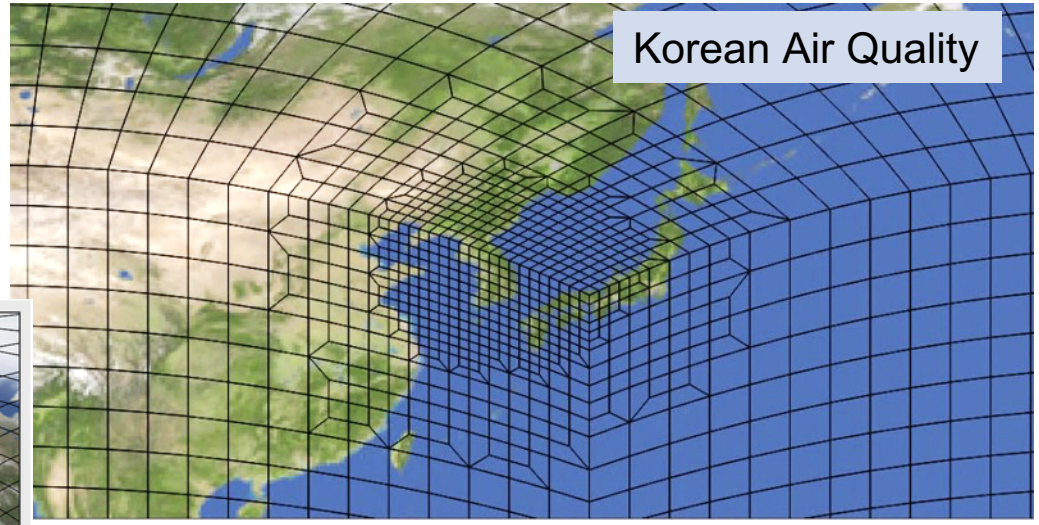
https://www2.acom.ucar.edu/workshop/musica-tutorial-2020

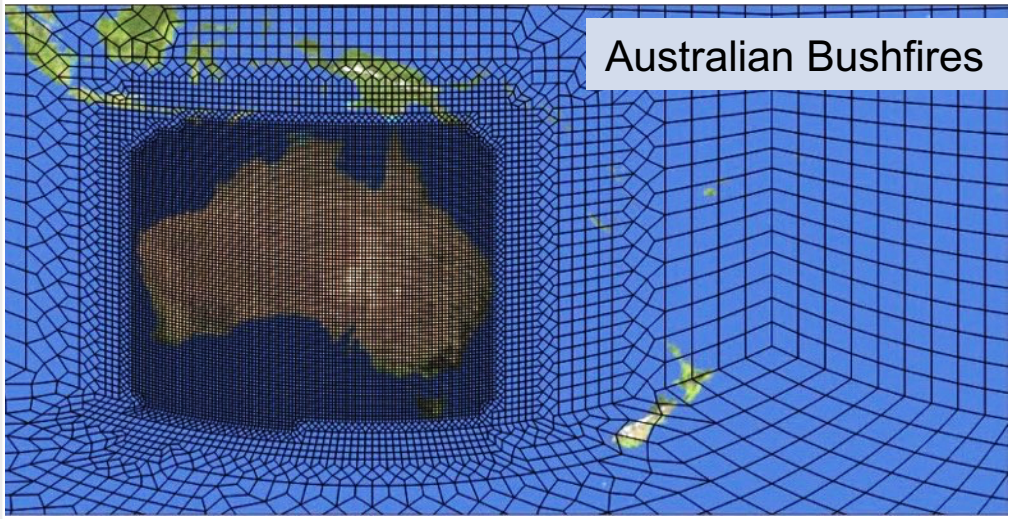


MUSICA-V0 User-specified Grids

Tools released with CESM allow users to create grids with arbitrary refined regions for use in MUSICA-V0







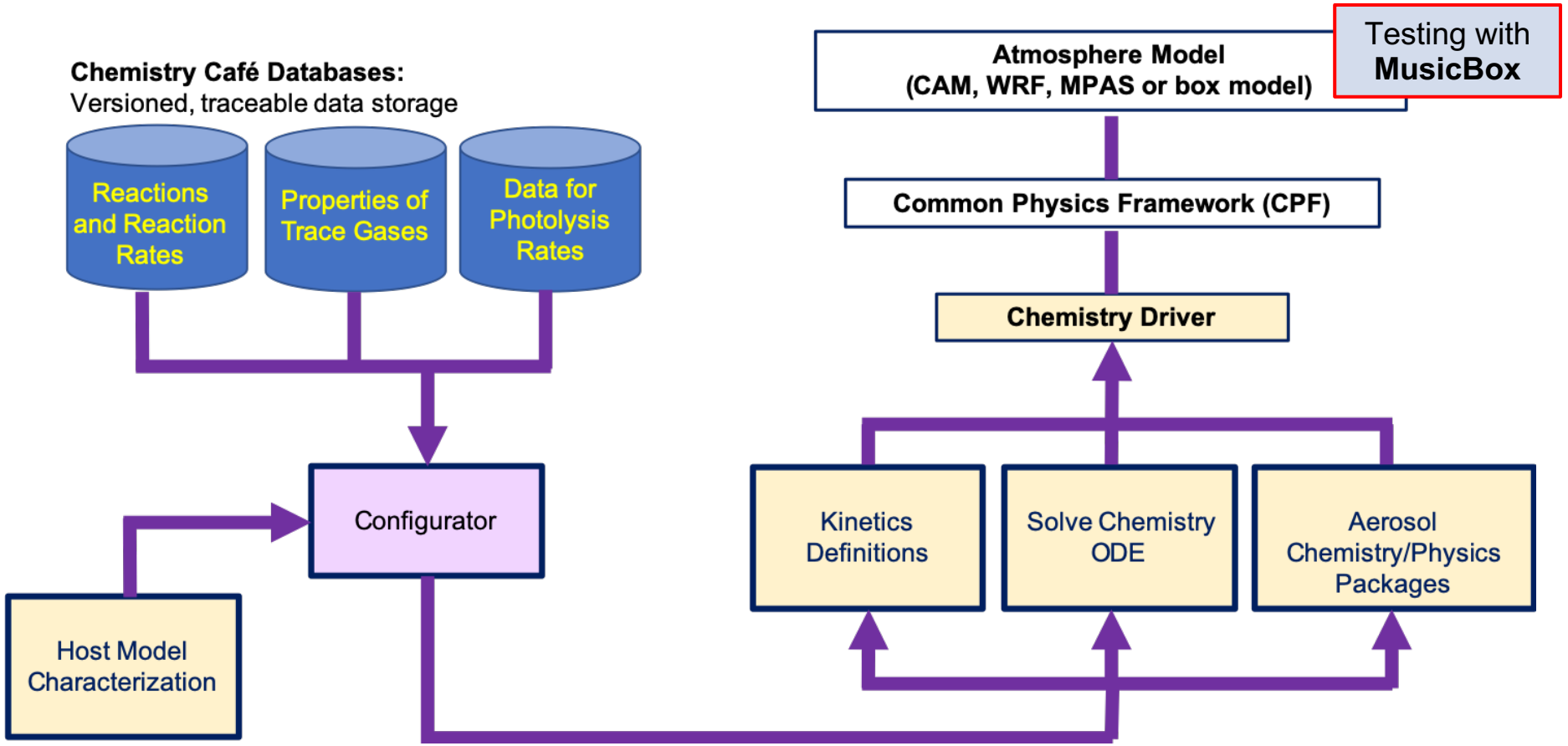
Model-Independent Chemistry Module (MICM)

MUSICA

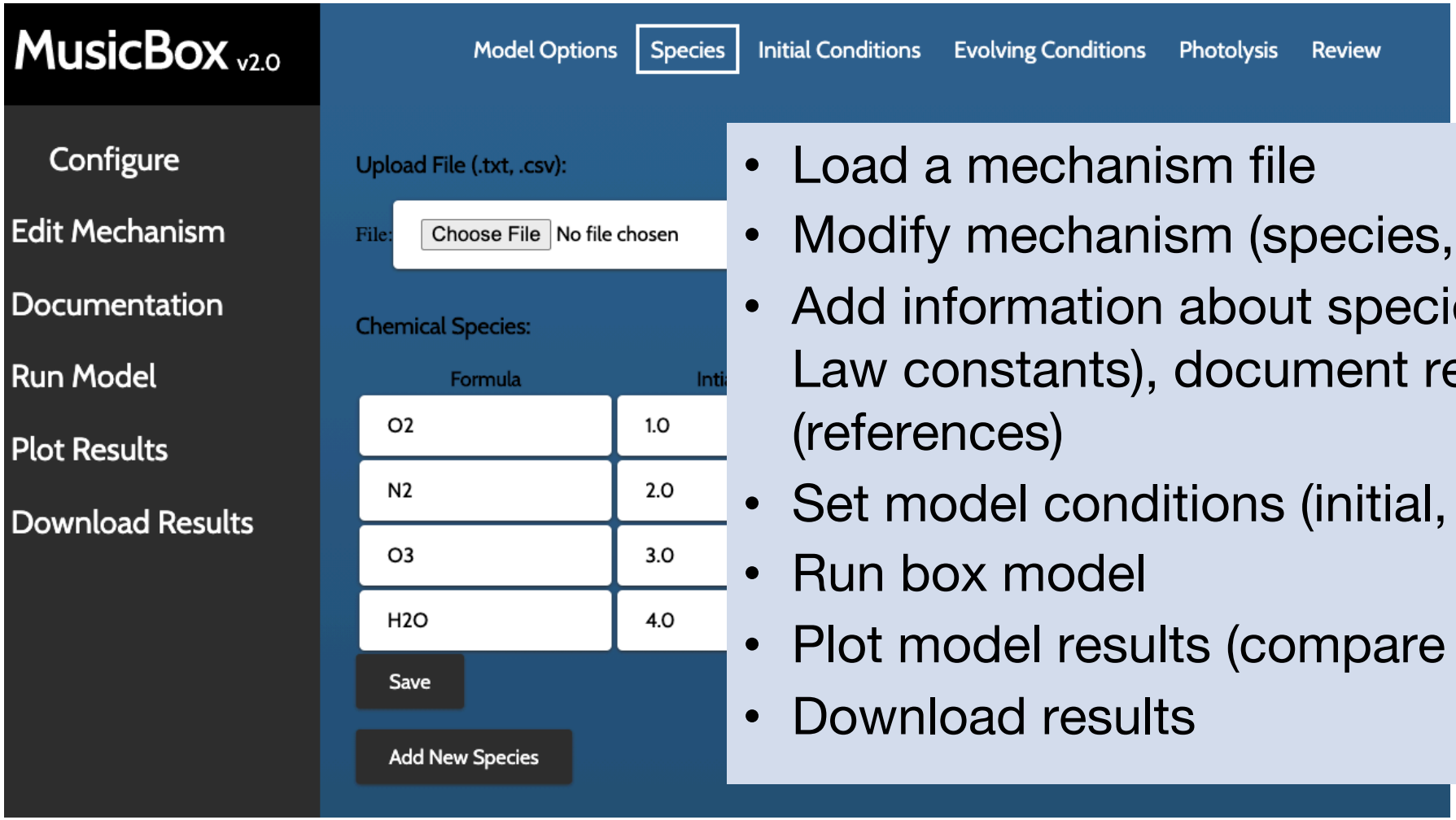
Will allow use of the same chemistry in different atmosphere models and offline meteorology (CTM)

Also allows easily changing the chemical mechanism

A box model using MICM is being developed: **MusicBox**



MusicBox: MICM in a box model



- Load a mechanism file
- Modify mechanism (species, reactions, etc.)
- Add information about species (e.g., Henry's Law constants), document reactions (references)
- Set model conditions (initial, time-varying)
- Run box model
- Plot model results (compare 2 mechanisms)
- Download results

Community use & development welcome: https://wiki.ucar.edu/display/MusicBox/, https://github.com/NCAR/MusicBox

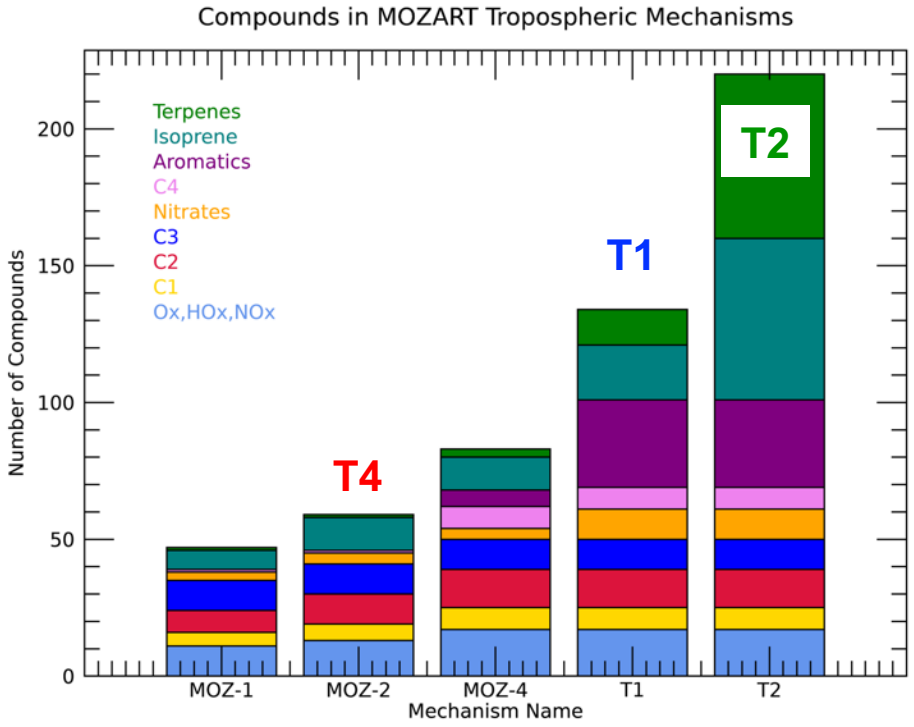
Applications for MusicBox

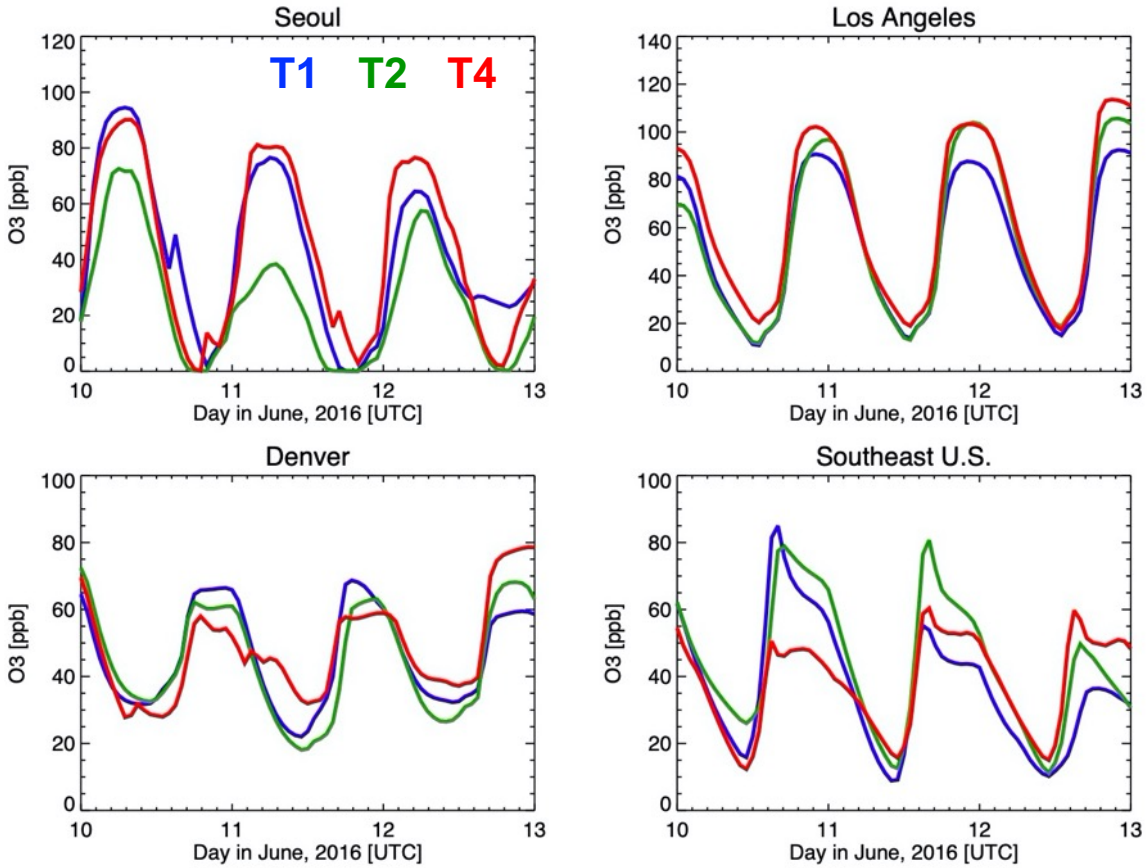
Evaluate and compare chemical mechanisms

- Different complexity (MOZART-T1, –T2 and MOZART-2)
- Different origin (SAPRC, GEOS-Chem, CB)

-> Community input welcome!

Comparison of MOZART mechanisms of different complexity
[*results from CAM-chem*]





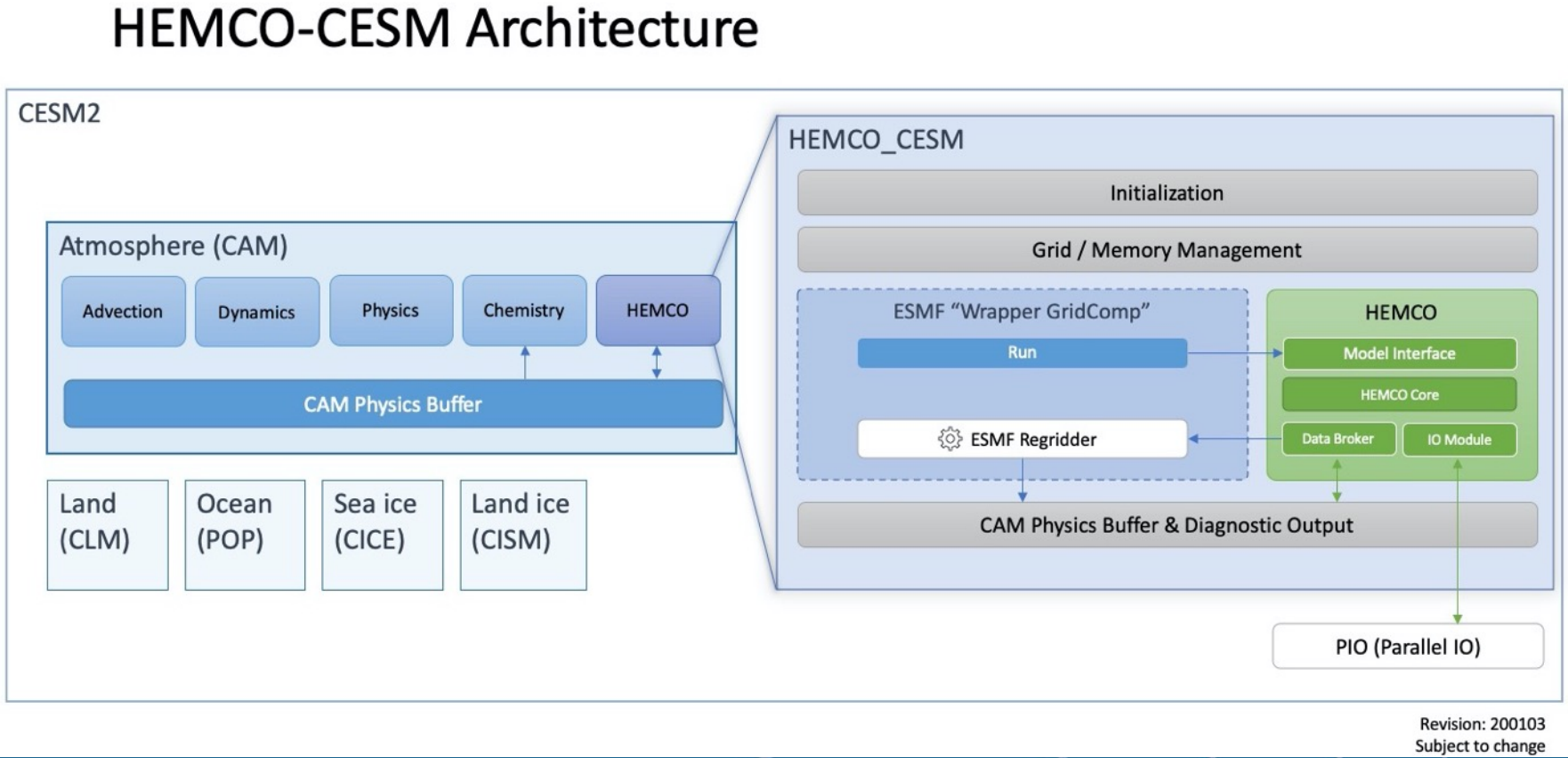
GEOS-Chem as a chemical module in CESM

Daniel Jacob (Harvard), Sebastian Eastham (MIT)

Coupling of GEOS-Chem to CESM is underway, with a functioning prototype in place
An opportunity to address dependencies of chemistry on physics in CESM
Enabling greater modularity, e.g., for dry deposition, wet scavenging

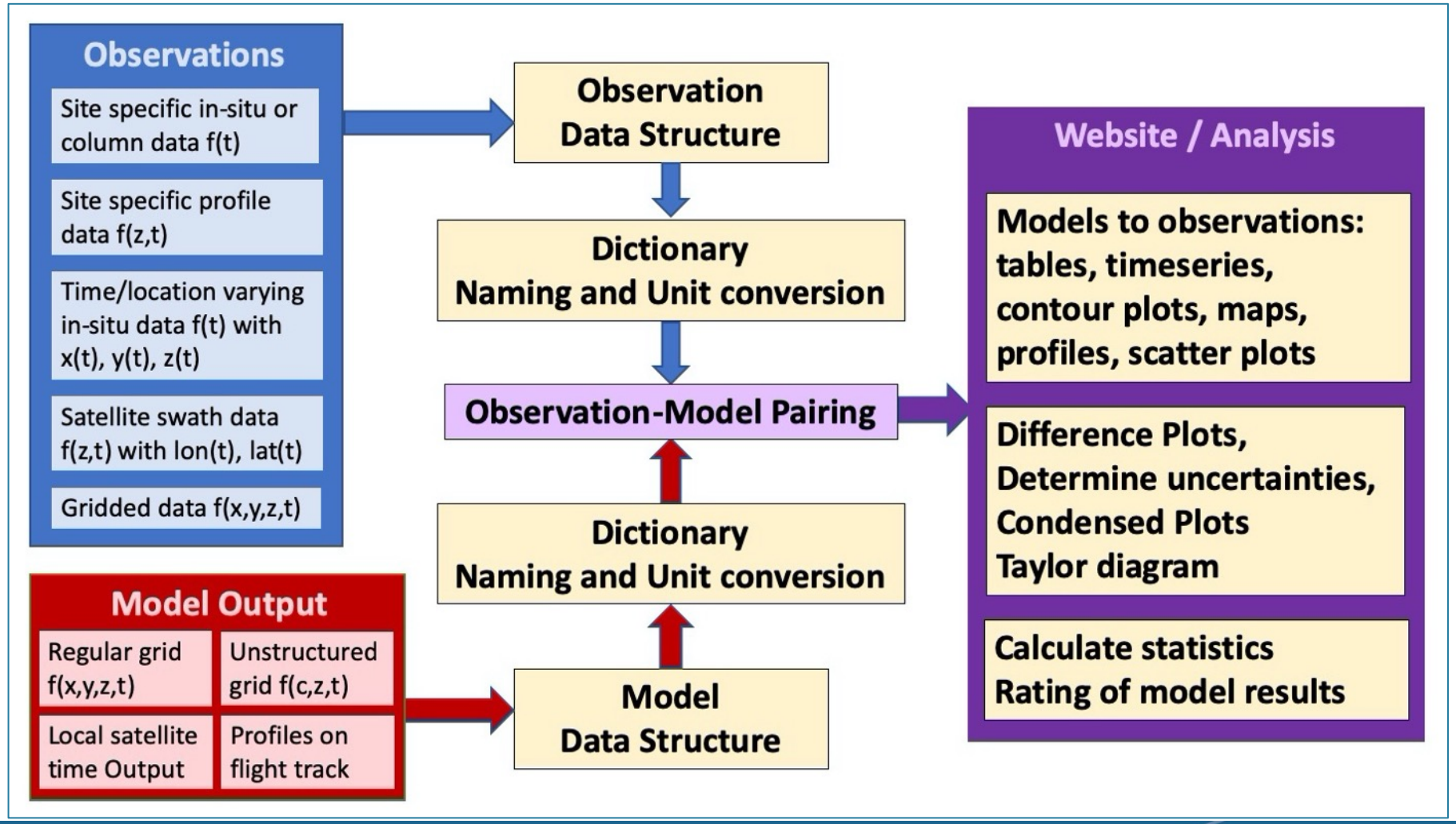
This includes implementation of the HEMCO emissions module in CESM

Enabling emissions data to be acquired from disk at arbitrary resolution, conservatively regridded



MELODIES for MUSICA: A modular framework to compare model results and observations of atmospheric chemistry [Funded by NSF Earthcube]

MELODIES: Model EvaLuation using Observations, DIagnostics and Experiments Software



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

Community input requested

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

Community Involvement

Visit the NCAR ACOM MUSICA website

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

To:

- Join email list to receive MUSICA updates
- Join working groups
- Learn about MUSICA and MusicBox Tutorials
- Contribute to MELODIES