

# MUSICA Tutorial Series 2021-2022: Introduction to MusicBox

**MUSICA: MULTI-Scale Infrastructure for Chemistry and Aerosols**



8 April 2022



# Agenda for the MusicBox Tutorial

- Introduction & Overview of MUSICA (Mary)
- Overview of MusicBox (Matt)
- Demonstration of MusicBox Interactive (Yang Li)
- Hands on Exercise (Mary)
- Introduce the command line version of MusicBox (Matt)

Mary Barth  
Senior Scientist  
NCAR/ACOM



Matt Dawson  
Software Engineer III  
NCAR/ACOM



Yang Li  
Assistant Professor  
Baylor University



## MusicBox Developers and Testers

Matt Dawson, Software Engineer III, NCAR/ACOM

2019-2021: Andrew Conley, Lead Technical Model Developer, NCAR/ACOM

2020-2021: Simon Thomas, Undergraduate student assistant

2021: Joana Olsen, Undergraduate student intern

Starting May 2022 we will have new student assistants contributing to MusicBox

If you would like to contribute to MusicBox development, please let us know!

# MUSICA: Multi-Scale Infrastructure for Chemistry & Aerosols

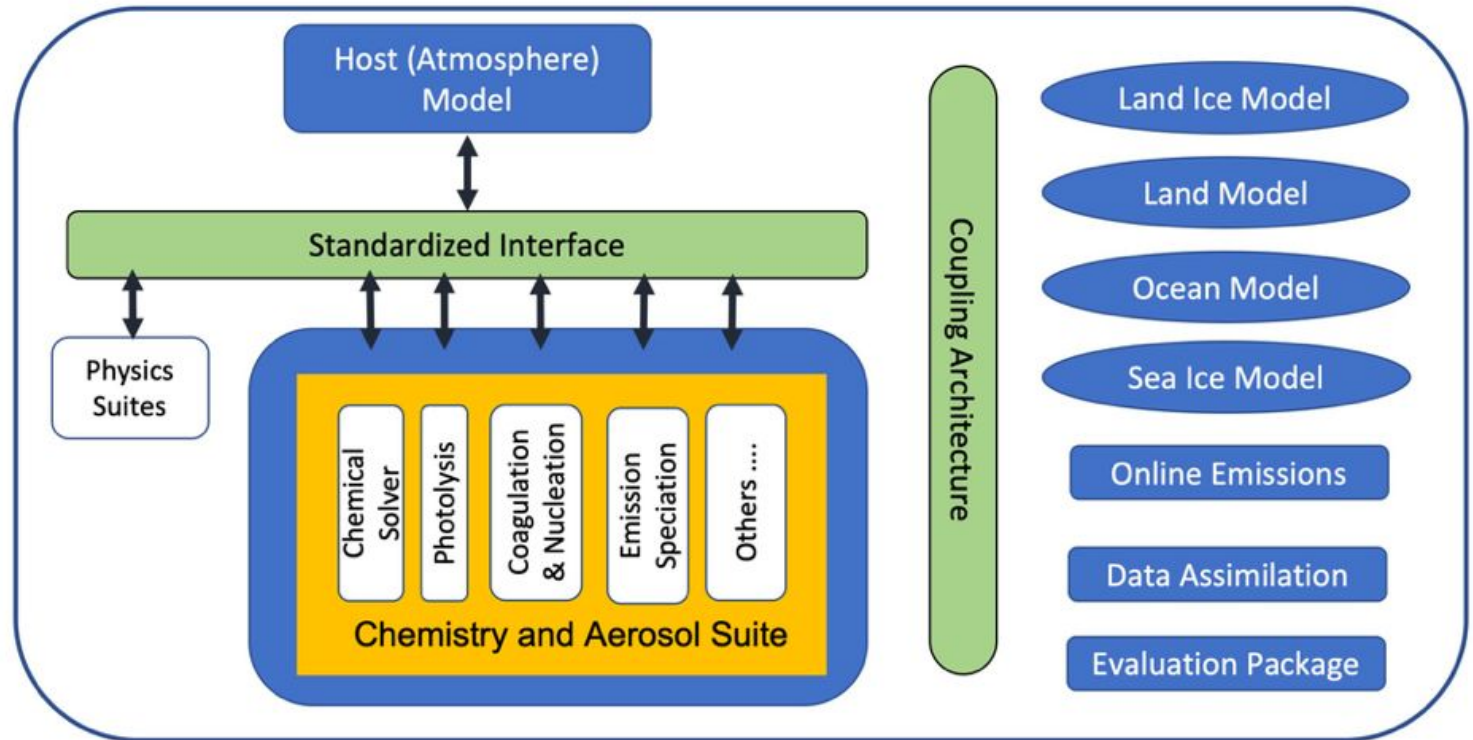
*A new model-independent framework, which will enable chemistry and aerosols to be simulated at different resolutions in a coherent fashion*

Will **facilitate use of a variety** of chemistry and physics schemes, and atmospheric models

**Coupled** to other **earth system** component models

**Whole atmosphere** framework: troposphere to thermosphere

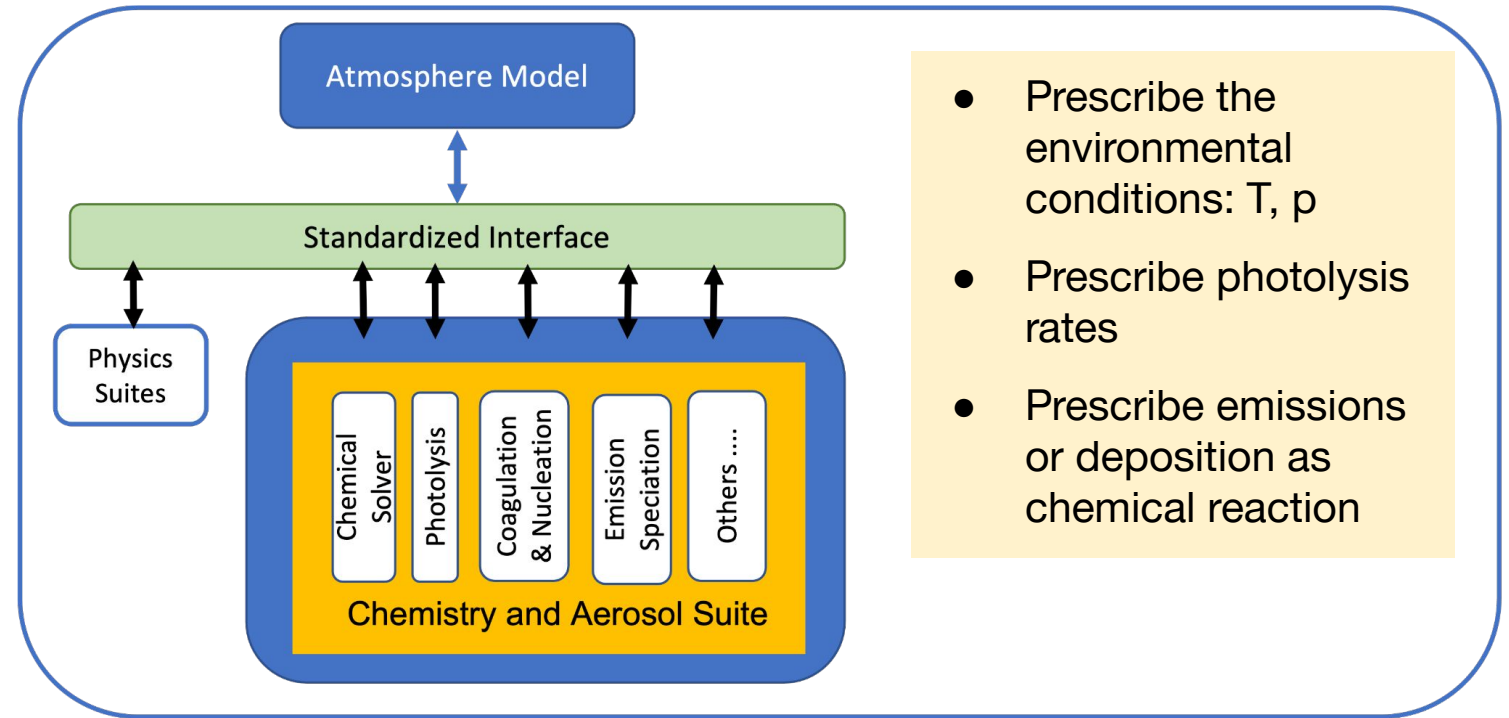
Coordinated with **SIMA**: System for Integrated Modeling of the Atmosphere



Web page: <https://www2.acom.ucar.edu/sections/multi-scale-chemistry-modeling-musica>

MUSICA Vision paper published in BAMS (Pfister et al., 2020: <https://doi.org/10.1175/BAMS-D-19-0331.1>)

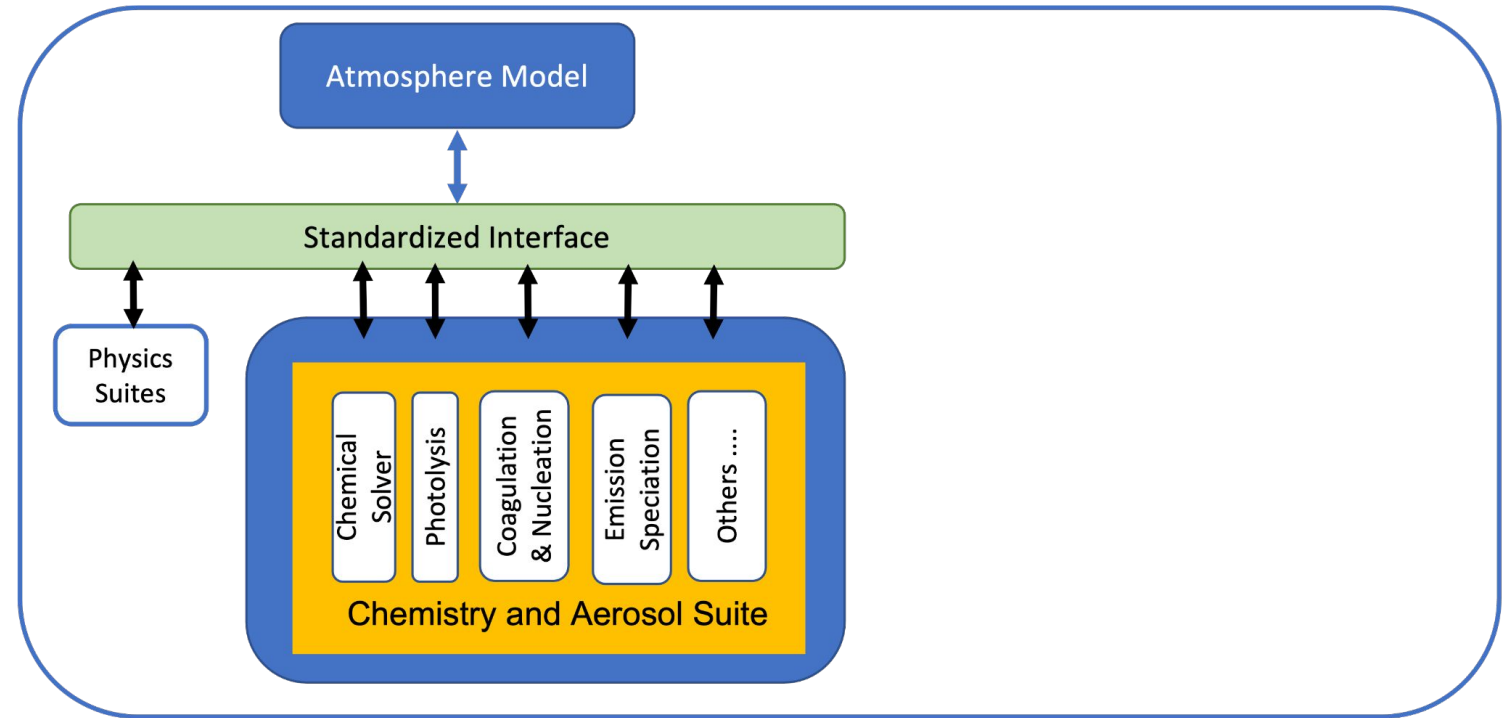
# MusicBox: A box model version of MUSICA



# MusicBox: A box model version of MUSICA

Enhance research by conducting simulations focused on the chemistry

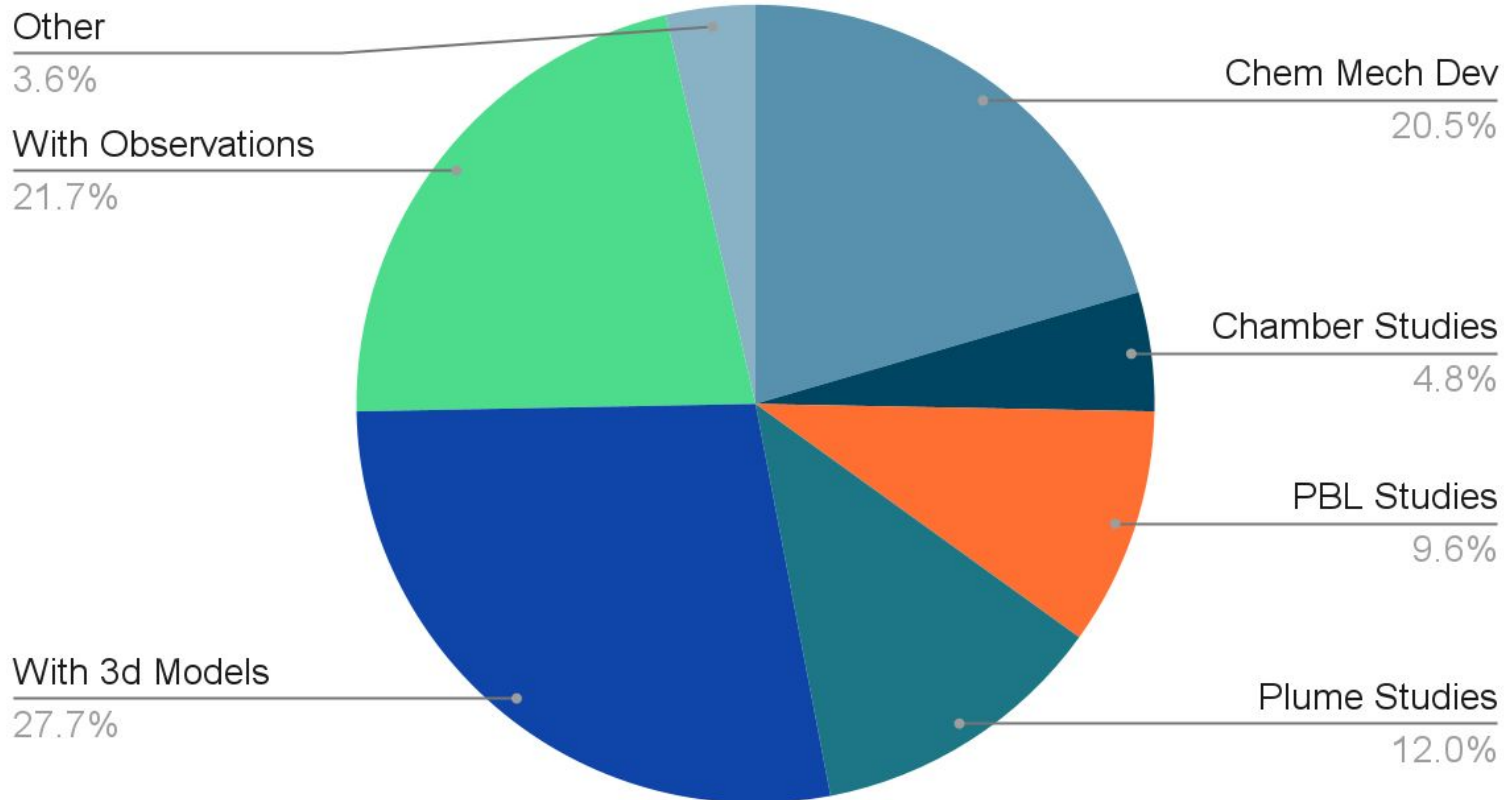
Provide a tool for teaching atmospheric chemistry in the classroom





# Potential Applications for MusicBox Research

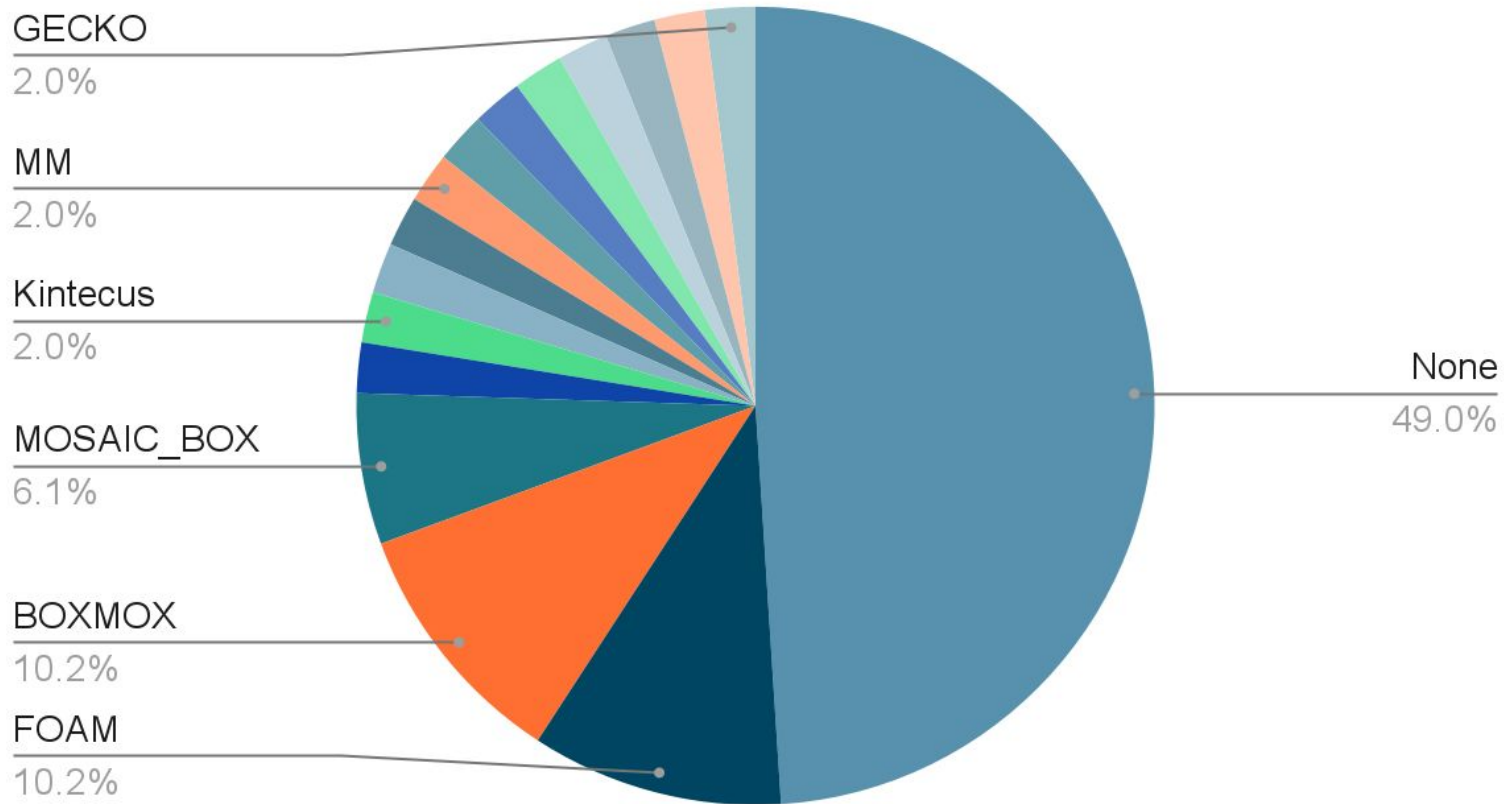
## Applications for Box Modeling



Based on 46 responses to the MusicBox Tutorial registration

# Have you used a box model before?

## Box Models Used Before



Based on 46 responses to the MusicBox Tutorial registration



# What do you like about these other box models?

- Ease of Use
- Run it from Web browser; easy installation
- Good documentation
- Flexibility, speed
- Free to download
- Ozone isopleth can be generated
- Ability to have steady-state diurnal cycle
- Plotting tools/Visualization for production and loss metrics
- 

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- 

Based on 46 responses to the MusicBox Tutorial registration

## MusicBox –

- Is free!
- Runs on a browser interface, and
- Runs via command line in a terminal window
- Has plotting capabilities
- Has flexibility
- Has documentation

# What is most difficult about using these other box models?

- Difficult to configure, I/O formats, accurate input data, preparing input files
- Manually input initial conditions
- Operating system compatibility; Needed different compilation options for different environments
- Not coupled to photolysis model or external source of photochemical inputs
- Not always easy to make changes
- Need to have a good understanding of atmospheric chemistry modeling
- Cost of software
- Feeling confident in the outputs
- Revising source code for changing mechanism

Based on 46 responses to the MusicBox Tutorial registration

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Based on 46 responses to the MusicBox Tutorial registration

## MusicBox –

- Multiple ways to provide input
- Can download configuration files for future use
- Runs in Docker
- Will be connected to the NCAR photolysis tool

## What features are not available with these other box models that you wished you had?

- Easily test chemical mechanism changes
- Implementation of photolysis calculations
- Having dynamic input data
- Be able to read NetCDF files as initial condition
- Aerosol chemistry; gas-particle partitioning
- Easy post-processing to calculate production and loss rates, etc.
- Constrain a species (e.g. NO<sub>x</sub>)
- 

Based on 46 responses to the MusicBox Tutorial registration

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- Constrain a species (e.g. NO<sub>x</sub>)
- 

Based on 46 responses to the MusicBox Tutorial registration

MusicBox –

### Under development

- Will be connected to the NCAR photolysis tool
- New types of reactions will be added:
  - heterogeneous
  - cloud, aerosol
- Analysis of results continues to be developed



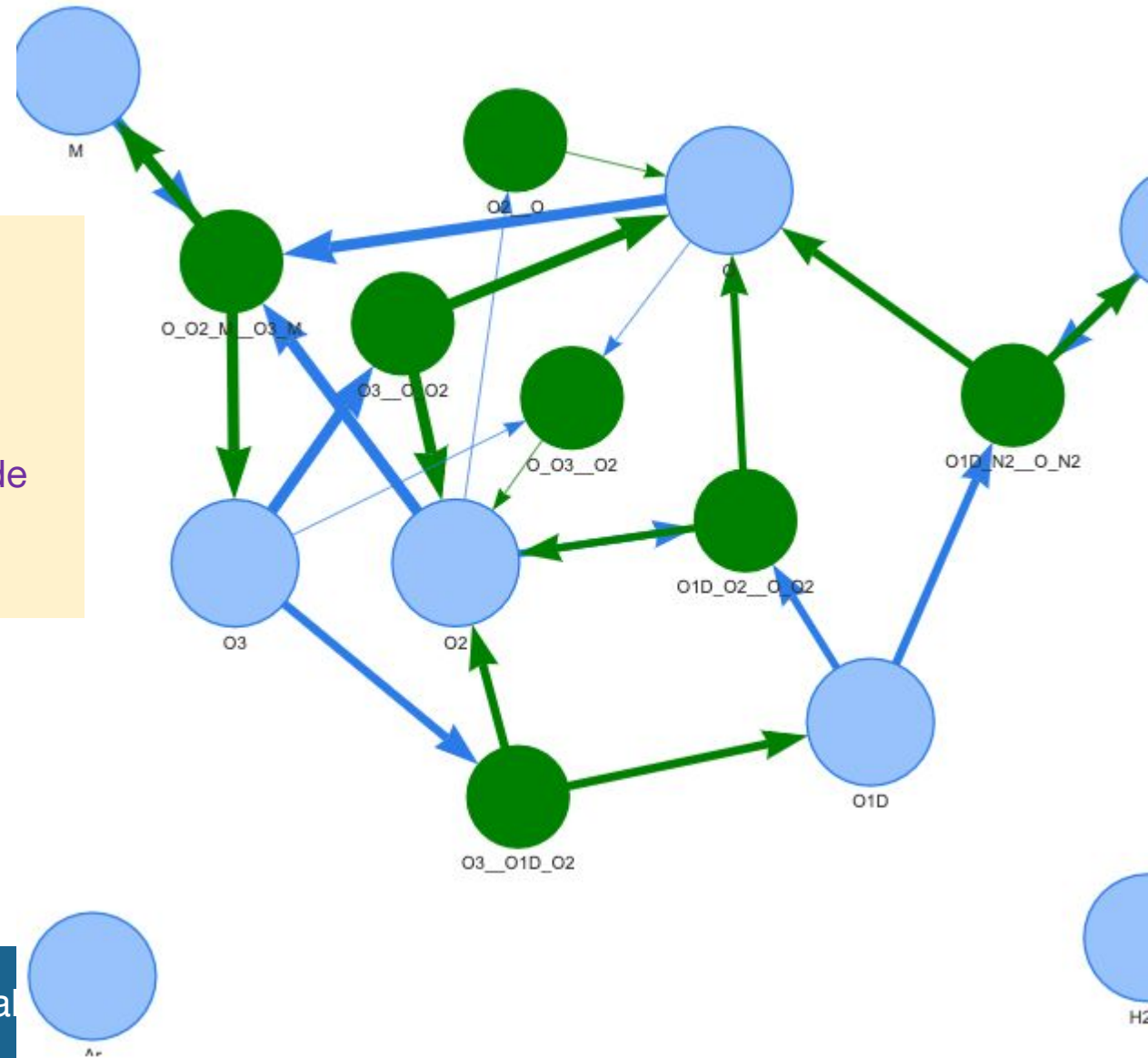
# Example analysis of Chapman Chemistry

## Analysis of Chapman Chemistry

Circles are individual trace gases

Arrows are reactions

Thickness of line related to magnitude  
of the reaction rate integrated over  
simulation



## MUSICA Goals

- To be **developed collaboratively** with university and government researchers
- To become the next-generation community infrastructure **for atmospheric chemistry & aerosol research**
- To contribute to both **advancing the science** and to providing **relevant and actionable information** for the development of mitigation policies or warning systems

## Community Involvement:

- Use released model configurations
- Use existing output
- Contribute to development
  - please join Working Groups

### Working groups:

- Model Architecture
- Emissions and Deposition
- Chemical Schemes
- Aerosols
- Physics, Transport, sub-scale Processes
- Whole Atmosphere
- Evaluation and Data Assimilation

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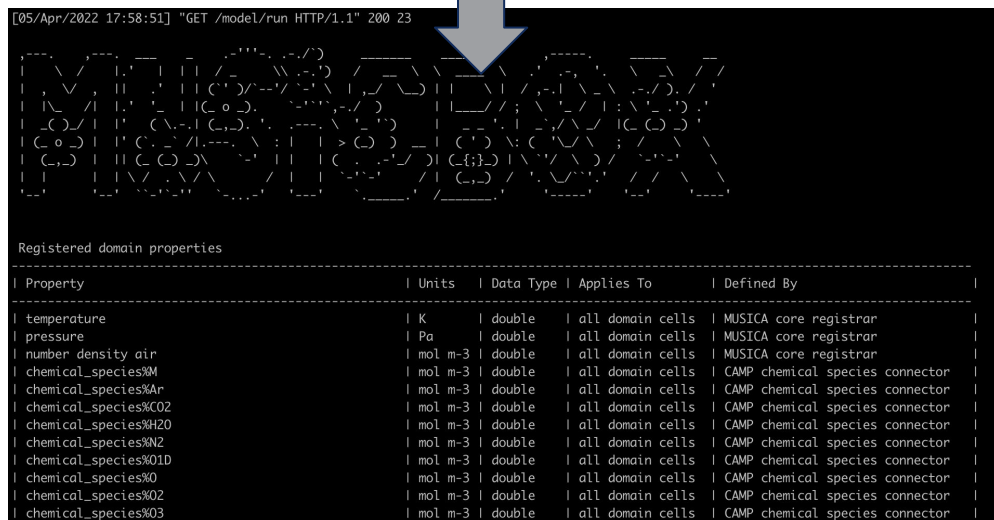


# MusicBox Design

## MusicBox command line (back-end)

Solves the chemical system

(also available directly to users for use in scripts)



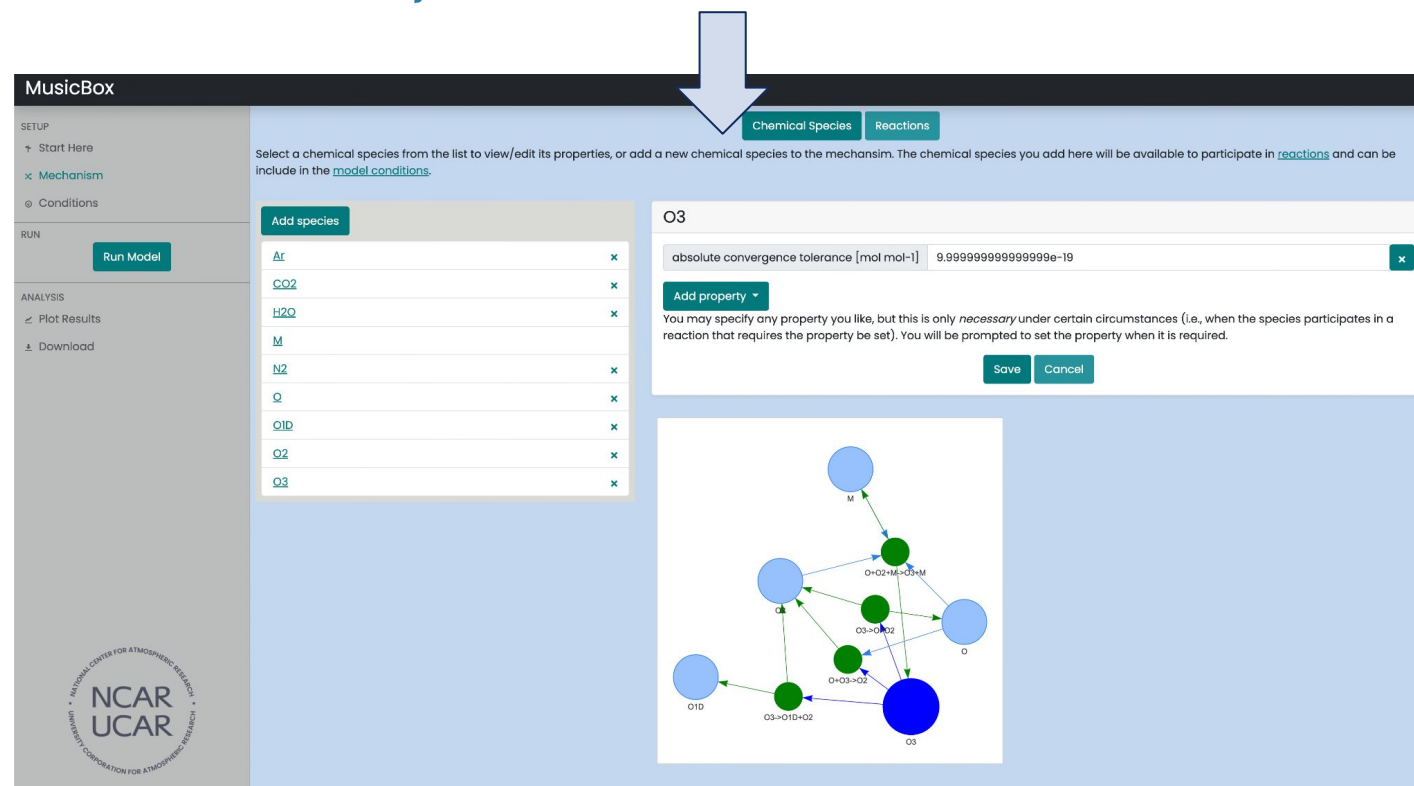
```
[05/Apr/2022 17:58:51] "GET /model/run HTTP/1.1" 200 23
```

Registered domain properties

Property	Units	Data Type	Applies To	Defined By
temperature	K	double	all domain cells	MUSICA core registrar
pressure	Pa	double	all domain cells	MUSICA core registrar
number density air	mol m-3	double	all domain cells	MUSICA core registrar
chemical_species%M	mol m-3	double	all domain cells	CAMP chemical species connector
chemical_species%Ar	mol m-3	double	all domain cells	CAMP chemical species connector
chemical_species%CO2	mol m-3	double	all domain cells	CAMP chemical species connector
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chemical_species%O3	mol m-3	double	all domain cells	CAMP chemical species connector

## MusicBox Interactive (front-end)

Interactively configures a chemical mechanism, environmental & chemical conditions, runs simulations, analyzes results



MusicBox

SETUP

- Start Here
- Mechanism
- Conditions

RUN

Run Model

ANALYSIS

- Plot Results
- Download

Chemical Species

Select a chemical species from the list to view/edit its properties, or add a new chemical species to the mechanism. The chemical species you add here will be available to participate in reactions and can be included in the model conditions.

Add species

- Ar
- CO2
- H2O
- M
- N2
- O
- O1D
- O2
- O3

O3

absolute convergence tolerance [mol mol-1] 9.999999999999999e-19

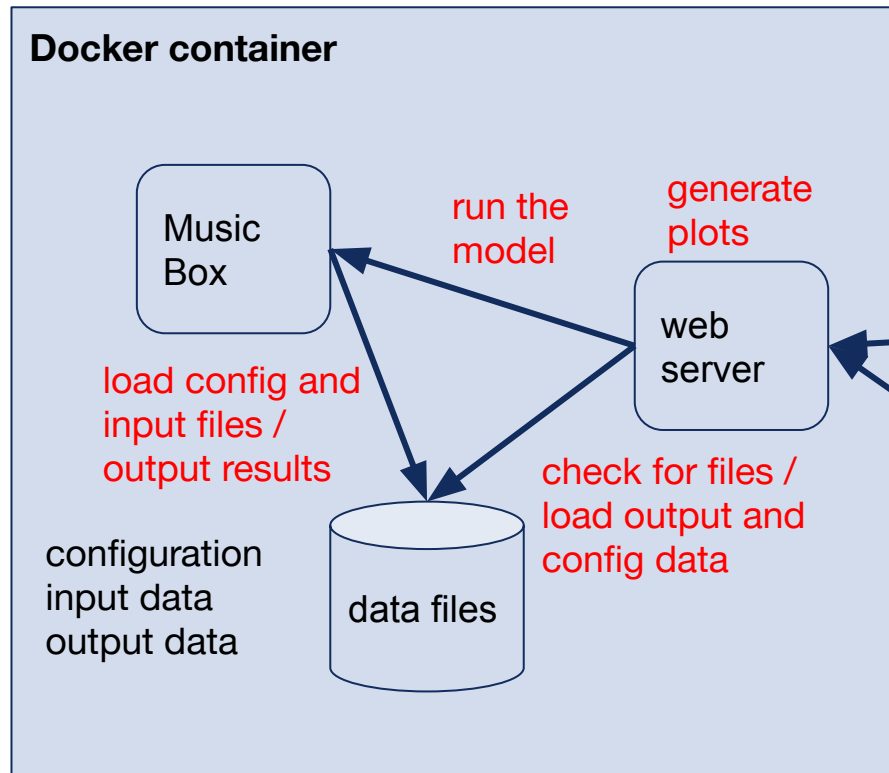
Add property

You may specify any property you like, but this is only necessary 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.

Save Cancel

Chemical reaction network diagram showing species O, O1D, O2, O3, and M with various reaction arrows.

# MusicBox Interactive (front-end)



handles requests:

- run model
- model status
- config data
- plots

logs:

- requests
- model output

**MusicBox v2.0**

SETUP

- Start Here
- Mechanism
- Conditions

RUN

Run Model

ANALYSIS

- Plot Results
- Download

Chemical Species

Reactions

Select a chemical species from the list to view/edit its properties, or add a new chemical species to the mechanism. The chemical species you add here will be available to participate in [reactions](#) and can be included in the [model conditions](#).

Species	Selected
CL2	x
CLO	x
CO	x
CRES	x
CRO	x
CXO3	x
ETH	x
ETHA	x
ETOH	x
FACD	x
FMCL	x
FORM	x
H2	x
H2O	x

- `docker run -p 8000:8000 -it --rm ncar/music-box`
- will soon be adapting MusicBox Interactive to be a multi-user hosted service

```
[07/Jul/2020 18:10:24] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:24] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:25] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:25] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:25] "GET /species HTTP/1.1" 200 6332
[07/Jul/2020 18:10:26] "GET /model_driver/mechanism_data HTTP/1.1" 200 4691
[07/Jul/2020 18:10:26] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:26] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:27] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:27] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:28] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:28] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:29] "GET /model_driver/check_status HTTP/1.1" 200 18
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[07/Jul/2020 18:10:30] "GET /model_driver/check_status HTTP/1.1" 200 18
[07/Jul/2020 18:10:30] "GET /model_driver/check_status HTTP/1.1" 200 18
```

# MusicBox - Testbed for MUSICA

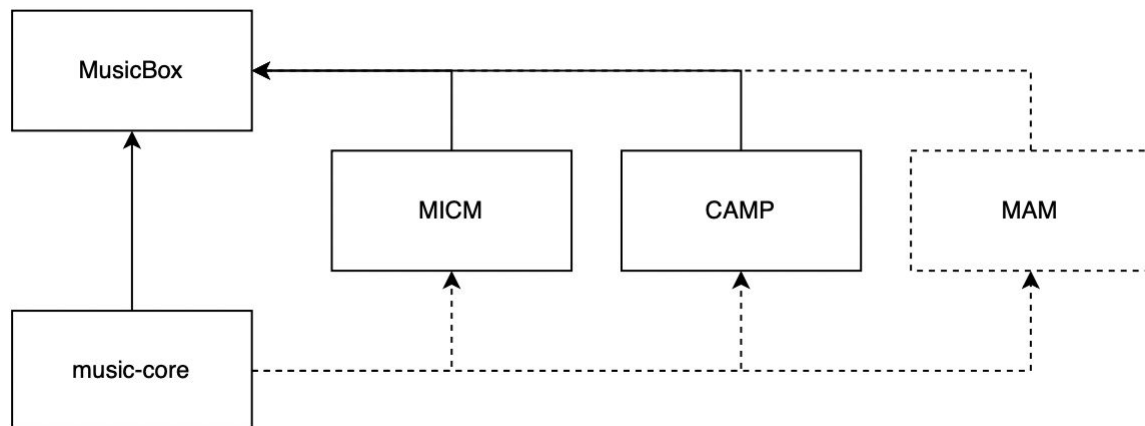
A testbed for science *and* software design!

Core MUSICA software design goals

- Science components that build as stand-alone libraries
- 80%+ code coverage by unit tests
- Run-time configurability



# MusicBox Library Structure



- libraries included as git submodules
- model components extend abstract `component_t` class
- `musica-core` library provides common utility functions and types

```
music-box/  
|—src/  
|  |—components/  
|    |—camp.F90  
|—libs/  
    |—musica-core @ 1d1a9fa  
    |—camp @ a54b863  
    |—micm @ 9fdec9c  
    |—mam @ abc1234
```

MICM = Model Independent Chemistry Module  
CAMP = Chemistry Across Multiple Phases  
MAM = Modal Aerosol Model

# Testing

```
Processing test/CMakeFiles/interpolator.dir/interpolator.F90.gcn
Finished .info-file creation
Test project /build
  Start 1: config
1/19 Test #1: config ..... Passed 0.01 sec
  Start 2: domain_cell
2/19 Test #2: domain_cell ..... Passed 0.01 sec
  Start 3: grid
3/19 Test #3: grid ..... Passed 0.01 sec
  Start 4: initial_conditions
4/19 Test #4: initial_conditions ..... Passed 0.01 sec
  Start 5: interpolator
5/19 Test #5: interpolator ..... Passed 0.01 sec
  Start 6: interpolator_linear_1D
6/19 Test #6: interpolator_linear_1D ..... Passed 0.01 sec
  Start 7: io_netcdf
7/19 Test #7: io_netcdf ..... Passed 0.01 sec
  Start 8: lookup_axis
8/19 Test #8: lookup_axis ..... Passed 0.02 sec
  Start 9: lookup_2D_axis
9/19 Test #9: lookup_2D_axis ..... Passed 0.01 sec
  Start 10: util_array
10/19 Test #10: util_array ..... Passed 0.01 sec
  Start 11: util_assert
11/19 Test #11: util_assert ..... Passed 0.04 sec
  Start 12: util_convert
12/19 Test #12: util_convert ..... Passed 0.01 sec
  Start 13: util_data_type
13/19 Test #13: util_data_type ..... Passed 0.01 sec
  Start 14: util_datetime
14/19 Test #14: util_datetime ..... Passed 0.01 sec
  Start 15: util_logger
15/19 Test #15: util_logger ..... Passed 0.01 sec
```



- goal of 80% unit test coverage for all component libraries
- automated testing for each commit via GitHub Actions
- test coverage analysis with codecov.io

README.md

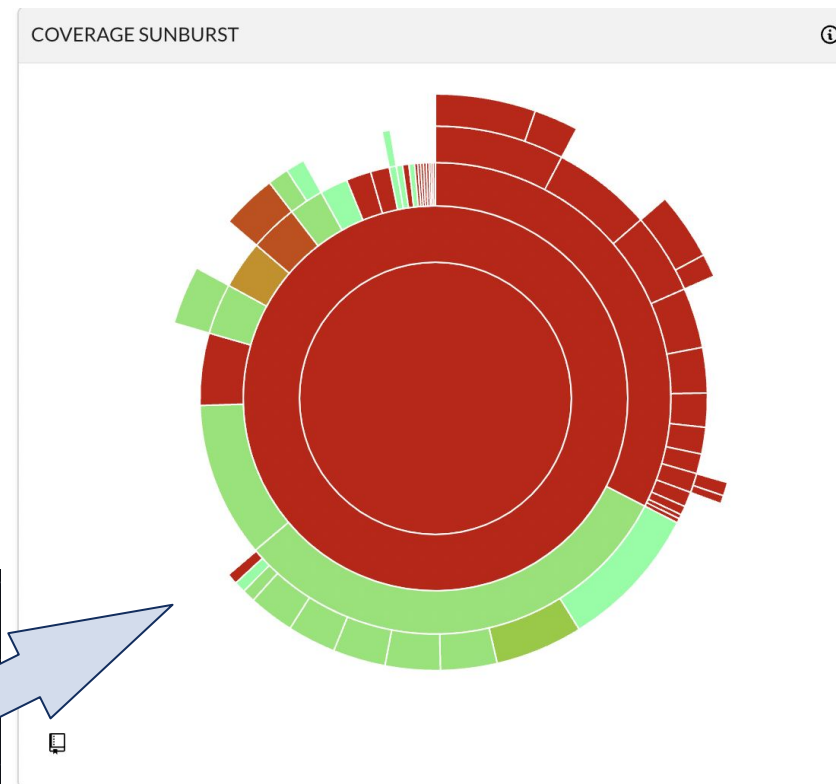
## musica-core

A library of model components and utilities.

license **Apache-2.0** build **passing** codecov **54%**

Copyright (C) 2020 National Center for Atmospheric Research

A working draft of the `musica-core` documentation can be found [here](#).



# Run-Time Configuration

```
[05/Apr/2022 17:58:51] "GET /model/run HTTP/1.1" 200 23
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Registered domain properties

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- Science components structured to remove hard-coded and build-time configuration
- Components register state variables and request accessors/mutators for use during solving

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To open the Hands-On Exercise document go directly to here:

<https://www2.acom.ucar.edu/sites/default/files/workshop/Hands%20On%20Exercises%20for%20the%20Tutorial.pdf>

Or go to the MUSICA Tutorial page, find the April 11, 2022 MusicBox Tutorial, and then the link the the document.

<https://www2.acom.ucar.edu/workshop/musica-tutorial-2021>

- April 8, 9-11am MDT (16-18 UTC): How to use MusicBox - **Separate registration required: Use [this form](#).**  
MusicBox requires [Docker Desktop](#). Please [install it](#) prior to the tutorial.  
[Hands-on Exercise document](#)



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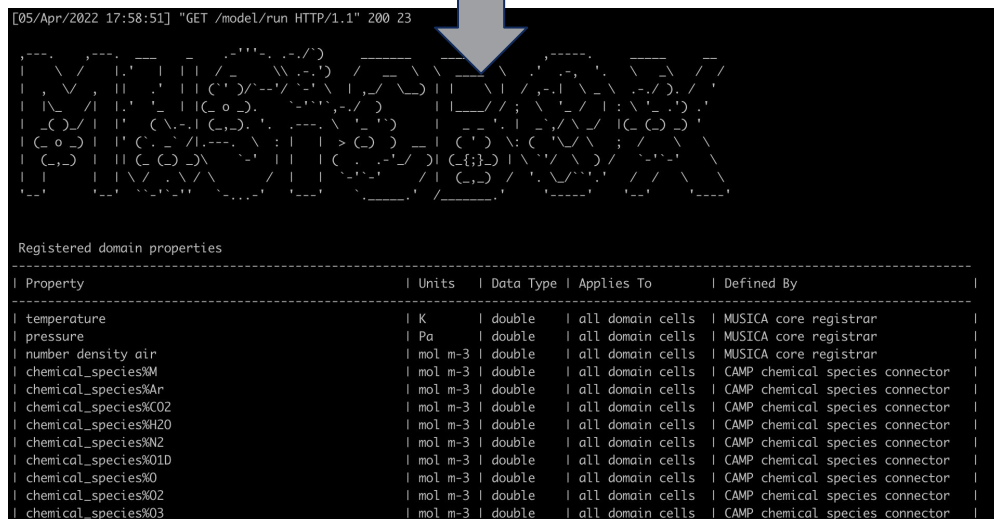


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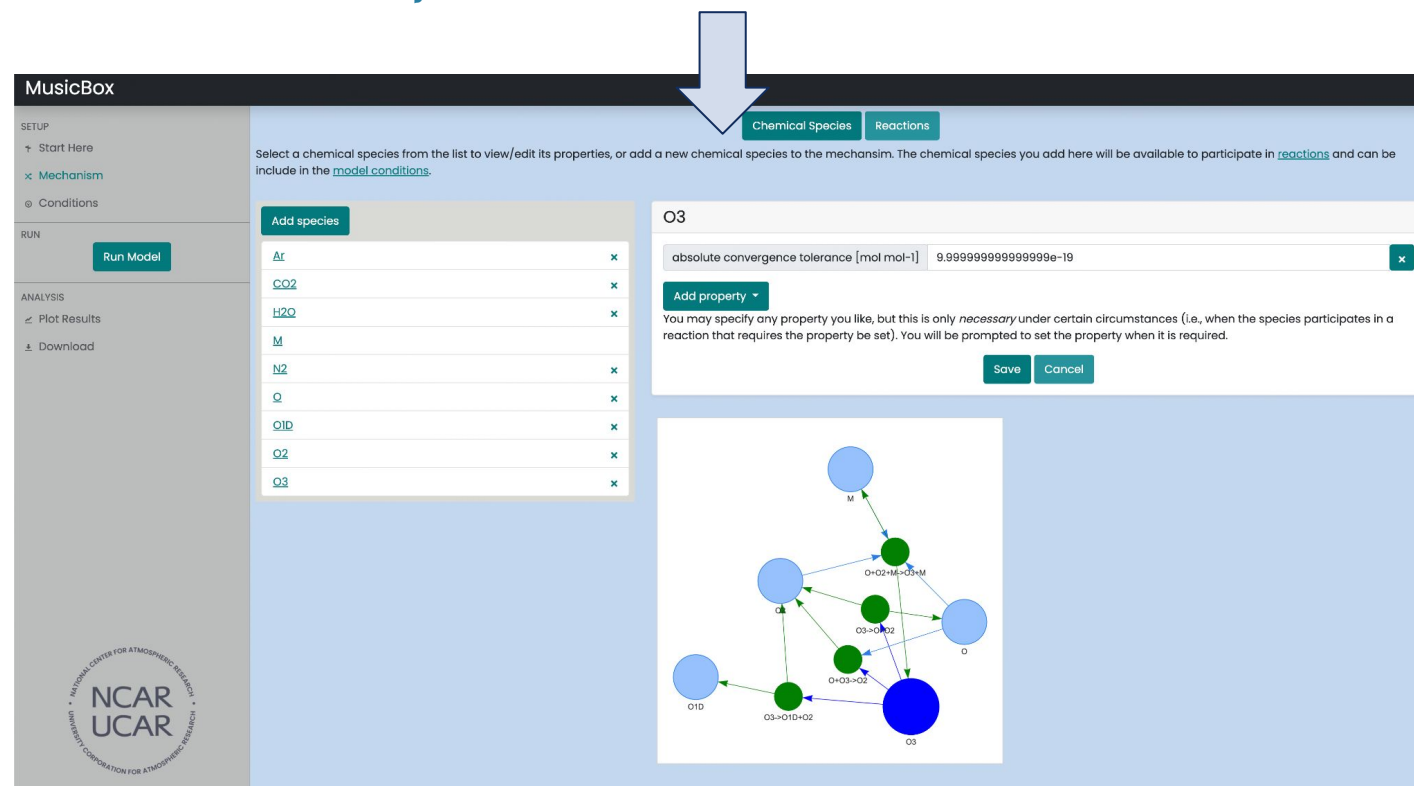


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## MusicBox Interactive (front-end)

Interactively configures a chemical mechanism, environmental & chemical conditions, runs simulations, analyzes results



The screenshot shows the MusicBox Interactive web interface. On the left is a sidebar with navigation links: SETUP (Start Here, Mechanism, Conditions), RUN (Run Model), and ANALYSIS (Plot Results, Download). The main panel has tabs for 'Chemical Species' and 'Reactions'. The 'Chemical Species' tab is active, displaying a list of species to add: Ar, CO2, H2O, M, N2, O, O1D, O2, and O3. Each species has a checkbox. To the right, the 'O3' species configuration panel is shown, with a field for 'absolute convergence tolerance [mol mol-1]' set to 9.999999999999999e-19. Below this is an 'Add property' button and a text box explaining that properties can be specified for species participating in reactions. At the bottom right, a chemical reaction network diagram is displayed, showing nodes for M, O, O1D, O2, and O3 with arrows indicating reaction pathways. The NCAR UCAR logo is visible in the bottom left corner of the interface.

## MusicBox command line

In MusicBox Interactive, select the Chapman Chemistry example, run the model and select Download > Download Configuration File.

In a terminal window:

```
$> mkdir mb-files
$> cp ~/Downloads/config.zip mb-files/
$> cd mb-files
$> tar -zxvf config.zip
$> docker run -it --mount src="$(pwd)",target=/mb-files,type=bind
ncar/music-box bash -c "cd mb-files/config; /build/music_box
my_config.json"
```

## *Thanks for attending the MusicBox Tutorial*

If you have any questions or suggestions for MusicBox, contact the MusicBox team:

If you would like to contribute to MusicBox, contact us!

[music-box-support@ucar.edu](mailto:music-box-support@ucar.edu)

### **Thanks to the MusicBox Developers and Testers:**

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2019-2021:

Andrew Conley, Lead Technical Model Developer, NCAR/ACOM

Simon Thomas, Undergraduate student assistant

2020: Joana Olsen, Undergraduate student intern

## What is your job position

46 responses

