Simulating Aerosol Chemistry with Graph Neural Networks

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April 25, 2024

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Motivation for Studying Aerosol Chemistry

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- 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?

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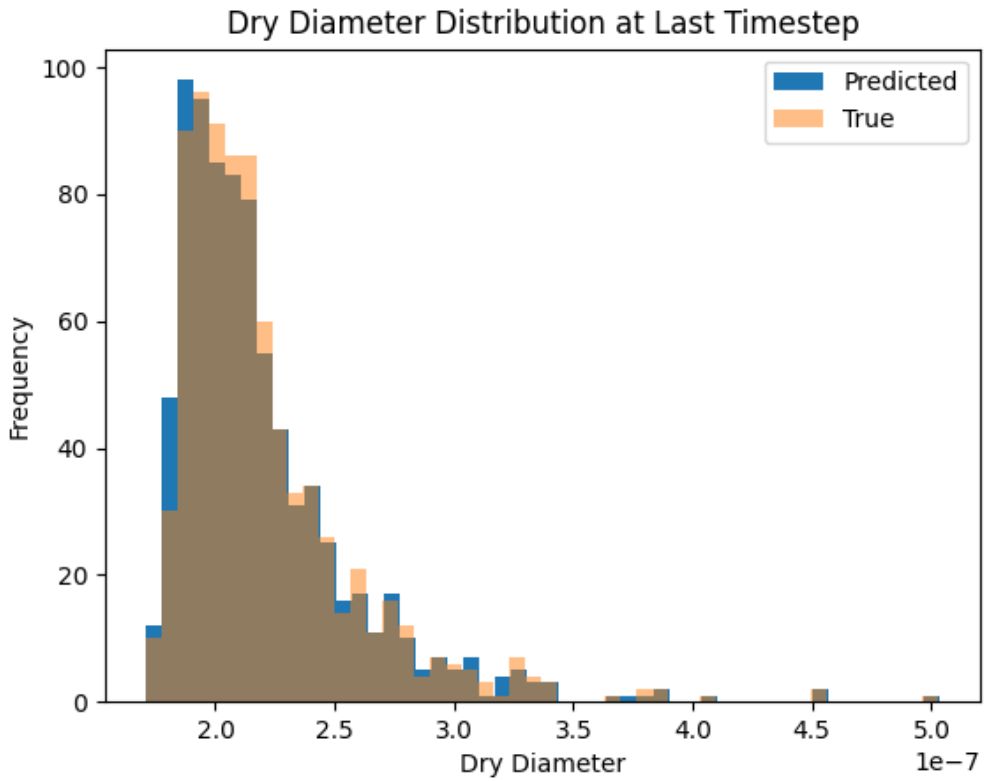

Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. MSE $\approx 8.126 \times 10^{-7}$ in rate of change rate. Time to predict ≈ 0.4 seconds

Graph Neural Networks (Scarselli et al. 2008)

Let $G = (V, E)$. Each node $v_i \in V$ has an associated feature vector x_i, and each edge $(v_i, v_j) \in E$ has an associated weight w_{ij}. At each message passing step t, the state of each node v_i is updated based on information from its neighbors.

$$m_i^{(t)} = \sum_{j \in N(i)} \text{MessageFunction}(x_i, x_j, w_{ij}) \tag{1}$$

$$h_i^{(t+1)} = \text{UpdateFunction}(h_i^{(t)}, m_i^{(t)}) \tag{2}$$

GNN Schematics

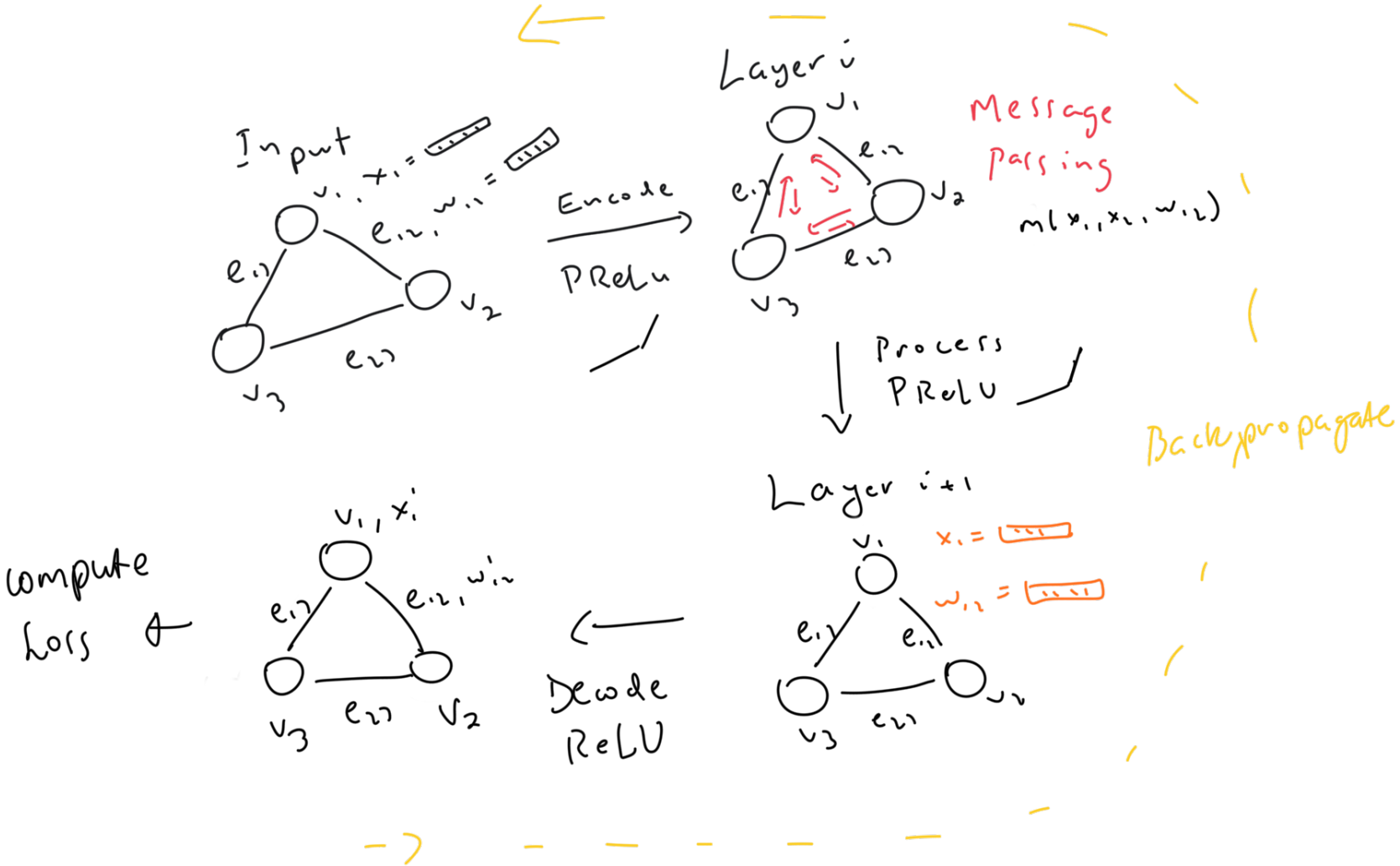

Figure: GNN scheme for Chem GNS

Parametric Rectified Linear Unit by He et al. 2015

Definition:

$$\text{PReLU}(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha x & \text{otherwise} \end{cases}$$

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Key Points:

- PReLU introduces a learnable parameter α to capture negative slope.

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Key Points:

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- When $\alpha = 0$, PReLU reduces to the ReLU activation function.
- PReLU allows for learning the optimal slope for negative inputs at each channel, improving model performance.

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

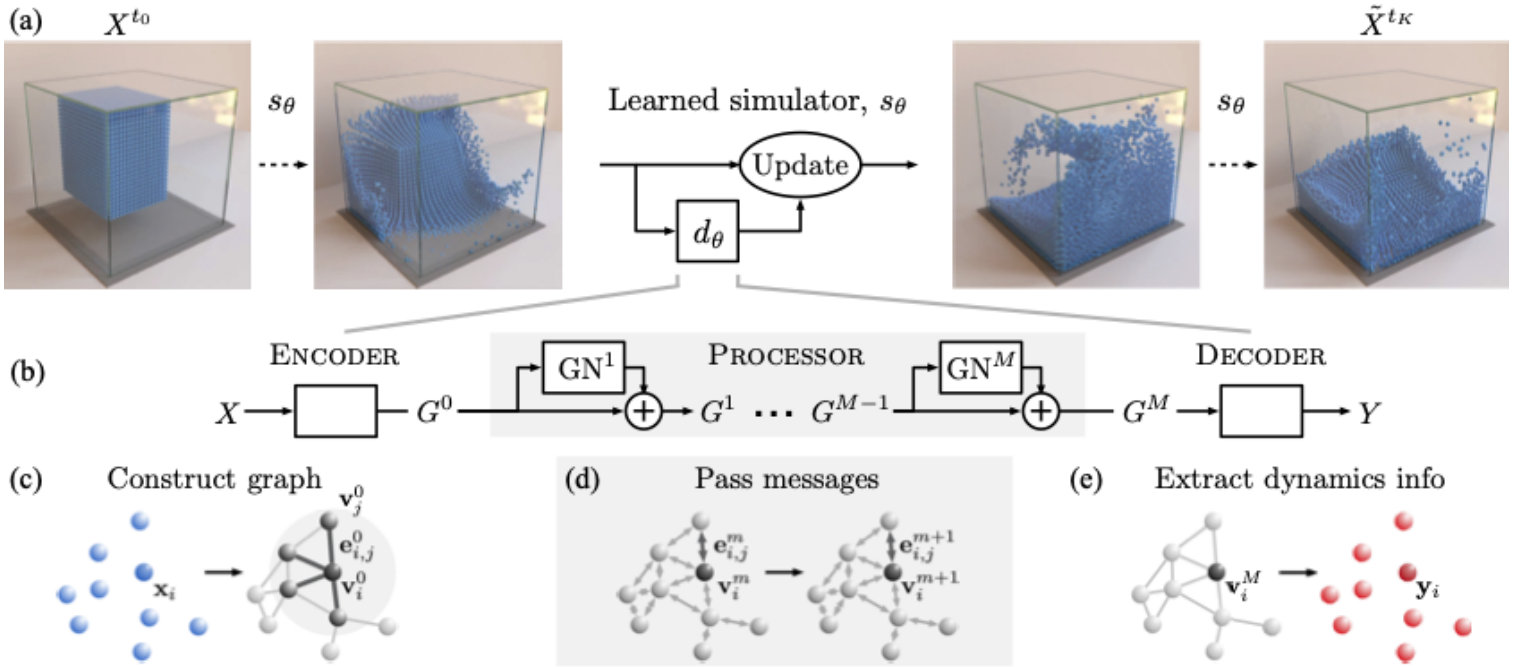
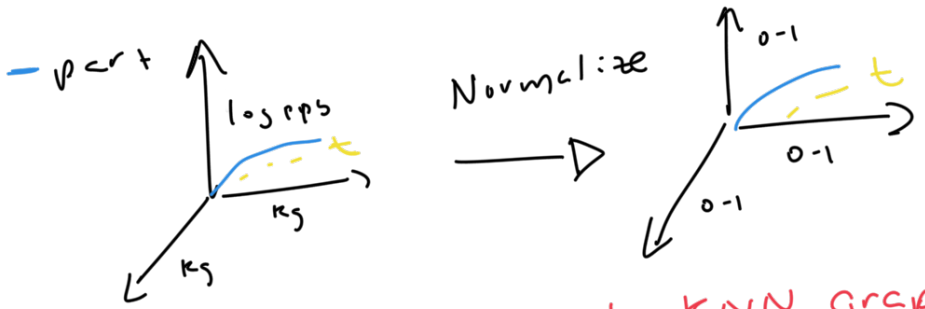


Figure: d_θ uses an "encode-process-decode" scheme, which computes dynamics information, Y, from input state, X

Chem GNS

Input at t per particle



Construct KNN graph k=2

node ◯ → "particle"

node feature → change from t-1 → t, differences from know minimax, node type, normalized material properties

edge → "displacements" and "distance" from neighbors Euclidean!

→ learned GNN to get input at t+1

Results from GNS Simulations: Water

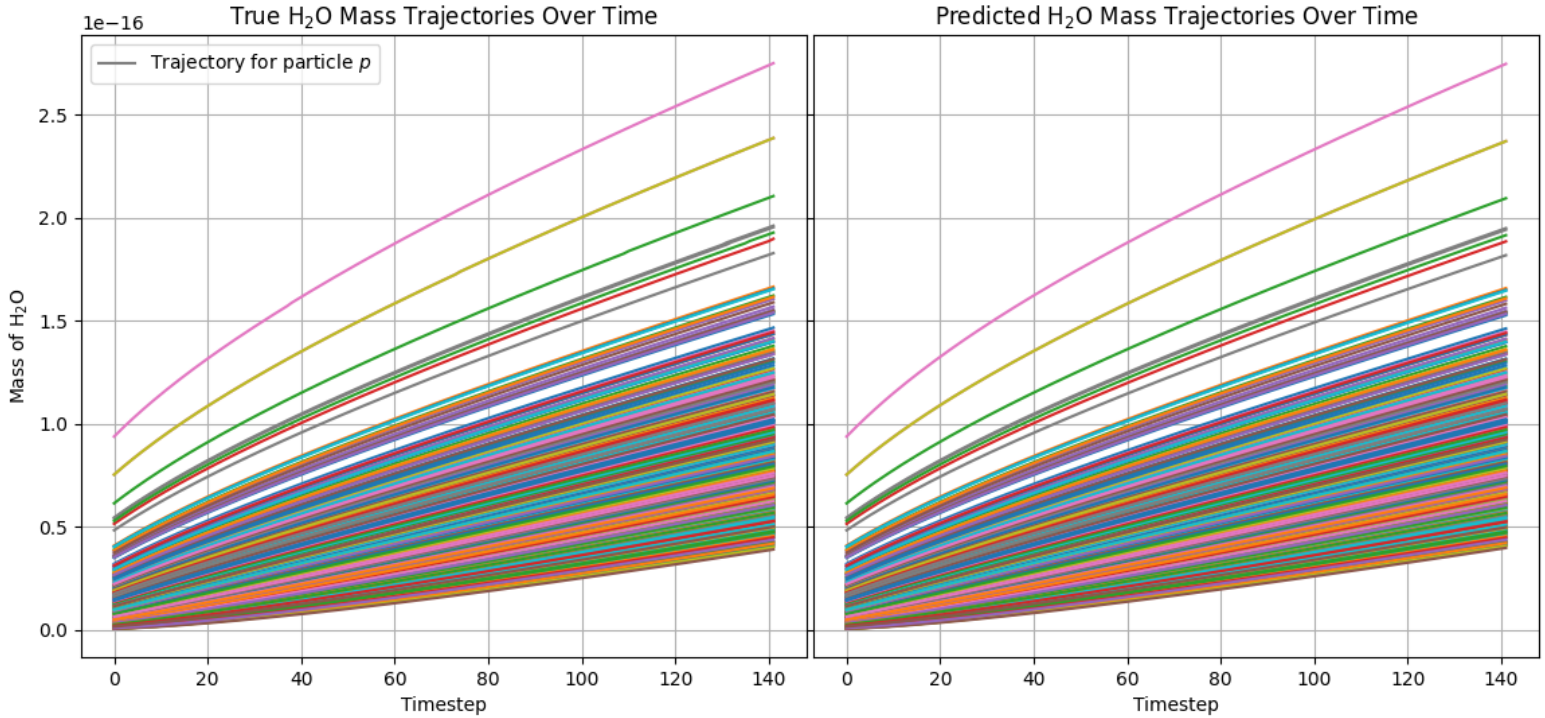


Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.004. Time to predict ≈ 0.4 seconds

Results from GNS Simulations: Sulfate

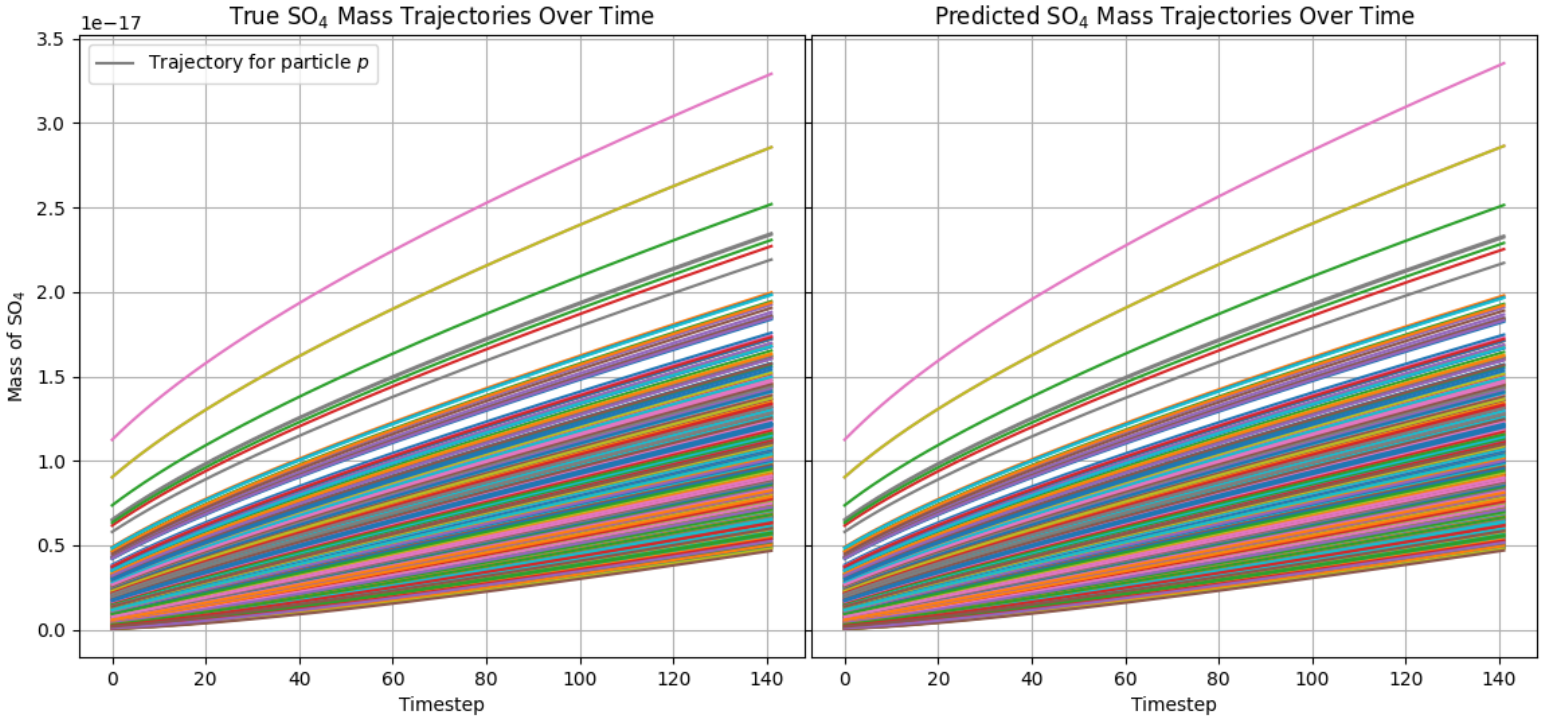


Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.007. Time to predict ≈ 0.4 seconds

Results from GNS Simulations: Sulfuric Acid

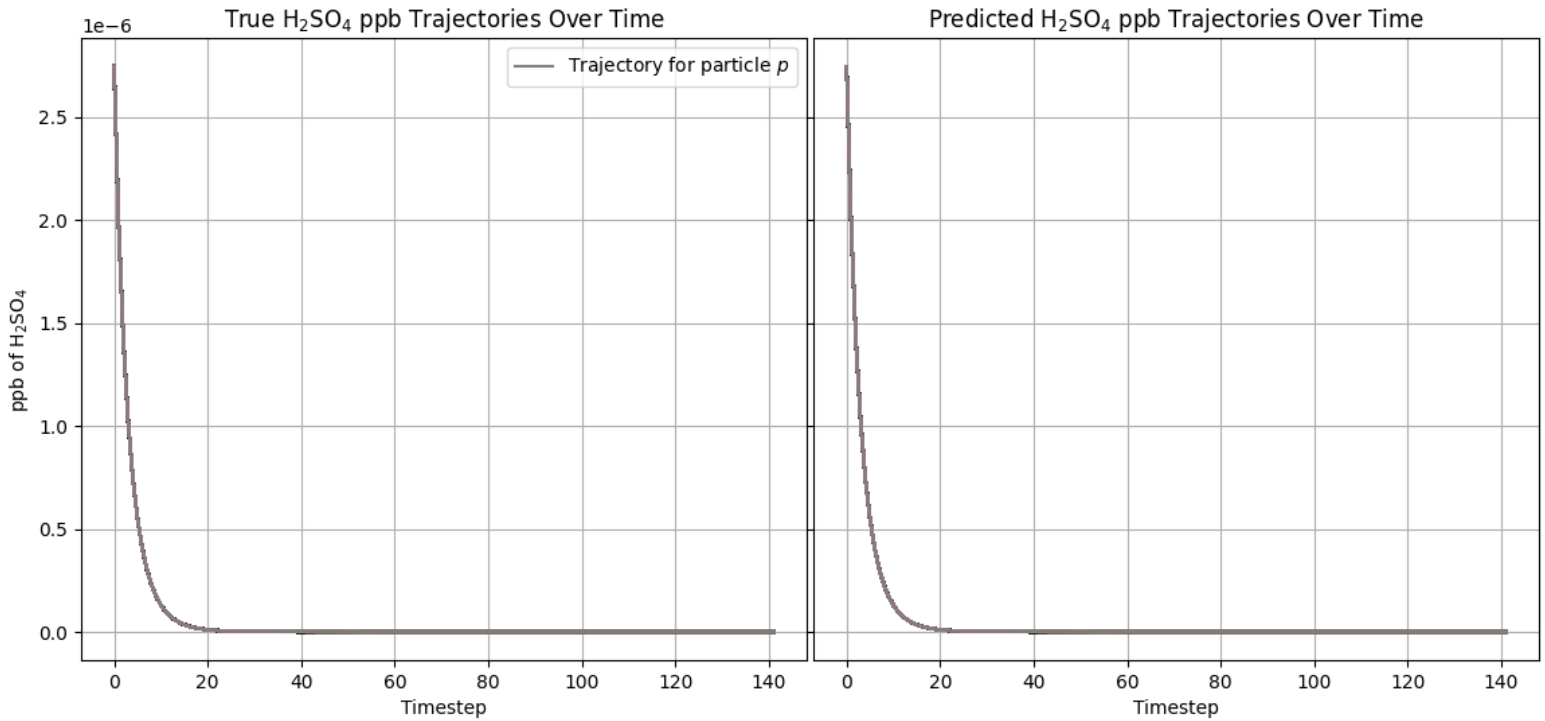


Figure: Results from Chem GNS on a simple particle-gas system. 142 timesteps, 808 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.011. Time to predict ≈ 0.4 seconds

Training on Different Examples

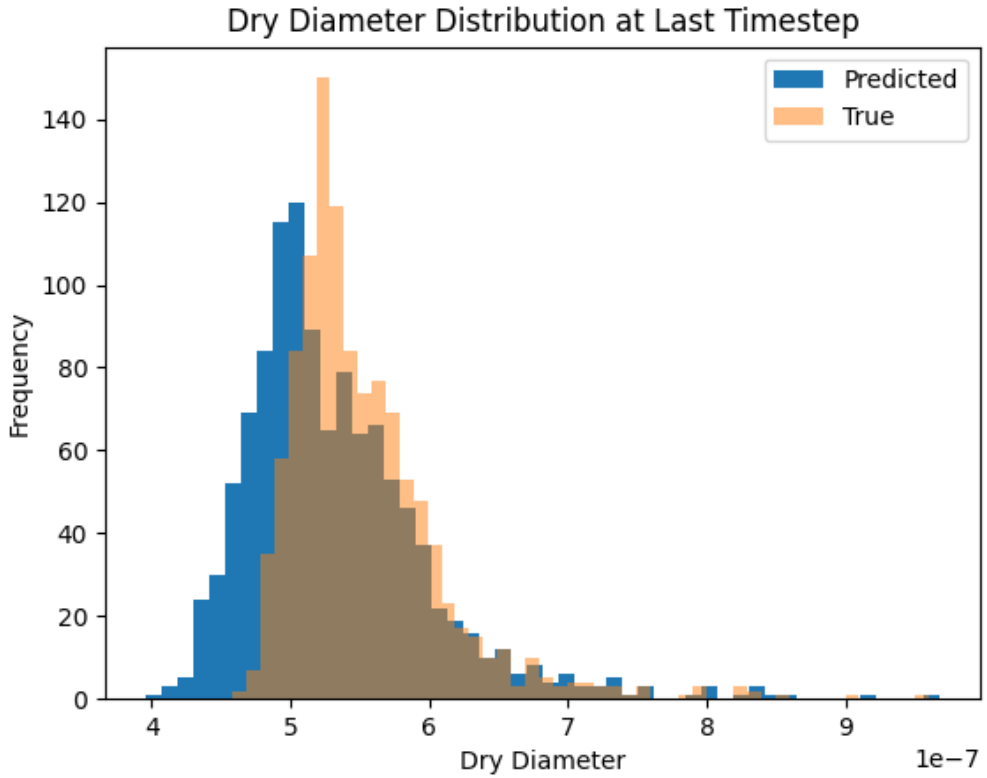


Figure: Results from Chem GNS trained on 9 different simple particle-gas systems. 142 timesteps, 1132 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. MSE ≈ 0.03 in rate of change rate. Time to predict ≈ 0.03 seconds

More Results from GNS Simulations: Water

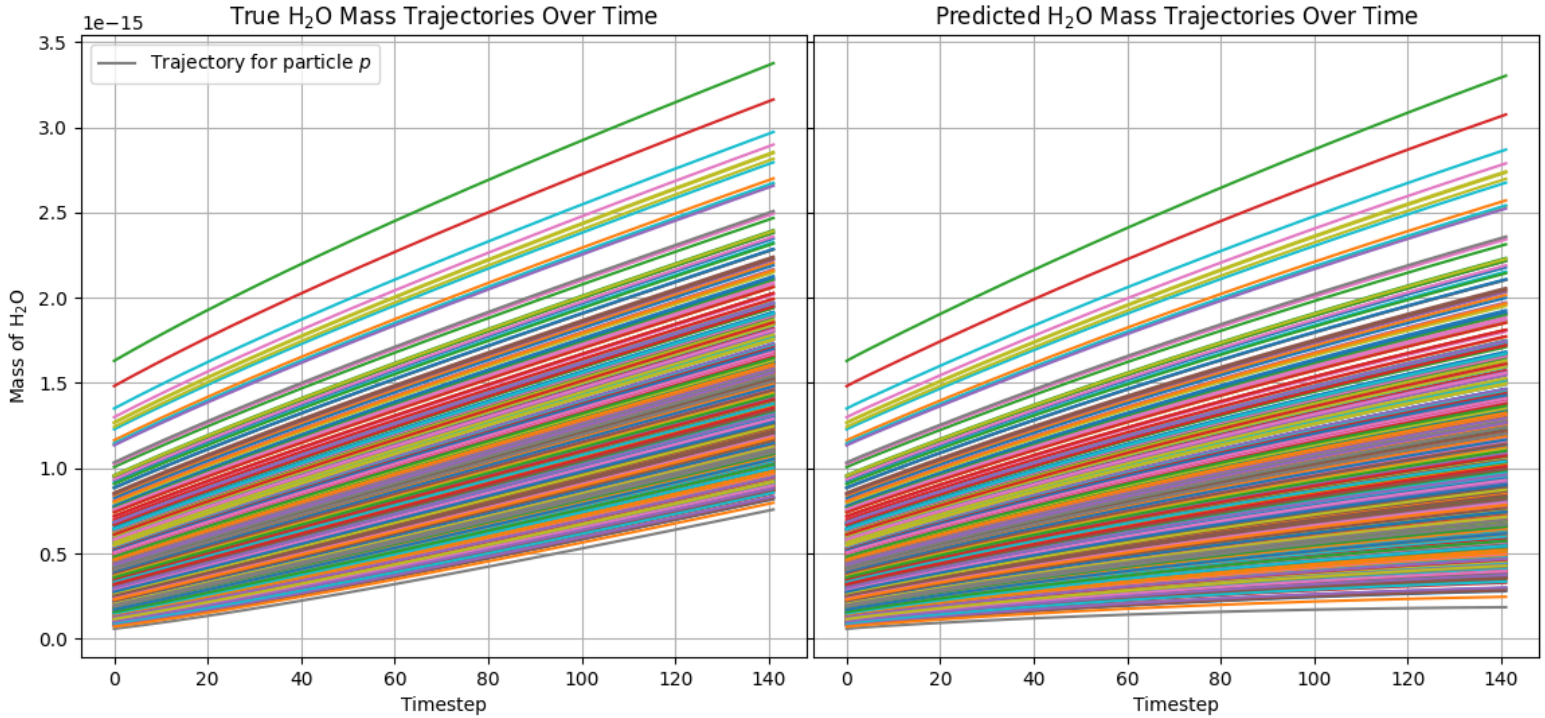


Figure: Results from Chem GNS trained on 9 different simple particle-gas systems. 142 timesteps, 1132 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.19. Time to predict ≈ 0.4 seconds

More Results from GNS Simulations: Sulfate

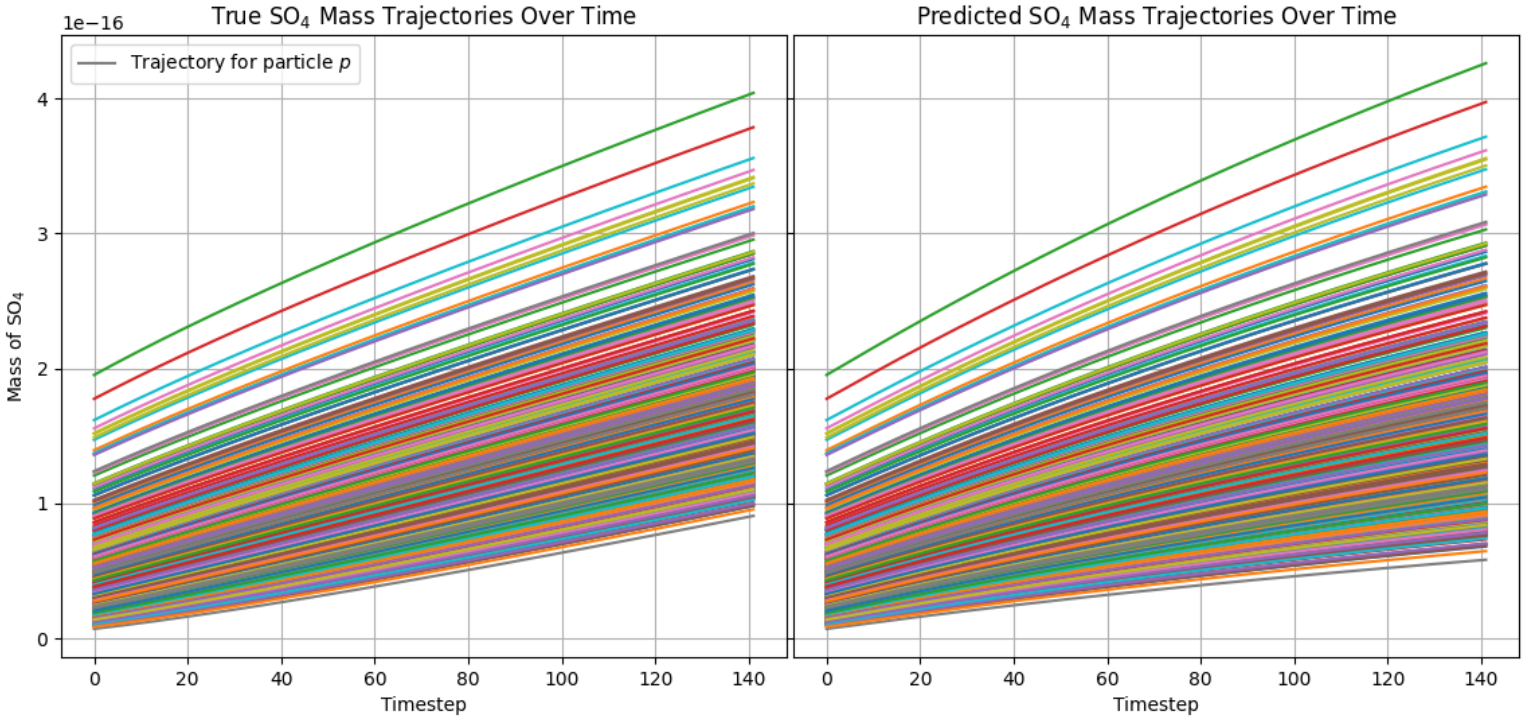


Figure: Results from Chem GNS trained on 9 different simple particle-gas systems. 142 timesteps, 1132 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.05. Time to predict ≈ 0.4 seconds

More Results from GNS Simulations: Sulfuric Acid

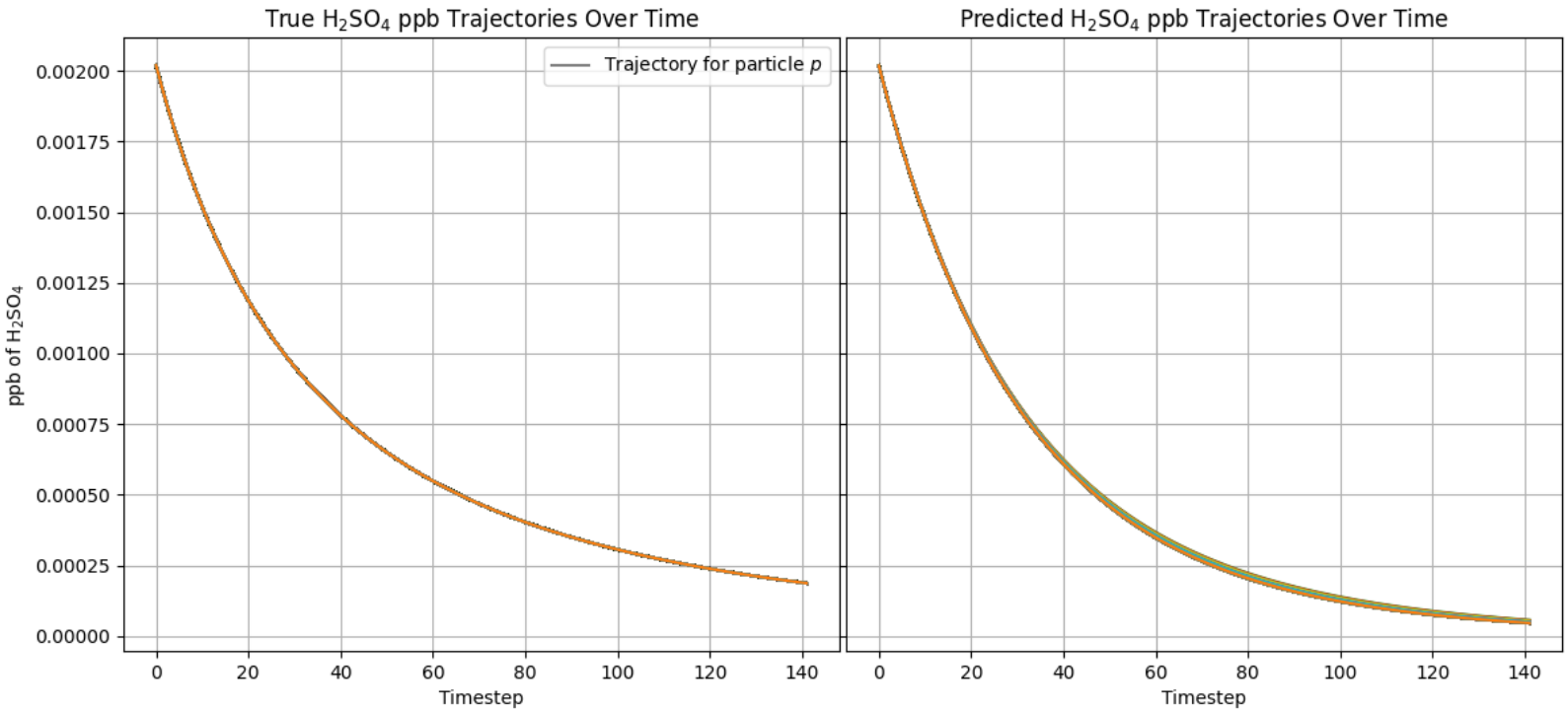


Figure: Results from Chem GNS trained on 9 different simple particle-gas systems. 142 timesteps, 1132 particles, 3 time changing features, 3 time fixed particle properties, 2 chemical types. NMAE ≈ 0.40. Time to predict ≈ 0.4 seconds

Future Directions

- Performance issues in high dimensions may require more careful selection of functions

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- Global nodes with environmental information

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- Making it bigger and better will require thinking outside Euclidean space
- If fasts speeds can be maintained, inclusion in climate models would be significant

References

- He, Kaiming et al. (2015). "Delving deep into rectifiers: Surpassing human-level performance on imagenet classification". In: *Proceedings of the IEEE international conference on computer vision*, pp. 1026–1034.
- Sanchez-Gonzalez, Alvaro et al. (2020). "Learning to simulate complex physics with graph networks". In: *International conference on machine learning*. PMLR, pp. 8459–8468.
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