An online-learned neural network chemical solver for stable long-term global simulations of atmospheric chemistry in S2S applications

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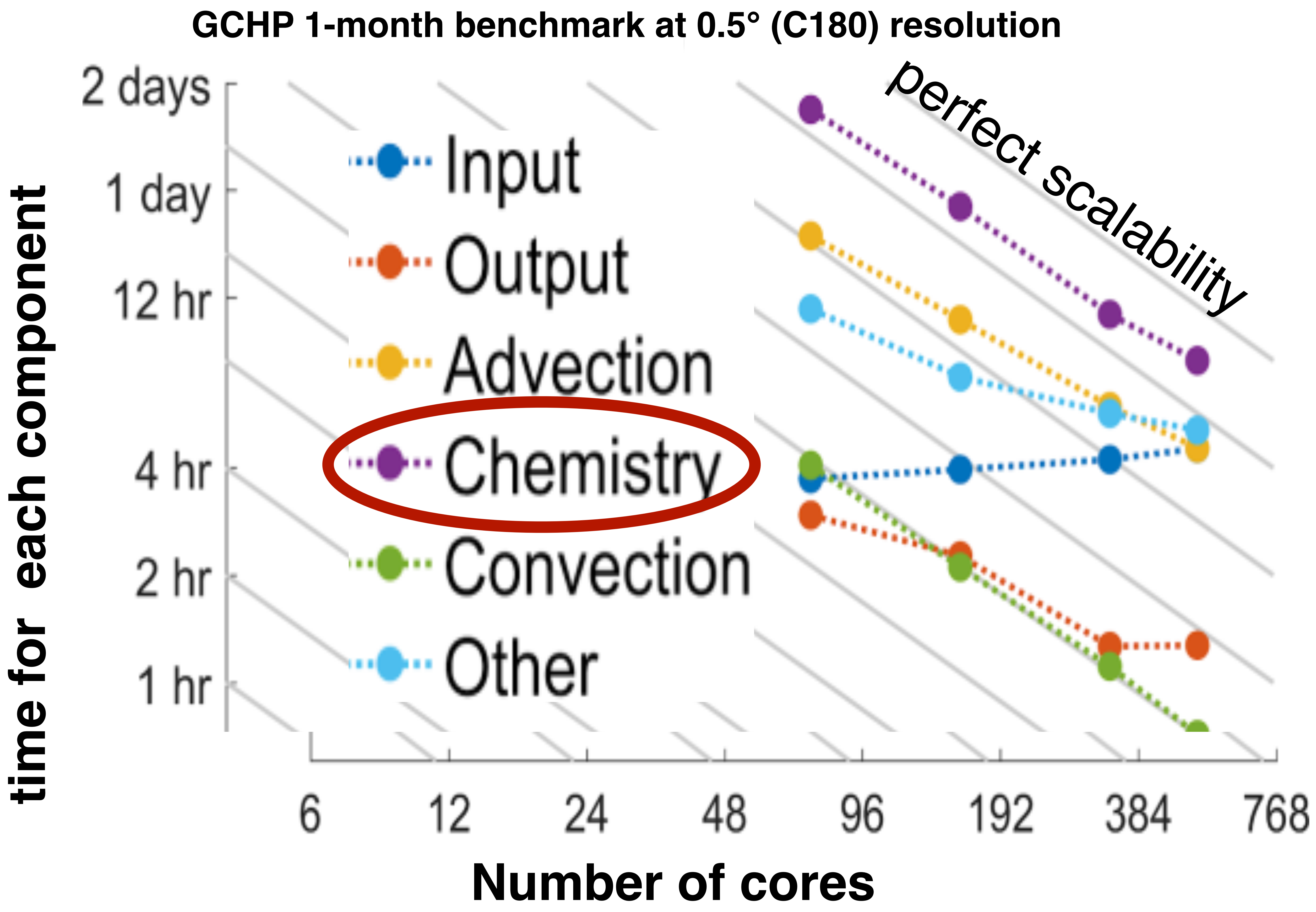
AMS 20220126

Global modeling of atmospheric chemistry is a grand computational challenge



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

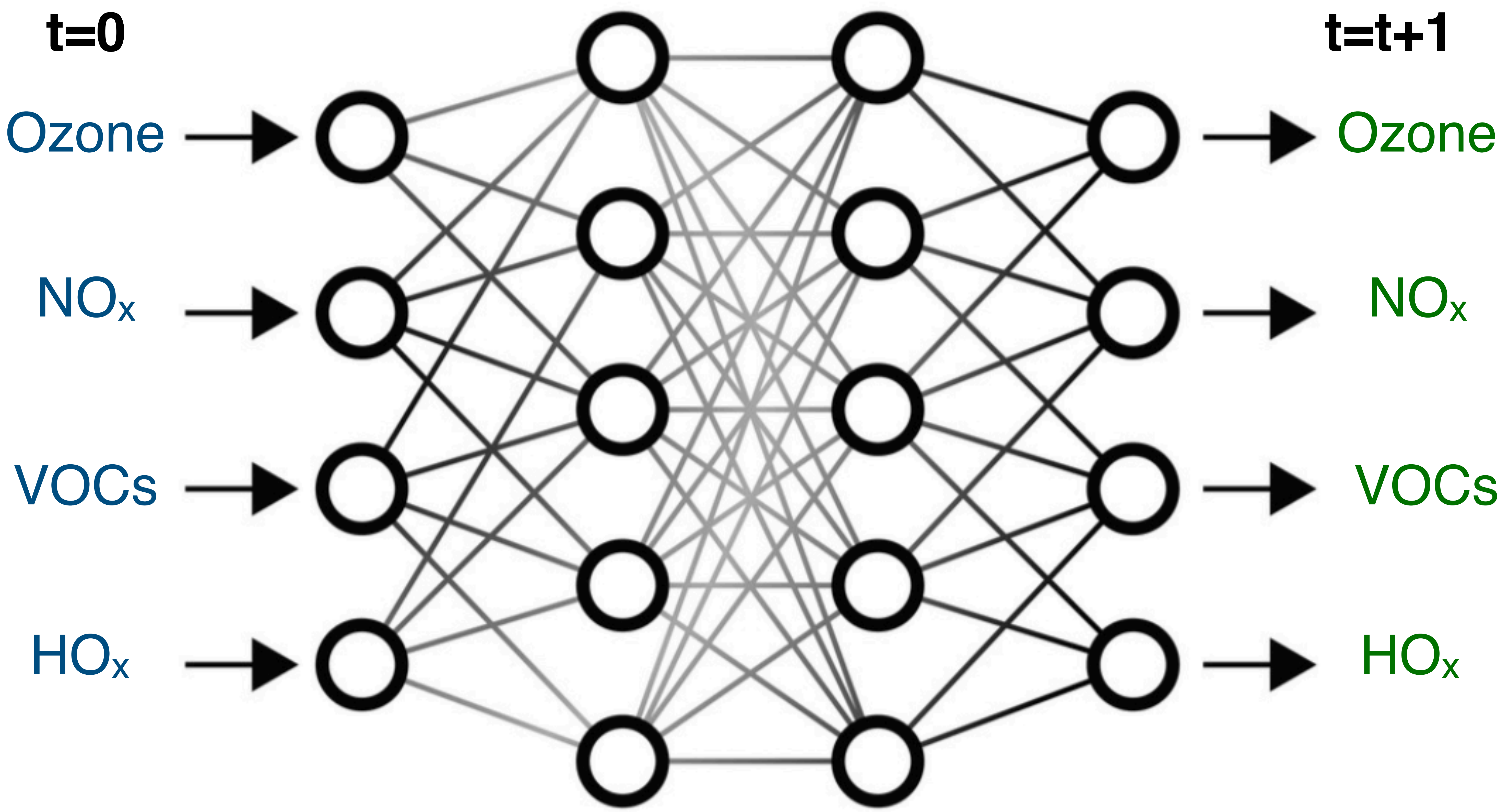
-Weather and climate models typically have **~4 variables**

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

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

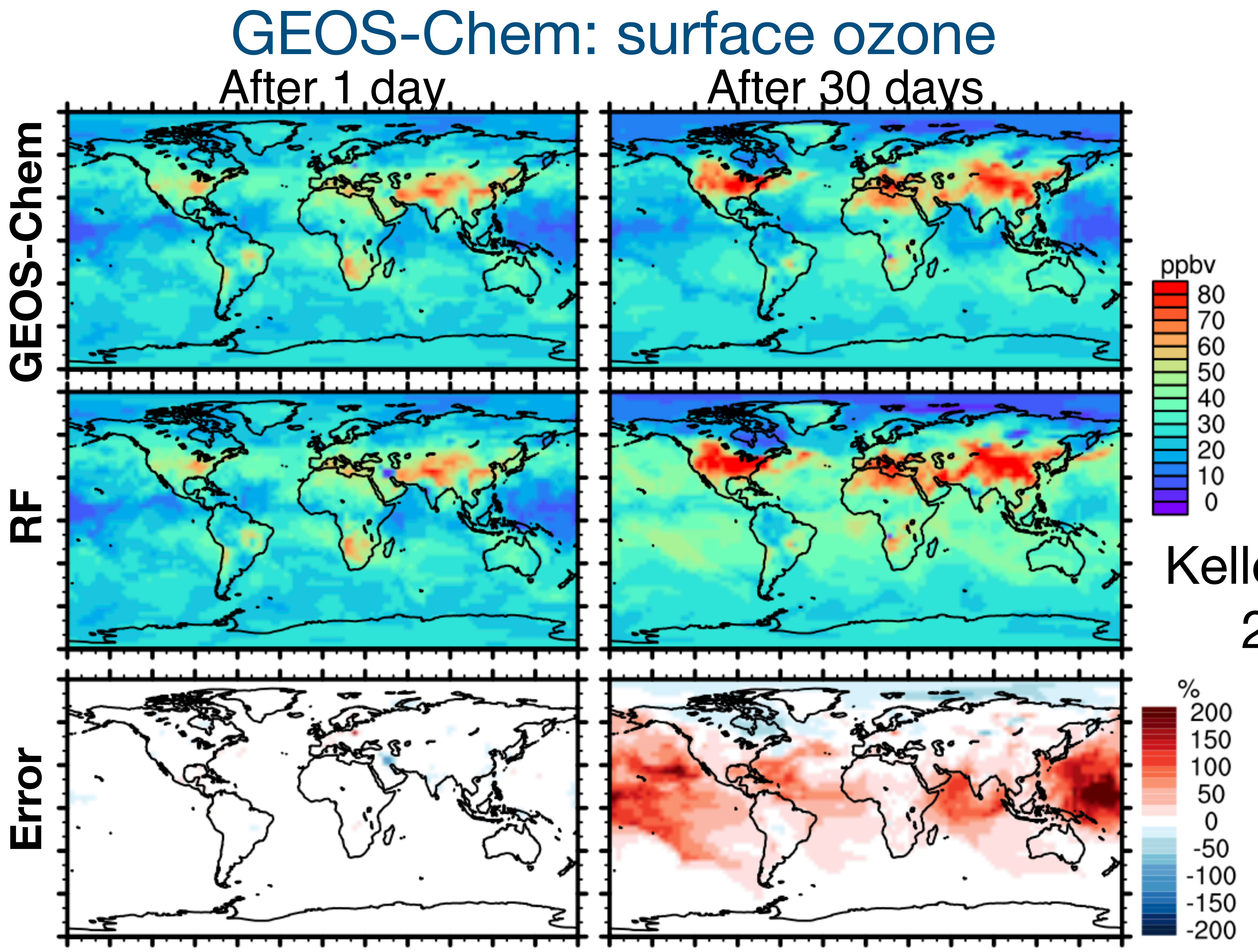
Eastham et al., 2018 GMD

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

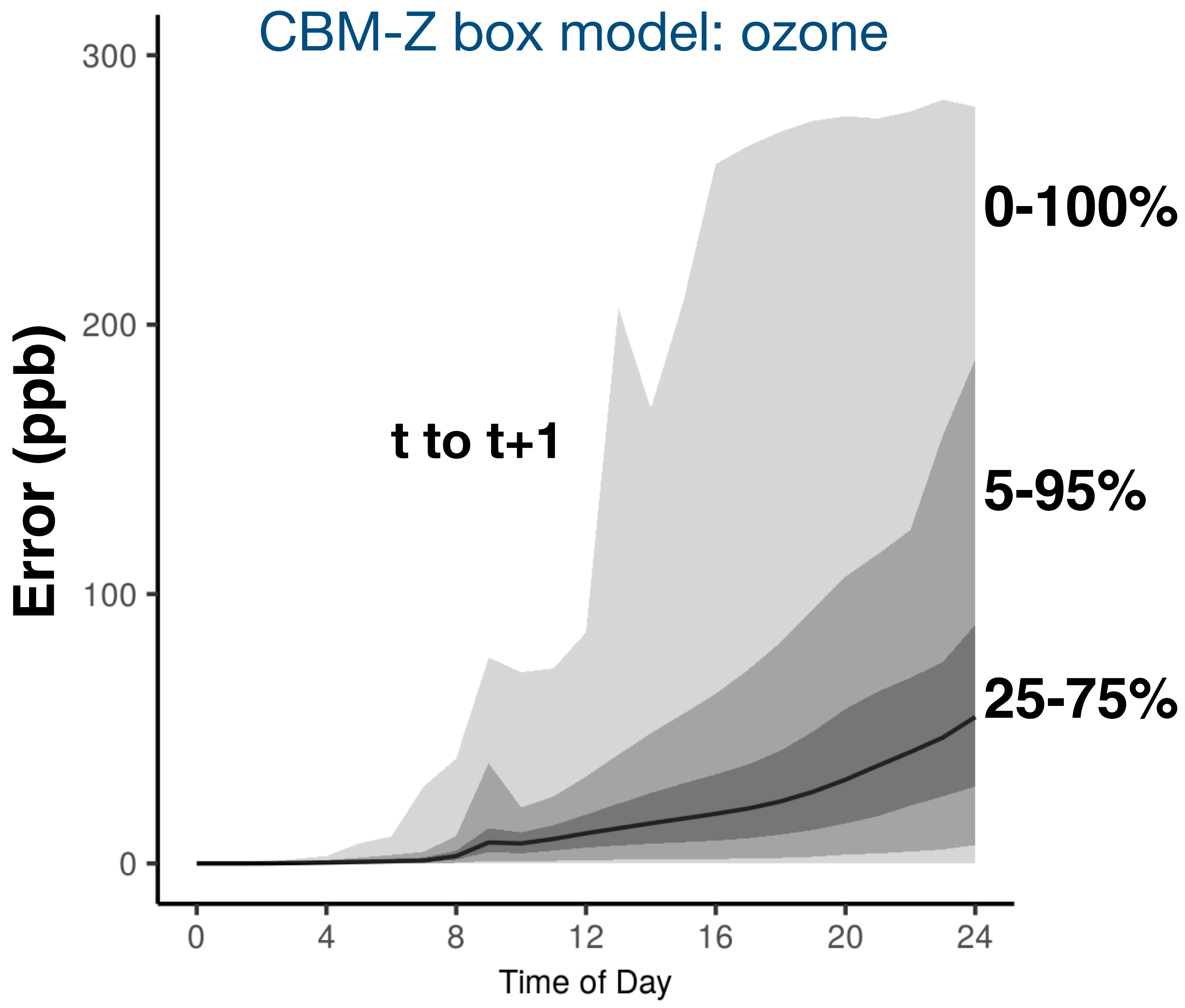


1. Nonparametric, **universal** function approximators
2. Learn to predict based on large dataset of **repeated** patterns
3. Proven to **speed up** solving ODEs at orders of magnitude (Malek and Shekari, 2006)

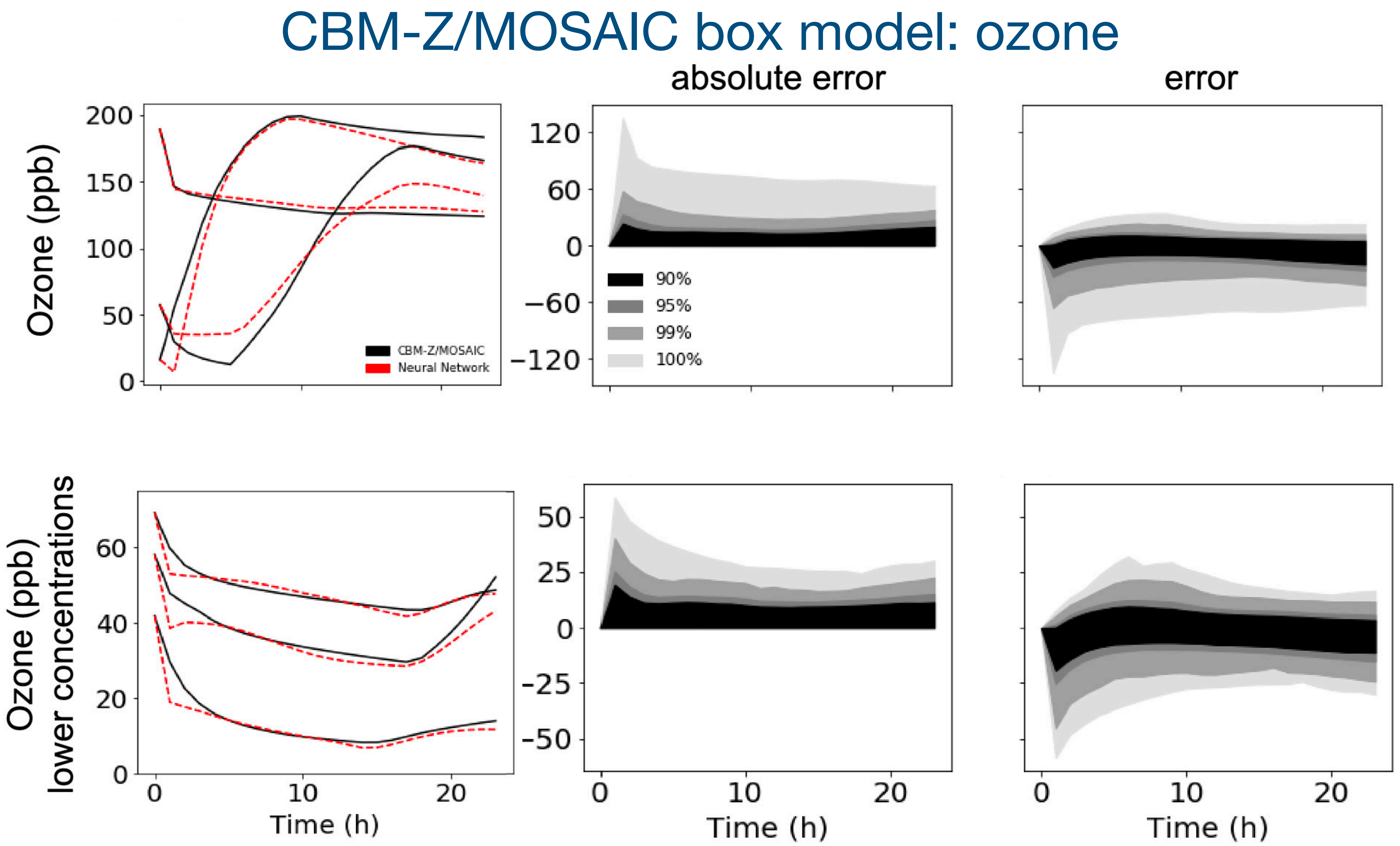
Past ML chemical solver attempts have encountered runaway error growth and have been limited to box model approaches



Keller and Evans, 2019 GMD



Kelp et al. 2018 ArXiv



Kelp et al. 2020 JGR

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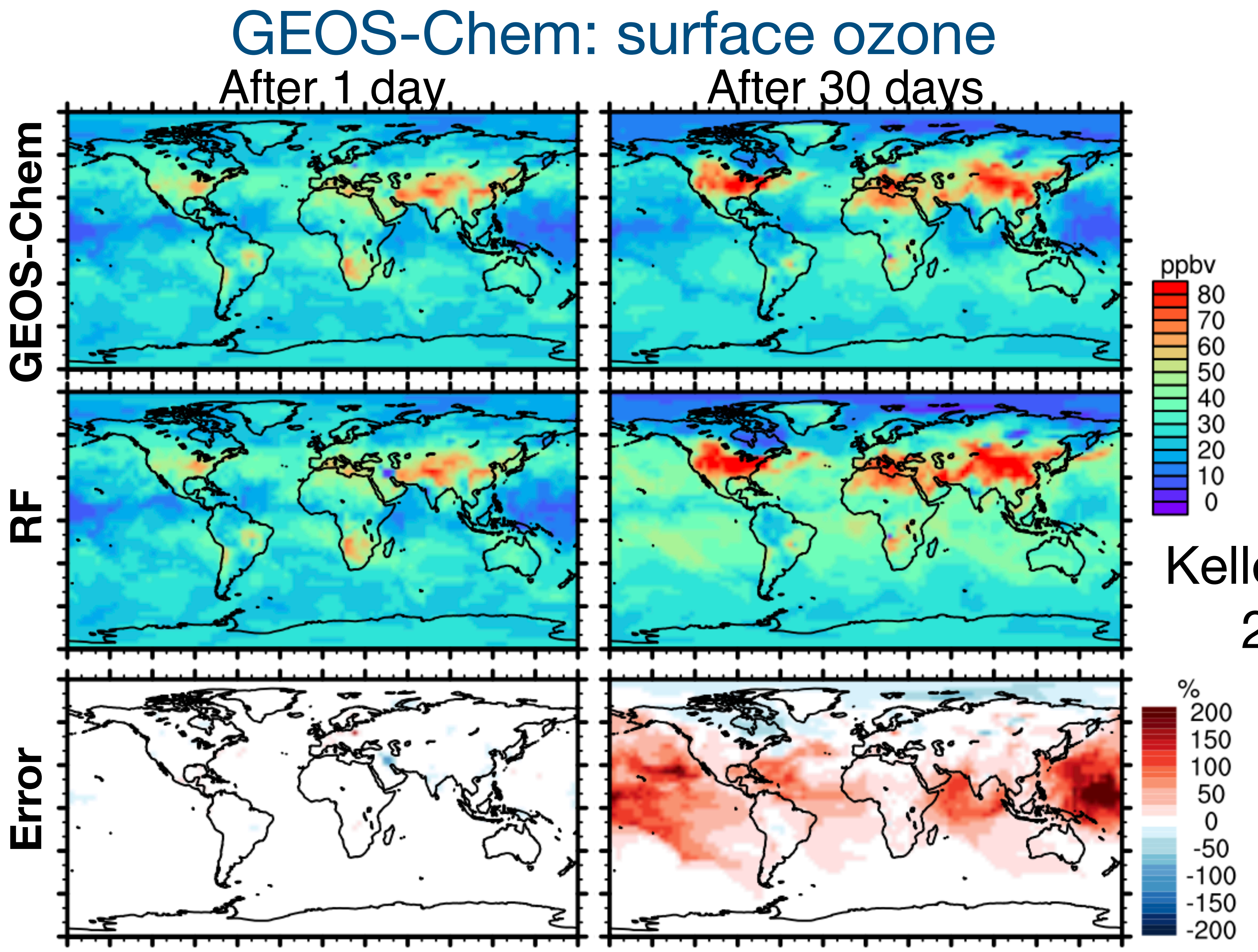

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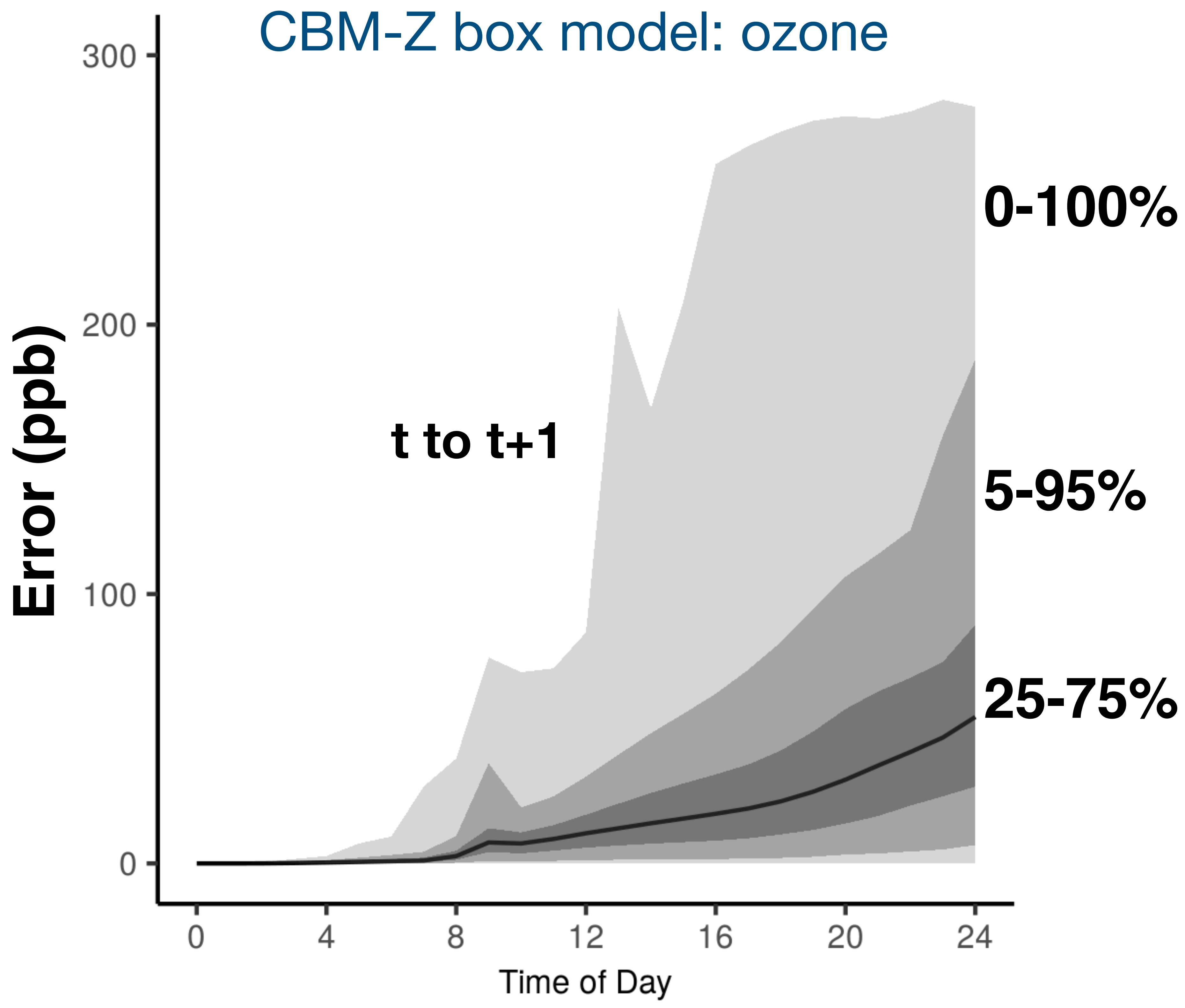

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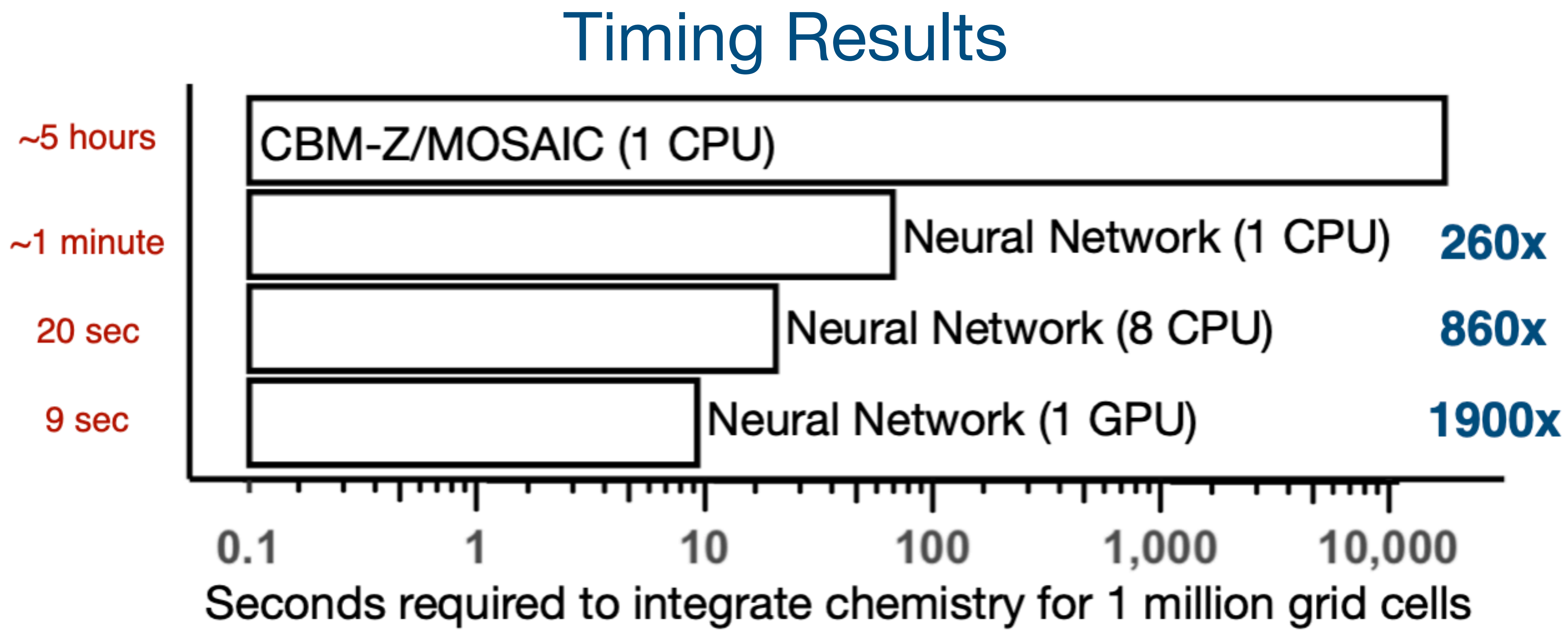
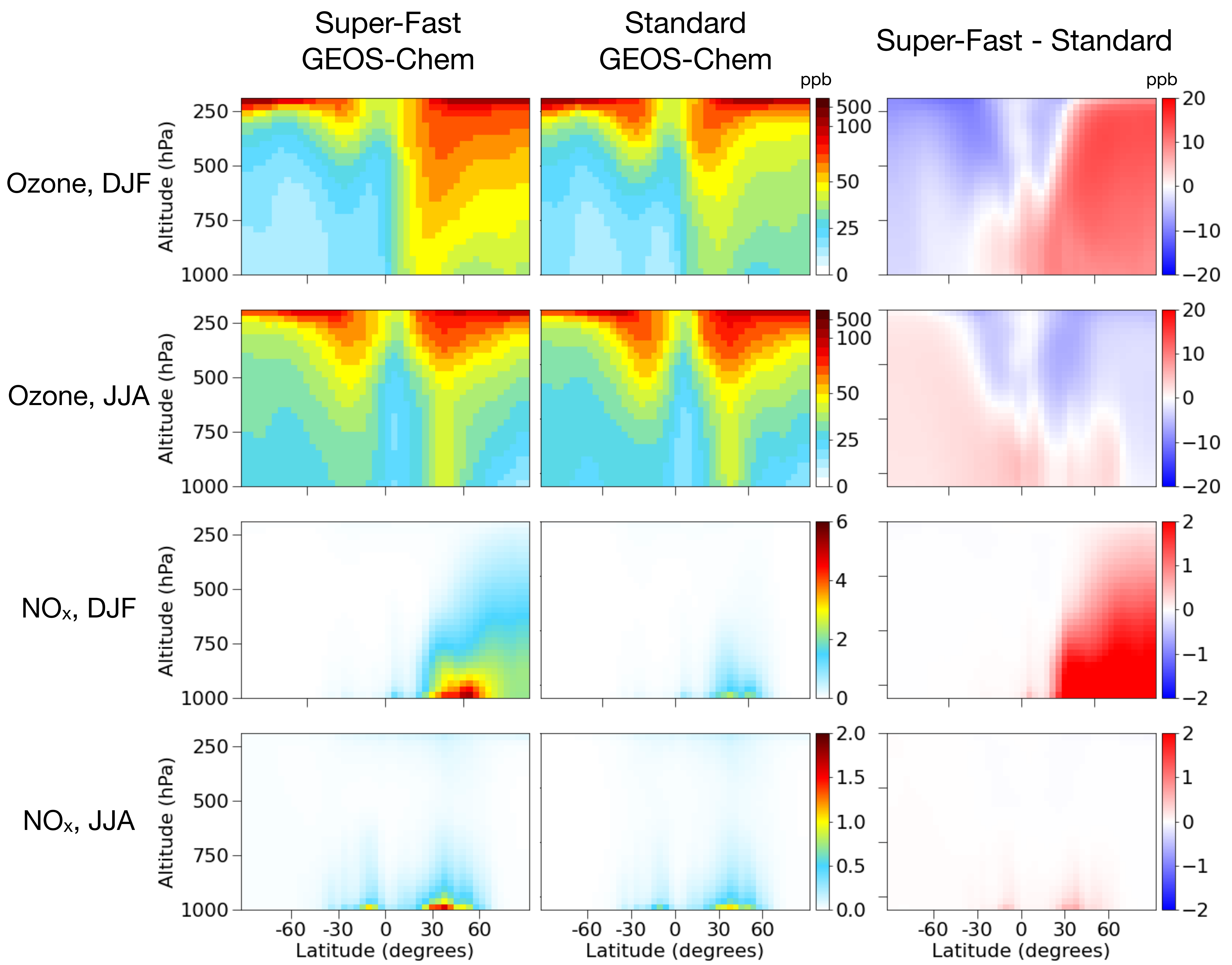


Kelp et al. 2020 JGR

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:

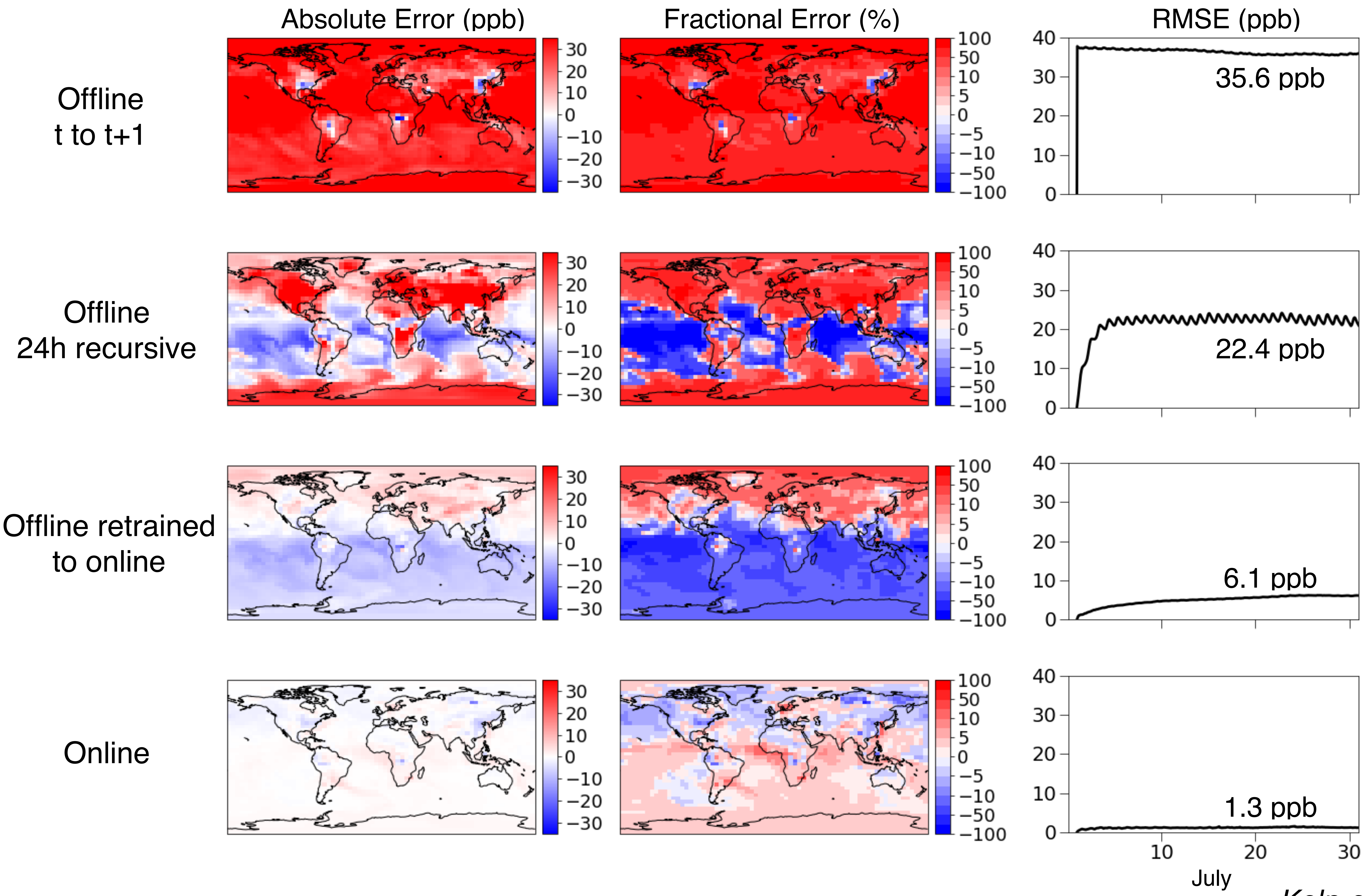
lon×lat×lev×days×hours = 46×72×~25×31×24 **->**~62 million samples

Training: 2016, Test: 2017

Kelp et al., in review

Online training improves accuracy and stability over offline training

Ozone



Train:
JJA 2016

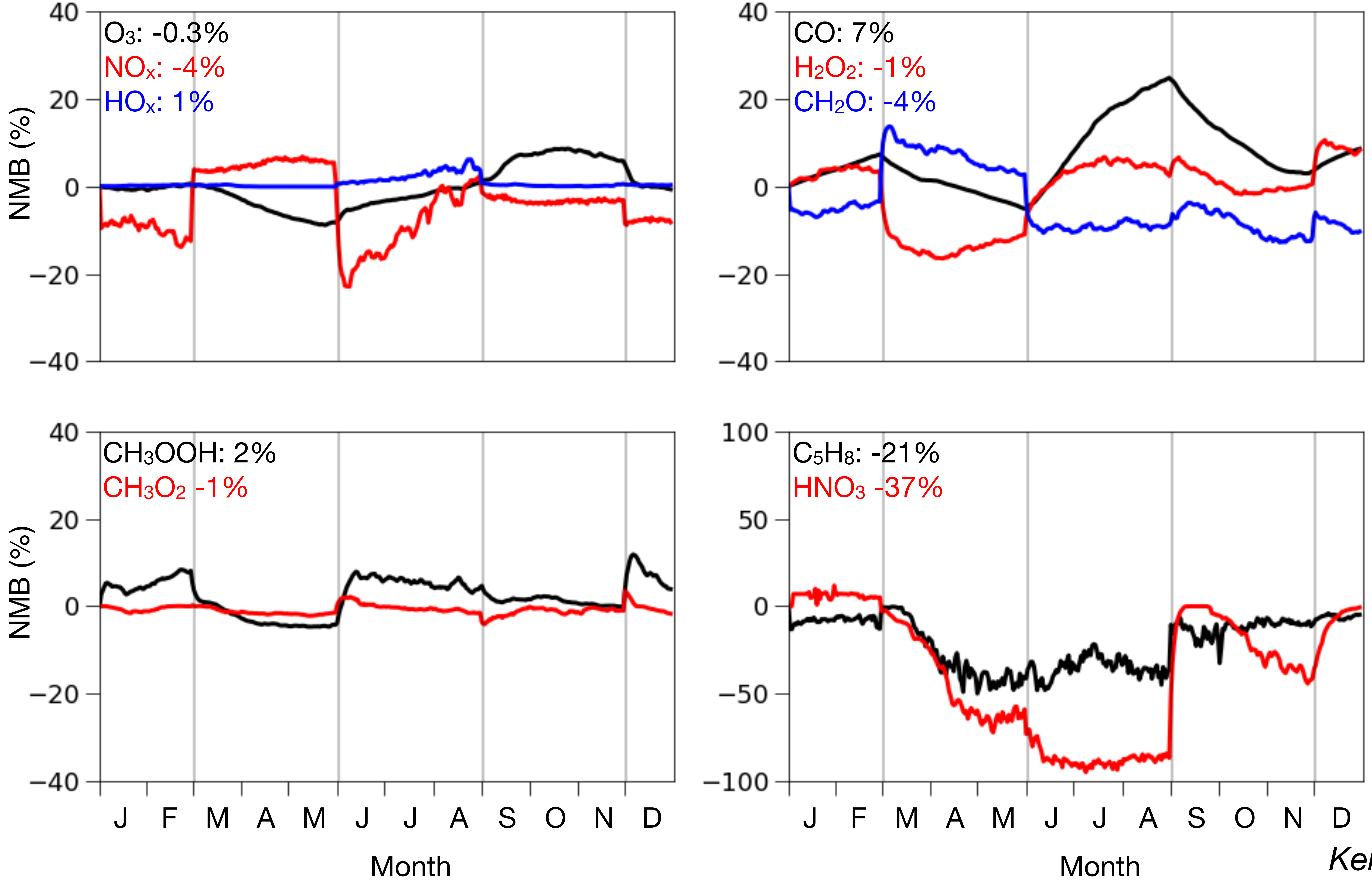
Test:
July 2017

Kelp et al., in review

ML solvers have different seasonal fits of accuracy

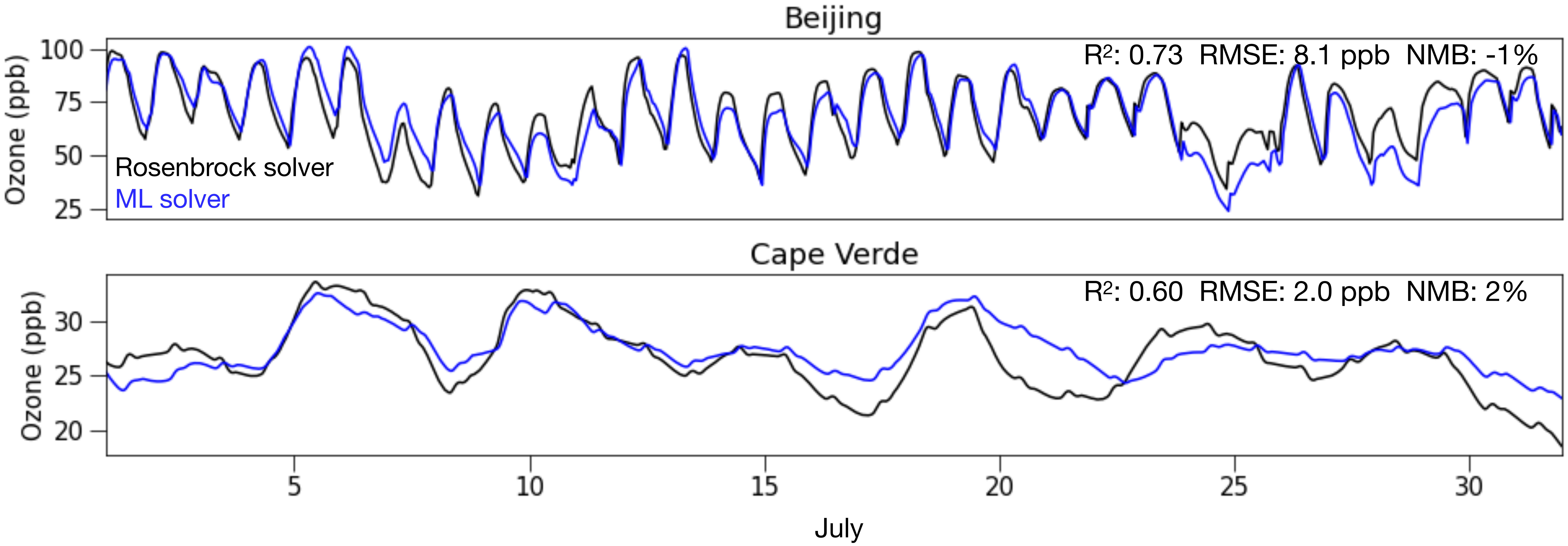
Separate ML solvers for:

- Species
- Season



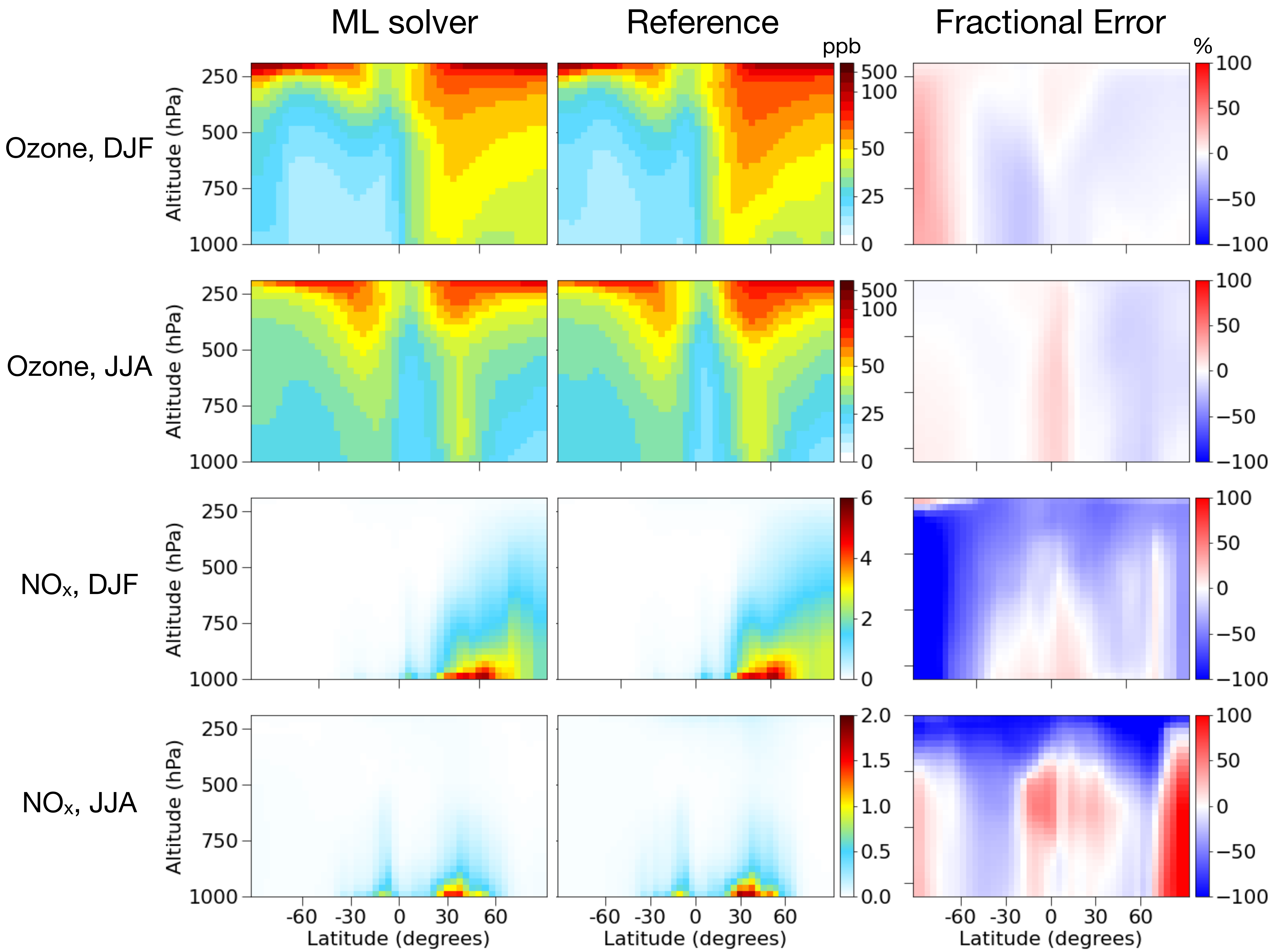
Kelp et al., in review

ML solver able to capture the diurnal and synoptic variability of ozone at polluted and clean sites



Kelp et al., in review

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



Kelp et al., in review

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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