Simulating Aerosol Chemistry with Graph Neural Networks

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May 18, 2024

Motivation for Studying Aerosol Chemistry

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- Regional variations
- Feedback mechanisms

Motivation for Simulation

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- MOSAIC: Model for Simulating Aerosol Interactions and Chemistry
- Computational complexity associated with the detailed representations of aerosol
- Closed-source

Can we do better?

Maybe

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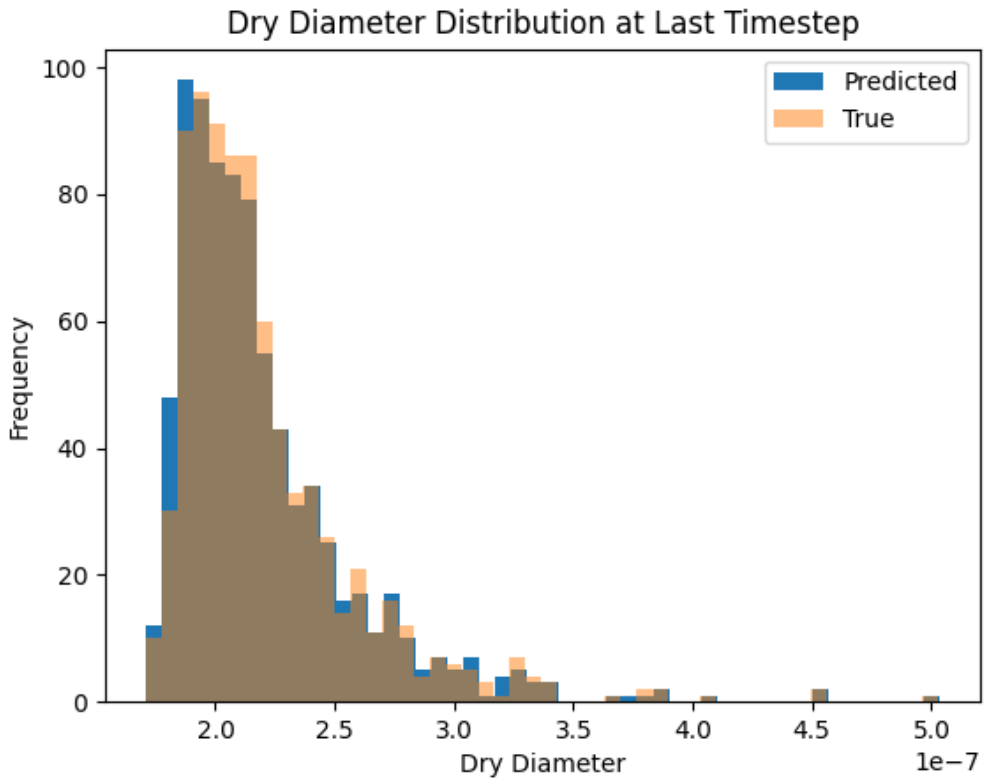

Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. MSE $\approx 8.126 \times 10^{-7}$ in rate of change rate. Time to predict ≈ 0.4 seconds

Our Contribution to Current GNS

- Inspired by Kumar and Vantassel 2022's Pytorch GNS: `https://www.geoelements.org/gns`

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- Prediction pipeline
- Data transformation pipeline
- Output analysis pipeline

Graph Neural Networks (Scarselli et al. 2008)

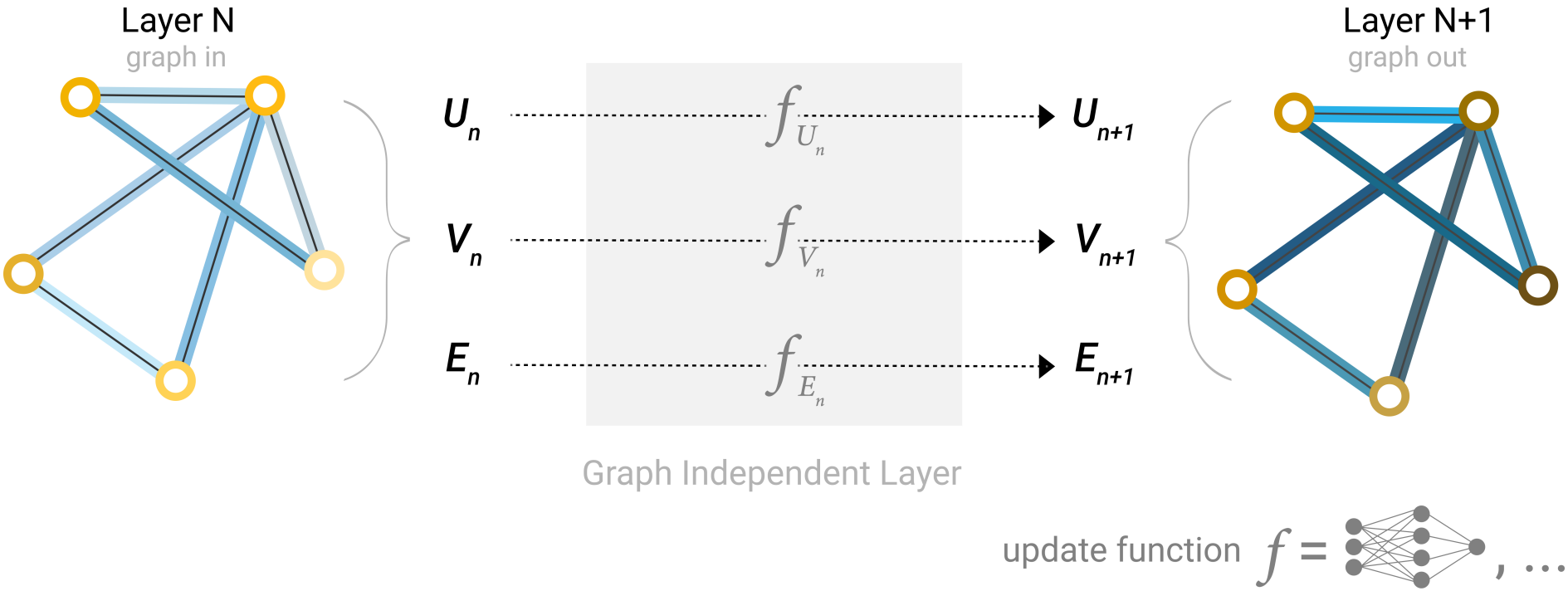
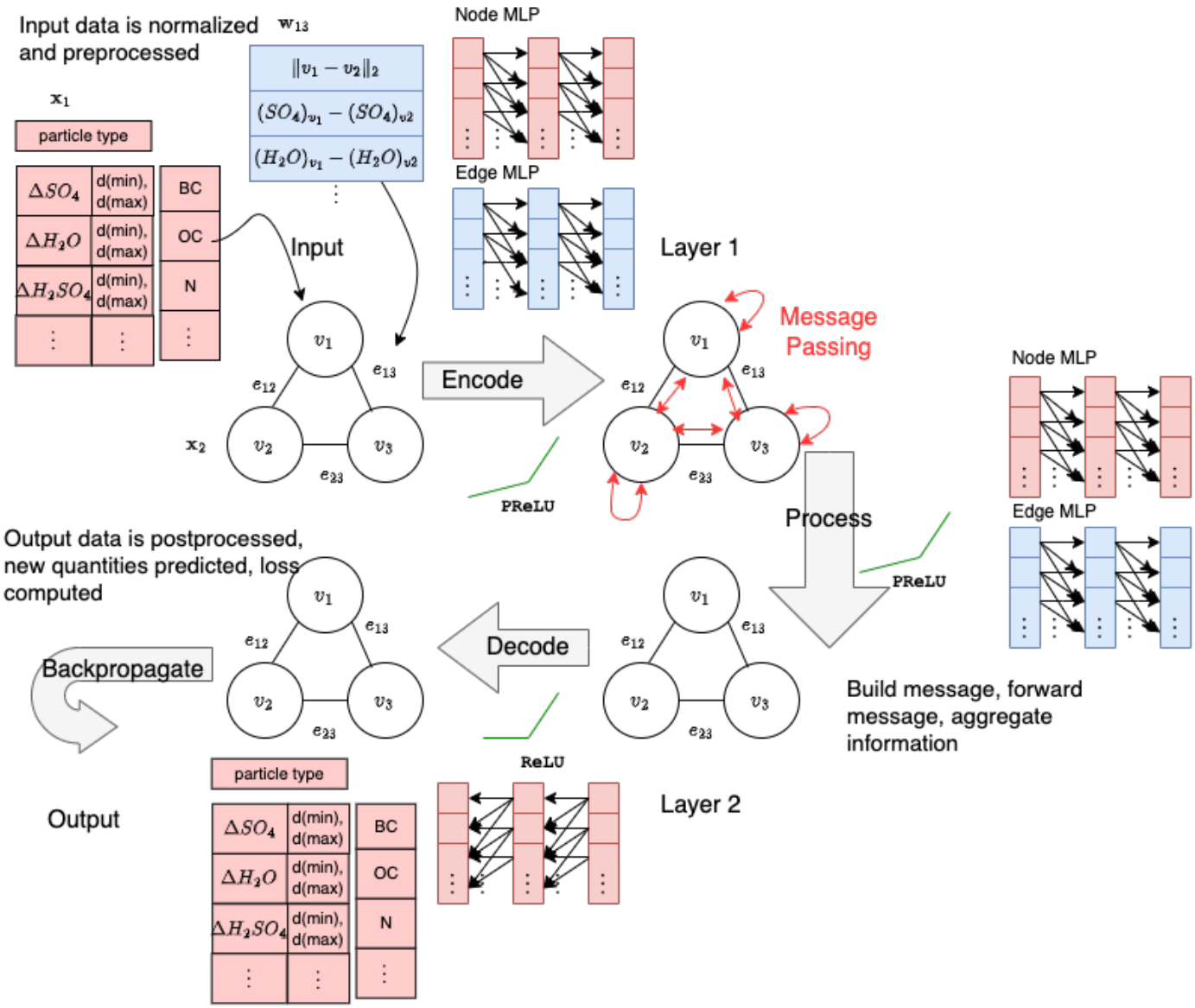


Figure: A single layer of a simple GNN. A graph is the input, and each component (V,E,U) gets updated by a MLP to produce a new graph. Each function subscript indicates a separate function for a different graph attribute at the n-th layer of a GNN model. *source*: `https://distill.pub/2021/gnn-intro/`

GNN Schematics



Graph Network Simulator (GNS) by Sanchez-Gonzalez et al. 2020

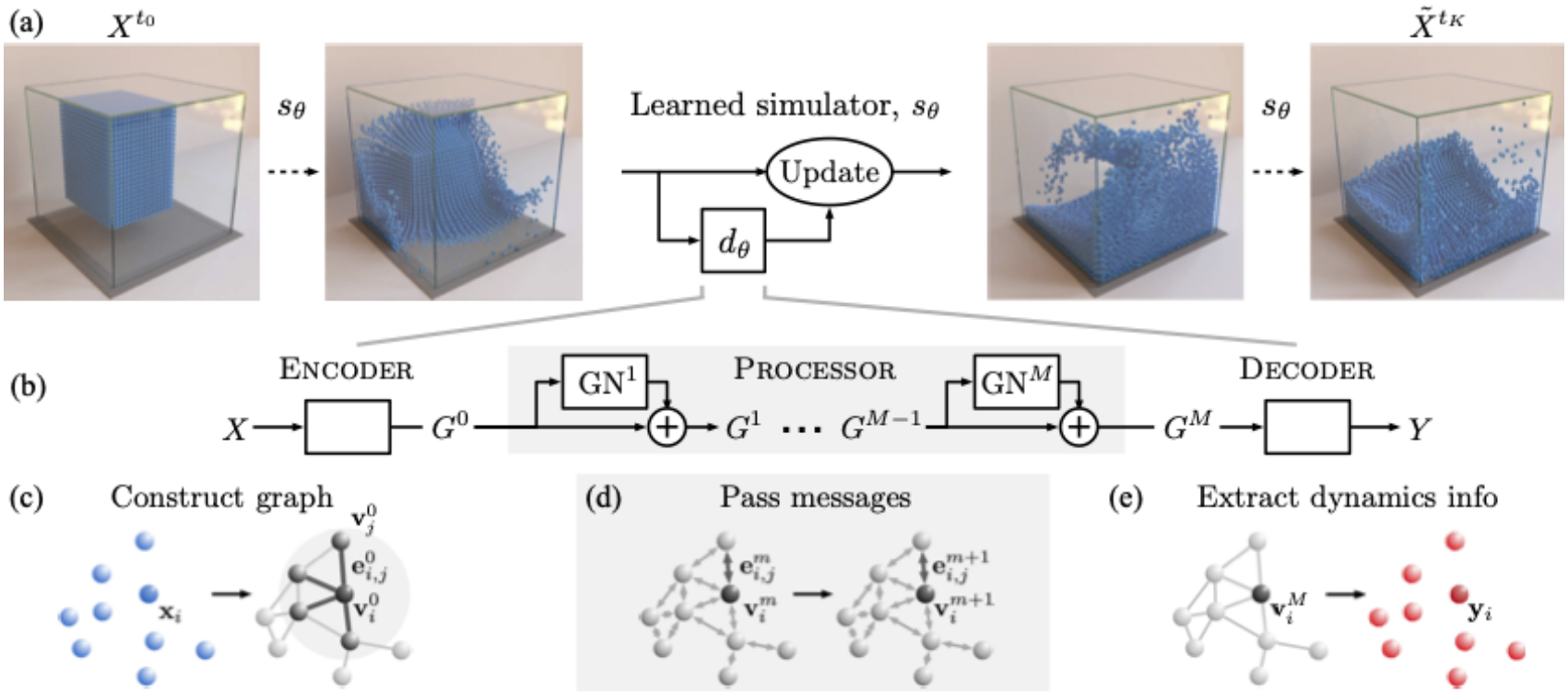


Figure: d_θ uses an "encode-process-decode" scheme, which computes dynamics information, Y, from input state, X

Chem GNS

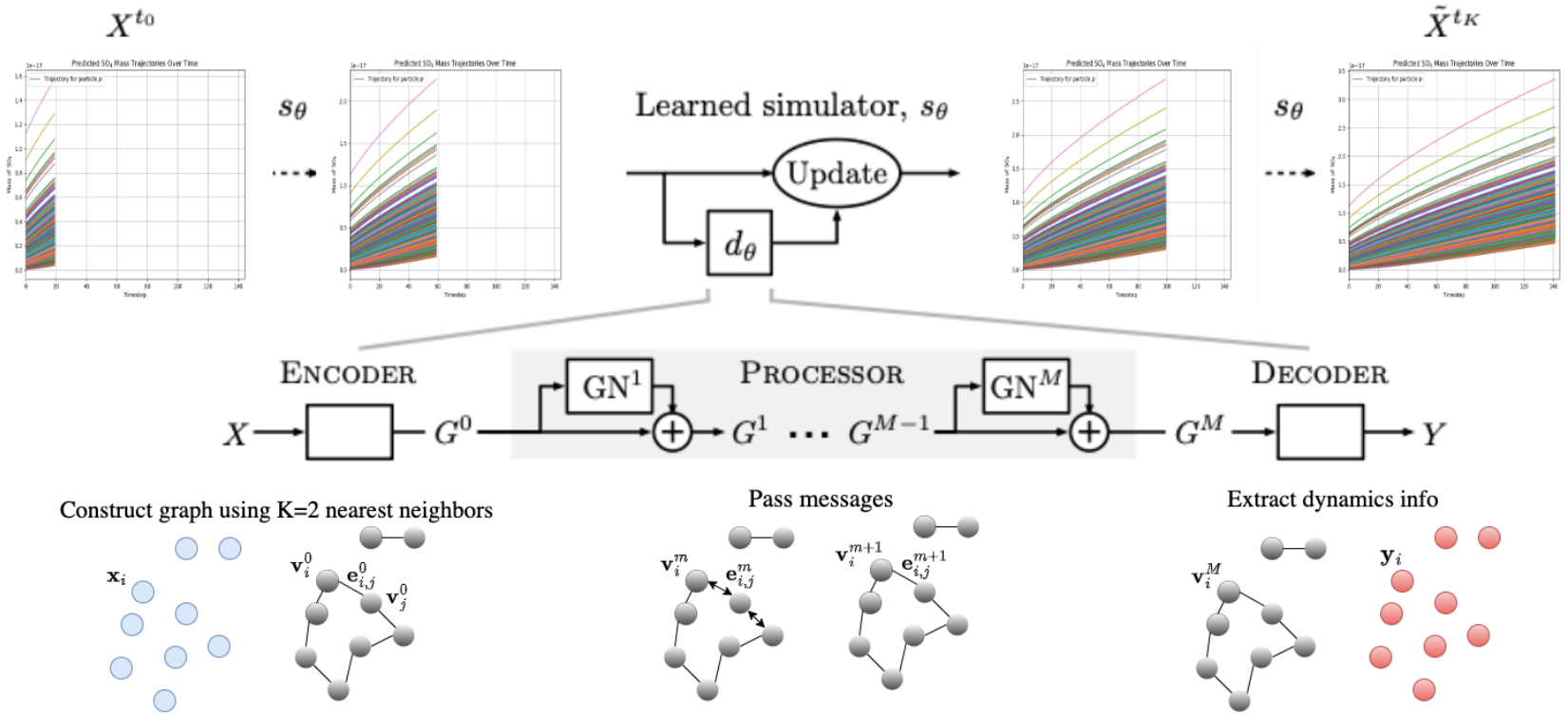


Figure: Uses an "encode-process-decode" scheme, which computes dynamics information, Y, from input state, X

Results from GNS Simulations: Water

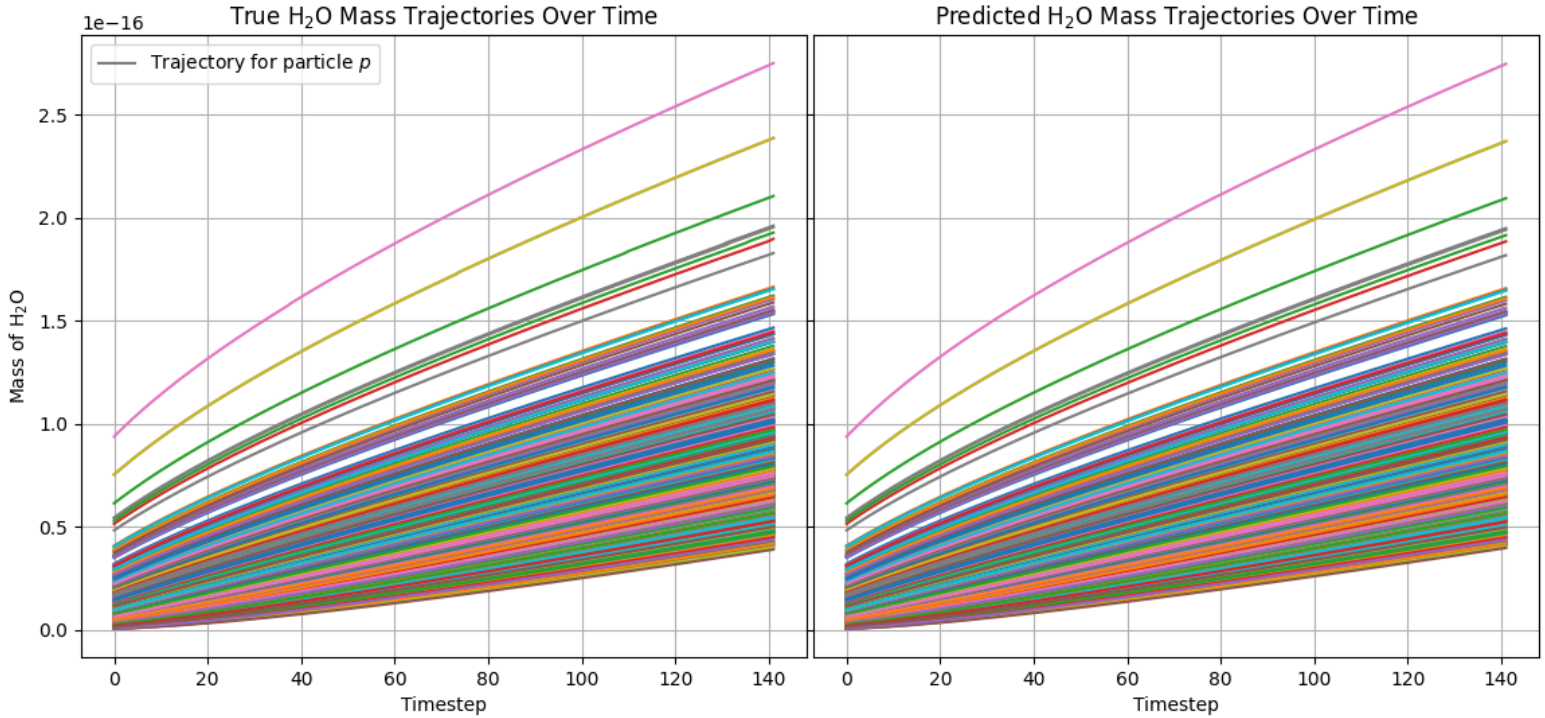


Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.004. Time to predict ≈ 0.4 seconds

Results from GNS Simulations: Sulfate

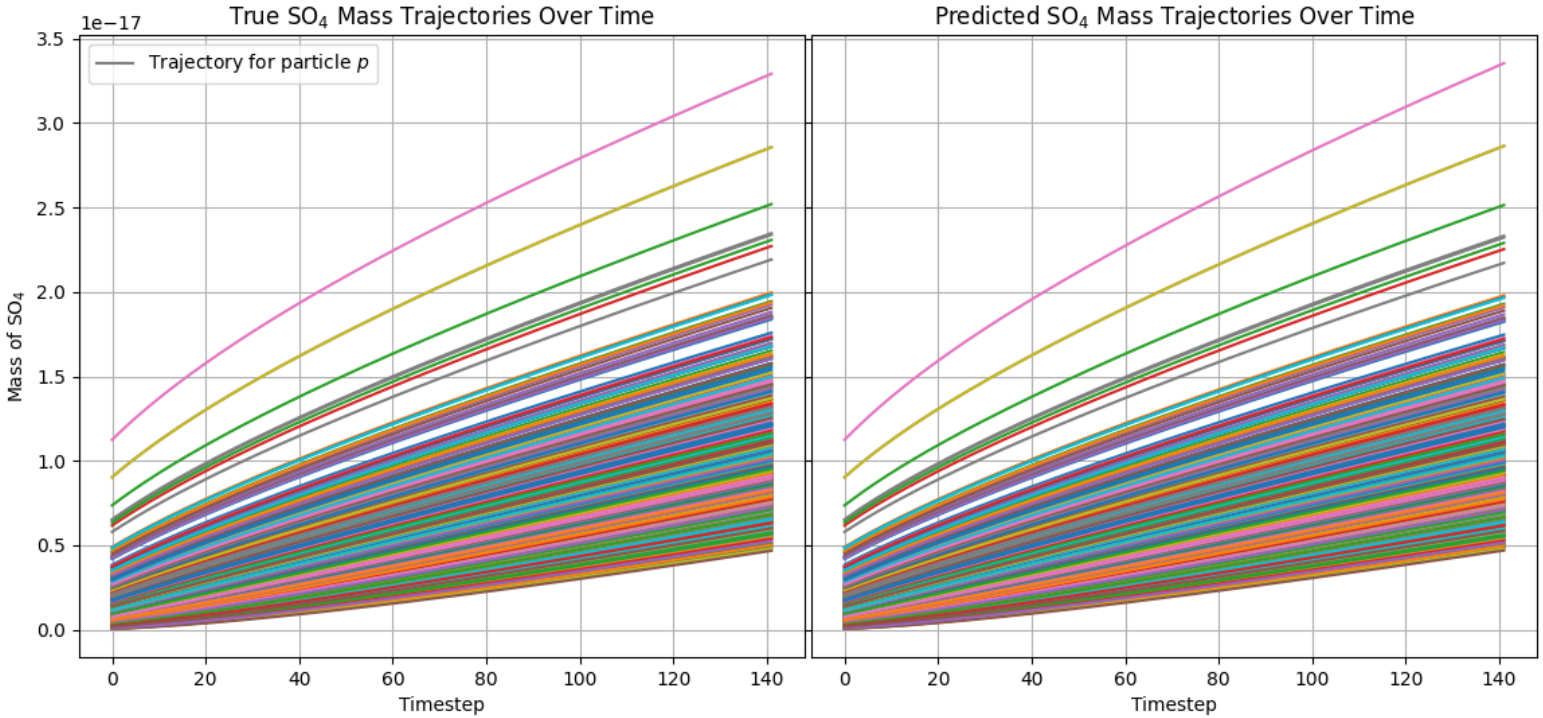


Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.007. Time to predict ≈ 0.4 seconds

Results from GNS Simulations: Sulfuric Acid

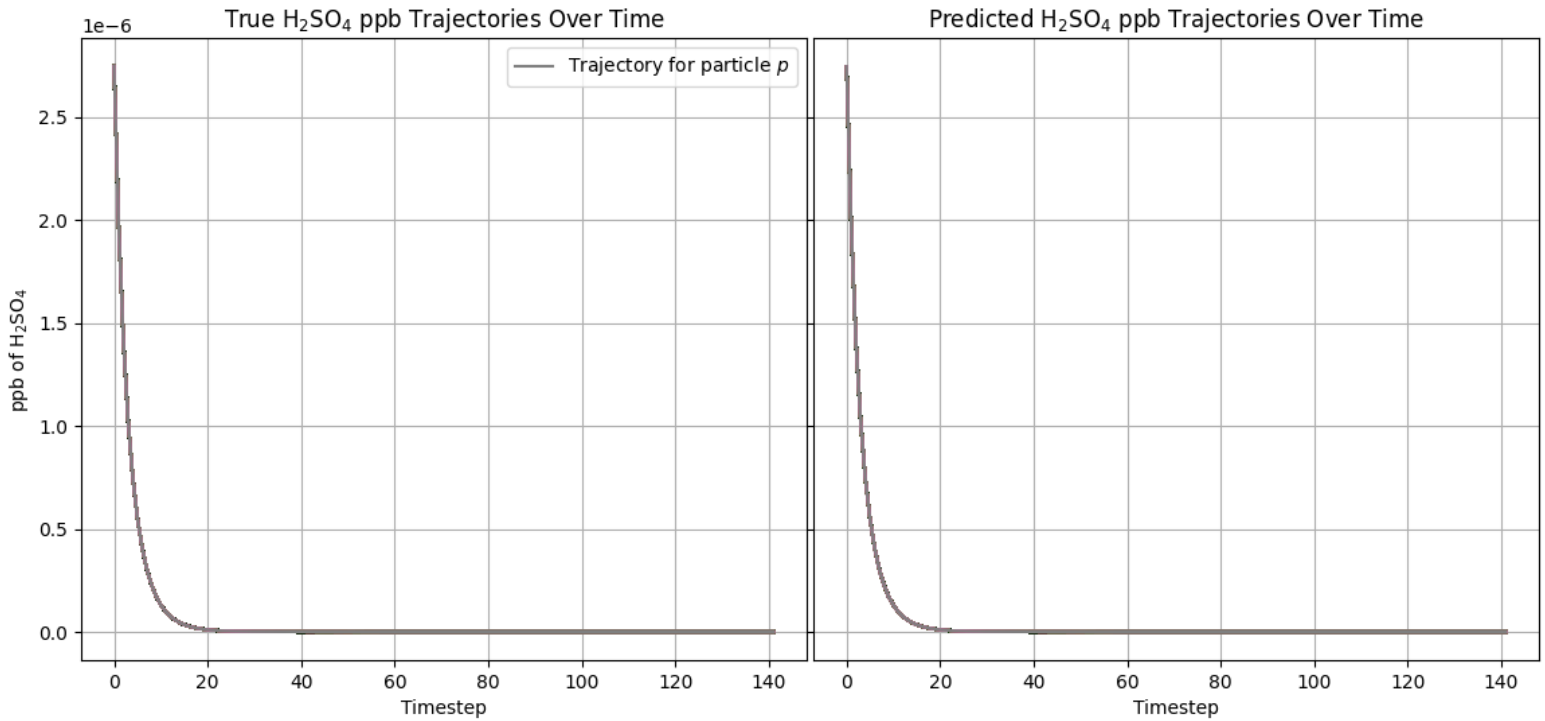


Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.011. Time to predict ≈ 0.4 seconds

Training on Different Examples

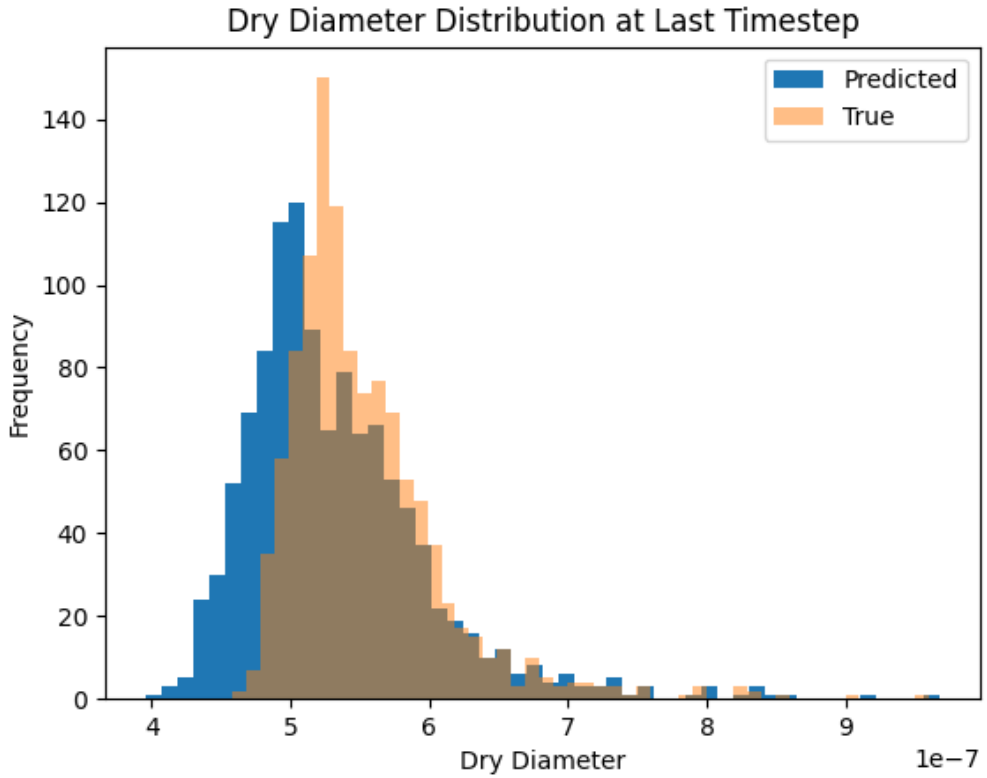


Figure: Results from Chem GNS trained on 9 different simple particle-gas systems. 142 timesteps, 1132 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. MSE ≈ 0.03 in rate of change rate. Time to predict ≈ 0.03 seconds

Future Directions

- Improve accuracy in high dimension non-linear space - may require more careful selection of functions

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- Global nodes with environmental information

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- Inclusion in climate models could be significant, if fast speeds can be maintained

References

- Kumar, Krishna and Joseph Vantassel (2022). "GNS: A generalizable Graph Neural Network-based simulator for particulate and fluid modeling". In: *arXiv preprint arXiv:2211.10228*.
- Sanchez-Gonzalez, Alvaro et al. (2020). "Learning to simulate complex physics with graph networks". In: *International conference on machine learning*. PMLR, pp. 8459–8468.
- Scarselli, Franco et al. (2008). "The graph neural network model". In: *IEEE transactions on neural networks* 20.1, pp. 61–80.