MUSICA*ctivities*

Newsletter

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 updates & news
- ❖ MUSICA updates
- ❖ MUSICA infrastructure plans
- ❖ MELODIES-MONET tutorial in Boulder
- ❖ MUSICA science: Early career scientist spotlight
- ❖ Presentations

Wenfu Tang (NSF NCAR) at the MUSICA tutorial in Nanjing China

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).

We want to hear what you are doing with MUSICA! Please send us contributions to the newsletter (please email gaubert@ucar.edu)

MUSICA Updates & news

❖ **MusicBox Interactive has new features**

The NSF NCAR MOZART Troposphere-Stratosphere (TS1) chemical mechanism is now available as one of the examples on the MusicBox Interactive web page (musicbox.acom.ucar.edu). Its initial and environmental conditions are set for an isoprene-rich environment in the Amazon. NSF NCAR is developing a tool to obtain MusicBox initial conditions from 3D chemistry transport model output. The initial version of the tool is currently being completed for WACCM output.

MusicBox emails:
For technical support: music-box-support@ucar.edu
For information exchange: music-box-info@ucar.edu can be used to share experiences, share example configurations, and ask questions of other users.

❖ **Job Offer at CERES/CSL in Boulder, Colorado**

Scientific Software Engineer/Associate Scientist position
Apply here before November 12 2024

❖ **MUSICA tutorial at Nanjing university**

The MUSICA tutorial at Nanjing University Sept 20-21 was attended in-person by 35 graduate students, postdocs and early career professors, primarily from China.
The tutorial materials are available at:
https://wiki.ucar.edu/display/MUSICA/Nanjing+Tutorial
These include instructions for configuring and running MUSICAv0 in CESM3 beta versions (https://wiki.ucar.edu/display/MUSICA/Custom+Grid+in+CESM3) which will continue to be updated as CESM3 is developed.
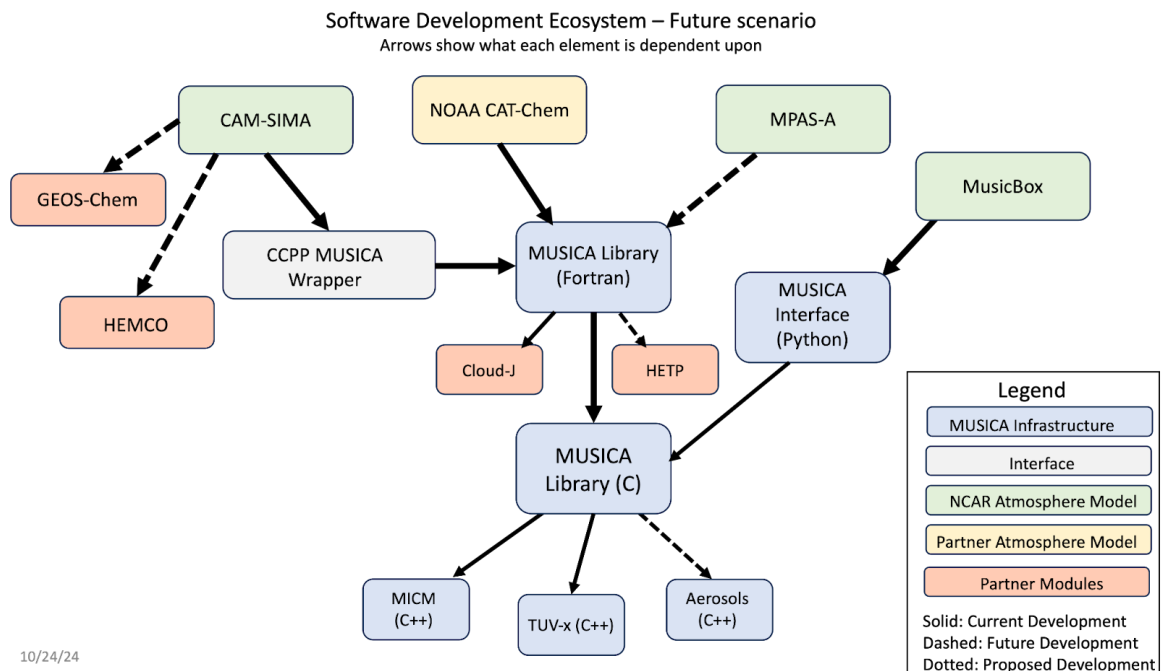
MUSICA Updates

❖ Developments in MUSICAv0

GEOS-Chem 14.4 is now available in MUSICA v0. Improvements over the version previously available are inclusion of nitrate photolysis and use of spectral element with regional refinement dynamical core. It also uses Cloud-J photolysis and HETP aerosol thermodynamics. GEOS-Chem 14.5, which includes expanded RCOOH, monoterpene, peroxynitrate and alkyl nitrate chemistry, will be available soon.

Cloud-J and HETP in MUSICAv0: Cloud-J photolysis and HETP aerosol thermodynamics are both new modules introduced in MUSICAv0. Cloud-J is an improved version of Fast-JX. HETP is a new version of ISORROPIA which uses modern Fortran. These modules are now available to work towards interfacing with CAM-chem allowing Cloud-J to be a potential alternative to TUV.

HEMCO in MUSICAv0: The Harmonized Emissions Component (HEMCO) is available for use with CAM-chem and GEOS-Chem in MUSICAv0. Work is in progress to make it the CESM default for emissions.

❖ Moving to the MUSICA Library Infrastructure

The basic construct of the MUSICA infrastructure includes Model Independent MUSICA Modules (MIMM) in a software library and MUSICA interfaces in Fortran, C, and Python, as shown in the schematic. This enables the MUSICA infrastructure to connect to any atmosphere model.

Software Development Ecosystem – Future scenario
Arrows show what each element is dependent upon

10/24/24

Moving to the MUSICA Library Infrastructure

The table below describes different atmosphere models that the MUSICA library infrastructure is currently being connected to or is planned to be connected.

Atmosphere Model & Status	Description	Why use this configuration?
NSF NCAR MusicBox Version 2.5.3 released MusicBox interactive Command-line version	Chemistry box model using prescribed atmospheric conditions. It currently runs gas-phase chemistry only.	Test chemical schemes; Classroom teaching or summer schools; Research focused on chemical sources and sinks
NSF NCAR CAM-SIMA MUSICA CCPP Wrapper connection to CAM-SIMA to be completed by Dec 2024 About CAM-SIMA	CAM-SIMA is CAM with the use of CCPP, which allows interoperability among schemes and easier maintenance of code.	Global with variable resolution capabilities in an Earth System Model
NSF NCAR MPAS-A-Chem GOCART-2G currently being implemented Full chemistry version being planned	MPAS-A is a standalone atmosphere model used for numerical weather prediction.	Can be run as a global or regional model, used with the JEDI DA system, and offline meteorology. LES capability is in development.
NOAA UFS/CATChem Under development About CATChem	CATChem is a chemistry driver and chemistry & aerosol components planned to connect to the NOAA UFS	Provides a consistent modeling system for air quality forecasting and research.

Acronyms:
CAM = Community Atmosphere Model
SIMA = System for Integrated Modeling of the Atmosphere
MPAS = Model for Prediction Across Scales
UFS = Unified Forecast System
CATChem = Configurable ATmospheric Chemistry
CCPP = Common Community Physics Package
JEDI = Joint Effort for Data assimilation Integration
DA = data assimilation
LES = large eddy simulation

MUSICA Infrastructure Plans

The NSF NCAR software engineers are moving forward with several development activities outlined here.

➢ Complete the implementation of MICM and TUV-x into CAM-SIMA, the next generation version of the Community Atmosphere Model (CAM) in CESM that will provide interoperability among dynamics and physics schemes.

➢ Continue development of abstract interfaces between aerosols and CAM physics schemes so that multiple aerosol schemes can be used in CAM. Abstract interfaces have been completed for aerosol-radiation, aerosol-cloud drop, aerosol-ice, and wet deposition processes. Work is continuing with cloud chemistry, dry deposition, and emissions during the next year.

➢ Continue the development of a toolbox to provide initial and environmental conditions to MusicBox from chemistry transport model output (see above).

➢ Apply MUSICAv1 (the CAM model with the MPAS dynamical core and TS1 chemistry) to the ASIA-AQ analysis.

❖ MUSICA Plans for interfacing with NOAA CATchem

➢ Complete documentation that describes how to implement the MUSICA library v1.0.0 into any atmosphere model. MUSICA library v1.0.0 is the version of the library that is implemented in CAM-SIMA.

➢ Add cloud chemistry to MICM.

❖ MUSICA Plans for interfacing with MPAS-A

➢ Complete the implementation of GOCART-2G into the standalone model MPAS-A.

➢ Design and implement the interface between the MUSICA library and the MPAS-A host model.

❖ Harvard University MUSICA Plans for the coming year

➢ Interface Cloud-J photolysis with the MUSICA Fortran library.

➢ Interface the HETP aerosol thermodynamics scheme with the MUSICA Fortran library.

➢ Modify GEOS-Chem to be CCPP compliant to connect with CAM-SIMA.

➢ Provide MICM-compatible GEOS-Chem chemistry mechanism files that can then be solved with MICM and therefore any atmosphere model.

MELODIES MONET Tutorial 2024

The MELODIES MONET tutorial, held at NCAR Oct 15-16, had about 50 online and in-person attendees.
It consisted of short lectures followed by hands-on exercises. Presentation and recordings are available here.
The python code is freely available on GitHub with documentation.

During the tutorial, participants got hands-on experience running the current capabilities of MELODIES MONET, as well as learned how to add new observations and model results to perform model evaluation for their own research.

MELODIES MONET has the goal to facilitate:
❖ Reading observational datasets with various spatial and temporal resolutions
❖ Reading model output from regional or global models with structured or unstructured grids.
❖ Matching variable names and units between observations and model output
❖ Matching observations and model results in space and time, applying observation operators and algorithms for quantitative comparison, as well as matching meteorological situations and other conditions.
❖ Plotting and analyzing comparisons: computing statistics with uncertainties, producing a performance matrix indicating limitations of comparisons.

MELODIES MONET v0.1 has been released:
https://melodies-monet.readthedocs.io/en/stable/

MUSICA Science

Development of a MUSICA Framework for Air Quality Research over the UK

Contributed by **James King** (*james.king@sheffield.ac.uk*)
School of Biosciences, University of Sheffield, UK

James King

James is a postdoc at the University of Sheffield in the UK with broad interests in climate dynamics, modelling, and mitigation. As part of Dr Maria Val Martin's research group, he is currently working on evaluating the unintended earth system consequences of nature-based carbon dioxide removal, including atmospheric chemistry, fires, and hydrology. James also has broader interests in climate policy, ethics, and communication. He was a NSF NCAR summer visitor in 2022 and enjoys working closely with NSF NCAR colleagues.

Project: A joint project is underway between the universities of Sheffield and Manchester in the UK to develop, test, and run MUSICAv0 over the country at ne30x16 (~7km) resolution. Having ported CESM2.2 to the UK's national HPC service ARCHER2, we are currently working to test and verify the model on the grid we have developed. We aim to evaluate the model against UK air quality observations, as well as running the model with domestic emissions inventories to compare to the CAMS-GLOB-ANT anthropogenic emission inventory.

UK_JAK_ne30x16

Further on in the project, the Manchester team (Dr Zhonghua Zheng with PhD students Zhiyi Song and Yuan Sun) plan to use MUSICA to simulate air pollution in UK cities, while the Sheffield team (Dr Maria Val Martin and James King, with PhD student Katie Rees) will be looking at the air quality and atmospheric chemistry implications of applying nature-based CDR strategies in the UK. They are grateful to the MUSICA team for developing this impressive model as well as for their patient technical advice!
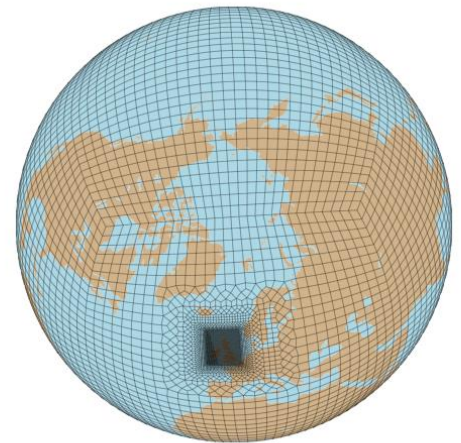
Workshop Presentations and Publications

Presentations

Amin Mirrezaei et al., Analyzing Ozone Pollution over Arizona: A Comparative Study of MUSICAV0 and WRF-chem Simulations. poster presented at the 29th Annual CESM Workshop. Boulder, CO. 10 June 2024.

Louisa Emmons, Simulating Air Quality with Regionally Refined Grids over Three Continents, 29th Annual CESM Workshop. Boulder, CO. 12 June 2024.

Wenfu Tang, The impacts on air quality of wildland-urban interface (WUI) fires versus wildland fires, 29th Annual CESM Workshop. Boulder, CO. 12 June 2024.

Noribeth Mariscal, Impact of Horizontal Resolution on Ozone Atmospheric Chemistry in Southeast Michigan during MOOSE, 29th Annual CESM Workshop. Boulder, CO, 12 June 2024.

Mary Barth, Updates on the Development of MUSICA, Joint WRF/MPAS Users Workshop. Boulder, CO, 2024.

Mary Barth, Current and Future Capabilities of Next Generation Multiscale Modeling for Atmospheric Chemistry, iCACGP-IGAC, Kuala Lumpur, Malaysia, September 2024.

Gabriele Pfister, Next generation atmospheric chemistry modeling with the Multiscale Infrastructure for Chemistry and Aerosols (MUSICA), CMAS conference 2024, Chapel Hill, NC, October 2024.