Advancing Atmospheric Chemistry Workflows in Python

https://linktr.ee/musica_documentation

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Mentors: Jian Sun, Kyle Shores, Matthew Dawson
Summer Internships in Parallel Computational Science (SIParCS)

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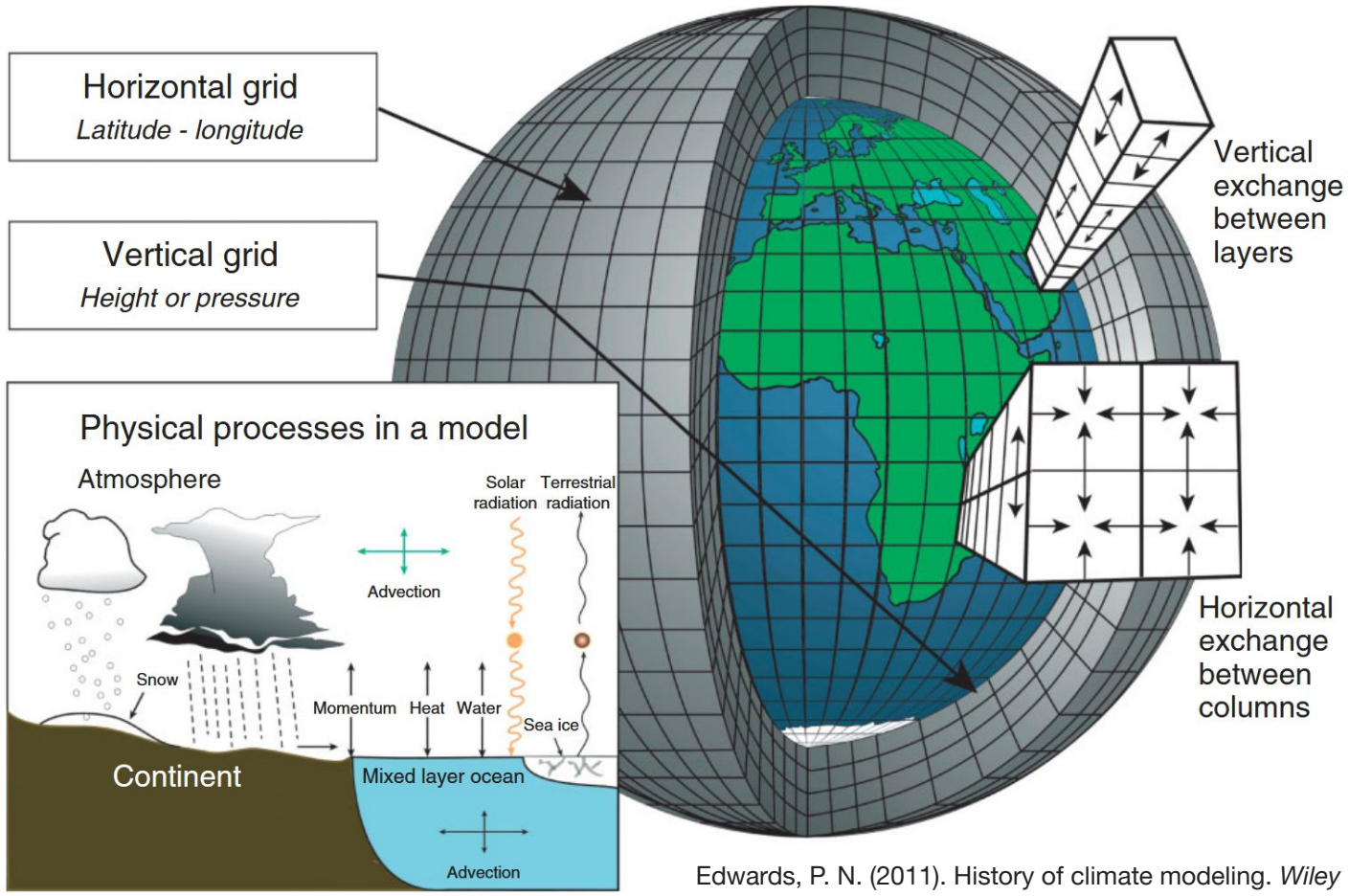
MUSICA Simulation Overview

MUSICA allows users to simulate chemical reactions in the atmosphere

- These simulations assume that the **air mass is isolated** and **well-mixed**.
- There are two types of grid cells in atmospheric models:
  - Horizontal grid cells
  - Vertical grid cells

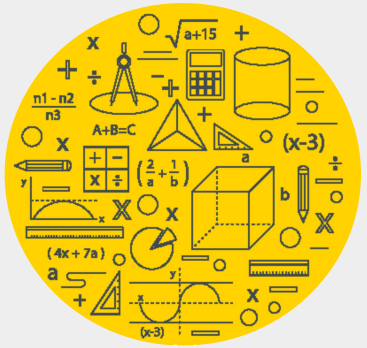


Edwards, P. N. (2011). History of climate modeling. *Wiley Interdisciplinary Reviews: Climate Change*, *2*(1), 128-139.

Intro to MUSICA System

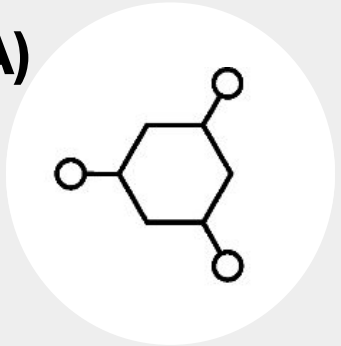
Model-Independent Chemistry Module (MICM)

- Chemistry solver
- Ordinary Differential Equation (ODE) integration



Multi-scale Infrastructure for Chemistry and Aerosols (MUSICA)

- Chemistry set up
- Mechanism configuration

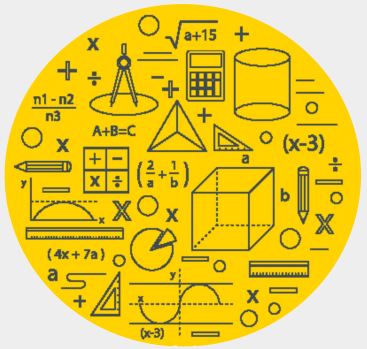


MusicBox

- Box model
- User friendly entry point

Intro to MUSICA System

Model-Independent Chemistry Module (MICM)



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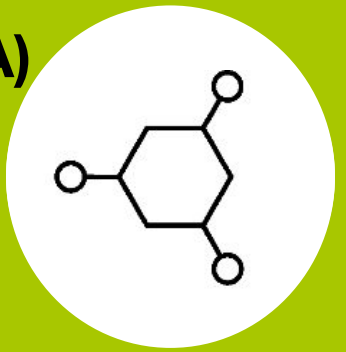
Multi-scale Infrastructure for Chemistry and Aerosols (MUSICA)



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MUSICA/MusicBox needs improved user guidance

Motivations:

- Incomplete documentation → limited user base ❌
- Gaps in support resources → complex use cases ❌
- Poor user knowledge outside the development team ❌

Objectives:

1. Clear and accessible documentation
2. Interactive tutorials with added performance features
3. A method for user engagement

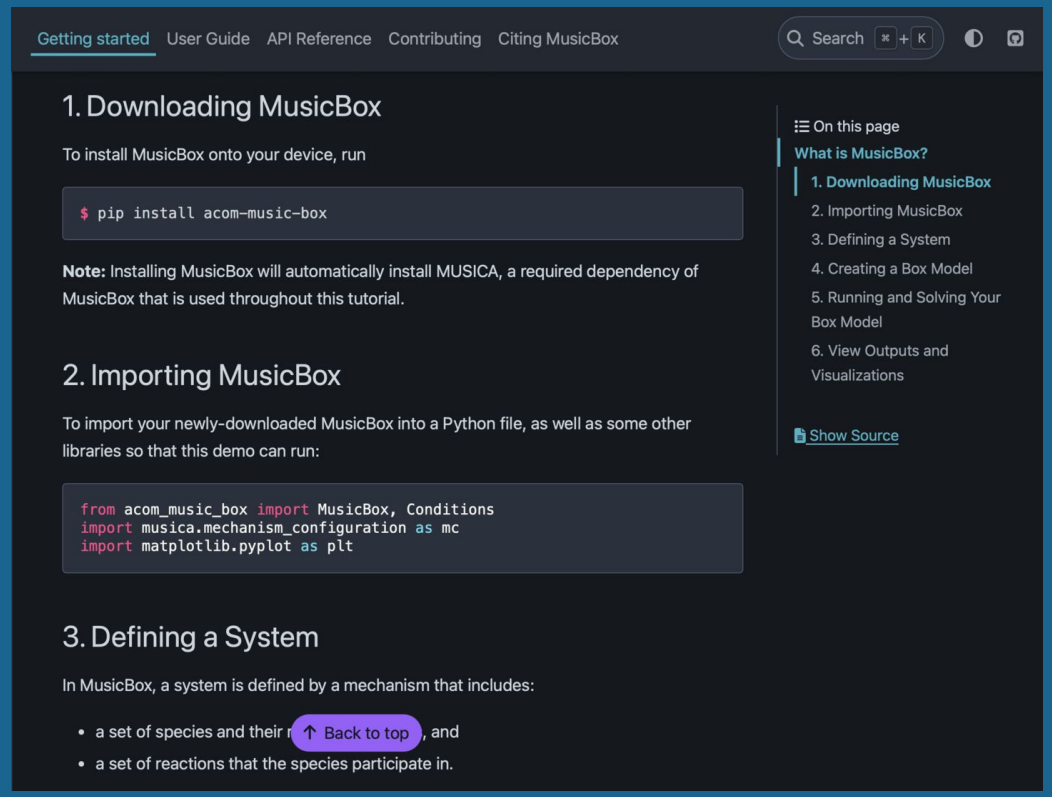
Enhance Documentation

- “Essentials” getting started guide
- Detailed user guide
- Python API reference
- Contributing guide

Build Tutorials

- MusicBox essentials
- Multiple grid cells
- Latin hypercube sampling
- Machine learning with Scikit-learn

MusicBox Essentials

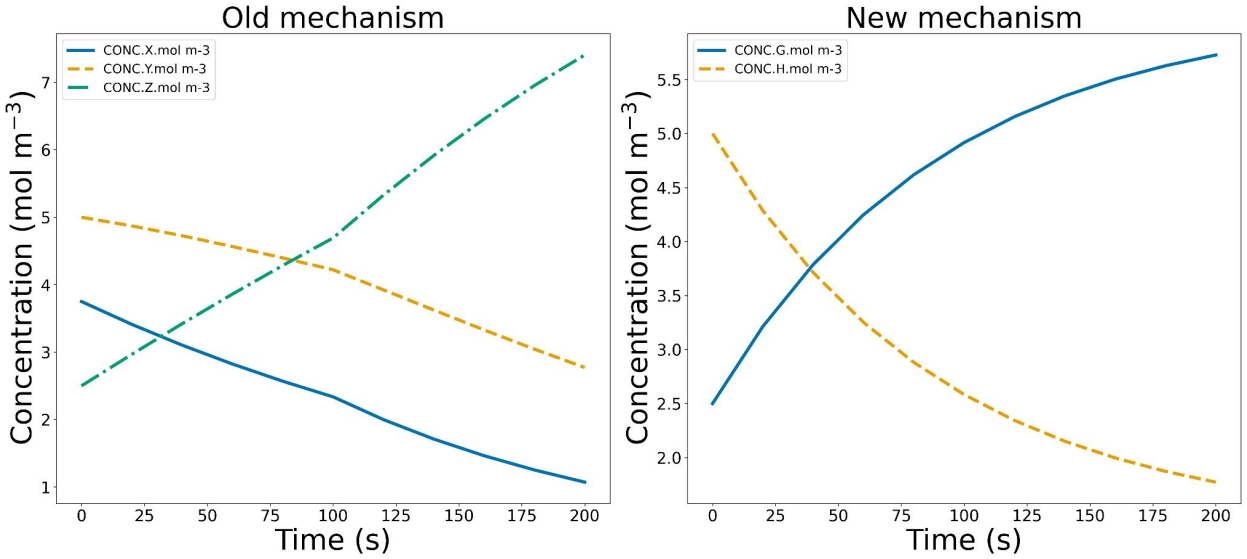


- Introducing the user to MusicBox
- Defining the species (chemicals), their phases (gas), reactions, and the mechanism
- Creating and solving the box model

view in browser **http://bit.ly/4nOMb6T**

interactive notebook **https://bit.ly/4IZSFOZ**

MusicBox Details: Overriding Mechanisms and Loading Box Models

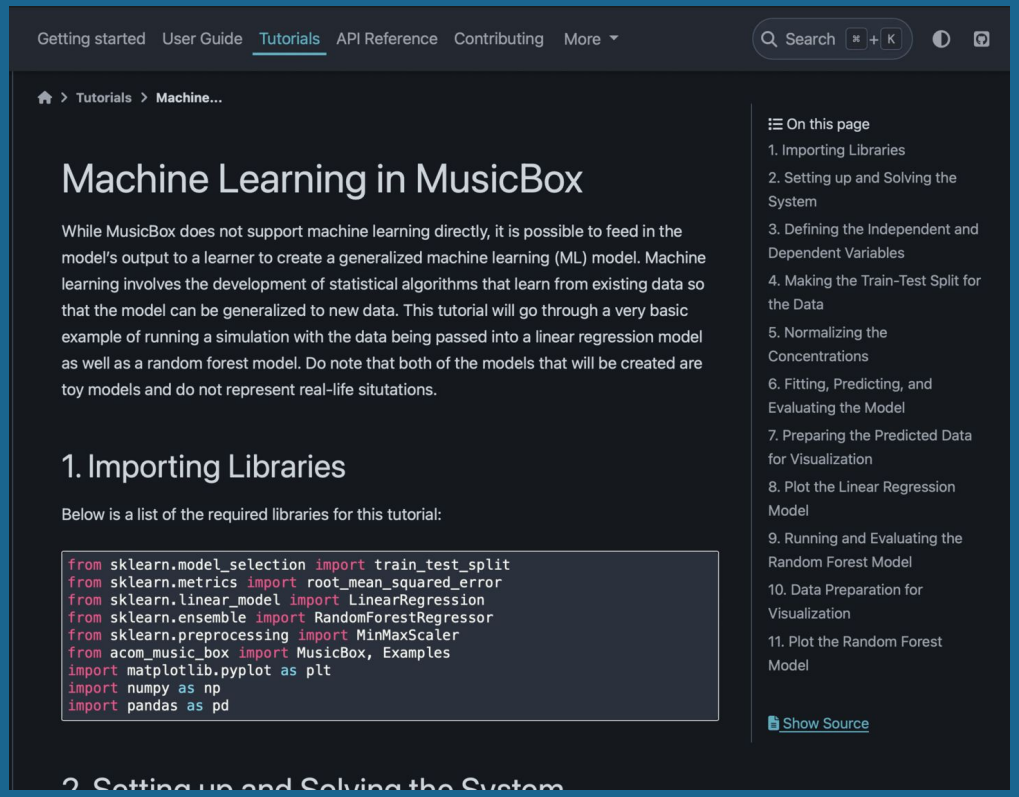


- Overwriting a mechanism replaces the entire chemical system:
  - species, conditions, simulation parameters

- Overwriting an old mechanism with a new one
- Loading a pre-made box model example
- Importing custom box model configurations

interactive notebook **https://bit.ly/3IDBIek**

MusicBox Details: Machine Learning with Scikit-learn

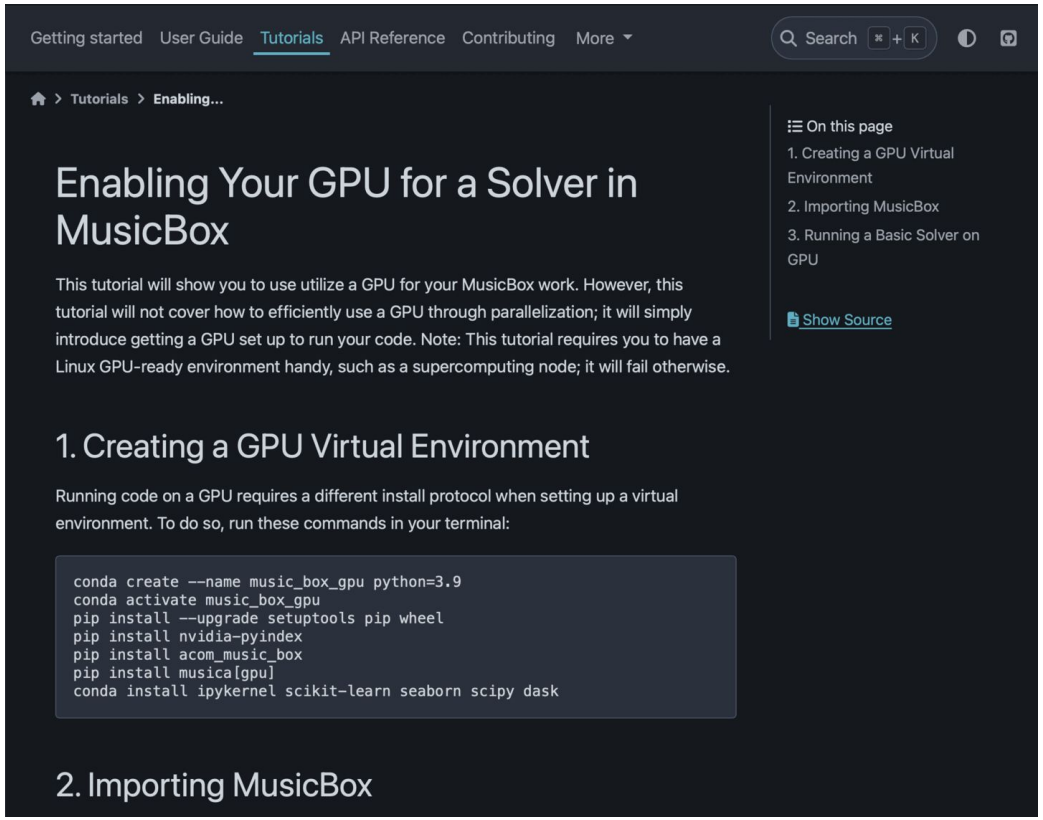


view in browser **http://bit.ly/3GQ5tYQ**

- Splitting the data into training and testing data
- Normalizing the concentrations
- Fitting, predicting, and evaluating with a linear regression and a random forest model
- Visualizing the predicted and actual concentration curves

interactive notebook **https://bit.ly/4m5Lx2U**

MusicBox & MUSICA Details: GPU Solver

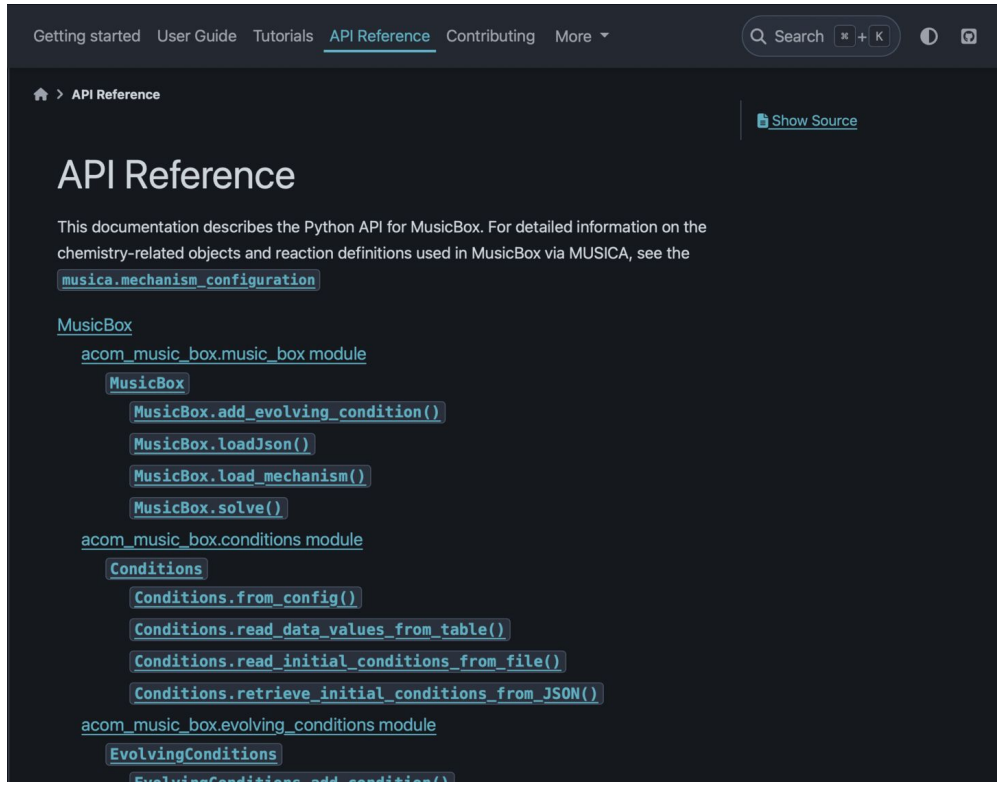


view in browser **http://bit.ly/3GDZVR8**

- Creating a new Conda GPU environment
- Verifying that a GPU is available to run on
- Running and visualizing a basic simulation

interactive notebook **https://bit.ly/4lPhpt0**

Documentation: API Reference and Contributing Guide



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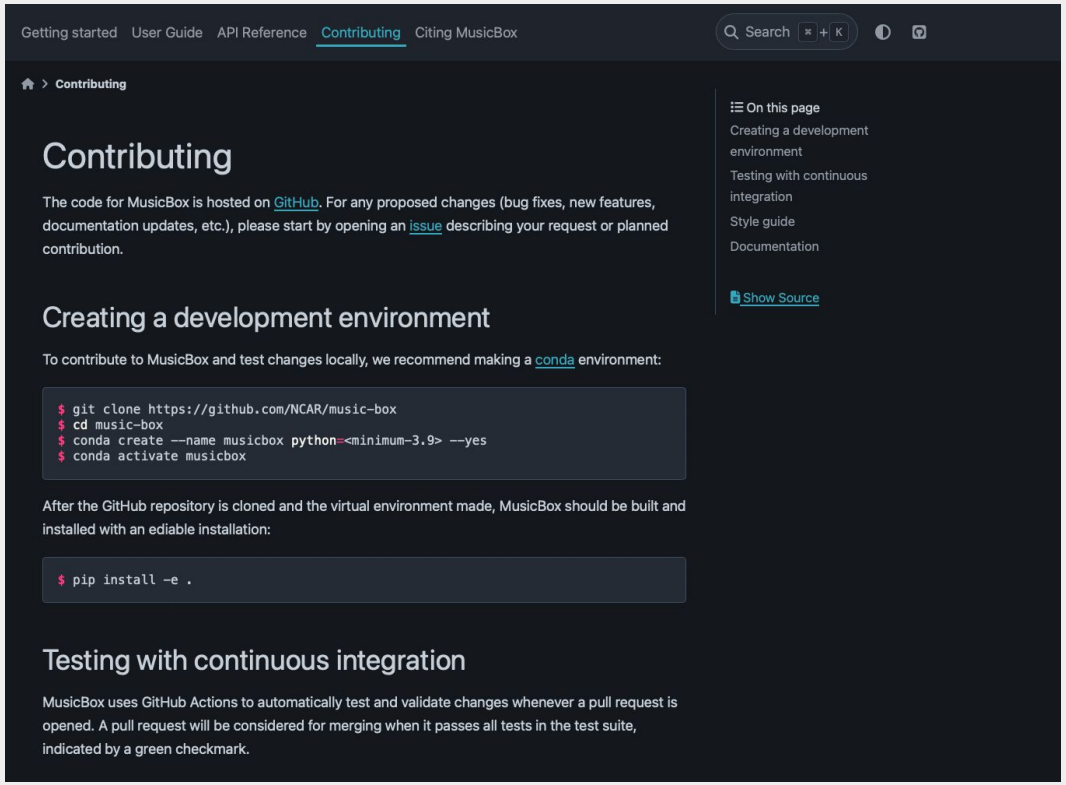

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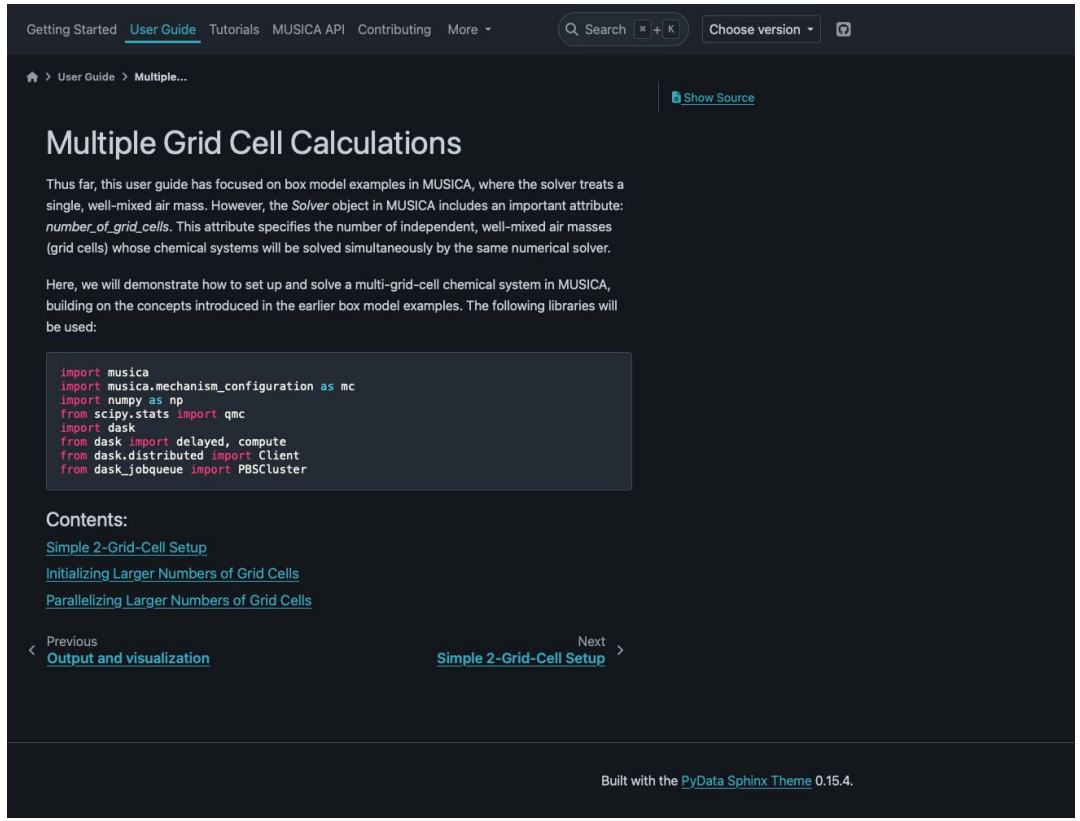
MUSICA Details: Multiple Grid Cells and Hypercube Sampling

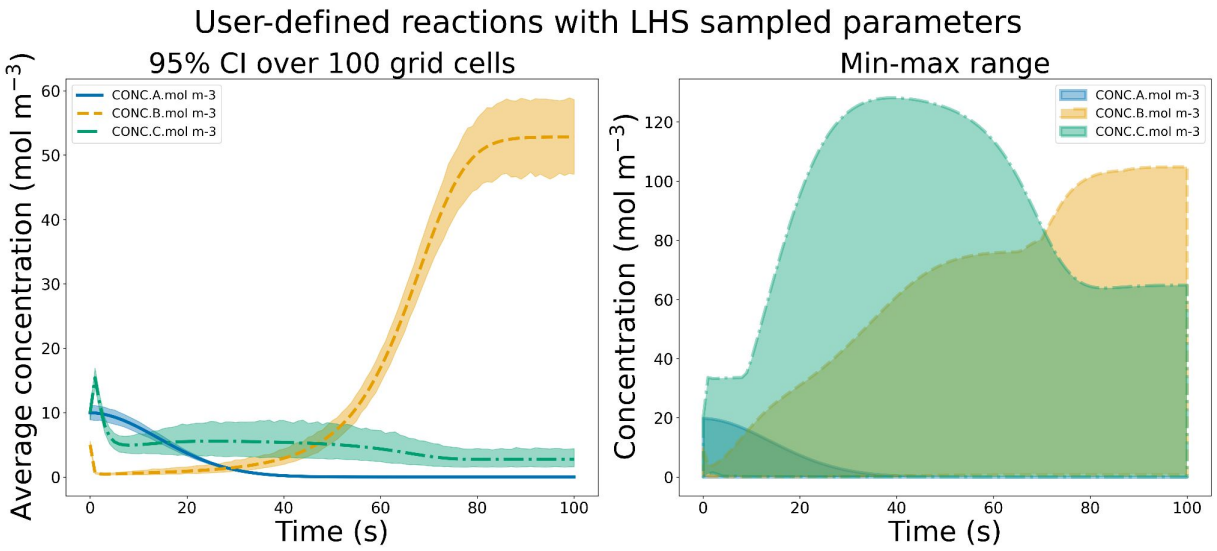


view in browser **http://bit.ly/4lJDkl7**

- Defining each of the grid cells both manually and through Latin Hypercube Sampling (LHS)
- Running the solver through every grid cell
- Plotting the concentration averages, ranges, and confidence intervals of all the grid cells

interactive notebook **https://bit.ly/3TMvJ9k**

MUSICA Details: User-Defined Reactions

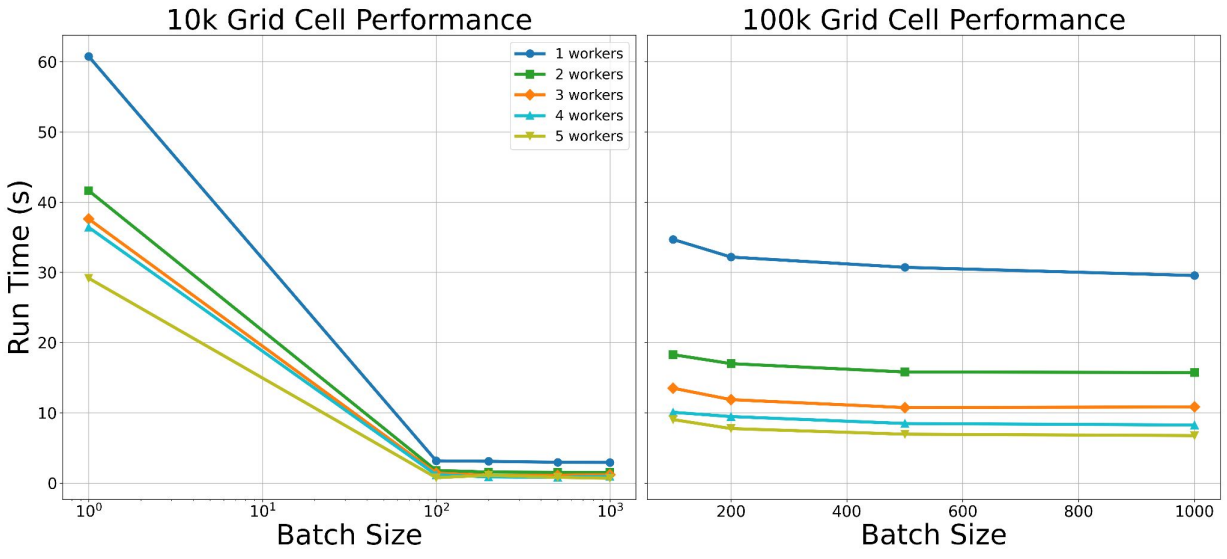


- The initial conditions and reaction rates are both randomized with LHS
  - Leads to a high variability between grid cells

- Defining the UserDefined, Emission, and FirstOrderLoss reaction classes
- Setting the user defined rate parameters
- Solving the system and visualize the concentrations between all the grid cells

interactive notebook **https://bit.ly/46h0nPy**

MUSICA Details: Multiple Grid Cells and Parallelization with Dask

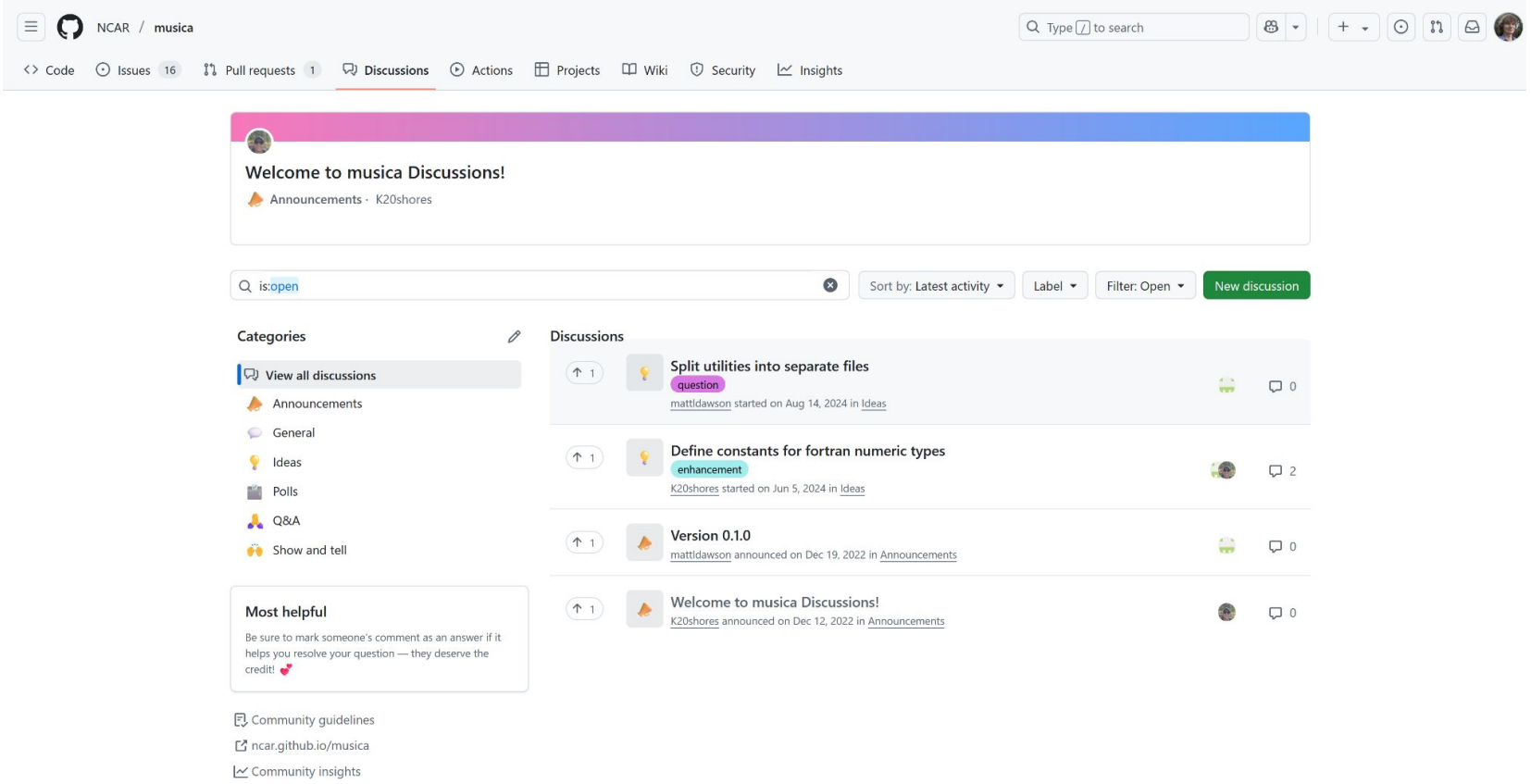


- Scaling tests performed on Derecho
- Parallelization recommended for > 10k grid cells
  - at least 4 workers
  - batch size > 100 cells at a time

- Parallelizing the solving of multiple-grid cells
- Local and PBSCluster implementations
- Batches grid cells due to low individual cost
  - 20x performance improvement optimizing 10k grid cells

interactive notebook **https://bit.ly/4lJBWiA**

Community Forum



MUSICA and MusicBox encourage the use of the community forums for:

- Q&A
- Discussions

Impacts

- Scientists at the **Indian Institute of Tropical Meteorology** are utilizing the tutorials to help students integrate MUSICA into their work
- Improved docs encouraged ACOM scientists to adopt MUSICA/MusicBox for their own projects
- Laid the groundwork for building a machine learning emulator, a key MUSICA goal

Summary and Acknowledgements

MUSICA and MusicBox systems have been enhanced with:

- Detailed documentation & interactive tutorial notebooks
- Additional performance features for multi-grid cell calculations
- Community forum

We gratefully acknowledge the support of:

- Our mentors Jian Sun, Kyle Shores, and Matthew Dawson
- Virginia Do and Jessica Wang
- CISL

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