MUSICActivities

NCAR ACOM

Newsletter

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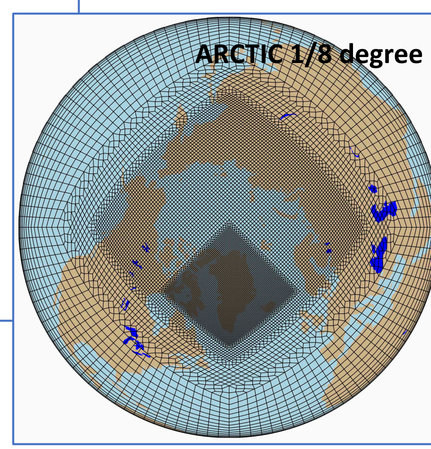
of the Multiscale Infrastructure for Chemistry and Aerosols - MUSICA

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

- Harmonized Emissions Component (HEMCO)
- Software Development
- MUSICA Library Release
- System for Integrated Modeling of the Atmosphere
- Conference and Workshop Presentations



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).

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

MUSICA Emissions Component

The Harmonized Emissions Component (HEMCO) 3.0, a versatile multi-model emissions component implemented within MUSICA/CAM-chem

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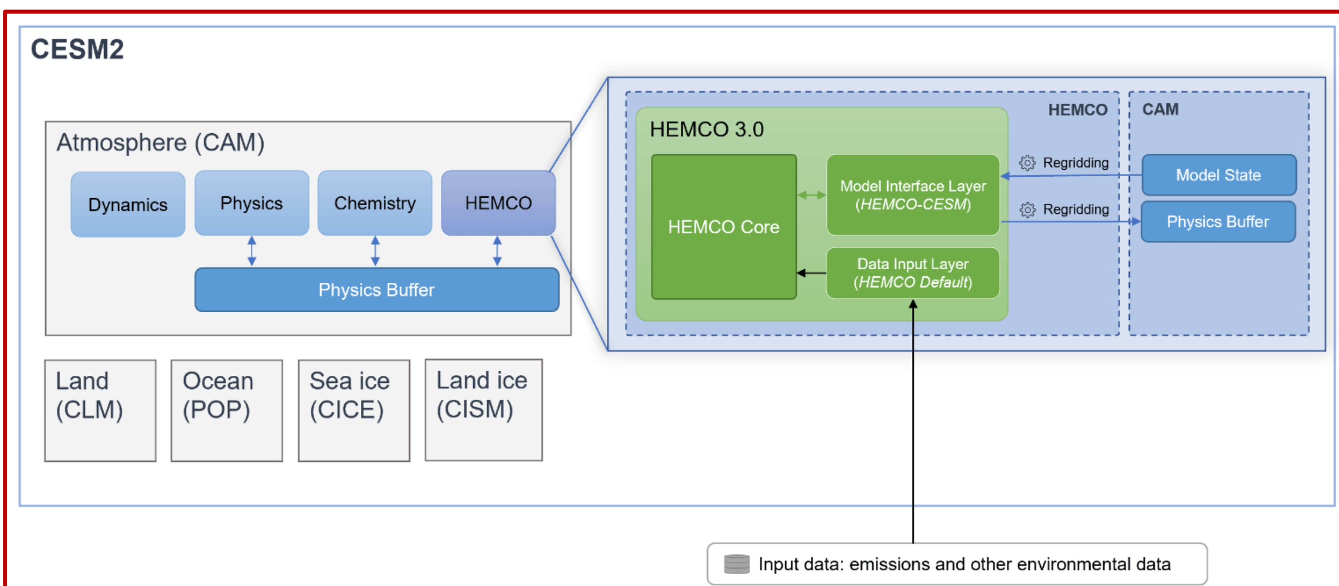
Introduction to HEMCO

The Harmonized Emissions Component (HEMCO) is a software component to compute emissions from a user-selected ensemble of emission inventories and algorithms. It allows users to re-grid, combine, overwrite, subset, and scale emissions from different inventories through a configuration file and with no change to the model source code or repeated pre-processing of source input.

HEMCO can operate in offline stand-alone mode but more importantly can be coupled to other models and work online as an emissions provider. It was originally designed by Keller et al. (2014) as an online emissions component for the GEOS-Chem chemical transport model but is now coupled to other models such as the GEOS ESM, WRF-GC, and now CESM2!



HEMCO 3.0 reference (Lin et al., 2021), Geoscientific Model Development, Sep 2021: https://gmd.copernicus.org/articles/14/5487/2021/gmd-14-5487-2021.html

MUSICA Emissions Component

HEMCO is functional in MUSICA/CAM-chem

HEMCO 3.0 has been coupled online to CAM to provide emissions to both CAM-chem and GEOS-Chem chemistry components within CESM2. It can be used independent of GEOS-Chem chemistry and works with the newest SE grids as well.

HEMCO within CESM is an independent component within CAM and can provide emissions to any CAM grid, using conservative ESMF re-gridding to map source inventory data to the model grid. HEMCO internally operates on a rectilinear latitude-longitude grid of user-defined resolution, which can be used to ensure consistency in emissions scaling and masking regardless of model resolution or grid. A description of this HEMCO grid is given in Section 2.4 of Lin et al.

HEMCO is publicly available for testing!

A tutorial presentation with slides and video, and additional resources, is available on the CAM-chem wiki at https://wiki.ucar.edu/display/camchem/HEMCO. Currently HEMCO requires a modified version of CAM within CESM 2.2 but work on integration into the trunk is ongoing and HEMCO will be available out-of-the-box in the future.

MUSICA Software Development

MUSICA Software development lifecycle and plan

The MUSICA team produced a document which describes the process followed by MUSICA software engineers and scientists to develop MUSICA software. It covers requirements gathering, design, implementation, and release to the community. This document is the result of an effort to define a Software Development Plan for MUSICA that began during our User Story Mapping Workshop in the summer of 2022. We encourage MUSICA community members to read and provide feedback on this approach, particularly if there are specific science developments you would like to see become part of MUSICA.

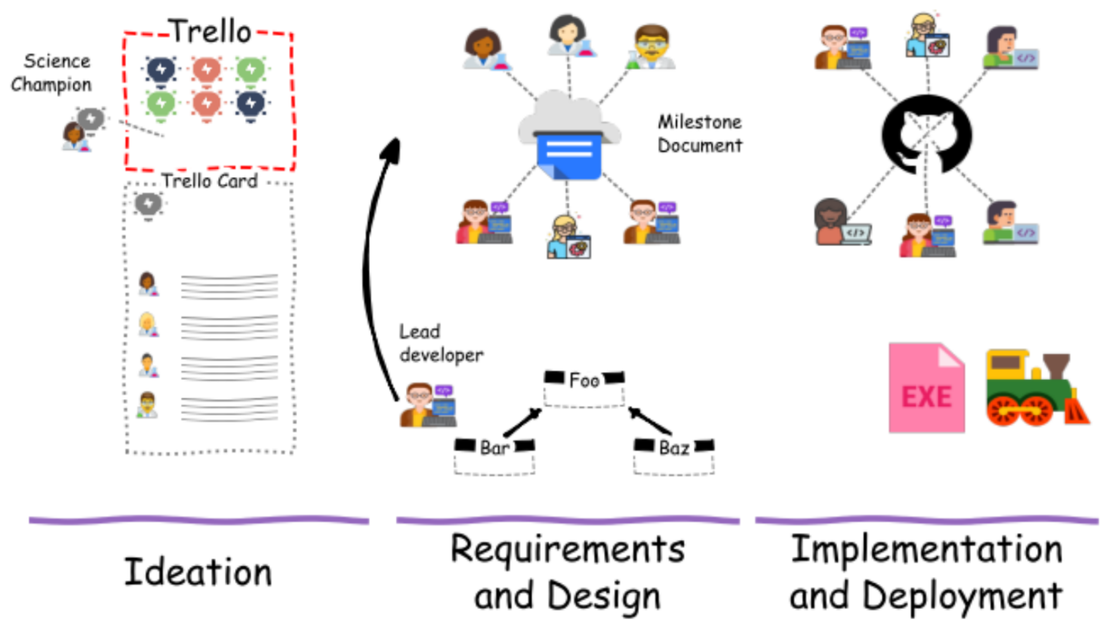


Figure. An overview of the steps for adding new functionalities to MUSICA. The approach is described at https://github.com/NCAR/musica/blob/main/docs/Software%20Development%20Plan.pdf

Steps for development

1. Write ideas on Trello board and discuss ideas among scientists
2. Identify science champion
3. Create milestone in milestone Google document listing requirements
4. Iterate with design lead to clarify requirements
5. Create design and implementation plan
6. Schedule milestone development
7. Execute implementation plan in sprints
8. Perform retrospective to evaluate product and process
9. Deploy product

MUSICA Library Release

With each newsletter, the MUSICA community can expect a new release of the MUSICA library. The MUSICA library will comprise all the aerosol and chemistry modules developed as part of the MUSICA project. This first release includes the TUV-x photolysis calculator, and the MUSICA-Core utility library, described in more detail below. Each version of MUSICA is described by semantic versioning.

MUSICA Library Release Version 0.1.0

- Repository: https://github.com/NCAR/musica
- Highlighted features or updates
  - Built and installed using modern CMake practices

TUV-x Version 0.3.0

- Repository: https://github.com/NCAR/tuv-x
- Description: The TUV-x photolysis calculator uses a wavelength-resolved radiation field to calculate photolysis rate constants and diagnostic dose rates using a number of algorithms for determining absorption cross-sections, quantum yields, and dose rates. The tool is configured using standardized input data provided at runtime. The radiation field can be provided by the user or calculated using the Delta-Eddington or n-Stream methods. The tool is usable as a stand-alone executable with photolysis rate constants and dose rates output to files, or through an API. It is suitable for embedding in a 3D atmosphere model.
- Highlighted features or updates
  - Refactored to be runtime configurable
  - Achieved 80% test coverage
  - Built and installed using modern CMake practices

MUSICA-Core Version 0.1.0

- Repository: https://github.com/NCAR/musica-core
- Description: MUSICA-Core is a collection of common utilities and algorithms needed by MUSICA software bundled into a single library. This library is agnostic of the model it is used in, but crucially is designed to allow runtime configurability of each of our models.
- Highlighted features or updates
  - Tool for accessing JSON configuration data
  - MPI wrapper functions
  - General-use string class
  - Assert functions
  - Built and installed using modern CMake practices

System for Integrated Modeling of the Atmosphere

MUSICA as part of the SIMA project

MUSICA is connected to the System for Integrated Modeling of the Atmosphere (SIMA) project through its implementation in the NCAR atmosphere modeling ecosystem. The SIMA project aims to unify existing NCAR community atmosphere modeling efforts to enable simulations of atmospheric processes and atmospheric interactions with other components of the coupled Earth system ranging from the surface to the ionosphere, and across scales from cloud-resolving weather to decadal climate studies. In November 2021, SIMA version 1 was released to the community. This initial version of SIMA includes configurations of the Community Atmosphere Model (CAM) with the spectral element dynamical core that has allowed Earth System Model simulations of polar climate and air quality in a variety of locations, as well as one-way coupling between WACCM-X and a geomagnetic grid mesh for magnetohydro-dynamics calculations

Recent developments in SIMA

One recent SIMA advancement will promote atmospheric chemistry studies that focus on links between the local, regional, and global scales (e.g., impacts of urban air quality on the regional and global scales). The SIMA project has implemented the Model For Prediction Across Scales (MPAS) non-hydrostatic dynamical core in CAM, giving CAM new functionality to resolve convective motions. Several tests are being conducted using a global MPAS mesh at 60-km grid spacing with regional-refinement to 3-km grid spacing over a specified region. An example application from the NSF-funded EarthWorks project demonstrates the capability of predicting precipitation amounts over the Pacific Northwest region of the US (see figure).

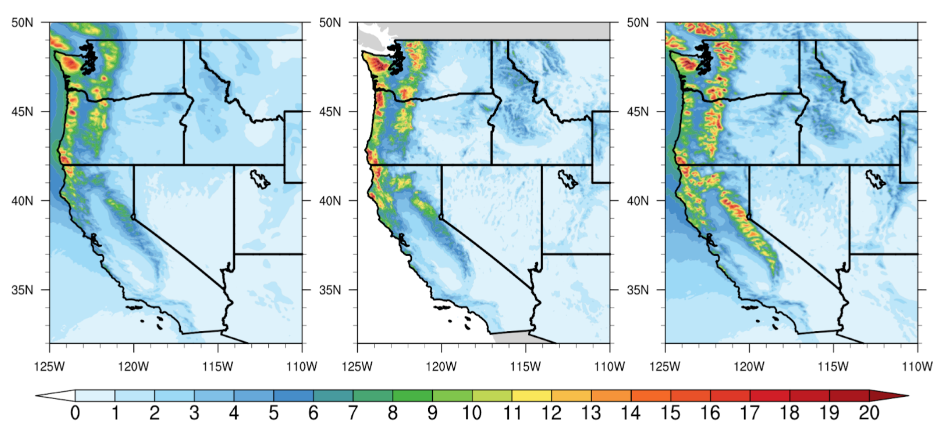


Figure. Wet-season (Nov-Mar) average precipitation rate (mm/day) over the western U.S. for 1999-2004. Left panel shows results from CESM-MPAS at 3-km grid spacing, middle panel observations from PRISM on a 4-km grid, and right panel results from WRF at 4-km grid spacing. CESM-MPAS has a small underestimation compared to the observations, while WRF tends to overestimate precipitation rate. The probability distributions of daily precipitation show that CESM-MPAS captures the PDF better than WRF, especially for more extreme precipitation. From X. Huang et al. GMD (2022).

Next Steps in SIMA Development

During the past year, the SIMA governance structure has been broadened to establish a SIMA steering committee, a SIMA Project Lead, a SIMA Scientific and Technical Co-Leads group, and a SIMA external advisory panel. Under this expanded structure, SIMA is taking a two-pronged approach for continued infrastructure development. The first is continuing to produce capabilities already identified as important. For example, there is planned work for enabling simulations with the SIMA-provided configuration of using the non-hydrostatic MPAS dynamical core in CAM using a global grid spacing of 3.75-km, which would provide the ability to perform sub-seasonal to seasonal forecasts in an Earth System Model. Other high-priority targets include refactoring CAM physics to be compliant with CCPP; developing an online, flexible regridding tool to improve input preprocessing for desired model grids; and enhancing the Model Independent Chemistry Module, while implementing it into CAM.

Another path for SIMA development is to identify and pursue a frontier-science application that will guide infrastructure development. NCAR has asked their staff to propose projects that require SIMA to develop additional functionality that can be utilized in investigations that will understand processes or predictability from local to regional to global scales and synthesize cross-disciplinary science. The SIMA developments for this science application should open the door for many other groups to apply SIMA for advancing their own science interests.

As SIMA development matures, we expect it will provide functionality to conduct exciting, new science in atmospheric chemistry from local to global scales. See more information about SIMA at *sima.ucar.edu*

SIMA Steering Committee:	G. Romine, D. Lawrence, G. Mullendore, H. Gilbert, P. Levelt, T. Hauser
SIMA Lead:	M. Barth
SIMA Scientific & Technical Co-Leads:	B. Skamarock, H. Liu, A. Herrington; SE Project Mgr: J. Powers
SIMA Project Management Lead:	D. Colegrove
External Advisory Committee:	A. Arellano (U. Ariz), S. Chen (U. Wash), L. Horowitz (GFDL), S. Merkin (HHU), C. Randall (U. Colo), D. Randall (CSU), R. Torn (U. Albany), C. Zarzycki (PSU)

Conference and Workshop Presentations

AGU 2022 Fall Meeting, Chicago

- **Matt Dawson,** Software Design for the MUlti-Scale Infrastructure for Chemistry and Aerosols (MUSICA).
- **Louisa Emmons,** Impacts of forest fires versus agricultural fires on air quality.
- **Sergio Ibarra Espinosa**, Air pollution simulation in South America using the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA).
- **Alma Hodzic,** Community effort to build a GeneralIzed Aerosol/chemistry iNTerface (GIANT) for Earth System Models to promote collaborative science.
- **Noribeth Mariscal**, Evaluation of Model Simulated Ozone and its Precursors Using High-Resolution Model Simulations during the Michigan-Ontario Ozone Source Experiment (MOOSE).
- **Rebecca Schwantes,** MELODIES MONET - A New Community Diagnostic Tool for Evaluating Air Quality and Atmospheric Chemistry Models Against Observations.
- **Ren Smith,** Evaluating the Modeled Representation of the Asian Summer Monsoon UTLS using Airborne In Situ Observations.
- **Wenfu Tang,** Application of the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) over Africa.
- **Jessica Wan,** Can Regional Marine Cloud Brightening Target Local Climate Change Impacts?

Atmospheric Chemical Mechanisms Conference, Davis

- **Louisa Emmons,** Multi-scale modeling of air quality and mechanism comparison with MUSICA (poster)
- **Rebecca Schwantes,** Plans For Enhanced Research Capabilities for Atmospheric Chemistry within NOAA's Unified Forecasting System