



Newsletter

Issue No. 10 April 2024

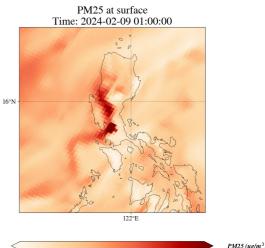
of the Multiscale Infrastructure for Chemistry and Aerosols - MUSICA

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 NSF NCAR (e.g., WACCM, CAM-Chem, WRF-Chem) paralleling other activities to streamline and unify model developments.

Summary of this issue

- MUSICA Forecasting for ASIA-AQ field study
- Music Box Interactive with PartMC
- MUSICA Library Release
- New presentations and publications

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



MUSICAv0 PM2.5 forecast map for NASA/NIER ASIA-AQ

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

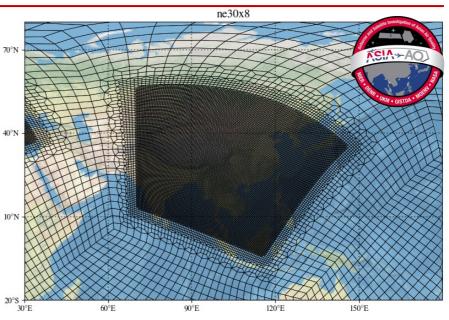
MusicBox is a box model using a model independent chemistry module.

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

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

MUSICA Forecasting for ASIA-AQ field study

number of Α models, including MUSICAv0, were used in flight planning for NASA Airborne the and Investigation Satellite of Asian Air Quality (ASIA-AQ) field experiment in February and March 2024.



ASIA-AQ consisted of airborne measurements from the NASA DC-8 and GIII in the Philippines, South Korea Thailand, focusing and on understanding local air quality, as well as interpreting satellite observations and improving model predictions of air guality. Chemical tracer forecasts were run with MUSICAv0 using a 12-km grid over most of Asia.



The CAM configuration of the model was used, simulating aerosols with specified oxidants, but a number of CO-like tracers were included to provide information on source contributions to the regions of interest. The forecasts were nudged to the GEOS-FP meteorological forecasts. The fire emissions were updated daily with FINNv2.5 near-real-time emissions using MODIS and VIIRS fire counts. Plots from the daily forecasts are available at: <u>https://www.acom.ucar.edu/asia-aq/forecast.shtml</u>. Full chemistry simulations are now being run to support analysis of the observations, with sensitivity simulations comparing several anthropogenic and biomass burning emissions inventories planned.

MUSICA Science

Music Box Interactive with PartMC

Contributed by Hunter Jiang (<u>hunterj3@illinois.edu</u>) University of Illinois Urbana Champaign

Hunter Jiang

Hunter, a freshman at the University of Illinois Urbana Champaign, is pursuing a major in computer science with an interest in environmental technologies and simulation software. He starts his collegiate journey with a clear vision to blend his passion for technology with impactful environmental research. This vision led him to join the innovative NCAR project MusicBox, under Student Push Innovation program of University of Illinois Urbana Champaign. Guided and mentored by Professor Nicole Riemer, Hunter is committed to bridging the gap between computational methodologies and atmospheric research. In MusicBox project, he is actively involved in the software development of MusicBox Interactive, where he made contributions to enhancing the platform's usability and functionality.



Project: Hunter's project is focused on advancing the capabilities of MusicBox Interactive. The core objective of this initiative is to enrich the platform's functionality and performance, enabling it to conduct more detailed and comprehensive atmospheric simulations.

Central to Hunter's efforts is the integration of the PartMC into MusicBox Interactive. This task encompasses a full-stack approach, involving the incorporation of aerosol configuration features into the MusicBox Interactive user interface and refining the backend architecture to allow for the use of PartMC. Through these enhancements, Hunter aims to elevate the platform's simulation precision and overall utility in atmospheric research.

MusicBox 2.3.4				
SETUP	Gas Species		Aerosol	Reactions
+ Start Here	Select a chemical species from the list to view/edit its properties, or add a new chemical species to the mechanism. The			
× Mechanism	chemical species you add here will be available to participate in reactions and can be include in the model conditions.			
© Conditions	Species		Phases	Representations
RUN Run Model			BC	
ANALYSIS	Add Species		Add property -	
∠ Plot Results	BC	×	You may specify any property you like, but this is only <i>necessary</i> under certain circumstances (i.e., when the species participates in a reaction that requires the property be set). You will be prompted to set the property when it is required.	
🛿 Flow Diagram	EC	×		
± Download	H2SO4	×		
NCAR	SOA1	×		
NCAR	SOA2	×		
	VOCI	×		
UCAR UCAR	VOC2	×		
localhost:5173				

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. Additionally, citing the software can easily be done by poking the "Cite this repository" button on Github.

TUV-x

Heating rates are now calculated with TUV-x! TUV-x now also includes a YAML option for configuration files, in addition to the existing JSON-based configurations. Several data sets and an example configuration have been added to the repository to handle photolysis rate constant calculations for WACCM simulations.

TUV-x On The Web

The new TUV-x Quick Calculator is implemented in alpha-test form on the web: https://www.acom.ucar.edu/Models/TUV/Interactive_TUV/tuv-x.shtml

MusicBox Interactive

- Try out the tool here: https://musicbox.acom.ucar.edu/home

More minor bug fixes have been addressed. The evolving conditions table now supports paging.

Model Independent Chemistry Module: MICM

Completing the port of the Rosenbrock solver to GPU with cuda is well on track. 48% of our defined issues are completed, but most of the remaining ones are small cleanup type issues while the work so far has been the majority of the work. Full GPU support is expected for the next release.

MUSICA

A fairly large refactor of our file structure has taken place, along with some updates to our cmake build system. The C-API to interact with MUSICA has been trimmed down and will be reflected in the CCPP wrapper for MUSICA shortly. Musica-core is now deprecated with needed functionally copied into TUV-x. This removes the dependency for json-fortran making installation easier.

Presentations

Gabriele Pfister, Next generation atmospheric chemistry modeling with the Multiscale Infrastructure for Chemistry and Aerosols (MUSICA). EGU General Assembly 2024.
Madankui Tao, Evaluating the Impact of Resolving Hourly Anthropogenic Emissions on Air Pollutant Simulations in the United States Using the MUSICAv0 Model, CESM Winter Working Group Meeting.
Haipeng Lin, The Harmonized Emissions Component (HEMCO) 3.0 as a

versatile multi-model emissions component implemented within MUSICA/CAM-chem, CESM Winter Working Group Meeting.

- Publications

P. Lichtig, B. Gaubert, L. K. Emmons, D. S. Jo, P. Callaghan, S. Ibarra-Espinosa, L. Dawidowski, G. P. Brasseur, G. Pfister. **Multiscale CO budget** estimates across South America: quantifying local sources and long range transport, *Journal of Geophysical Research: Atmospheres*, https://doi.org/10.1029/2023JD040434

H. Lin, L. K. Emmons, E. W. Lundgren, L. H. Yang, X. Feng, R. Dang, S. Zhai, Y. Tang, M. M. Kelp, N. K., Colombi, S. D. Eastham, T. M. Fritz, D. J. Jacob. Intercomparison of GEOS-Chem and CAM-chem tropospheric oxidant chemistry within the Community Earth System Model version 2 (CESM2), EGUsphere [preprint], https://doi.org/10.5194/egusphere-2024-470.