Advancing Atmospheric Chemistry Workflows in Python

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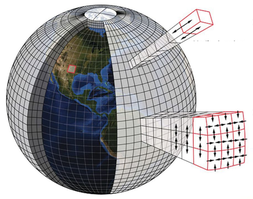
BACKGROUND

Atmospheric Chemistry Simulations:



adapted from Kotamarthi et al. [2021]

- assume that the **air mass is isolated** and **well-mixed**
- horizontal and vertical grid cells

MICM MUSICA MusicBox

Problem: Limited documentation and user knowledge restrict MUSICA and MusicBox accessibility

Goal: Update documentation to include comprehensive guides and tutorials

Updates will make MusicBox and MUSICA easier to use and broaden their user base

OBJECTIVES

1. Develop clear and accessible **documentation**
2. Build interactive **tutorials** with **added performance** features
   - **Latin hypercube sampling** for multi-grid cell input
   - **Parallelization** of multi-grid cell simulations
   - **Machine learning** model based on simulation data
3. Implement a method for **user engagement**

Key Tools

binder jupyter

ENHANCEMENTS

Tutorial Series

Created comprehensive tutorials guiding users from installation to complex simulations in both tools

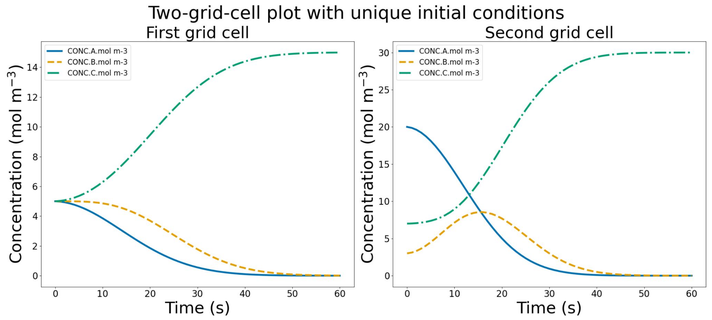


Fig 1. Overwriting a mechanism replaces the entire chemical system, including the species, conditions, and simulation parameters.

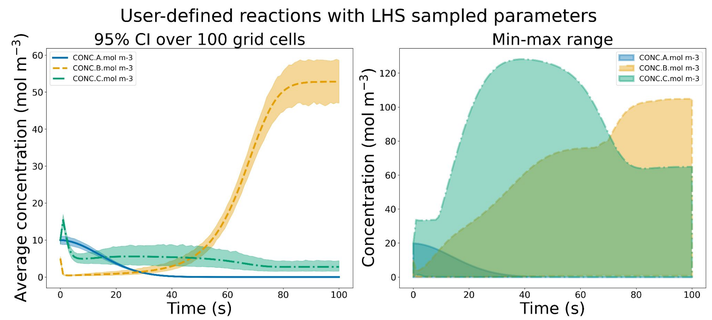


Fig 2. The initial conditions and reaction rates are both randomized with LHS. This leads to a high variability between grid cells.

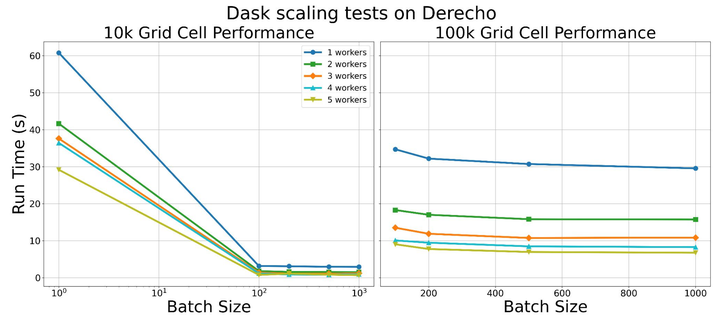


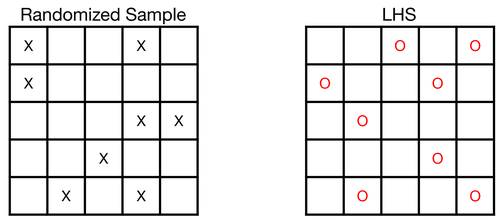
Fig 3. Scaling tests on NCAR Derecho parallelizing 10k and 100k grid cells with Dask. Batch sizes of ≥100 and using 4+ workers achieve the best run-time efficiency.

Documentation

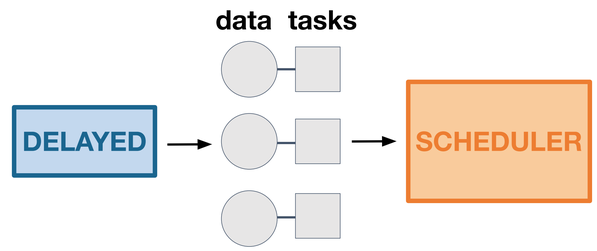
Expanded documentation to address previous gaps and enhance user accessibility

METHODS

Latin Hypercube Sampling (LHS):



Parallelization:



IMPACTS

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

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