Making MUSICA

The Multi-Scale Infrastructure for Chemistry and Aerosols

Adapted from "The Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA)," by **Gabriele G. Pfister** (NCAR), **Sebastian D. Eastham, Avelino F. Arellano, Bernard Aumont, Kelley C. Barsanti, Mary C. Barth, Andrew Conley, Nicholas A. Davis, Louisa K. Emmons, Jerome D. Fast, Arlene M. Fiore, Benjamin Gaubert, Steve Goldhaber, Claire Granier, Georg A. Grell, Marc Guevara, Daven K. Henze, Alma Hodzic, Xiaohong Liu, Daniel R. Marsh, John J. Orlando, John M. C. Plane, Lorenzo M. Polvani, Karen H. Rosenlof, Allison L. Steiner, Daniel J. Jacob**, and **Guy P. Brasseur**. Published online in *BAMS*, October 2020. For the full, citable article, see DOI:10.1175/BAMS-D-19-0331.1.

Empirical evidence and modeling studies support that dynamical and chemical coupling occurs across the range of spatial and temporal scales inherent in the Earth system. However, these couplings are inadequately accounted for in current chemical transport models.

As a result, the predictability of local air quality from regional models is limited by the insufficient representation of large-scale feedbacks and the prescribed land and ocean state, while predictability of future atmospheric trace constituents is hampered by either the coarse resolution of global chemical climate models or the initial and boundary conditions impacting limited-area regional models. Also, predictions of weather and climate often neglect the two-way interactions with atmospheric trace constituents.

To meet future challenges, such as establishing early warning systems and developing adaptation and mitigation strategies, modeling systems will need to 1) change spatial scales in a consistent manner, 2) resolve multiple spatial scales *in a single simulation*, 3) couple model components that represent different Earth system processes, and 4) easily mix and match model components as needed for a specific application. This requires moving away from the fractured modeling activities of the past and bridging the gap between regional chemical weather models and global chemical climate models. It requires coupling from the local emission scale all the way up to the global forcing scale within a single framework.

Limitations in current modeling systems as they relate to the different MUSICA Working Group topics.

This vision motivates the development of Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA). MUSICA is not a single model, but a set of infrastructure concepts and requirements with rigorously defined standards that will enable studying atmospheric composition across all relevant scales. It describes a unified and modular framework with consistent scale-aware modeling approaches (i.e., approaches that are not dependent on model resolution and that can be applied to any Earth system model). It will account for feedbacks between all components of the Earth system, thereby permitting the exploration of

Model architecture

- Physical and chemical processes are typically packaged together into a single monolithic code base with complex data interdependencies, but this slows down scientific advancement and also prevents fair comparisons and rigorous assessments of different process treatments. This inflexible approach further complicates modifying or replacing different process modules in models.

Emissions and deposition

- Current models require extensive preprocessing of emissions inventory files to match the model horizontal resolution, the model chemical scheme, etc. This also consumes disk space, challenges incorporating feedbacks of dynamics and meteorology on emissions, and often requires users to develop their own regridding tools.
- Using offline inventories introduces inconsistencies between land use and vegetation information used in the model and that used to generate the different types of anthropogenic and natural emissions.
- Current dry deposition schemes crudely parameterize the dependence on meteorology and biophysics, leading to poor understanding of the impact of dry deposition on atmospheric chemistry and vegetation.

Chemical schemes

- Current chemical mechanisms are not flexible and are targeted toward a limited scale and application.
- Mechanism development, which is based on a set of handwritten equations, starting simple and adding complexity as needed, is becoming more challenging as complexity increases.

Aerosols

- Modules that calculate aerosol processes are typically strongly tied to the aerosol representation of the host model, which complicates porting aerosol process treatments between host models with different aerosol representations. The required level of complexity increases when considering aerosol–cloud interactions or interstitial and cloud-borne aerosol species.

Physics, transport, subgrid processes

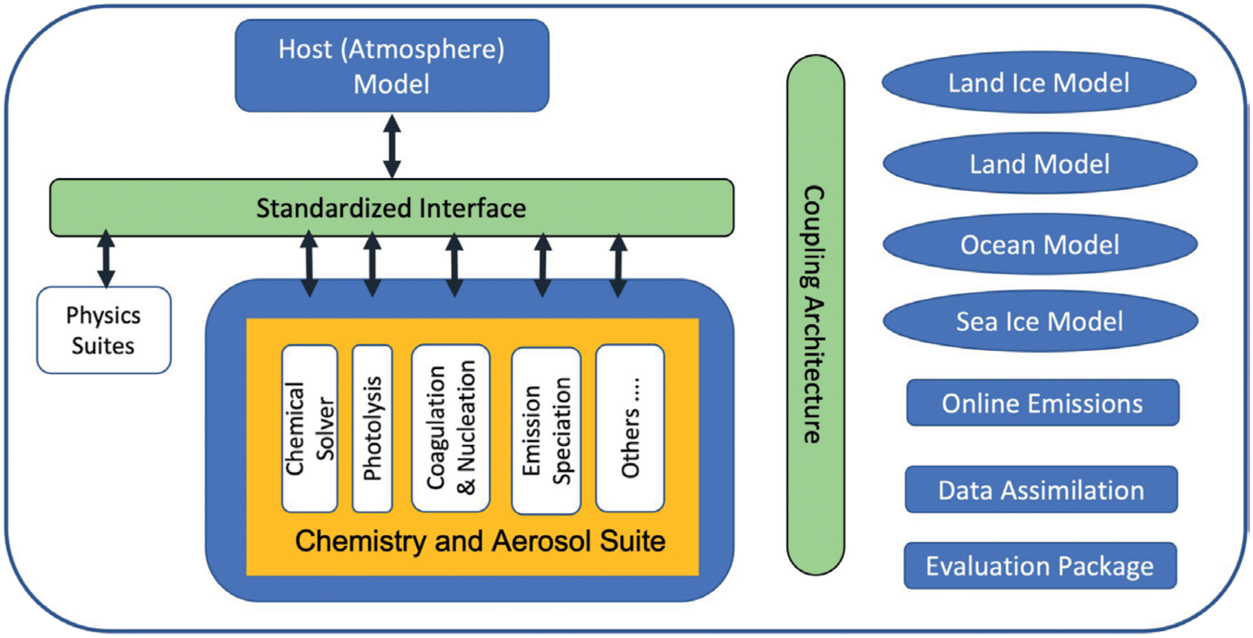
- Subgrid physics processes can be sensitive to the grid mesh sizes and therefore are often tuned within a limited range of spatial scales for optimizing model results.
- Most chemistry transport models assume that each grid cell is well mixed, although it has been shown with large-eddy simulations that reactants can be segregated, causing effective reaction rates to be different from those in the well-mixed grid cell.
- Currently, boundary layer parameterizations are employed by the chemistry transport model and constituents are transported as passive tracers. However, fast chemistry alters trace gas vertical gradients, which affects their transport efficiency.

Whole atmosphere

- Gravity waves are a dominant driver of the vertical constituent transport and circulation of the middle and upper atmosphere, connecting the whole atmosphere to solar processes and Earth's surface. These waves must be parameterized, as their 10–100-km scales are too small to be resolved on a global mesh, but there is evidence through recent research that their transports are severely underrepresented in models.

Model evaluation and DA

- Current evaluation packages are limited in scope and inflexible at incorporating new observational datasets.
- The inability to conduct a more advanced ensemble analysis and prediction via stochastic parameterization across scales and chemical species leads to insufficient characterization of model skill.
- Not considering multiscale coupled chemical DA leads to suboptimal exploitation of information content in observations and in accounting for chemical feedback processes.
- Mismatches in the representation of observational and model data result in systematic errors in model evaluation and source attribution.



interactions between atmospheric chemistry and weather and climate. Evaluation and data assimilation will be essential components of MUSICA.

To date, the lack of coordination between the different atmospheric chemistry models has made it difficult to accurately assess the benefits of different model components. MUSICA's flexible modular design will break down the problem of simulating atmospheric composition into the representation of individual processes that are described by separate modules. MUSICA can be configured in different ways appropriate for the scientific question at hand. This design will facilitate direct intercomparison of individual modules in a single framework, facilitating the quantification of uncertainties in individual processes and the codevelopment of individual components.

MUSICA will enable exploration of new science topics addressing important, frontier issues by overcoming constraints posed by limited-scale awareness in current models and frameworks. MUSICA is envisioned to become a central tool for research and for operational applications, and thus applicable to a wide range of users. This requires the system to be open source, transferable, efficient, and user friendly. The framework is built to address the needs of the wider community.

MUSICA and its components are being developed by the atmospheric research community

MUSICA defines a framework to integrate chemistry into any atmospheric host model. It includes coupling to emissions, evaluation, and data assimilation tools, and enables linking to other Earth system components, all through well-defined standardized interfaces. All physics and chemistry processes operate on individual columns; cross-column processes have to be handled by the host model.

under the coordination of the NCAR Atmospheric Chemistry Observations and Modeling (ACOM) Laboratory and in support of the NSF Atmospheric and Geospace Sciences (AGS) Atmospheric Chemistry program. Several strategic partnerships are being developed to participate in the effort (see www2.acom.ucar.edu/sections/musica-governance for a list of members).

Infrastructure design

The specific goal of MUSICA is to produce a new modular and flexible infrastructure that will enable chemistry of gases and aerosols to be simulated over all relevant atmospheric scales in a single, coherent fashion. Coupling of a stand-alone chemistry component to other atmospheric processes (e.g., aerosol–cloud interactions or convective scavenging) and Earth system components (e.g., land–sea atmospheric exchange) will leverage community-developed software tools. The Common Community Physics Package (CCPP, https://dtcenter.org/community-code/common-community-physics-package-ccpp), which will be adopted by MUSICA, includes a metadata standard that allows a model build system to check that all required fields are present.

At the heart of MUSICA is the Chemistry and Aerosol Suite, which provides updates to chemical states of gases and aerosols within the

Past and Current Approach	Future Approach including MUSICA
Impacts of the Asian monsoon on weather and climate	
Hemispheric to global impacts determined without resolving convection or surface air quality over the monsoon region.	More realistic predictions resolve local air quality and convection in the monsoon region consistently with global impacts.
Exploiting the future constellation of geostationary satellites for atmospheric composition	
Global analysis is at resolutions coarser than that of observations, and regional analysis doesn't consider the benefits of the entire constellation and those of polar-orbiting satellites.	Matching measurement resolution over the key regions together with global feedbacks results in more seamless prediction of long-range transport and more accurate source attributions between regions of the globe.
Subseasonal to seasonal predictions of air quality and weather	
Global simulations hamper fully resolving regional climate-relevant phenomena, with limited accuracy and information content at human impact scales as well.	Global coupled predictions with strategically placed high resolution over key areas (e.g., El Niño region) improves simulated regional climate variability, air–sea coupling, and exposure-relevant scales.
Stratospheric intrusions	
Global models offer coarse resolution near the upper troposphere–lower stratosphere, while regional models are dependent on boundary conditions.	Higher horizontal and vertical resolutions over tropopause-fold regions will allow better representation of frontal passages and the filaments associated with intrusions.
Long-range pollution transport and urban air quality	
Global models providing boundary conditions to regional models only consider one-way transport and are inconsistent in nature.	Seamless two-way feedback connects the local to global and global to local scales.
Intercontinental/global-scale transport of chemical layers	
Coarse vertical and spatial resolution and associated numerical diffusion prevents simulation of the layered structure of the troposphere.	Adaptive model resolution preserves chemical layers and enables assessment of their global impacts.
Aerosols seeding extreme events (e.g., hurricanes)	
High resolution over impact regions but coarse resolution over aerosol source regions and/or from lateral boundary conditions leads to poor aerosol prediction and affects feedback on extreme-event predictions.	High resolution is enabled over both impact and aerosol source regions in a consistent framework with fully enabled feedback of meteorology, chemistry, and dynamics, and between ocean and atmosphere.
Feedback loop of climate change on trace gas and aerosol gas concentrations	
Global simulations with coarse resolution over high-emissions regions impact the accuracy of simulated pollutant life cycles and land–sea–atmosphere exchange.	Global feedbacks with increased spatial resolution over high-emission regions better represent the life cycles of short-lived pollutants and land–sea–atmosphere exchange.
Gravity wave processes impacting stratosphere and mesosphere temperature and mixing	
Global simulations with general circulation, chemistry, and climate are dependent on parameterized wave sources, characteristics, and transport; or costly high-resolution "nature runs."	Better resolution of the gravity wave spectrum within the refined region couples with a more internally consistent gravity wave parameterization on the global grid.
Effect of megacities on global atmospheric composition and climate	
Disconnected spatial and temporal scales compound the problem of separate models for local/regional and global impacts.	A fully coupled system accounts for detailed chemistry/emissions over megacities and enables quantifying their impacts on remote regions (e.g., the Arctic) and the global atmosphere.
Chemical data assimilation (CDA) and evaluation	
CDA in models is generally done separately from meteorological DA and limited to updating atmospheric concentrations. Evaluation tools have been developed separately from DA.	CDA will be codeveloped as integral part of MUSICA with the objective of updating concentrations and inputs (e.g., emissions) efficiently. Commonalities between DA and evaluation will be addressed in parallel.
Air quality (AQ) under a changing climate	
Use downscaling methods to provide meteorological and chemical initial and boundary conditions to a regional AQ model.	Conduct an ensemble of simulations under various future scenarios with a single self-consistent model with sufficient resolution to simulate key AQ metrics.
Cobenefits of greenhouse gas emission reduction policies	
Conduct separate inconsistent simulations using regional or global AQ models and global climate models to investigate impacts on AQ and climate change from the move toward a net-zero-emissions future.	Conduct simulations under net-zero future scenarios with a single self-consistent model with sufficient resolution to simulate key AQ metrics and accurately simulate climate change.
Top-down emission estimates	
Either coarse resolution or inconsistency in modeling and emissions when constraining sources and sinks of long-lived species.	Improved accuracy and consistency by simulating transport and chemistry of long-lived species consistently across all scales.
Land surface coupling	
Coarser-resolution climate models are limited in their representation of land–atmosphere couplings, such as biogenic emissions and dry deposition of atmospheric constituents. Many regional models lack full coupling between land and atmosphere processes.	Land–atmosphere coupling and regionally finer resolution improves representation of meteorology, biogenic emissions, and wet and dry deposition (e.g., simulating effect of acid rain on vegetation).

Examples of new science applications enabled by MUSICA.

broader atmospheric simulation framework. It is to be incorporated through the CCPP to enable its connection to any physical component that is compliant with the interface. Any atmospheric dynamics model that uses CCPP will be able to use those physical components.

MUSICA will be capable of coupling to biogeochemistry treated in land and ocean models and provide a platform for both short-term air quality predictions and fully coupled Earth-system simulations. Closely tied to the development of MUSICA is the development of community tools for processing input data such as interpolating emissions onto flexible model grids, a common model evaluation and diagnostics framework, and data assimilation capabilities.

MUSICA components and working groups

The seven existing MUSICA working groups invite members from the community to become active members. Each group focuses on a different topic: model architecture; emissions and deposition; chemical schemes; aerosols; physics, transport, and subgrid processes; whole atmosphere; and model evaluation and data assimilation. The groups discuss expected developments, challenges, and scientific gains anticipated with respect to their topic, and how limitations in current modeling systems can be overcome.

MUSICA is designed to be implemented under different configurations with, for example, different dynamical cores and different formulations of physical and chemical processes. This could include offline systems such as the GEOS-Chem High Performance model or online systems such as the ECMWF Integrated Forecast System. Once the models are adapted for compliance with CCPP and the principles underlying MUSICA, code and knowledge exchange could be significantly accelerated.

Evaluation of the first MUSICA simulations is still underway, but the infrastructure is now at a stage where assessment of individual processes and scale awareness is possible, and the increased value of a multiscale framework can be tested. It also provides a framework conducive to active engagement with the community.

As for data assimilation, the adoption of MUSICA Version 0 with existing capabilities (e.g., Data Assimilation Research Testbed) is envisaged to be straightforward and will require less than two years to develop and implement. We also foresee that development of an observation package can be leveraged across different activities (model development, evaluation and testing, data assimilation).

Community involvement and outlook

The development of MUSICA represents an exciting challenge that necessitates strong community involvement and partnerships among different organizations and different disciplines, ranging from laboratory studies and field experiments to statistics and computational sciences, and from molecular chemistry to space physics. The community was invited at an early stage to engage in the development and design of the MUSICA framework. The new capabilities represented by MUSICA will deepen existing, and establish new, working relationships in the research community with a variety of users ranging from the research community to stakeholders. MUSICA will contribute to both advancing the science and providing relevant and actionable information for the development of mitigation policies or warning systems.

Within the next few years, MUSICA will gradually replace the current suite of community chemistry models supported by NCAR and is envisioned to also integrate the capabilities of other modeling capabilities in the community. It will provide efficiencies through consolidation of model development and training efforts and provide a single point of entry for the majority of end-users. The transition phase will be dictated by the progress of MUSICA in providing, at a minimum, the capabilities of current models. The transition will be accompanied by educational activities including user guides and in-person and online tutorials.

The capability of MUSICA to unify various spatiotemporal scales and couple to other Earth system components, as well as its process-level modularization, will allow advances in both fundamental and applied research in atmospheric composition, air quality, and climate, with MUSICA also envisioned to become a platform that addresses the needs of policymakers and stakeholders.

Website: *https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica*

BAMS: What would you like readers to learn from this article?

Guy Brasseur (NCAR): *Global and regional chemical transport models have been extremely useful to investigate the influence of emissions, transformations, transport, and deposition processes of chemical species in the atmosphere. To make further progress, however, the time has come to develop new computational approaches and move the frontier of knowledge further ahead. MUSICA should be a prototype for a new generation of chemical models.*

Gabriele (Gabi) Pfister (NCAR): *Atmospheric chemistry modeling is entering into an exciting era regarding how the next generation models will be built and the new science that will be made possible.*

Mary Barth (NCAR): *The right tool has been found to answer our science questions. The MUSICA model concept is visioned to address atmospheric chemistry from global to regional to local scales. There will be no need to learn how to use different models!*

BAMS: How did you become interested in the topic of this article?

Gabriele (Gabi) Pfister (NCAR): *Air quality has captured my interest early on in my career and it became increasingly clear that we need models that bridge the scales from global to street-level and capture the feedbacks with weather and climate if we want to advance our understanding.*

Kelley Barsanti (University of California, Riverside): *I started my academic career studying the chemistry of aerosol formation on a molecular level, using models based on fundamental thermodynamics. As a postdoctoral fellow at NCAR, I learned more about how aerosol formation was represented in large-scale regional to global models. I was quite surprised at the disconnect between the scales, and really, the critical information lost as you go to longer spatial and temporal scales. I have since spent most of my academic career using experimental observations and chemically detailed models to develop better parameterizations of gases and aerosols in chemical transport models.*

Alma Hodzic (NCAR): *For many years I have been interested in the global impacts of aerosol particles that are produced from activities happening at the local/urban scales, and this multiscale modeling framework will allow me to study these impacts.*

BAMS: What surprised you the most about the work you document in this article?

Nicholas Davis (NCAR): *It is really surprising and exciting to see so many people from so many different backgrounds all recognize the need for a fundamentally new approach to modeling, such as MUSICA.*

Gabriele (Gabi) Pfister (NCAR): *The countless opportunities for new science the next generation of models will open to us.*

Guy Brasseur (NCAR): *The MUSICA initiative shows that addressing the question of scale interactions in a single modeling framework becomes possible and will therefore lead to new scientific knowledge. It also opens the way to model architectures that are really modular and will provide flexibility for different groups who will be able to adapt the modeling framework for their own needs.*

BAMS: What was the biggest challenge you encountered while doing this work?

Seb Eastham (Massachusetts Institute of Technology): *Communication. With so many different specialities talking, sometimes you almost need a translator in the room to get everyone on the same page. That goes double when considering that MUSICA is as much about software engineering as it is about science.*

Kelley Barsanti (University of California, Riverside): *I am part of the "chemical schemes" working group, and the ongoing challenge we face is managing chemical complexity. We need to be able to represent hundreds of different molecules in the atmosphere, just one of which can undergo 10^5–10^6 reactions and form 10^4–10^5 products. Reducing the number of explicitly represented compounds and products, lumped compounds and products, and chemical reactions—while adequately reproducing or predicting the amounts and properties of these compounds and products—is an ongoing challenge.*

Gabriele (Gabi) Pfister (NCAR): *The demands from a software engineering perspective are significant, and so are the demands for developing scale-aware parameterizations. It's going to be a challenging project but hugely rewarding.*