



Newsletter

Issue No. 9 January 2024

of the Multiscale Infrastructure for Chemistry and Aerosols - MUSICA

MUSICA is a computationally feasible global modeling framework currently in development that allows for the simulation of large-scale atmospheric phenomena, while still resolving chemistry at emission and exposure relevant scales (down to 4 km). MUSICA will replace and extend the current community chemistry modeling efforts at NCAR (e.g., WACCM, CAM-Chem, WRF-Chem) paralleling other activities at NCAR to streamline and unify model developments.

Summary of this issue

- Update on the Vision for MUSICA Development
- The impact of horizontal resolution on surface ozone concentration using Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA-V0)
- MUSICA Library Release
- NCAR is hiring a MUSICA scientist

New! MUSICA Library Release Version is available at https://github.com/NCAR/musica

MUSICAv0 is an initial configuration based on the CESM Community Atmosphere Model with chemistry using the Spectral Element with Regional Refinement dynamical core.

MusicBox is a box model using a model independent chemistry module.

MELODIES is a modular framework to compare model results with observations.

MUSICA is part of **SIMA** (System for Integrated Modeling of the Atmosphere).

Update on the Vision for MUSICA Development

The pathway to developing MUSICA continues to be tweaked as new ideas are brought to the project. Currently available incarnations of MUSICA include (1) <u>MUSICAvO</u>, a 3-d global chemical transport modeling capability in CESM for global to regional scale simulations that runs with both MOZART and GEOS-Chem chemistry, (2) <u>MusicBox</u> for performing box model chemistry calculations, and (3) <u>MELODIES</u>, which is a framework for model output evaluation and analysis. <u>MUSICAv1</u>, which uses the MPAS non-hydrostatic dynamical core in CESM, is now being tested and evaluated for global simulations with high resolution over regional to local scales with interactive chemistry.



As noted in the MUSICA Library Release notes, software libraries (MICM, TUV-x) for the envisioned MUSICA framework are becoming functional. How do these libraries fit in the development plan of the MUSICA ecosystem? The schematic above shows the MUSICA ecosystem under current (solid lines) and future (dashed lines) development. At the center of the ecosystem is the MUSICA library that comprises the collection of science-component libraries at the bottom (MICM, TUV-x, Aerosols, Cloud-J, and ISORROPIA) and exposes their functionality to the atmosphere models at the top (CAM-SIMA in CESM, NOAA CAT-Chem, GEOS-Chem, and MPAS-A that are written in Fortran) and middle (FastEddy and MusicBox). The front page of this newsletter states that MUSICA is part of SIMA, which is shown in the schematic by the upper left box "CAM-SIMA". Yet, MUSICA software will also be usable in other atmosphere models in the future either through the Fortran or Python interface, or directly to the MUSICA library (C). The interface is being developed to maximize modularity and interoperability of atmospheric chemistry and aerosol processes, and to provide standardized processes for incorporating new science components. Note that this is the current version of the MUSICA Ecosystem. We expect it to evolve over time based on changing needs.

MUSICA Science

The impact of horizontal resolution on surface ozone concentration using Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA-V0)

Contributed by **Amin Mirrezaei** (<u>amirrezaei@arizona.edu</u>) Department of Hydrology and Atmospheric Sciences, University of Arizona, Tucson, AZ, USA

In short

Arid/Semi-arid environments, like Phoenix, Arizona, exhibit unique seasonal and spatial variability in ozone precursors including NOx, as well as anthropogenic, and biogenic VOCs that needs to be better captured to improve AQ forecast of surface O_3 in the region.

Multiscale air quality modeling is a tool to address the limitations on spatial and temporal coverage of current satellite and surface measurements. In this study, MUSICAv0 model with refined resolution over CONUS (ne30x8 ~14km) is compared with WRF-chem model with two nested grid domains consisting of 9 km and 3 km horizontal grid over Arizona.

Findings

- MUSICAv0 overestimates HCHO during afternoon periods relative to PAMS and WRF-Chem.
- MUSICAv0 has lower NO₂ than 9km and 3km WRF-Chem.
- The combination of higher HCHO and lower NO₂ in the afternoon results to a shift in chemical regime in MUSICAvO to NOx-limited and subsequently to an overestimation of O₃.

Mohammad Amin Mirrezaei



Amin is currently a 2nd year PhD student in Atmospheric Science at the University of Arizona.

He attended CESM tutorial and visited NCAR in the summer of 2023. Amin's research focuses on regional to global air quality modeling, along with satellite data, to quantify the relative contributions of different emission sources to ozone pollution and global CH_4 budget.



AGU Poster Reference: <u>https://agu.confex.com/agu/fm23/meetingapp.cgi/Paper/1426610</u> M. A. Mirrezaei, W. Tang, L. Emmons, Y. Guo, B. Gaubert, and A. F. Arellano, "The impact of horizontal resolution, chemistry and emission on surface ozone concentration using Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICAv0)", to be submitted.

MUSICA Library Release

Checkout updates to the various components that make up the MUSICA library below! The MUSICA library will comprise all the aerosol and chemistry modules developed as part of the MUSICA project.

• TUV-x

New functionality

- Read radiator optical properties from a NetCDF file
- Output the version of TUV-x

Minor changes and bug-fixes

- Updated build scripts for Derecho
- Fixed interpolation error handling
- Fixed error in equal-interval grid spacing

TUV-x On The Web

The new TUV-x Quick Calculator is implemented in alpha-test form on the web: <u>https://www.acom.ucar.edu/Models/TUV/Interactive_TUV/tuv-x.shtml</u> There are no updates since the October 2023 release.

MusicBox Interactive

Try out the tool here: <u>https://musicbox.acom.ucar.edu/home</u>

Several updates have come including a more responsive menu for mobile devices, various minor bug fixes, and the release of more interactive graphics and a flow diagram.

Model Independent Chemistry Module: MICM

MICM now fully supports the TS1 gas-phase chemical mechanism. Initial tests comparing a box-model version of the CAM-CHEM MOZART solver showed very close agreements over a single time step. Differences are related in this case to floating point roundoff and different solver schemes (Rosenbrock of MICM, a single step backward Euler for the CAM-CHEM solver).

MUSICA

- No large updates in the musica library took place this release cycle, but the versions of MICM and TUVx were updated.

Workshop Presentations and Publications

Presentations

- Louisa Emmons, <u>Simulating Air Quality with MUSICAv0 for the Geostationary</u> <u>Constellation</u>.
- Mary Barth, <u>Representing Convective Transport of Trace Gases and Aerosols</u> <u>Using Multiscale Modeling</u>.
- Rebecca Buchholz, <u>Multi-scale Modeling for the 2019/2020 Extreme Wildfire</u> <u>Season in Australia</u>.
- Noribeth Mariscal, Ozone Atmospheric Chemistry in Southeast Michigan during the Michigan-Ontario Ozone Source Experiment (MOOSE).
- Wenfu Tang, <u>Global Expansion of Wildland-Urban Interface (WUI) and WUI fires</u>.
- AGU Town Hall: Louisa Emmons, Mary Barth and the MUSICA community <u>Next-Generation Modeling of Atmospheric Composition with the Multi-Scale</u> Infrastructure for Chemistry and Aerosols (MUSICA
- Sergio Ibarra Espinosa, <u>Road transportation emissions in Brazil between 1960 and</u> <u>2100 and impacts on air quality</u>
- Amin Mirrezaei, <u>The impact of horizontal resolution</u>, <u>chemistry</u>, <u>and emissions on</u> <u>surface ozone concentration using Multi-Scale Infrastructure for Chemistry and</u> <u>Aerosols (MUSICAv0)</u>

MUSICA Job

NSF NCAR seeks to fill a scientist II or III position to lead a multidisciplinary team that develops, maintains, and uses NSF NCAR's Whole Atmosphere Community Climate Model (WACCM) within ACOM's Multi-Scale Infrastructure for Chemistry Modeling (MUSICA) activities. <u>Apply here</u>



The incumbent will contribute to and foster a culture of scientific excellence within ACOM and NSF NCAR, support the scientific and university communities, and seek opportunities to lead and participate in research projects on a scale commensurate with that expected of a national center.

- If Scientist II The candidate will conduct research and exercise leadership responsibilities while guided and mentored by senior staff. However, independent thinking and initiative are essential and strongly valued.
- If Scientist III The candidate will conduct research and exercise leadership responsibilities. The candidate's work will be largely self-directed with support from senior staff as needed. Independent thinking and initiative are essential and strongly valued.