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

Summary of this issue

- MUSICA Air Quality simulations during KORUS-AQ

- Software Development Planning - User Story Mapping

- MUSICA tutorials and publications

- Conference and Workshop Presentations

ARCTIC 1/8 degree
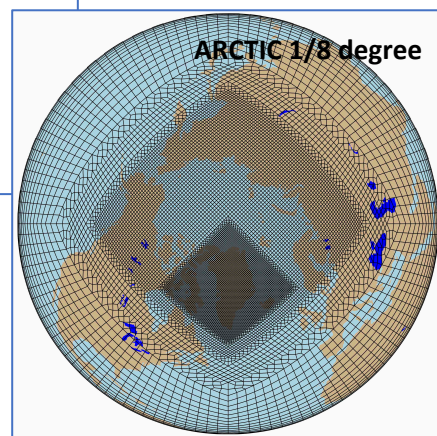
New! Information on existing MUSICAv0 grids is available at https://wiki.ucar.edu/display/MUSICA/Available+Grids

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.

To contribute to the newsletter, please email alma@ucar.edu

MUSICA Science

Comparison of Urban Air Quality Simulations during the KORUS-AQ campaign by Regionally Refined vs Global Uniform Grids With the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) Version 0

Contributed by **Duseong S. Jo** (cdswk@ucar.edu)
NCAR/ACOM, Boulder, CO
Submitted to J. of Advances in Modeling Earth Systems

■ In short

MUSICAv0 has been applied to simulate air quality over South Korea using a custom grid capability. Two global grids (ne30 (~112 km) and ne60 (~56 km)) and two regional refinement grids (ne30x8 (~14 km) and ne30x16 (~7 km)) are constructed to investigate the effects of grid resolution on air quality simulation during the KORUS-AQ campaign. Simulation results are compared for a comprehensive suite of chemical species including O_3, CO, SO_2, NO_X, other nitrogen compounds, and VOCs with different reactivities. Anthropogenic and biogenic emissions are also investigated with different model configurations.

Duseong S. Jo

Duseong graduated from Seoul National University in 2017 and did his postdoc at CU and NCAR. He is now working at NCAR as a Project Scientist 1.

Duseong's research focuses on 1) secondary organic aerosol modeling, 2) radiative and health effects of aerosols, 3) chemical mechanism development, and 4) aerosol changes under future climatic scenarios.

■ Findings

This work shows that grid resolution is important for chemical species with a high spatial gradient of emission flux and high reactivity. Furthermore, OH reactivities can be changed up to 3 times according to grid resolution over urban areas, which can affect OH levels and the lifetime of chemical species. Oxidation pathways of VOCs can be significantly changed due to grid resolution, which is important for organic nitrates and secondary organic aerosol formation. Emission inventory with up-to-date information is important for chemical species regulated by air quality policies such as SO_2. Imposing the diurnal cycle on monthly emissions is also essential for nighttime chemistry and chemical species with strong diurnal variations (e.g., O_3, NO_X, NO_3).

MUSICA Software Development Planning

■ User Story Mapping

On July 18–19, 2022, a group of 18 people participated in two User Story Mapping sessions intended to kick-off the creation of a comprehensive Software Development Plan for the MUSICA project. The group included members of MUSICA Leadership, ACOM scientists and software engineers, and University partners. The outcome of the meeting was a collection of MUSICA User Personas, and a software development "backbone" that will provide the high-level organization of the MUSICA Software Development Plan.

■ The concept

User Story Mapping is an Agile development process that structures individual development tasks into a 2D grid. This arrangement of tasks enables stakeholders to visualize how each individual task contributes to the overall project, and facilitates the organization of development into versions and group-oriented, two-week working plans called sprints. Crucially, user stories focus software development on the needs of users; every development task is directly related to a User Story, and collections of User Stories form a comprehensive User Journey of interactions with MUSICA software.

More information on User Story Mapping can be found at:
https://help.easyagile.com/easy-agile-user-story-maps/Best-Practice.1999339979.html

■ The outcome

Over the course of two 3-hr sessions, the team developed a set of 12 User Personas, or representative users of MUSICA software, that include demographic information as well as psychographic information like interests, frustrations and motivations for using our products. Examples of User Personas include *graduate students* using MUSICA for their research, *educators* teaching atmospheric chemistry, or *chemical weather forecasters* applying MUSICA.

These User Personas were then used to develop a User Journey or high-level set of discrete interactions (or "Epics") a user has with MUSICA software in chronological order. The goal was to come up with a User Journey that is applicable to all of our User Personas (from educators to research scientists; box-model to 3D model users). The team accomplished this goal on the second day of the workshop, developing a set of 9 Epics that form the "Back-bone" for our development plan. Under each of these Epics in the User Story Map, are specific User Stories, or specific product features that contribute to the high-level Epic. For MUSICA, we have replaced User Stories with Milestones, as these are still relatively complex features.

The scientists in the group began drafting Milestones and will continue to add more over the coming weeks. After a more-or-less comprehensive set of Milestones is included, they can be organized vertically into versions, the first of which will represent the minimum viable product (MVP). The remaining Milestones will be grouped into subsequent versions and on a continuing basis.

■ Moving forward

As scientists continue to add User Stories to the User Story Map, software engineers will work with them to iteratively clarify the product features needed to support each story. They will then develop a design and detailed implementation plan, along with a timeline, to deliver the needed features.

The hope is that this approach will lead to develop a software design, more accurate estimates of development time for MUSICA products, highly collaborative software development, a system that is designed with user needs as the primary consideration, and development that always contributes directly to the overall MUSICA Software Development Plan.

■ Upcoming

MUSICA software engineering plans to release updated versions of MUSICA features on a quarterly basis coinciding with the newsletter publication. The next release will be in December 2022 and will feature TUV-x, an extended version of the Troposphere Ultraviolet and Visible code that calculates actinic fluxes and photolysis rates from the surface to the upper atmosphere.

MUSICA Tutorials and Publications

■ MUSICA Tutorial Series Continue

On September 6-8, 2022, Louisa Emmons gave an informal tutorial at the University of Leeds on running MUSICAv0. Students, postdocs and professors from the University of Leeds and University of Sheffield attended. The participants had a wide range of experience with models, including having expertise running CESM and WRF-Chem, to researchers relatively new to 3D chemistry modeling. The sessions covered running MUSICAv0 on the Leeds computer, visualizing and using unstructured grid output, and creating your own grid.

Dr Maria Val Martin
@MValMartin

Fantastic day 1 at the 1st @NCAR_ACOM Musica workshop in Leeds with Louisa Emmons. Hosted by @EnvLeeds & @CEMAC_Leeds #atmosphericchemistry #modeling @NCAR_Science #NSF

The presentations relied on material from previous tutorials sessions (https://www2.acom.ucar.edu/event/workshop/musica-tutorial-2021) as well as instructions specific for the computers at Leeds. We look forward to ongoing collaborations with this group!

MUSICA Publications

- Schwantes et al., 2022: Evaluating the Impact of Chemical Complexity and Horizontal Resolution on Tropospheric Ozone Over the Conterminous US With a Global Variable Resolution Chemistry Model, *Journal of Advances in Modeling Earth Systems*, https://doi.org/10.1029/2021MS002889

- Tang et al., 2022: Effects of fire diurnal variation and plume rise on U.S. air quality during FIREX-AQ and WE-CAN based on the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICAv0), *Journal of Geophysical Research: Atmospheres*, http://dx.doi.org/10.1029/2022JD036650

Conference and Workshop Presentations

iCACGP - IGAC Conference 2022

Abstracts can be found at : https://www.icacgp-igac-2022.org/

- Vertical Transport of Trace Gases and Aerosols: Contrasting WRF-Chem, CAM-chem, and MUSICAv0 Results with Field Campaign Observations by Mary Barth.

- Regional-scale modeling in a global model with MUSICAv0: MUlti-Scale Infrastructure for Chemistry and Aerosols by Louisa Emmons.

- Application of the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) over Africa by Wenfu Tang.

- Air pollution simulation in South America using the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) model by Sergio Ibarra-Espinosa.

- Multi-scale Modeling Over Australia for the 2019/2020 Extreme Wildfire Season by Rebecca Buchholz.

- Simulations of Air Quality in South America: effects of boundary conditions and model intercomparison by Pablo Lichtig.

CESM Workshop 2022

- Recent developments in MUSICA by Louisa Emmons.

- Evaluations of Model Simulated Ozone and its Precursors in MUSICA-V0 Against In-situ and Airborne Measurements over CONUS by Noribeth Mariscal.

- Comparing the regional-scale model variability of MUSICA with a regional model (WRF-Chem) over CONUS by Wenfu Tang.

- Influence of Asian Summer Monsoon Eastward Shedding Events on Upper Tropospheric Chemical Composition by Doug Kinnison and Jun Zhang.

- Evaluating the representation of the Asian summer monsoon UTLS composition in CESM using airborne in situ observations by Ren Smith.

Conference and Workshop Presentations

Joint WRF / MPAS Users' Workshop 2022

- What is MUSICA? How does MUSICA compare to WRF-Chem? And going to higher resolution by Wenfu Tang.

AeroCom / AeroSAT Workshop 2022

- On October 10-14, 2022 Michael Schulz (U. of Oslo), Alma Hodzic (NCAR), and collaborators organized two 2-hr sessions during the AeroCom workshop to discuss ideas and foster collaborations for the development of community aerosol-chemistry interfaces within weather and climate models. The meeting sought to engage the European aerosol modeling community in the effort of building the GeneralIzed Aerosol/chemistry iNTerface (GIANT) project that has been started in the US.

- Participants reviewed the existing solutions used to separate aerosol code from host models, and identified the need to build stand-alone libraries of aerosol modules, well-defined interfaces between aerosol modules and host models, and unit and science testing to provide both portable and robust aerosol code.

- The next steps will consist of developing software engineering solutions, unit testing, and organizing additional Hackathons withing the GIANT project.

More information can be found at the MUSICA web page:
https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica