

Regional simulations of chemistry within MUSICA and new chemical model developments

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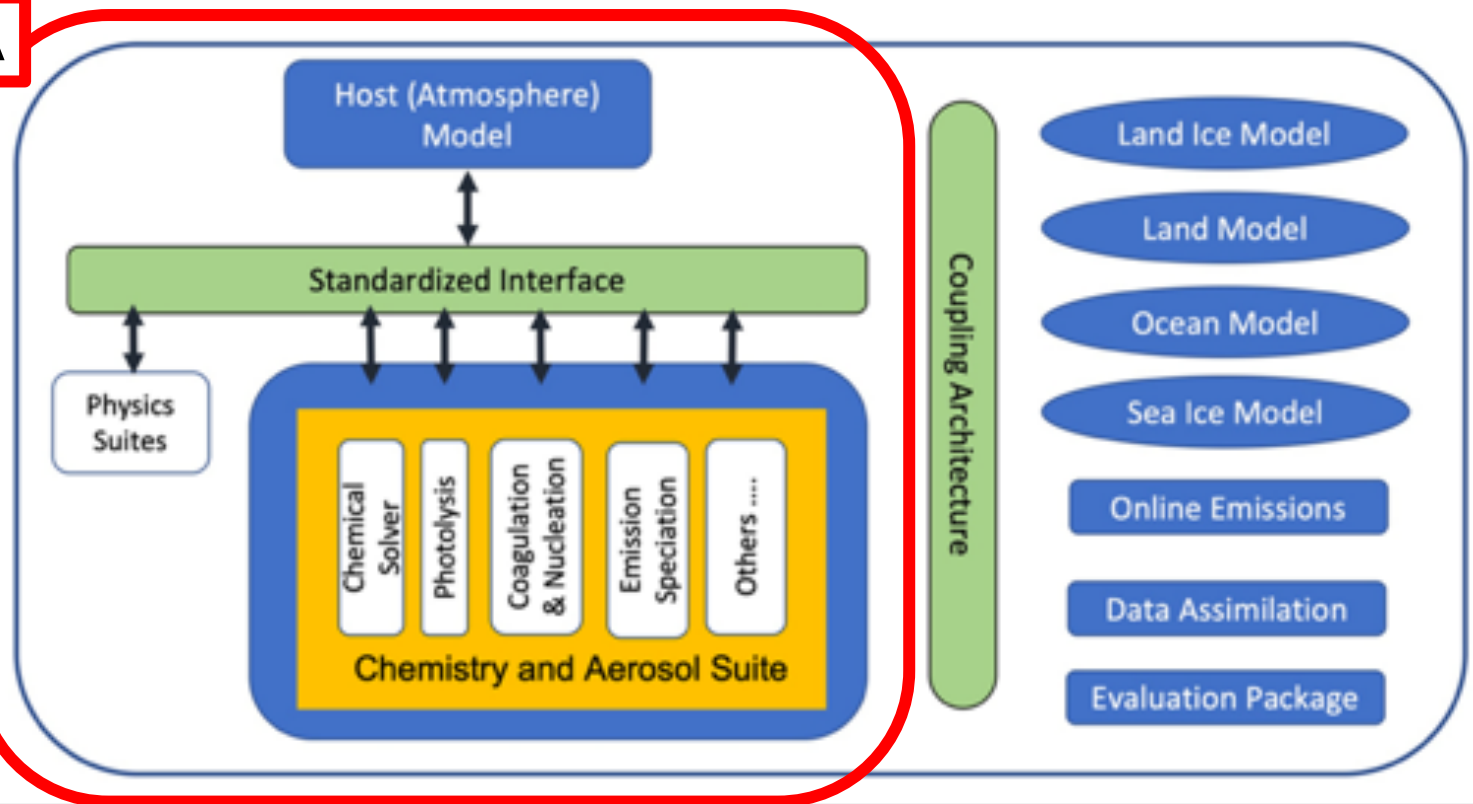
MUSICA: MULTI-Scale Infrastructure for Chemistry & Aerosols

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

Goal to develop model configurations based on a user's individual science question / familiarity (e.g., CAM, WACCM, chemical transport model)

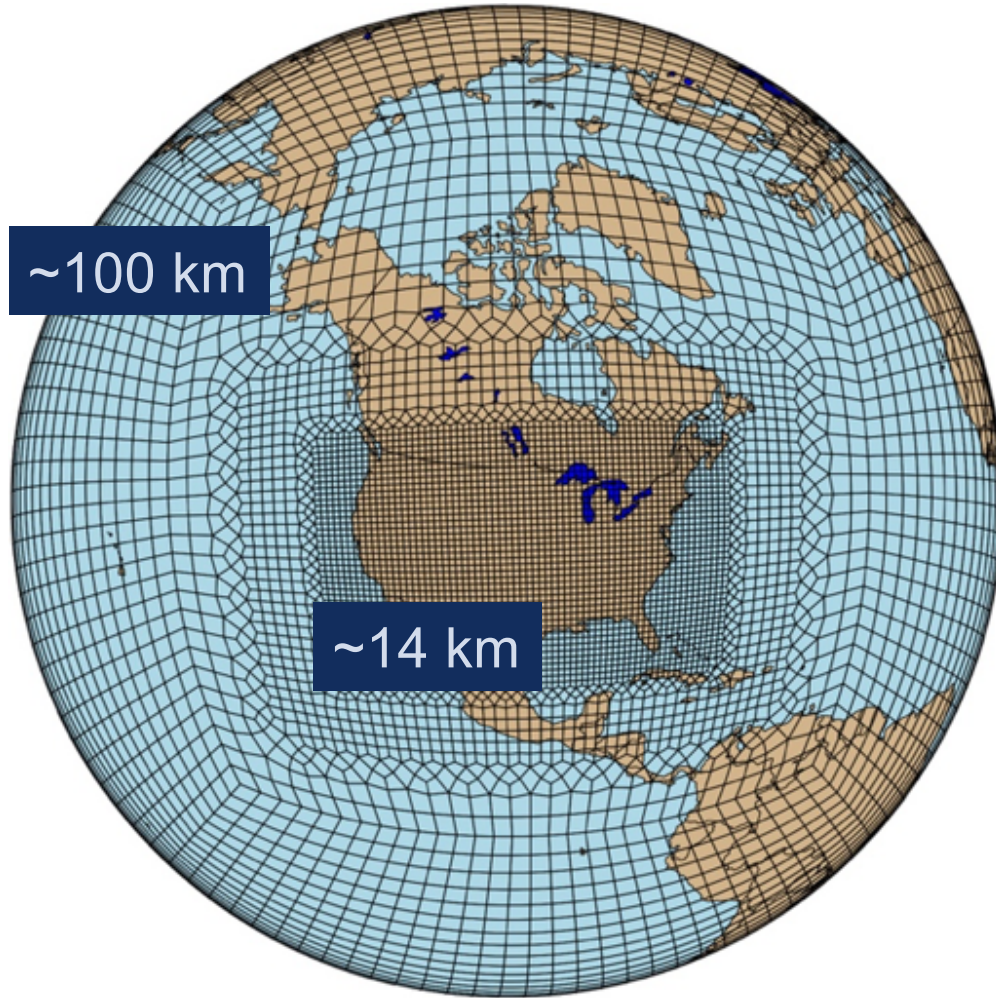
Development of the framework is underway in many labs at NCAR and within our community partners

SIMA



<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>)



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

Model Setup: MUSICA Framework

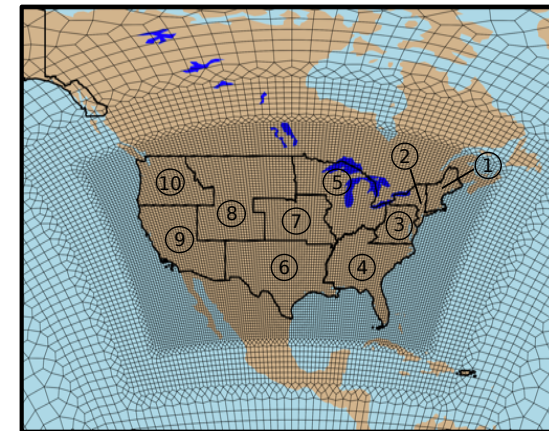
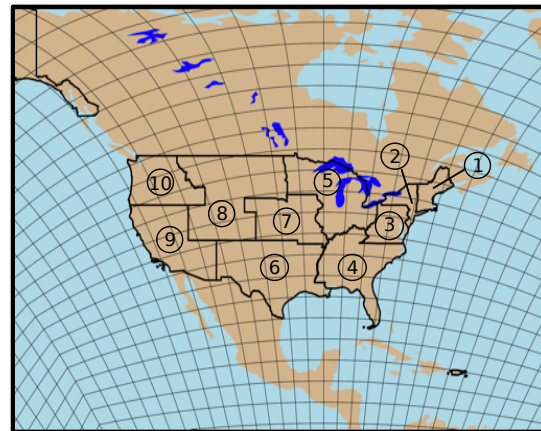


MUSICA.v0 allows for modeling of the formation and fate of trace pollutants at different resolutions and using various chemical mechanisms

Horizontal Scale:

- Global 1° degree cubed-sphere
- Global 1° with 1/8° degree over CONUS

Resolution Improvement



Lacey et al., *in prep*

Model Setup: MUSICA Framework



MUSICA.v0 allows for modeling of the formation and fate of trace pollutants at different resolutions and using various chemical mechanisms

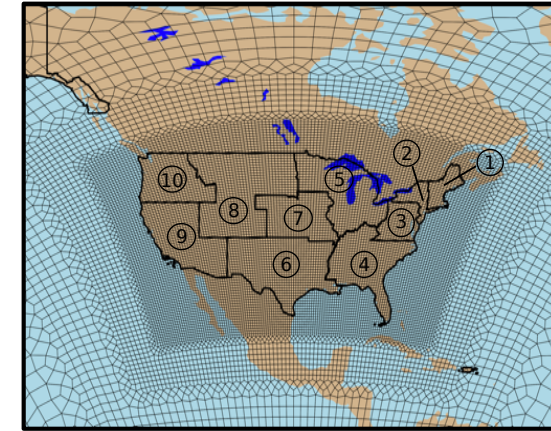
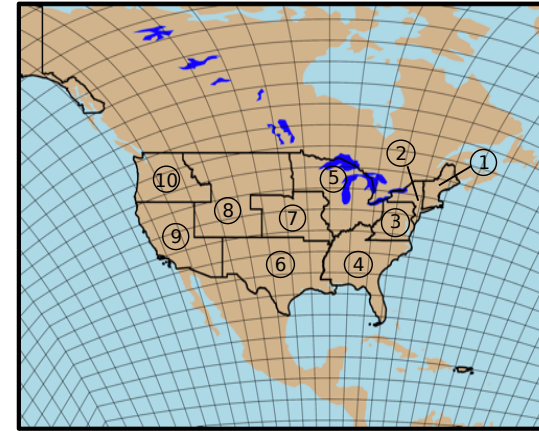
Horizontal Scale:

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Chemical Complexity:

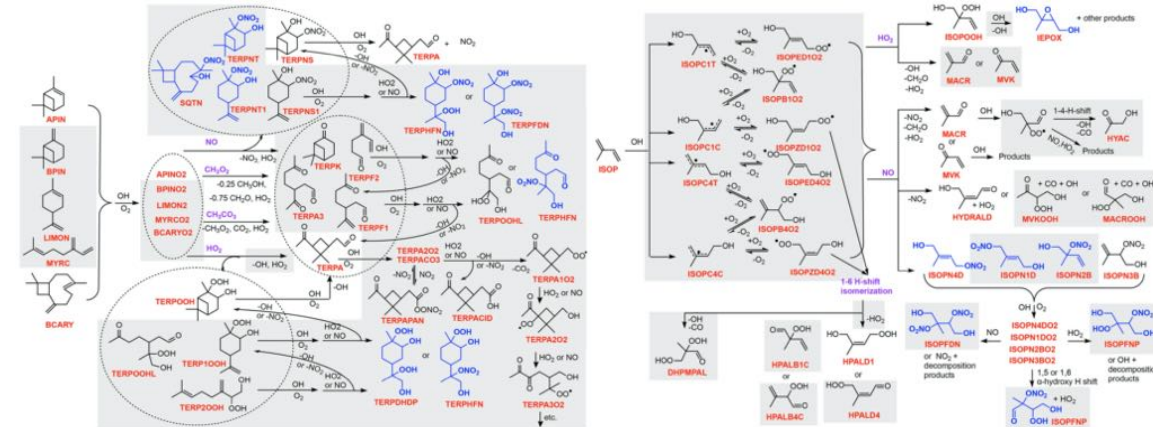
- MOZART TS1 – 151 species
- MOZART TS2 – 237 species (improved isoprene and terpene chemistry, Schwantes et al., 2020)

Resolution Improvement



Lacey et al., *in prep*

Chemical Complexity



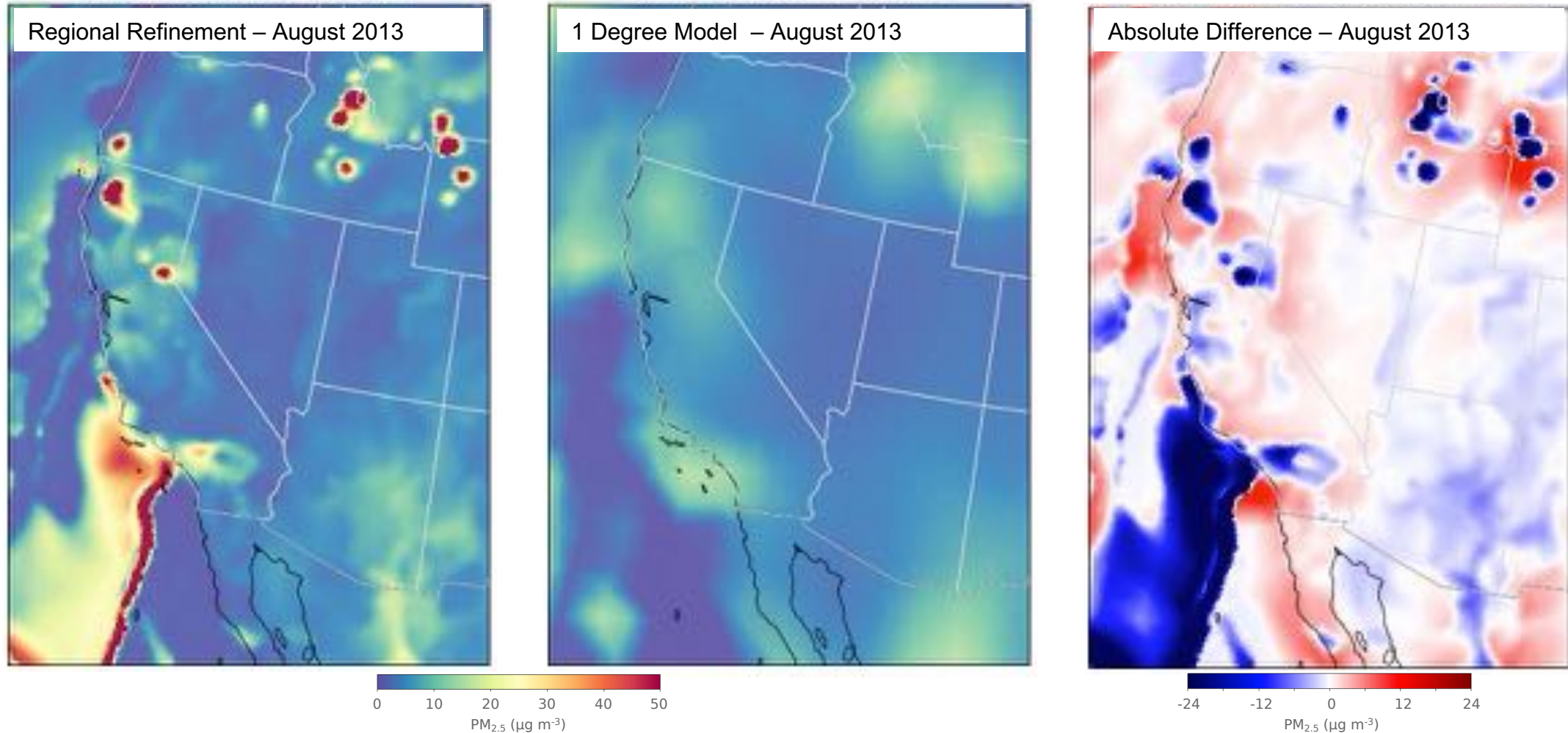
Schwantes et al., 2020 ACP

Results: MUSICA.v0 – Resolution Significance

Wildfires and other localized sources are becoming increasingly important w.r.t. ambient air quality

Resolution has a large impact on estimates of surface $PM_{2.5}$ as seen from the Rim Fire in 2013

Lacey et al., *in prep*

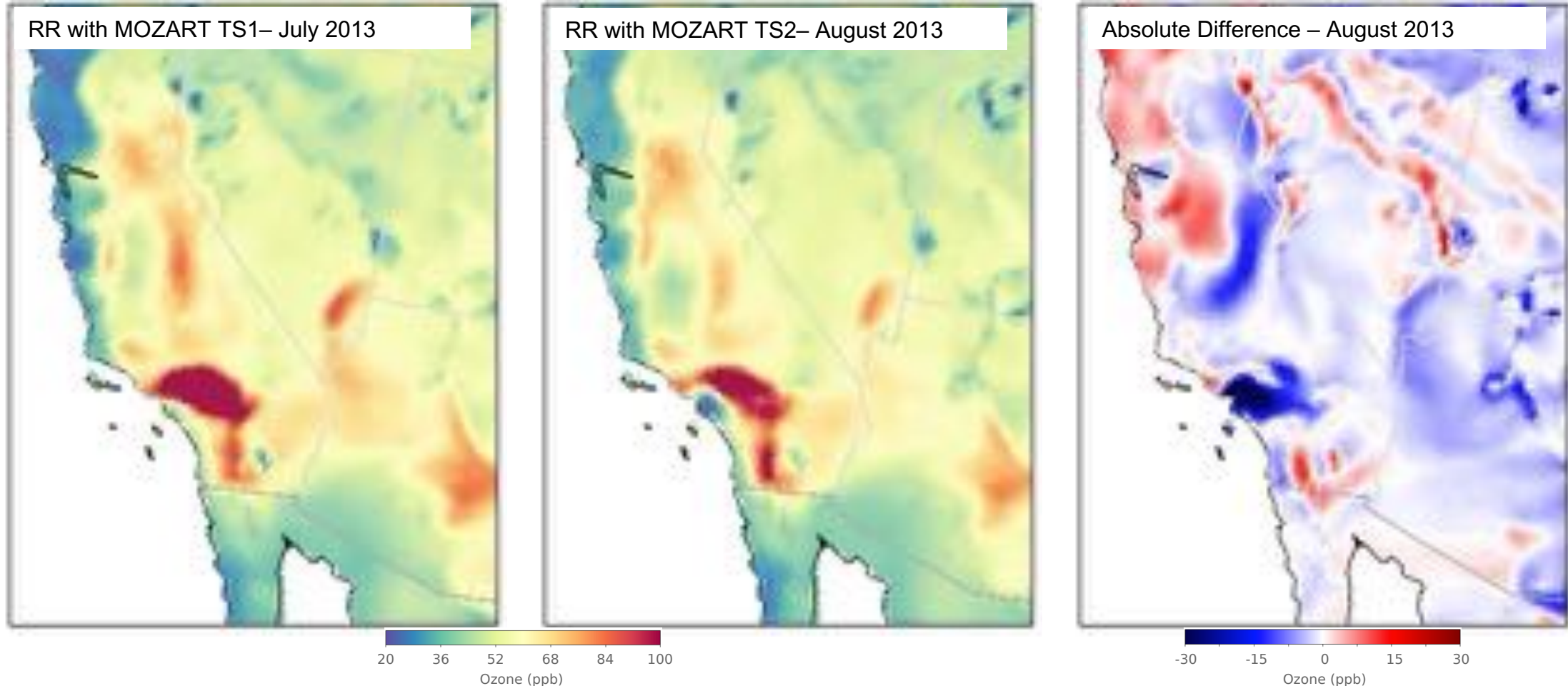


Results: MUSICA.v0 – Impacts of Chemical Mechanism

The MOZART TS2 mechanism provides improvements in oxidation of isoprene and monoterpenes as well as adding high-NO_x pathways for several other species

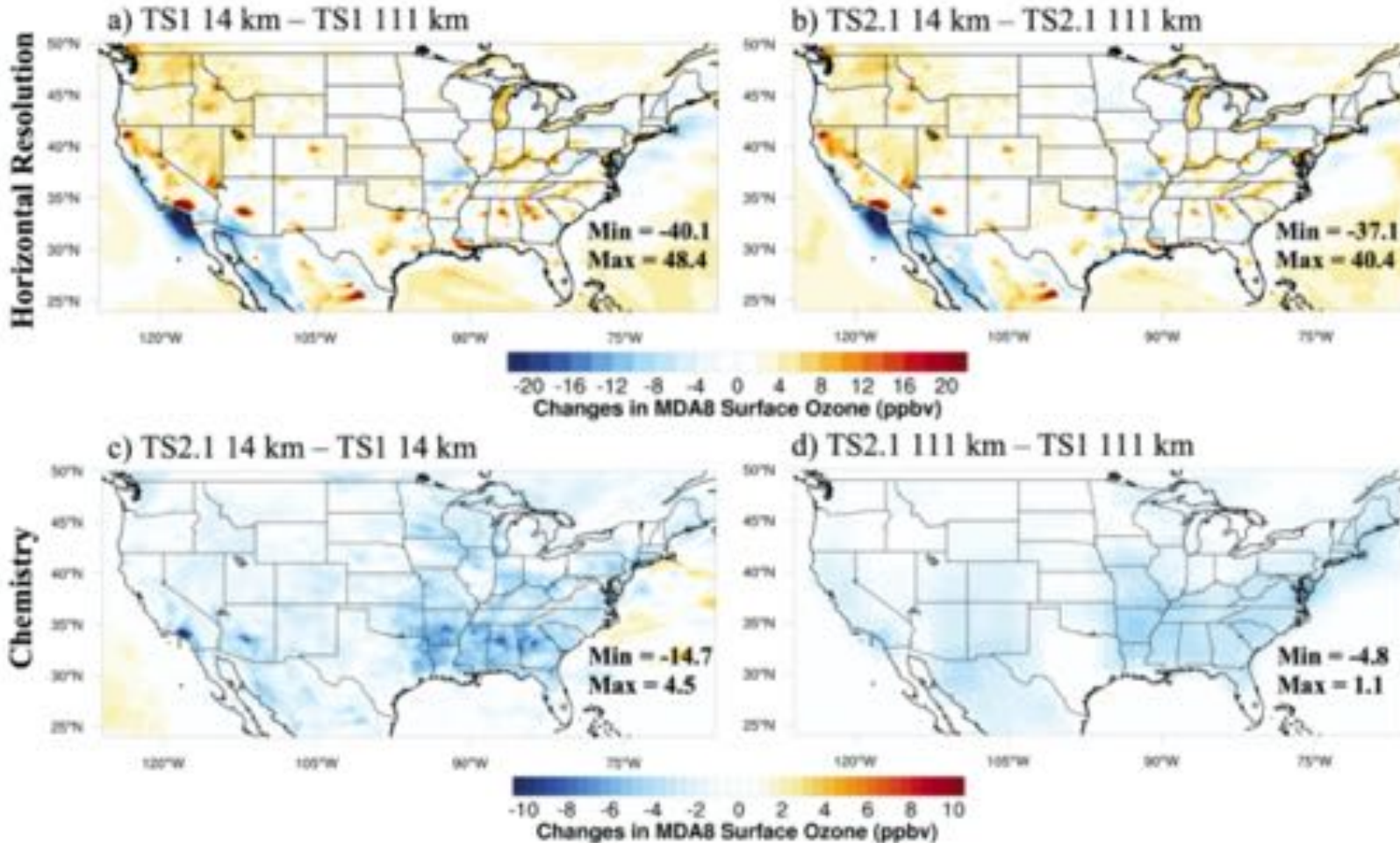
We can see some of these changes over California that has a mix of anthropogenic and biogenic emission sources and as the outflow from Los Angeles and other cities

Lacey et al., *in prep*



Results: MUSICA.v0 – Impacts on Pollutant Concentrations

In general, the results show that the changes due to shifts in resolution are similar in magnitude to the changes in chemical complexity, especially at higher resolution.



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>

Results: MUSICA.v0 – Impacts on Pollutant Concentrations

In general, the results show that the changes due to shifts in resolution are similar in magnitude to the changes in chemical complexity, especially at higher resolution.

Shifts in ozone bias (ppb)

Shifts in PM_{2.5} bias (µg m⁻³)



Regional and seasonal analysis also highlights potential areas for model improvement

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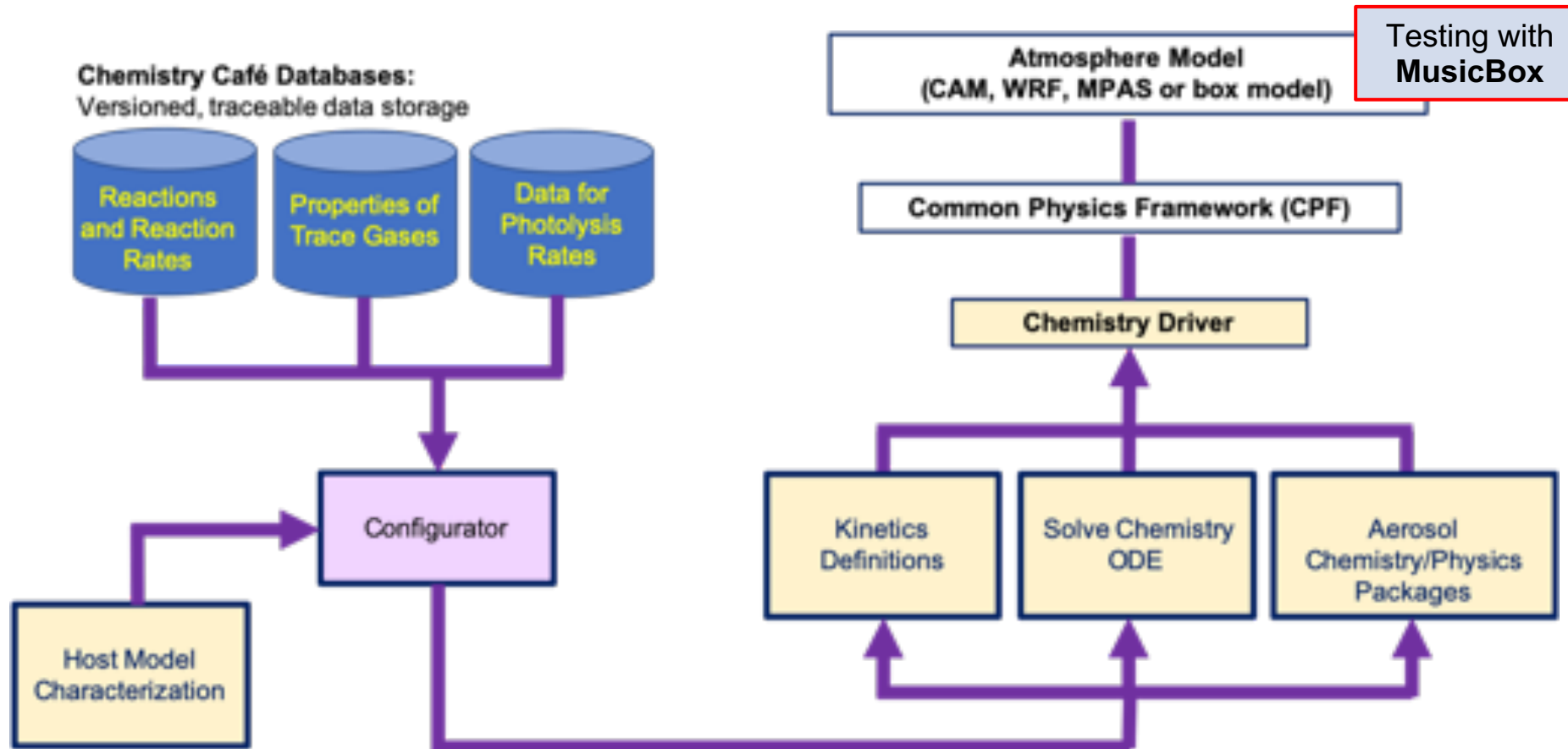
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Model-Independent Chemistry Module (MICM)

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 v2.0

Model Options **Species** Initial Conditions Evolving Conditions Photolysis Review

Upload File (.txt, .csv):

File: No file chosen

Chemical Species:

Formula	Initial Concentration
O2	1.0
N2	2.0
O3	3.0
H2O	4.0

- 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>

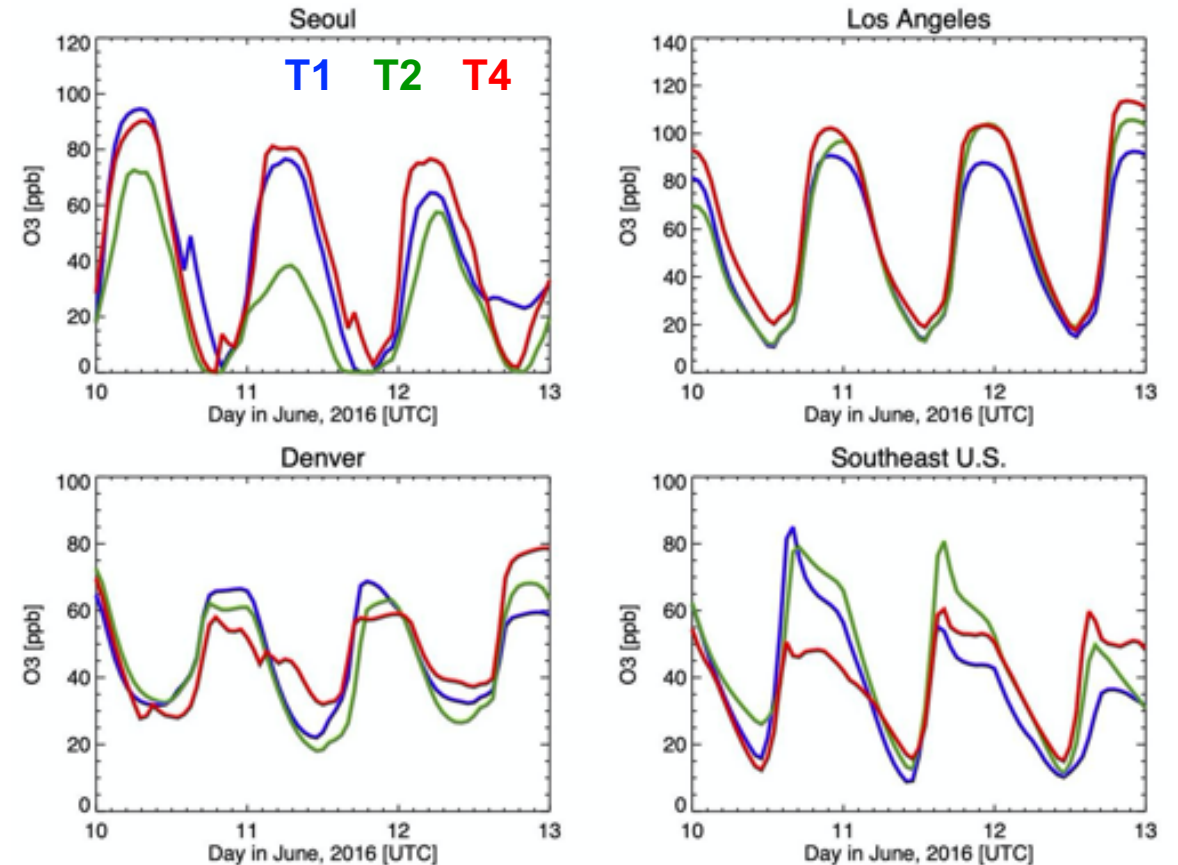
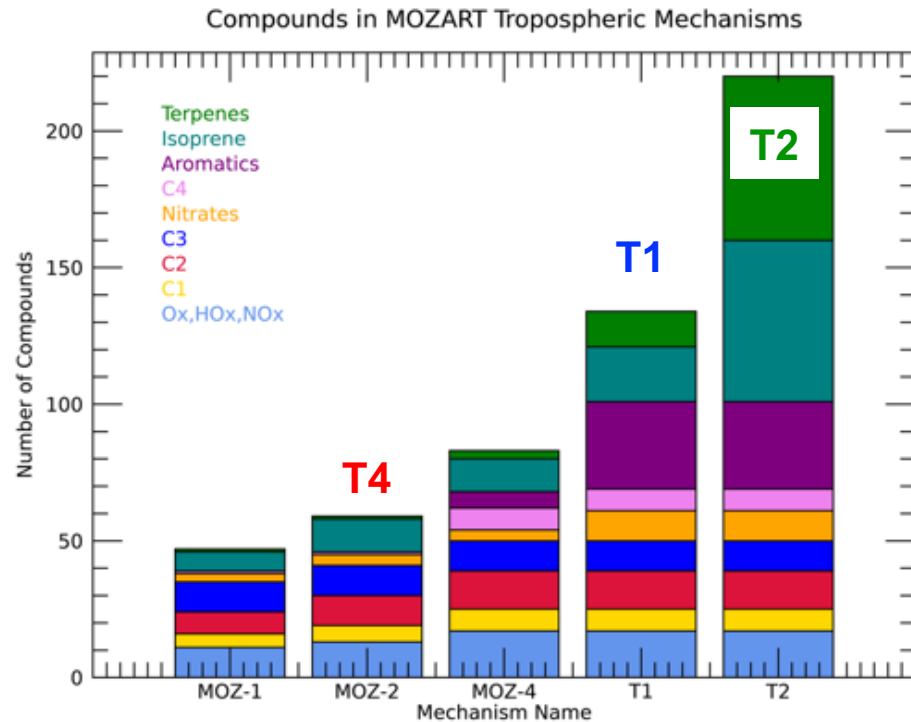
Applications for MusicBox

Evaluate and compare chemical mechanisms

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

-> **Community input welcome!**

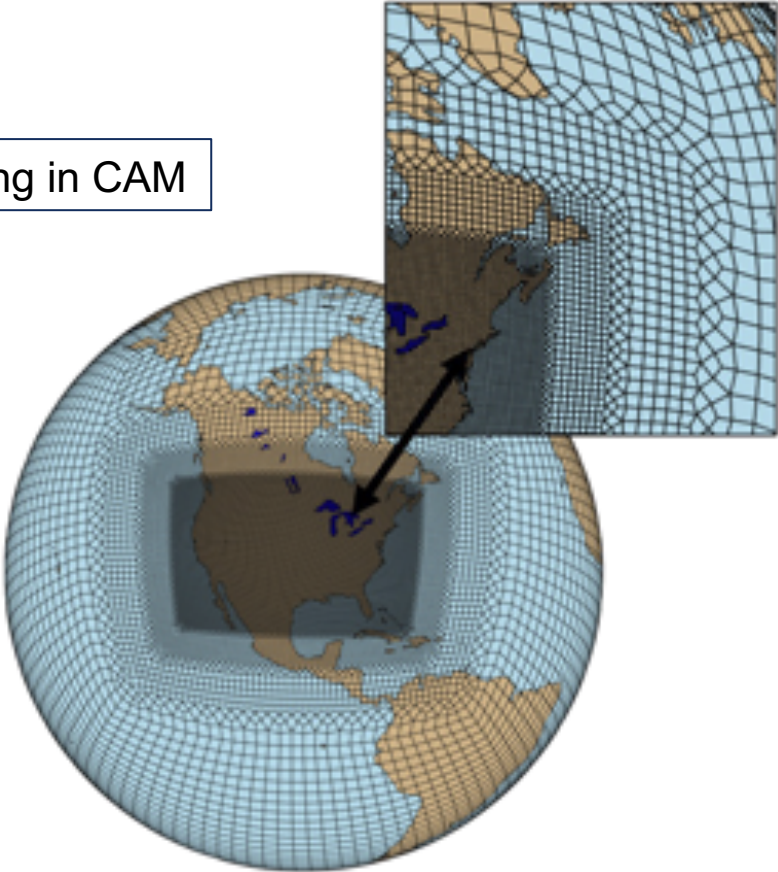
Comparison of MOZART mechanisms of different complexity
[results from CAM-chem]



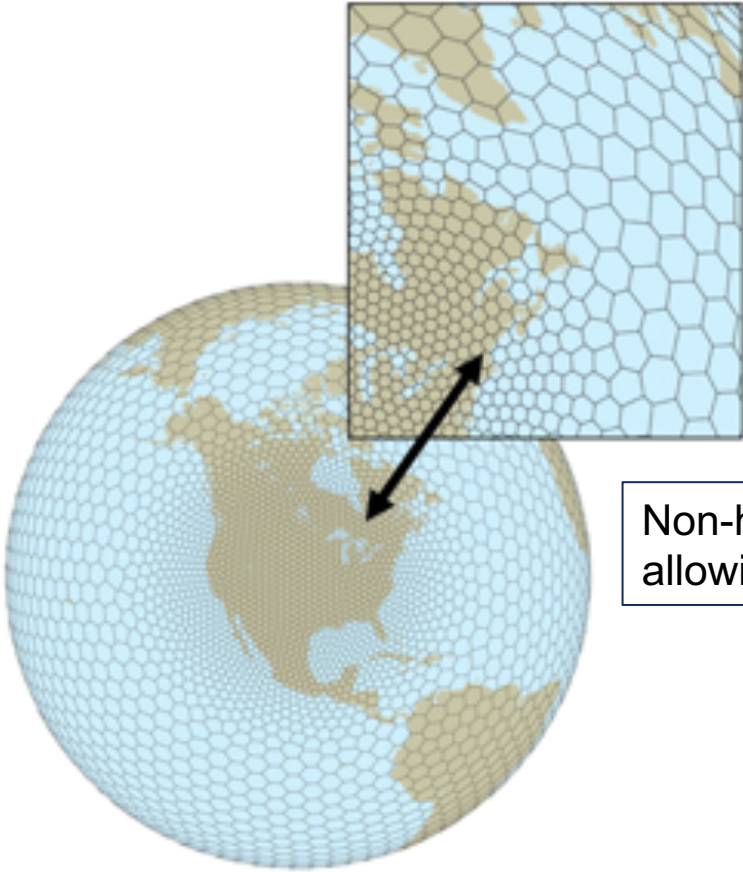
Ongoing Development: MUSICA.v0

Spectral Element
(cubed sphere)

Currently running in CAM



MPAS
(hexagonal mesh)

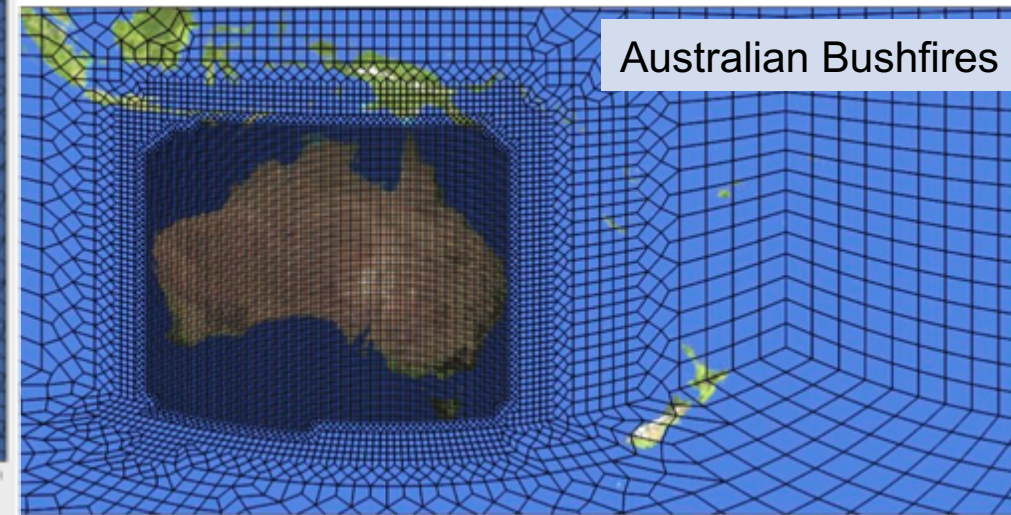
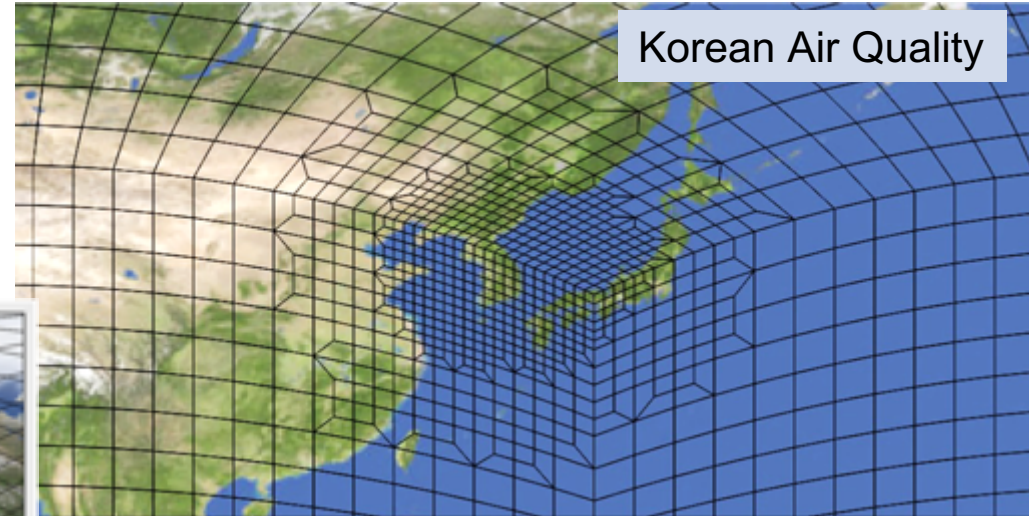
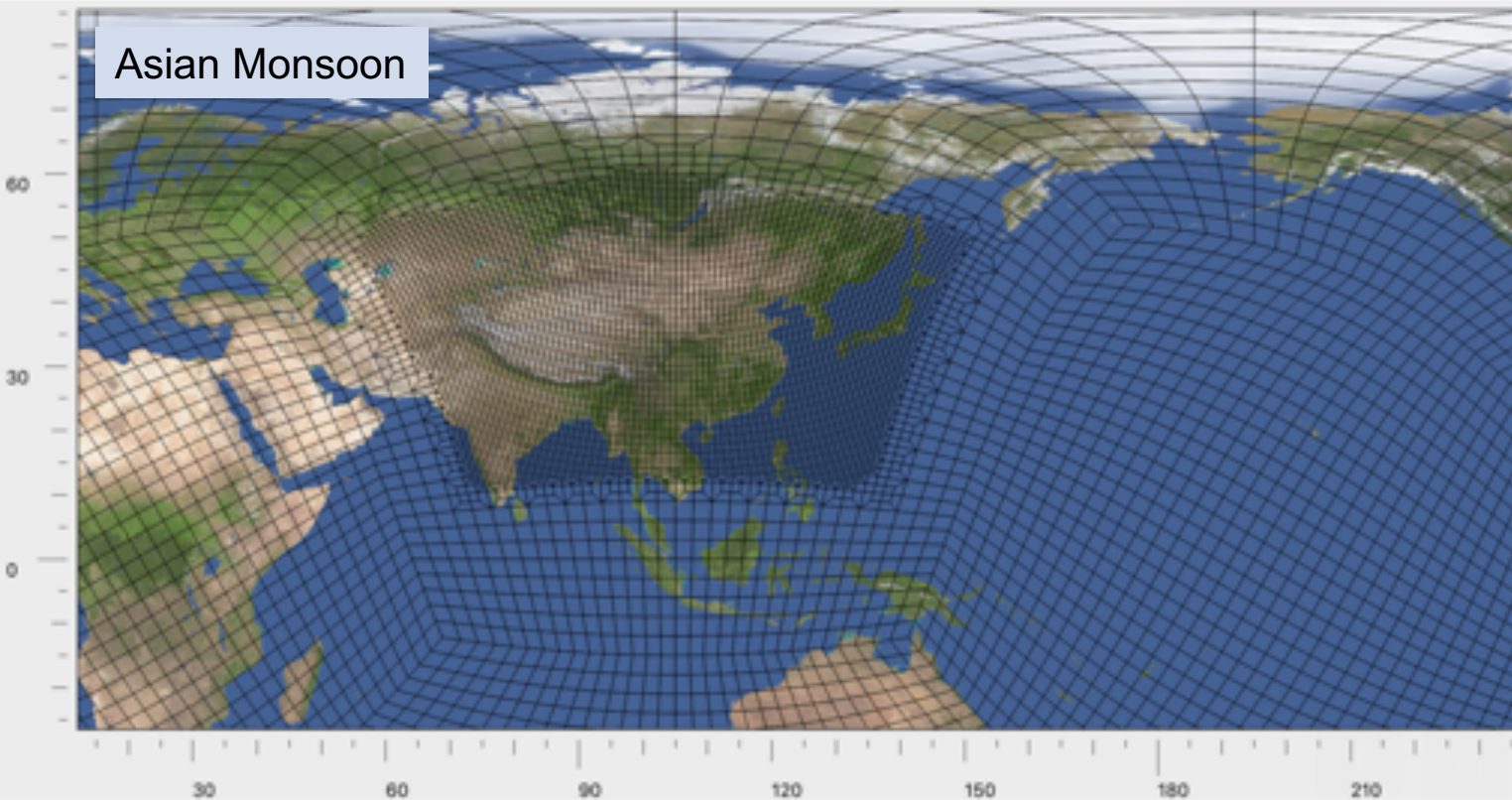


Non-hydrostatic
allowing for finer scales

Ongoing Development: MUSICA.v0

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

<https://wiki.ucar.edu/display/MUSICA/Generating+variable+resolution+grids>



Conclusions

- MUSICA and SIMA allow for the simplified evaluation of model complexity impacts on atmospheric state within a single **framework**
- Initial experiments show that both horizontal scale and chemical complexity are of equal importance for estimating non-linear species such as ozone and PM2.5
- MICM and MusicBox are tools that can be used to aid in answering some of these questions before implementation into a 3D model
- Community support is present and needed to continue development of MUSICA based on the various model components that are all involved

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