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

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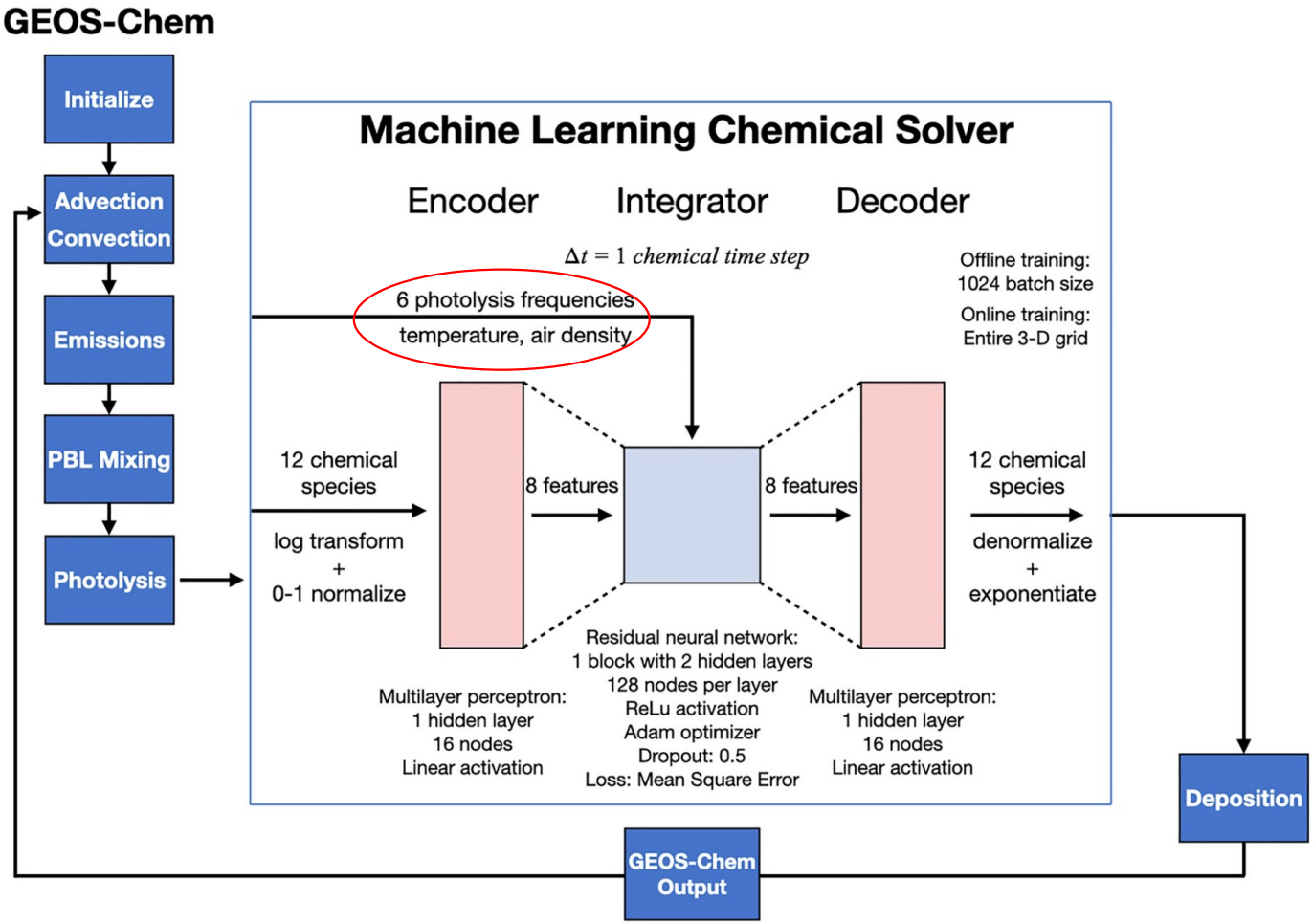
Objective

- Numerical solver for atmospheric chemistry is slower, dominating the cost of atmospheric simulation
- A ML solver for global model
  - Fast
  - Stable for year long simulaiton, because error grownth is significant in long-term ML inference
  - Reinitialization of chemical concentraion (due to non-chemistry effect)

Data

- Use a simplified chemistry scheme.
  - In the standard model: 228 species, 724 reactions
  - Simplified scheme: 12 species, 21 thermal reactions and 6 photolysis reactions.
  - KPP Rosenbrock solver simulation as baseline.

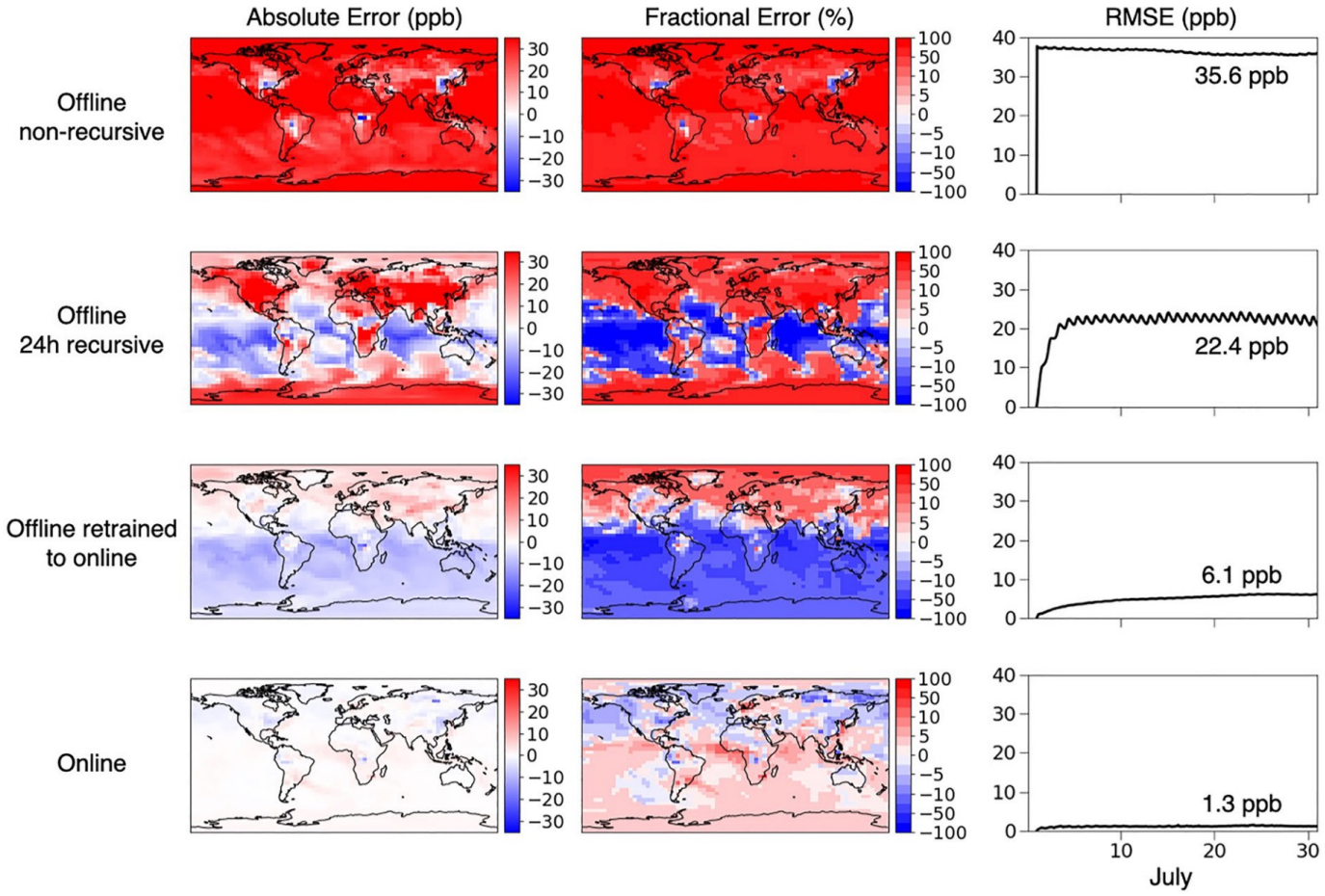
Network Architecture



Details

- 12 different solvers for each species to prioritize each species individually.
- Hardcoded reaction: OH formation: log normalization
- Recurssively training for a 24-h evolution:
  - Train 1h time step
  - Apply non-chemistry effect.
  - Recurrently for 24h.
  - (Only for training)
- Compare different training procedure
  - Offline
  - Offline-Online
  - Online (run python training code within fortran model)

Result



Capture day-night change

Not enough to fix bias learned form offline

Non-random order of training, Capture temporal evolution