these new species following the diagram in Figure S8. After running the new version of the model for 12 months, our reduced algorithm shows consistent improvement in performance, reducing the chemical integration time by 53% and maintaining error <0.5% in the boundary layer and 2-3% in the free troposphere and stratosphere (Figure 6c).

## 4. Conclusions

The high computational cost of chemical integration is a long-standing limitation in global atmospheric chemistry models. Typical chemical mechanisms include over 100 species coupled on short time scales. Previous research has proposed a variety of ways to speed up the chemical operator, all involving some loss of accuracy or generality. In this study, we have presented a machine learning-guided adaptive method that can reduce the chemical integration time ~~by 50% when compared to the full chemical mechanism~~ while ~~maintaining error <2% for important species and~~ retaining full diagnostic capability.

In our algorithm, we first partition the mechanism species in into chemically logical blocks using a machine learning approach that analyzes production/loss rates and chemical linkages between species. We then assemble these blocks into an ensemble of submechanisms to encompass the range of chemical environments in the atmosphere. The model picks locally on the fly which submechanism to use based on species' production and loss rates. The original mechanism can thus be greatly reduced in most environments while maintaining complexity where needed. ~~Our method can reduce the chemical integration time by 50% while incurring errors of less than 2%, with no error growth over multi-year global simulations.~~ Updates to the original mechanism can be accommodated by assigning new species to the existing blocks without having to reconstruct the suite of submechanisms.

Our method has many advantages over previously proposed approaches to reduce chemical mechanism: (1) it is chemically logical; (2) it can save 50% computer time in chemical integration with errors lower than 2% for important species; (3) it is stable (no error growth over time) for 8-year simulations; (4) it retains full diagnostic information of concentration and rates; and (5) it is scale-independent. Our algorithm can significantly ease the computational bottleneck of chemical kinetics in global atmospheric chemistry models.

**Code availability**. The standard GEOS-Chem code is available through https://doi.org/10.5281/zenodo.1343547 (version 12.0.0) and https://doi.org/10.5281/zenodo.3950473 (version 12.9.1). The updates for the adaptive mechanism can be found at https://doi.org/10.7910/DVN/KASQOC.

**Data availability**. All datasets used in this study are publically accessible at https://doi.org/10.7910/DVN/KASQOC.

**Author contribution.** L. Shen and D. Jacob designed the experiments and L. Shen carried them out. L. Shen and D. Jacob prepared the manuscript with contributions from all co-authors.