An Online-Learned Neural Network Chemical Solver for Stable Long-Term Global Simulations of Atmospheric Chemistry

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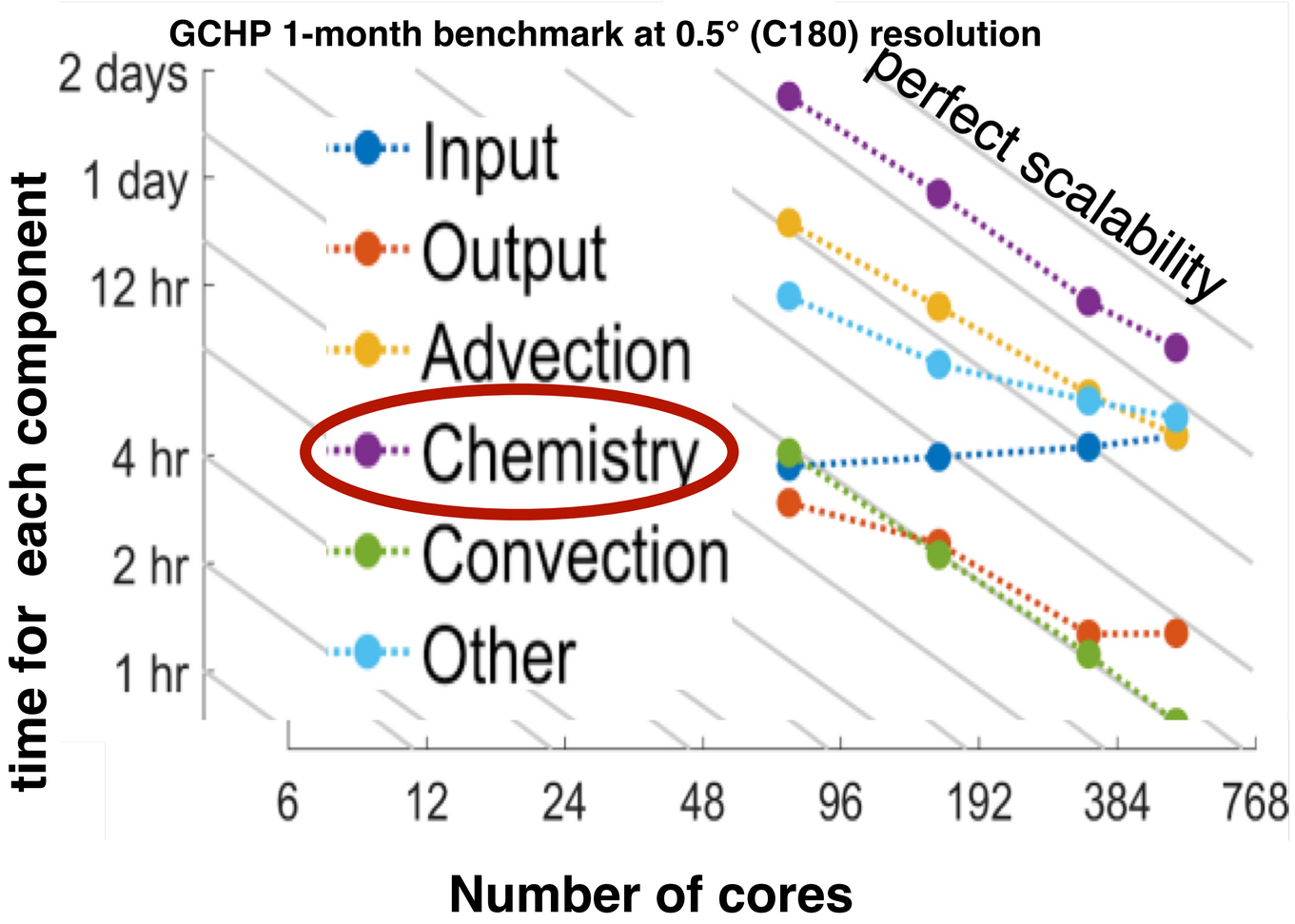
Global modeling of atmospheric chemistry is a grand computational challenge



-Chemistry **dominates** the cost of a simulation (**~40%**) even though ideally scales

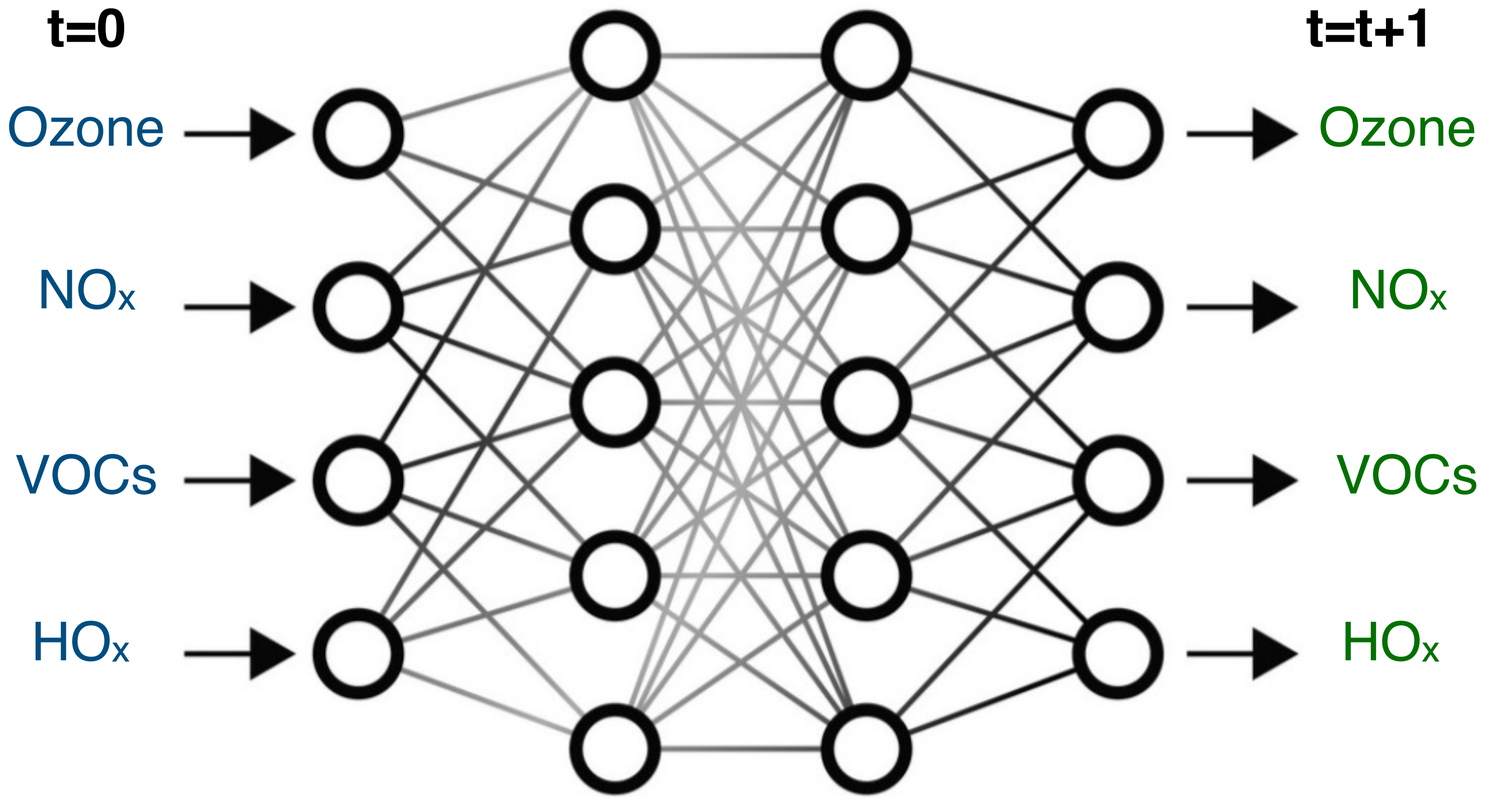
-Weather and climate models typically have **~4 variables**

-Chemistry models have **hundreds** of evolving species

Bottom Line: Adding chemistry into an Earth system model becomes computationally infeasible

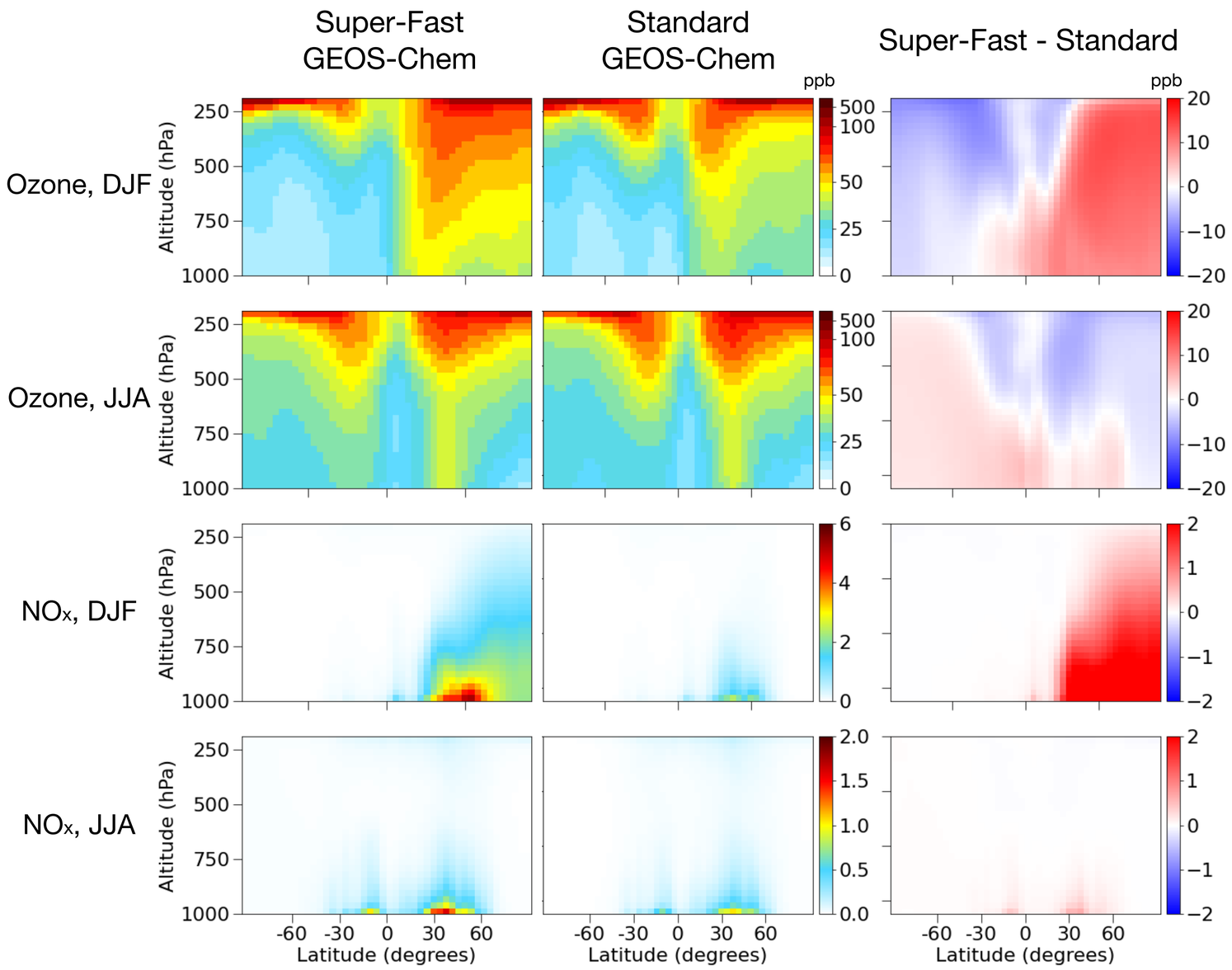
Eastham et al., 2018 GMD

Machine learning (ML) methods can provide a solution to this problem



1. Nonparametric, **universal** function approximators
2. Learn to predict based on large dataset of **repeated** patterns
3. Proven to **speed up** solving ODEs at orders of magnitude (Malek and Shekari, 2006)

The ‘Super Fast’ chemical mechanism will allow us to better define ML methods and understand limitations in a full 3-D global modeling framework



- Global mechanism with 12 species [Brown-Steiner et al., 2018]
- Benchmarked in GEOS-Chem v12.0.0
- 4x5° resolution

1-hour chemical time step output

20 variables:

2 physical var: T, air density

6 photolysis frequencies

12 gas-phase species

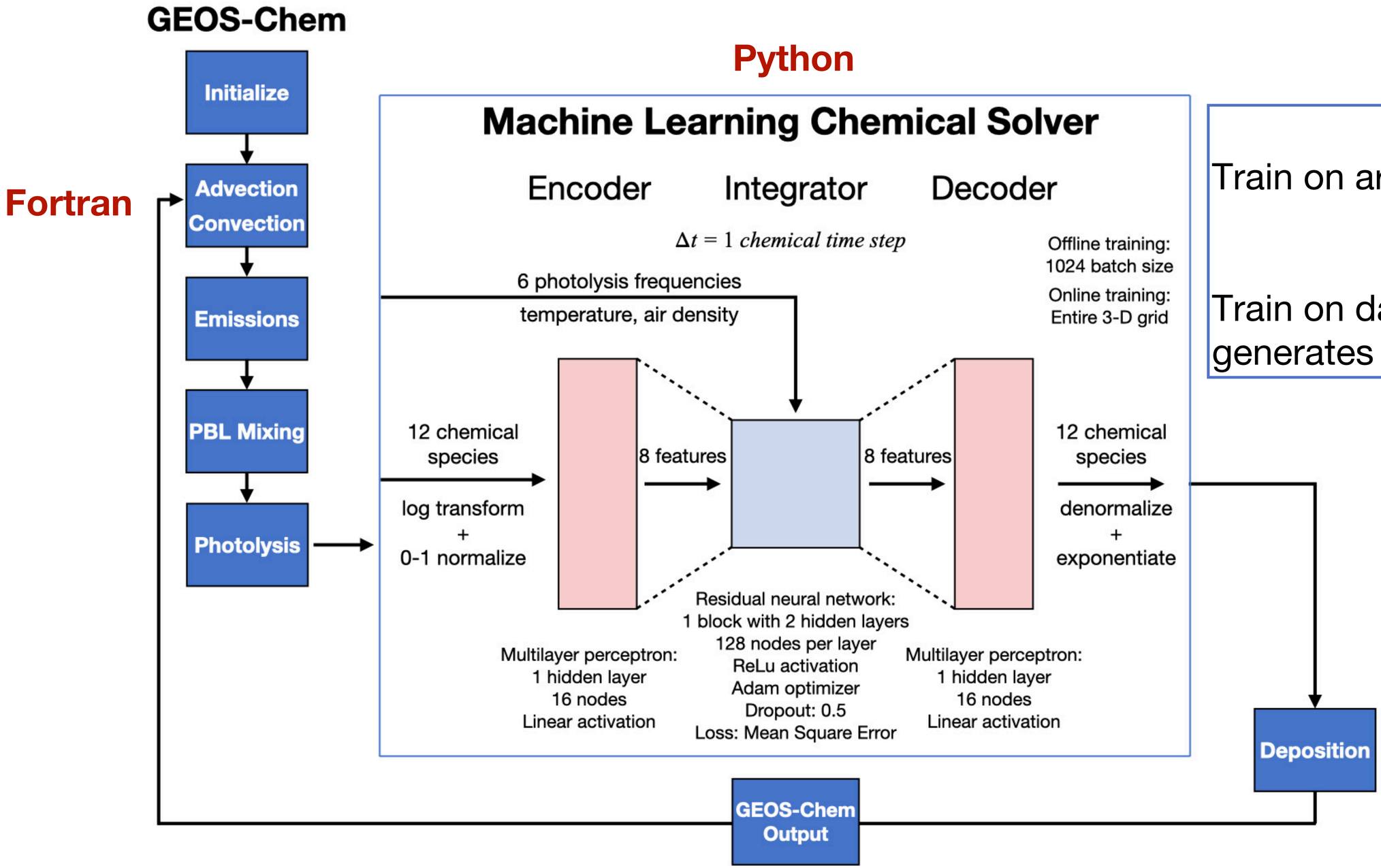
1 month dataset would contain:

lon×lat×lev×days×hours = 46×72×~25×31×24 **->**~62 million samples

Training: 2016, Test: 2017

Kelp et al., 2022

We train ML solvers online synchronously with a GEOS-Chem simulation to train on representative conditions in sequence



Offline:
Train on archived dataset

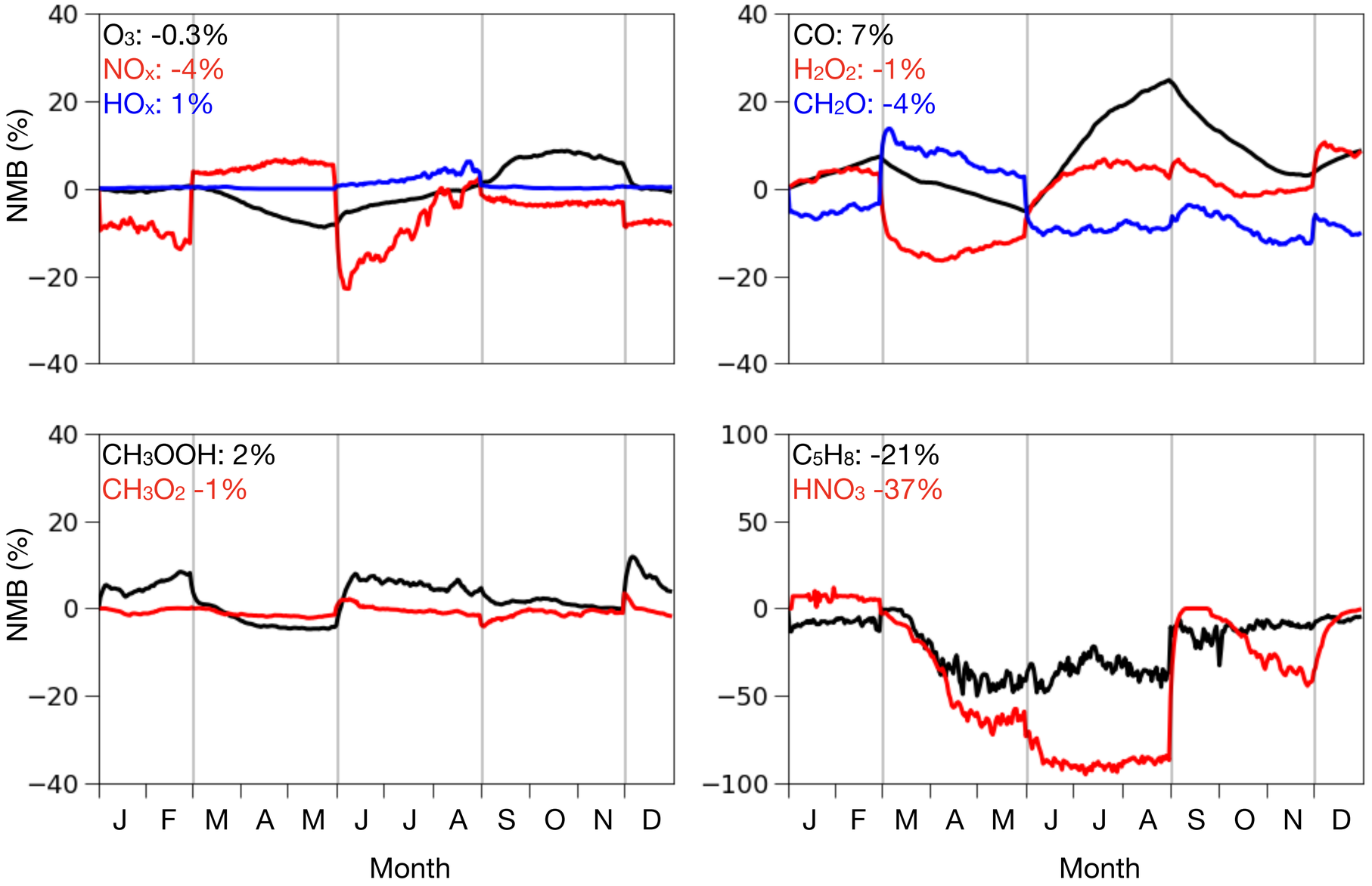
Online:
Train on data as GEOS-Chem generates it

Kelp et al., 2022

Simulation are stable and average errors for the year are <10%, but ML solvers have different seasonal fits of accuracy

Separate ML solvers for:

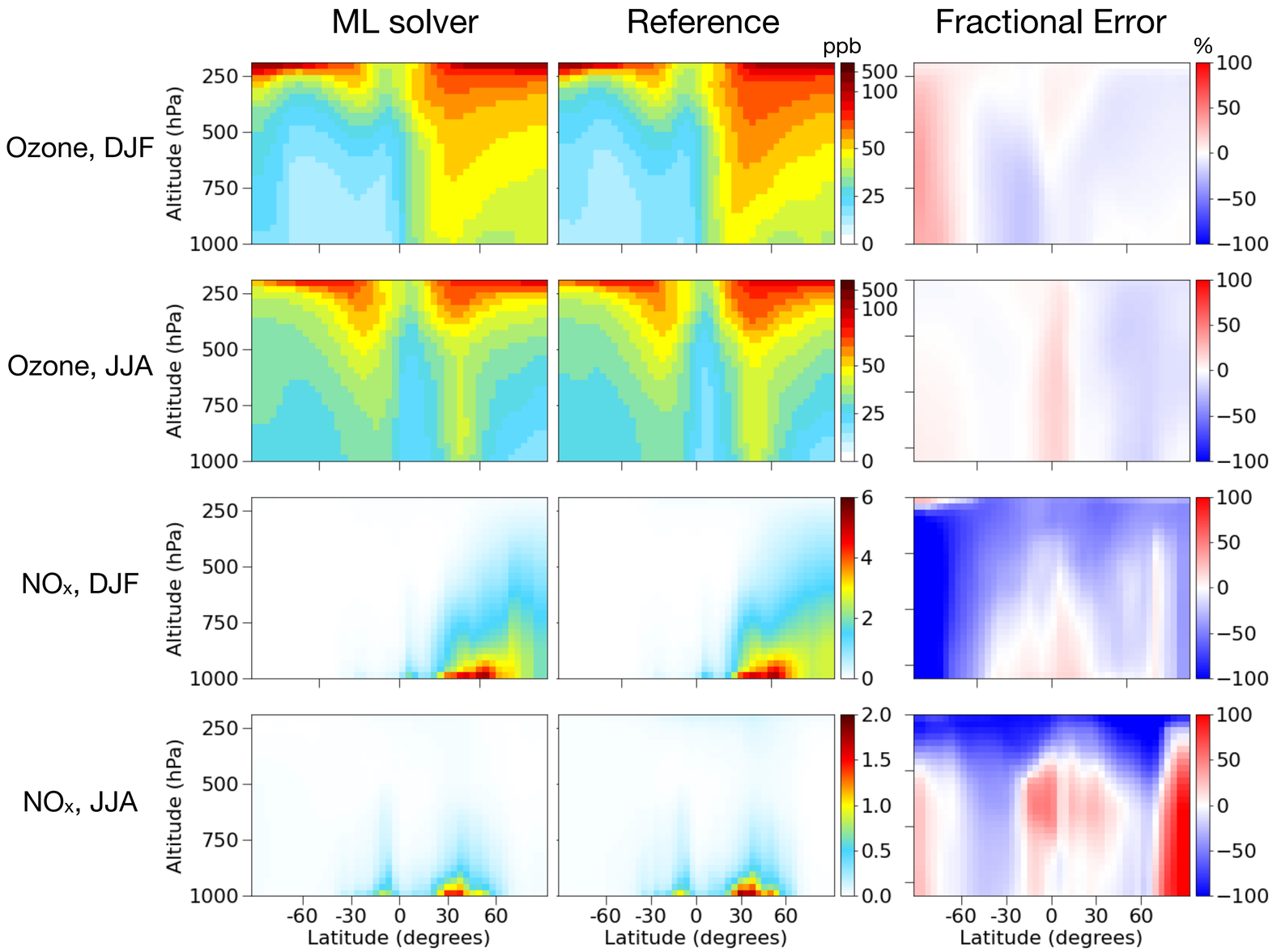
- Species
- Season



Error does not accumulate over the course of a year

Kelp et al., 2022

Errors are largest at remote latitudes and high altitudes due to chemical error accumulation as air ages



Kelp et al., 2022

Takeaways

- Application of ML chemical solver in global 3-D atmospheric chemistry models may require online training.

- **Stable** year-long global simulation of chemistry can be achieved with a ML solver applied to the Super-Fast mechanism in GEOS-Chem.

- Computational speedup is five-fold relative to the reference Rosenbrock solver in GEOS-Chem.

- Large regional biases for ozone and NO_x under remote conditions where chemical aging leads to error accumulation.
  - Regional biases remain a major limitation for practical application, and ML emulation would be more difficult in a more complex mechanism.

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