Simulating atmospheric chemistry in a Julia-based climate model

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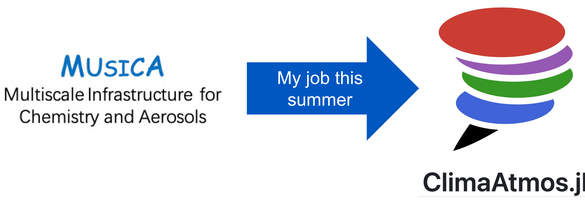
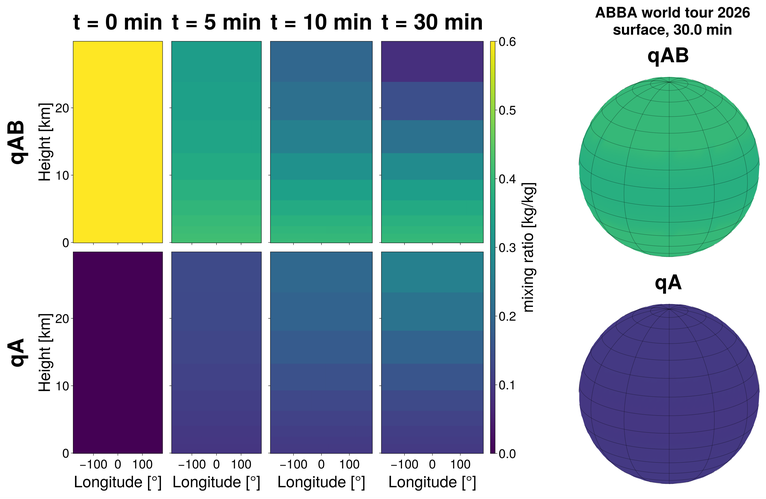
Overview

The CliMA (Climate Modeling Alliance) initiative is building a modern Earth system model that leverages recent computing advances and is written in the Julia scientific programming language. The atmospheric component of CliMA, ClimaAtmos.jl, does not yet include any representation of the chemical processes that determine atmospheric composition. This summer, we built a representation of atmospheric chemistry in CliMA using NCAR's Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA). MUSICA as an optional extension to Clima facilitates flexible representation of chemistry, where different chemical mechanisms can be chosen based on desired use case. We maintain this mechanism-agnostic feature in CliMA, allowing different chemical mechanisms to be flexibly chosen depending on the application and processes of interest.



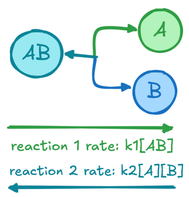
Equilibrium chemistry goes global

After initial tests on the Bomex single column model, we ran similar tests for a global aquaplanet simulation – on a laptop! ClimaAtmos.jl allows for an easy transition from single column to global aquaplanent simulation (prescribed, zonally-symmetric sea surface temperatures), requiring only a new configuration file change and initial conditions. ABBA on the aquaplanet converges to the analytical solution.

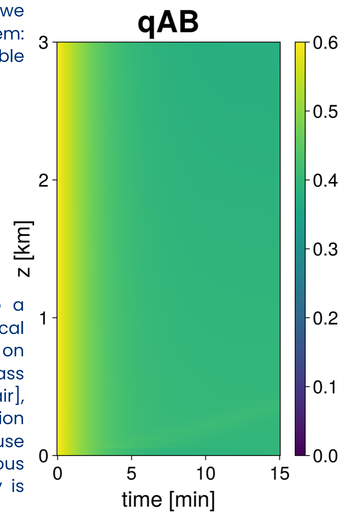


First steps: equilibrium chemistry

As a `hello world` for chemistry we test a simple equilibrium system: the "ABBA" model with reversible decomposition AB ⇌ A + B.



This mechanism equilibrates to a steady state that has an analytical solution. This solution depends on air density: with an initial mass mixing ratio of qAB = 0.6 [kg/kg air], the analytical steady-state solution for qAB at the surface is ~0.4. We use the analytical solution at various levels to validate that chemistry is working in a single column run.

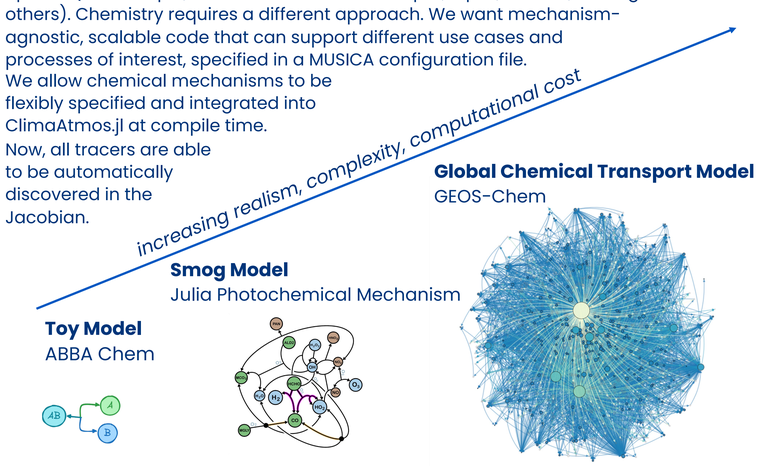


Mechanism-agnostic, flexible chemistry

Before chemistry, CliMA had only a small number of set prognostic tracer options (for example, concentration of water vapor, liquid, and ice, among others). Chemistry requires a different approach. We want mechanism-agnostic, scalable code that can support different use cases and processes of interest, specified in a MUSICA configuration file.

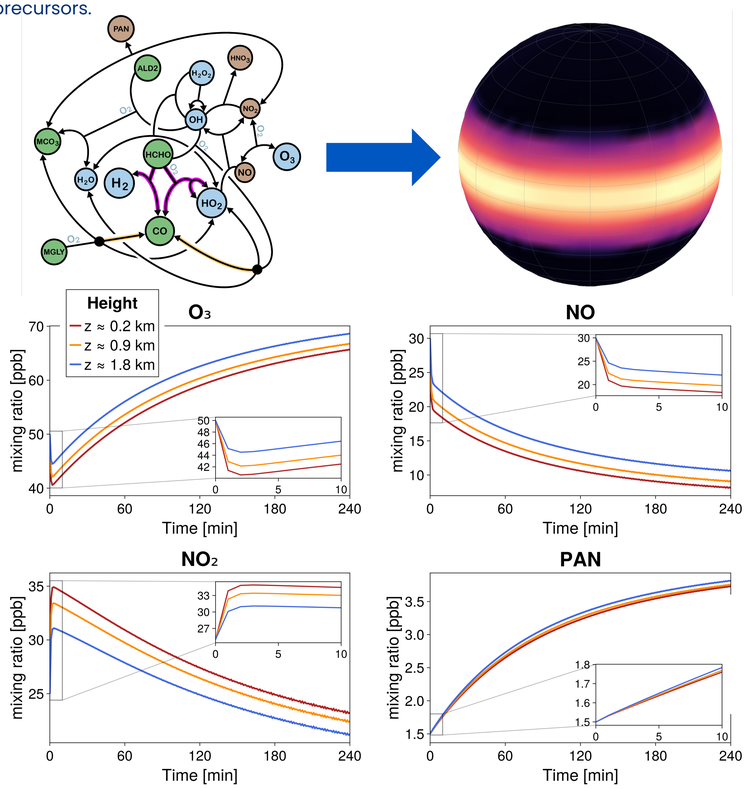
We allow chemical mechanisms to be flexibly specified and integrated into ClimaAtmos.jl at compile time.

Now, all tracers are able to be automatically discovered in the Jacobian.



Julia photochem on CliMA's aquaplanet

We use the **Julia photochemical mechanism** (JPM) to represent a real process: photochemical ozone formation, also known as smog, which degrades air quality. Though simplified, JPM contains the essential aspects of daylight ozone chemistry in the troposphere, including cycling of nitric oxides NO and NO_2 with O_3 as well as other highly reactive radical species formed from volatile organic precursors.



The Julia photochemical mechanism through Musica.jl in CliMA captures essential behavior of tropospheric ozone chemistry. This includes fundamental nonlinear responses on different timescales: initial titration of O_3 before sustained production.

Next steps: photolysis, updrafts and beyond

With flexible chemistry from MUSICA, CliMA can now support the representation of many processes: aerosol chemistry, the UV-shielding ozone layer, and methane chemical sinks, among others. With the ability to resolve subgrid processes in updrafts, it could potentially capture plume chemistry of wildfires or urban cores. Key processes besides kinetics and transport still need to be implemented: photolysis, deposition, and emissions. Next we will couple NCAR's TUV-x photolysis with RRTMGP.jl, CliMA's implementation of the RTE+RRTMGP radiative transfer model (Pincus et al., 2019; Lopez-Gomez et al., 2020).

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