Atmospheric Chemistry Modeling using Machine Learning

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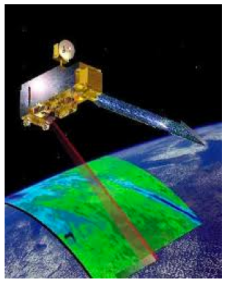
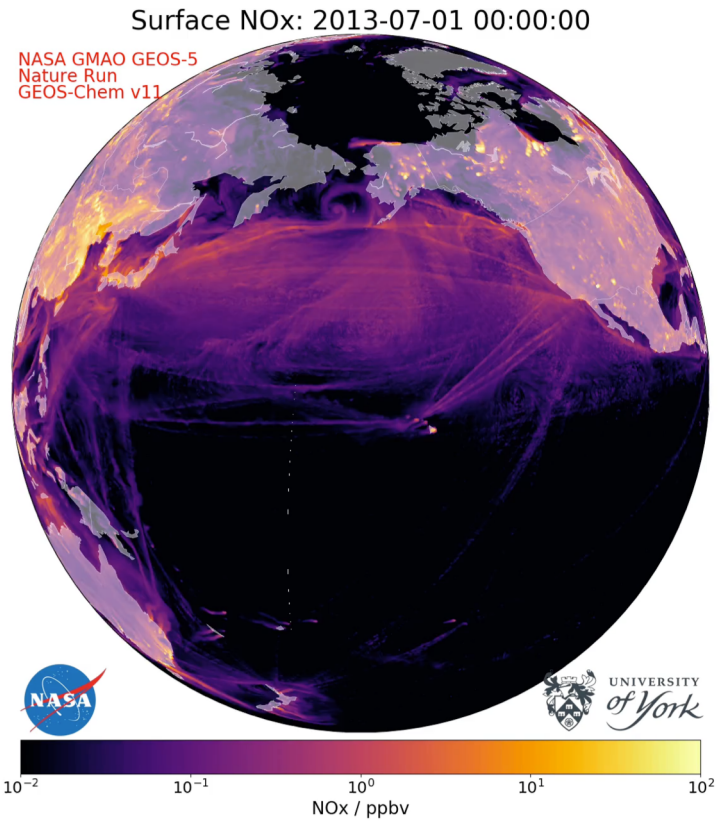
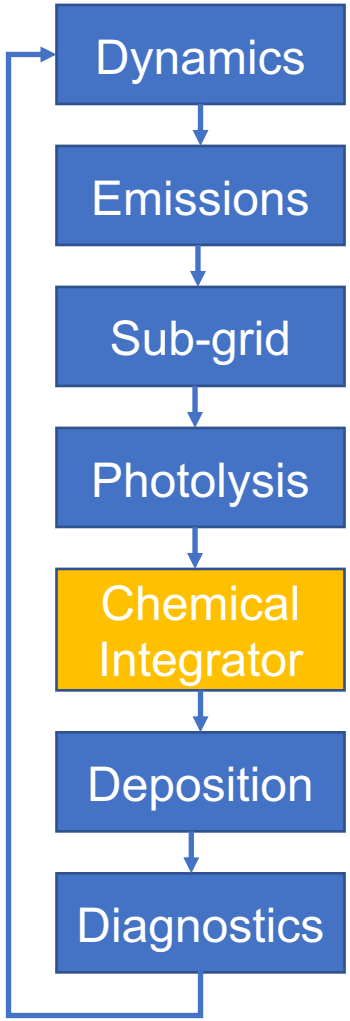
Modeling of atmospheric chemistry is very complex



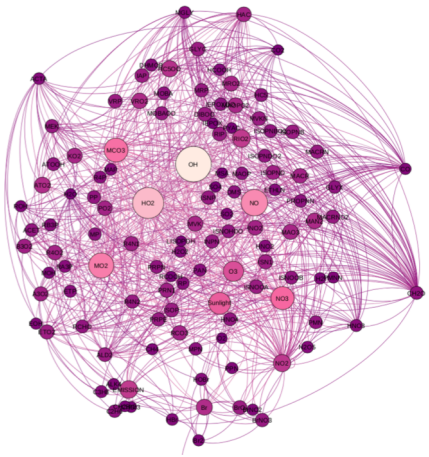


Need 3’500 CPUs for 25 km^2 simulation

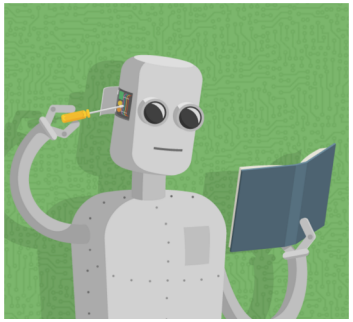
Replace chemical integrator with model trained by machine learning



Conventional: GEOS-Chem solver



Alternative: random forest, neural net, ?

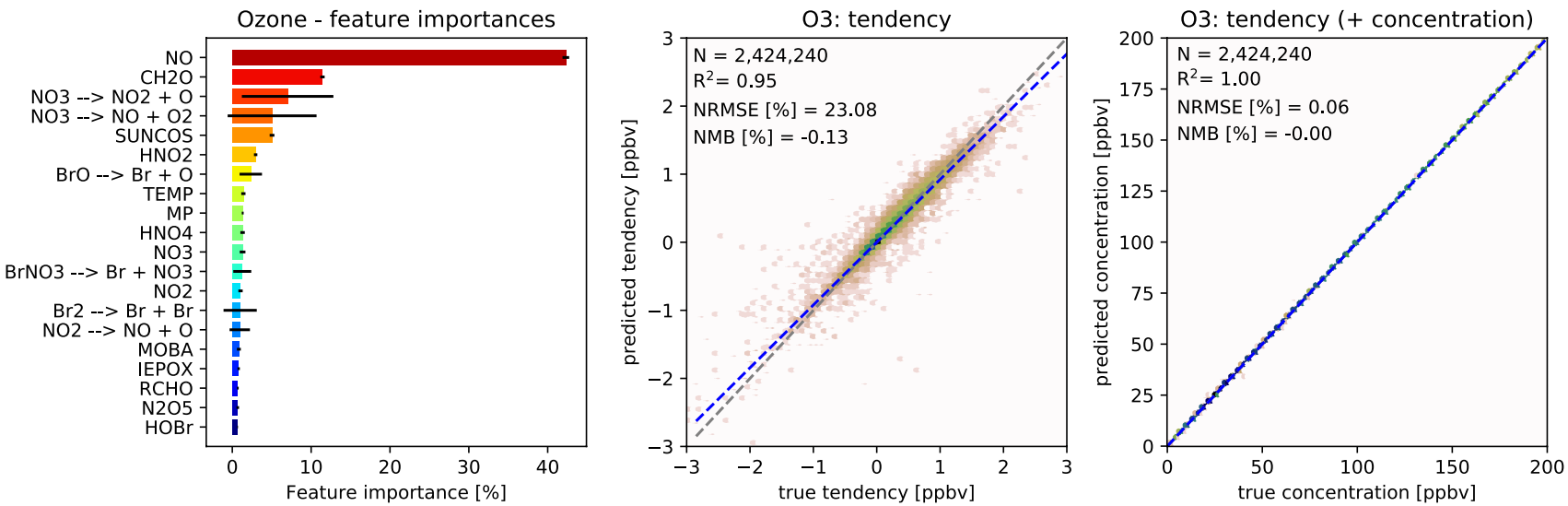


Random forest emulator

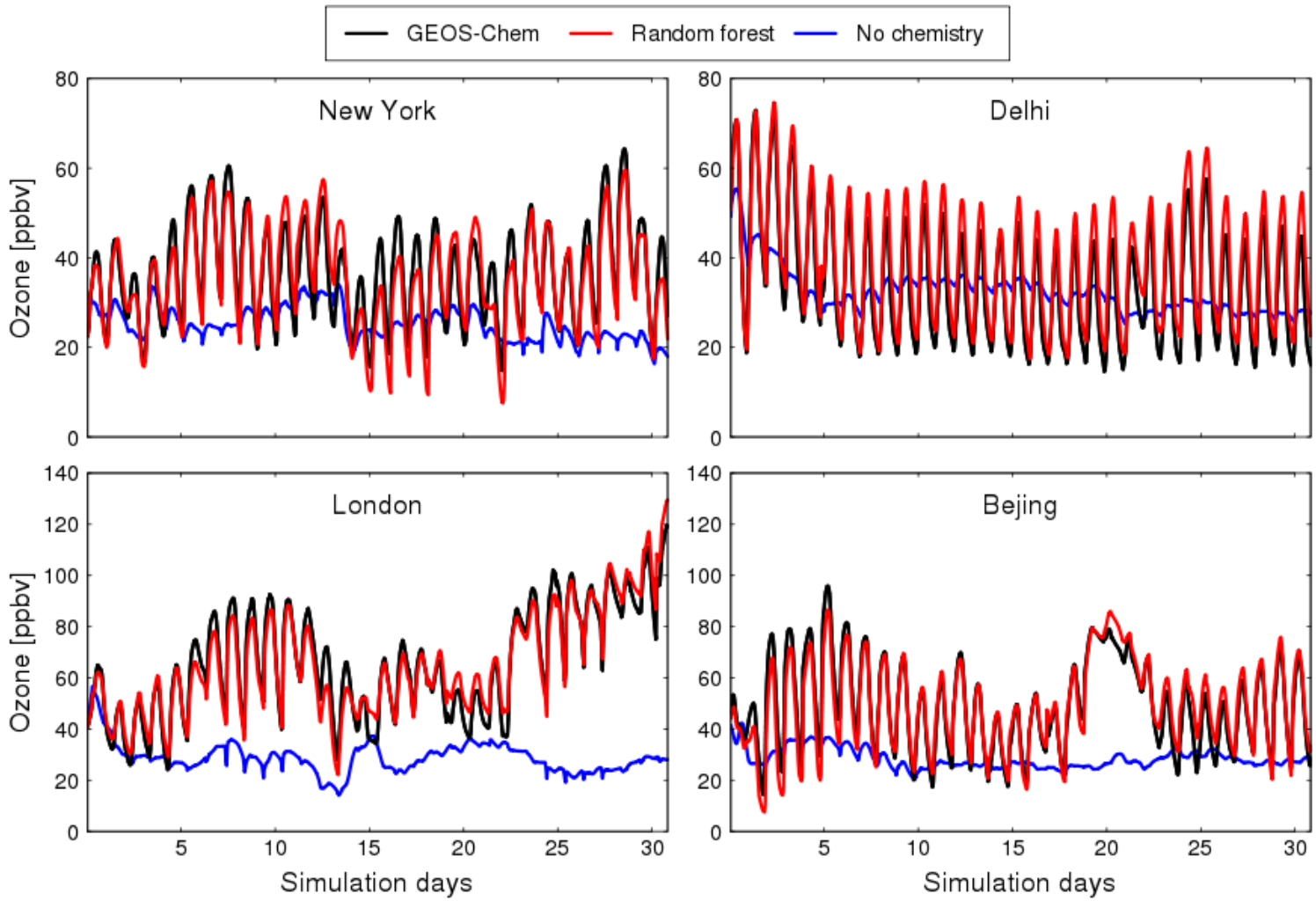
- 51 chemical species
- 68 photolysis rates
- 7 meteorology fields

→ Change in concentrations due to chemistry

- Training data from full chemistry model: 2.4 x 10^8 sets
- Random forest: 30 trees, 10’000 leaves

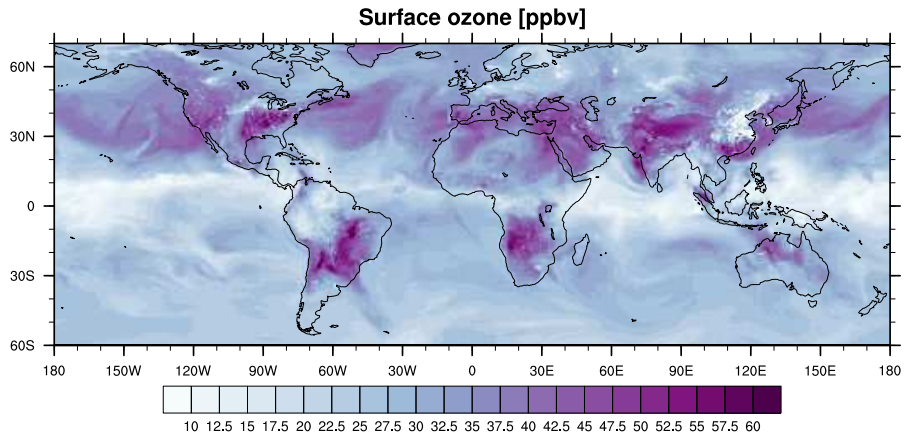


Machine learning model accurately predicts surface concentrations of ozone



Summary

- Developed a random forest model to simulate atmospheric chemistry
- Now working on more efficient implementation into the full model



Keller, C. A. and Evans, M. J.: Application of random forest regression to the calculation of gas-phase chemistry within the GEOS-Chem chemistry model v10, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2018-229, in review, 2018.

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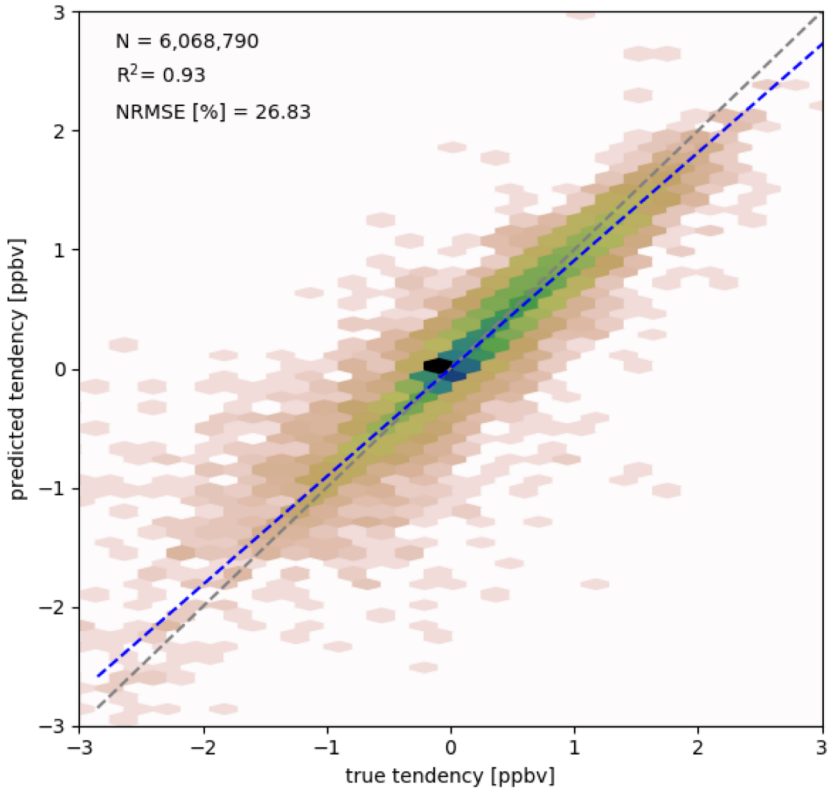
Gradient booster and GPUs: >100 times faster…

Random forest: 1h 30min



XGBoost (+GPUs): 45s