Orders-of-Magnitude Speedup in Atmospheric Chemistry Modeling through Neural Network-Based Emulation

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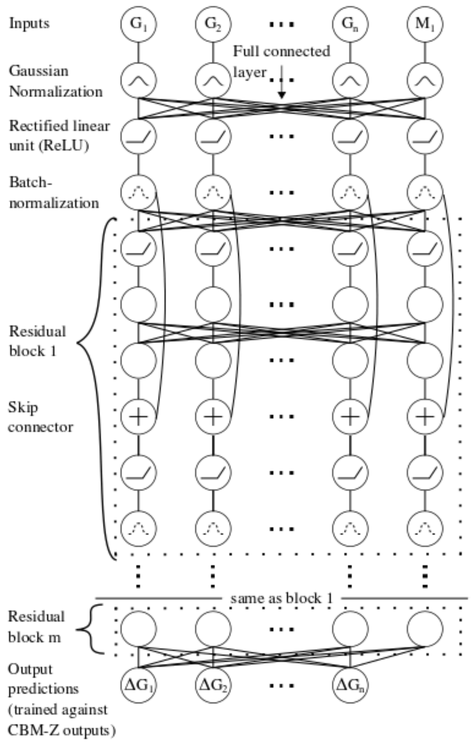
Background

Chemical transport models, often used to simulate air pollution transport, transformation, and removal, are **computationally expensive**, largely because of the computational intensity of the chemical mechanisms: systems of coupled differential equations representing atmospheric chemistry. Here we investigate the potential for machine learning to **reproduce the behavior of a chemical mechanism with reduced computational expense.**

Methods

- We created a **17-layer residual multi-target regression neural network** (Fig 1., right) to emulate the Carbon Bond Mechanism Z (CBM-Z) gas phase chemical mechanism.
- We trained the network to match CBM-Z predictions of changes in concentrations of **77 chemical species** after one hour, given a range of chemical and meteorological input conditions.



Conclusions and Future Work

- The network can match CBM-Z predictions of changes in concentrations with root-mean-square error (RMSE) of **less than 2 ppb** (median RMSE = 0.02 ppb)
- Achieves a **250x computational speedup**. An additional 17x speedup (for a total of 4250x) is achieved by running the neural network on a graphics processing unit (GPU).
- The neural network is able to reproduce the emergent behavior of the chemical system over diurnal cycles using Euler integration, but additional work is needed to **constrain error propagation** before neural network-based chemical solvers can be used in chemical transport models.

Results

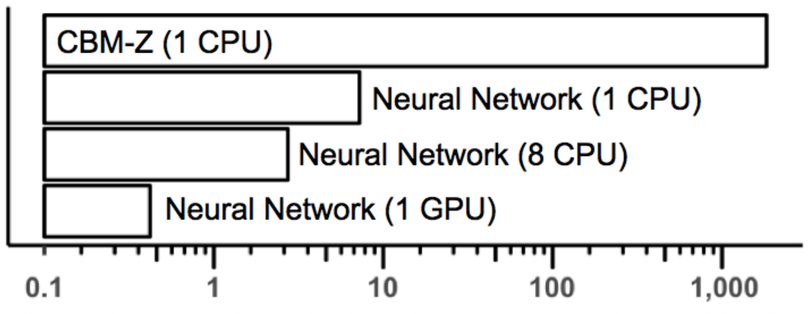


Fig 2. Time required for one million independent simulations using either CBM-Z using one CPU core, the neural network using one or eight CPU cores, or the neural network using one GPU.

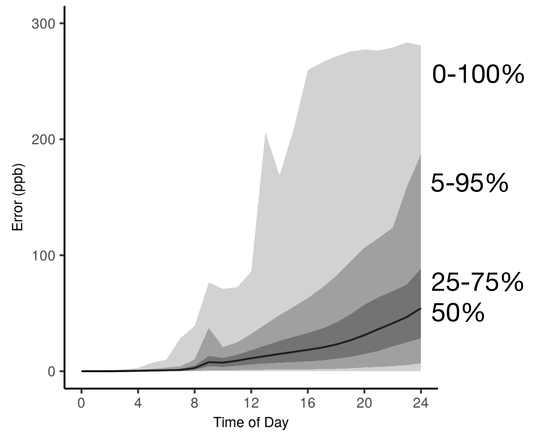


Fig 3. Neural network vs. CBM-Z error values in O_3 diurnal cycles initialized with 10,000 randomly generated initial conditions. The maximum observed error must be dramatically reduced before this approach is viable for use in chemical transport models.

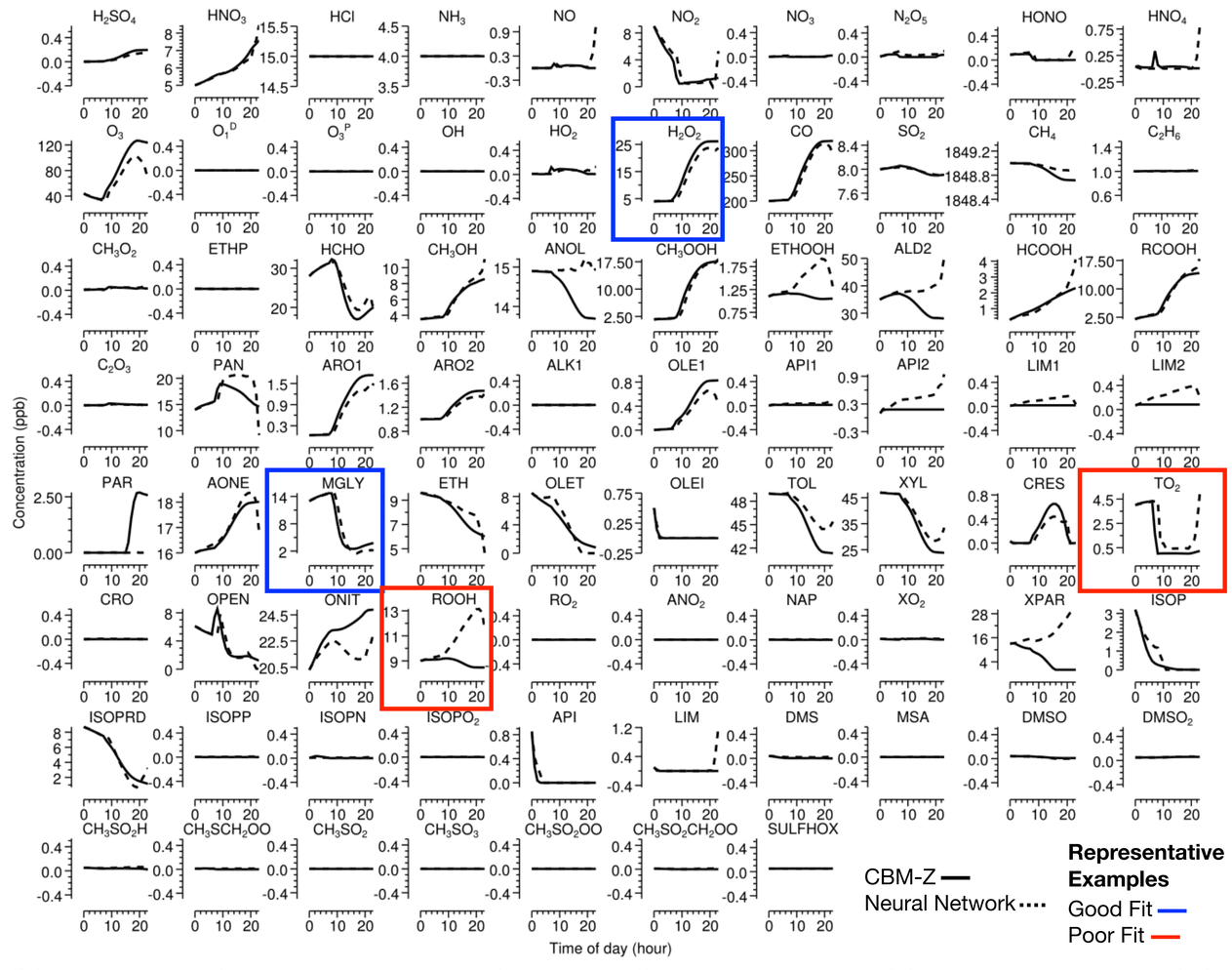


Fig 4. CBM-Z vs. neural network comparison of simulated diurnal patterns based on representative urban baseline concentrations.

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