Simulating Hadronic Interactions with Conditional Normalizing Flows

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Introduction

High Energy Physics (HEP) simulations, such as those generated by GEANT4 simulation toolkit, play a pivotal role in understanding particle interactions and predicting experimental outcomes. Traditional Monte-Carlo methods are computationally expensive and slow, prompting the exploration of newer techniques such as deep generative models. This project investigates the usage of Conditional Normalizing Flows (CNFs) as a deep learning model for modeling hadronic interactions. We propose a recursive normalizing flow to simulate a proton interacting with carbon material using the GEANT4 simulated data. This work shows a step towards building a fully differentiable and data-driven simulation model for hadronic interactions for High Energy and Nuclear Physics.

Methods

The dataset is the simulated result of a 31 GeV incoming proton ($\boldsymbol{p}^+$) colliding with a stational carbon material, which is produced by the GEANT4 simulation toolkit. The toolkit generates events which are an instance of $\boldsymbol{p}^+ + C$ collision given an incoming particle kinematic. Each event returns a cascade of particles and their resulting kinematics.

The total dataset is **4** Million events, with 10% used as the testing and validation dataset respectively. The number of final state particles ranges, so the results were previously filtered for interactions where the leading two particles were $\pi^+\pi^-$ in any order.

Our model is a masked autoregressive flow which combines normalizing flows and autoregressive estimation. A chain of bijectors, or invertible functions, alter a normal distribution $p_0(z_0)$ to achieve the target distribution $p_k(z_k)$. The densities are one dimensional conditional distributions: $p(z_0, \ldots, z_n) = \prod_i^n p(z_i|z_{i-1}, \ldots, z_0)$. Our model uses 20 bijectors whose invertible function is determined by the Mask Autoencoder for Density Estimation (MADE) block, which is trained.

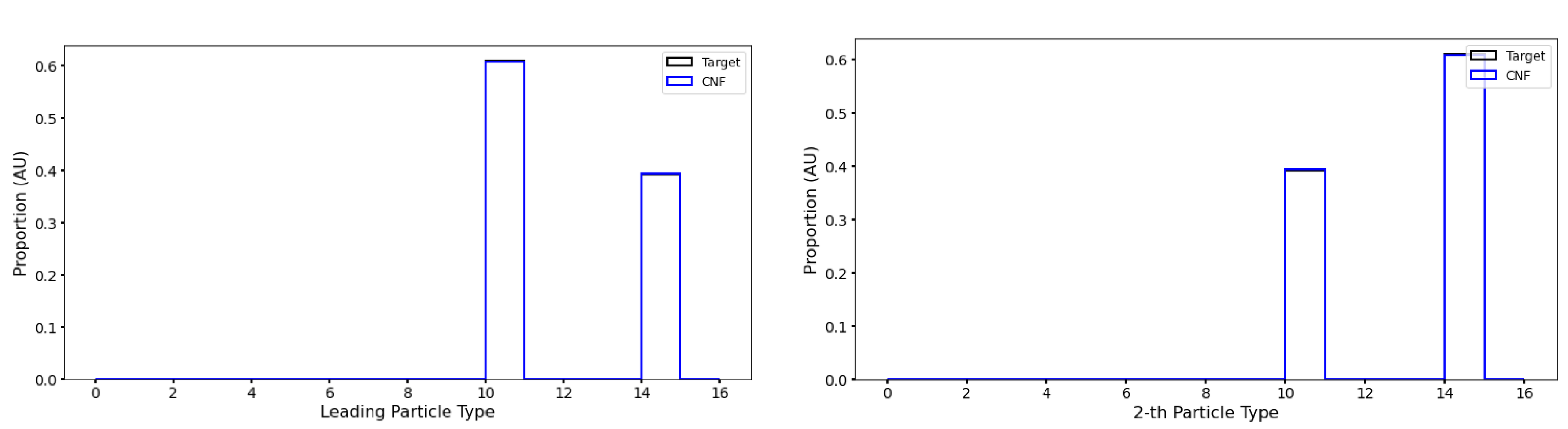
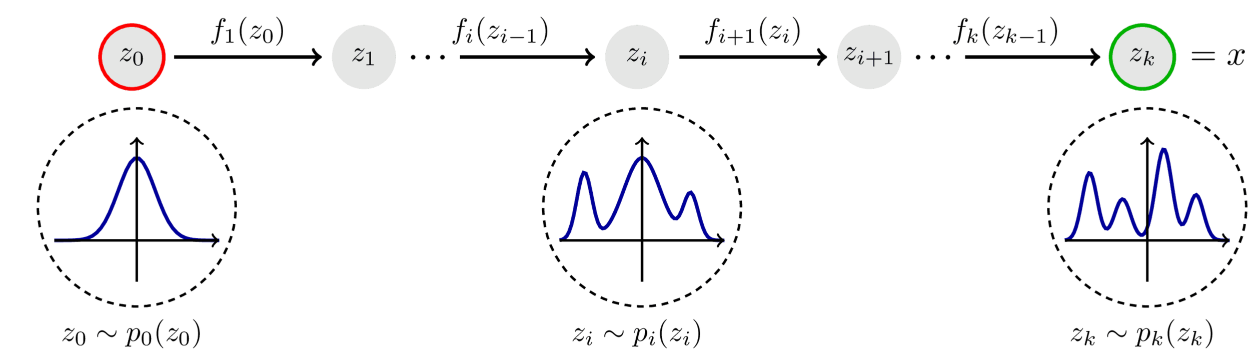


Fig 1: Predicts the particle types very closely. These particle types correlate exactly to the $\pi^+\pi^-$mode we expect. Within simple cases such as this, we see accurate performance.



Incoming particles kinematics are used to predict leading particles final state kinematics $(Energy,\ p_x, p_y, p_z)$. This final state kinematics is subtracted from the incoming particle kinematics to find the remaining 4-momenta in the system. This remaining 4-momenta is recursively fed back into the CNF model to find the 2nd particle final state kinematics.

In addition, we use the Adam optimizer with learning rate at 10^{-3} to $10^{-5}$and with polynomial decay.

Results

Leading Particle

The CNF model trains and produces particle kinematics from the conditional training dataset. The epoch with the lowest Wasserstein Distance was used to generate 100,000 events for comparison with the GEANT4 toolkit generated data in Figure 2 and 3.

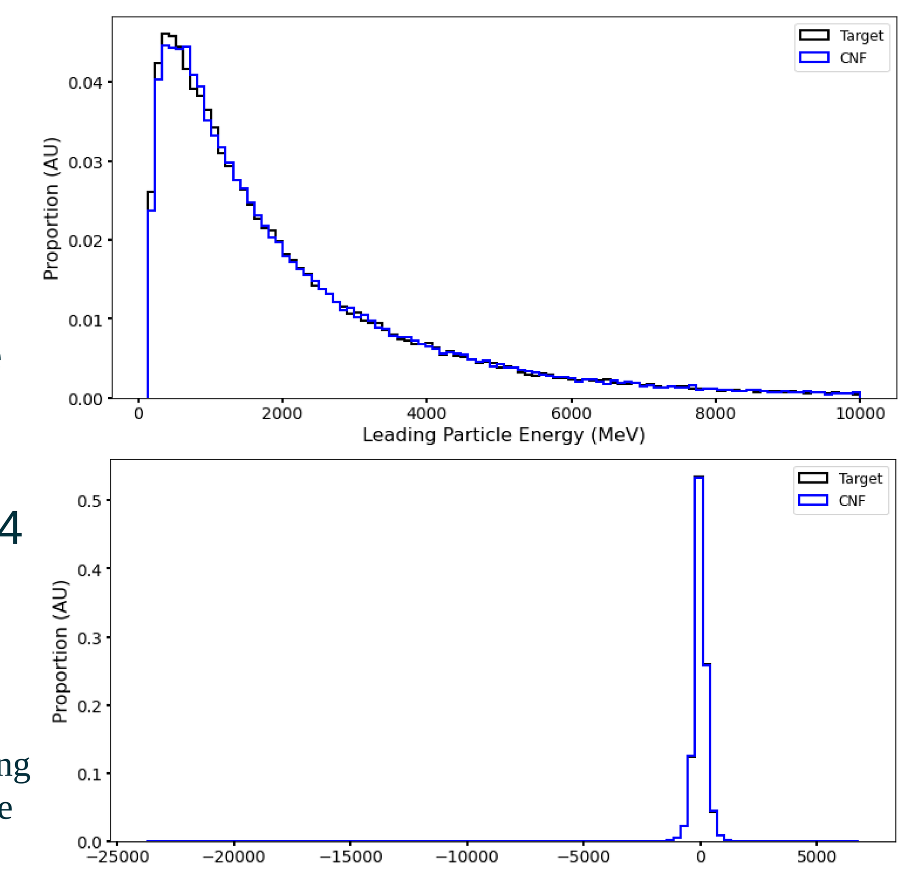


Fig 2: Predictions for the p_y, and p_z momentum density distributions overlaying the target distributions for the first particle generated from event (leading particle)

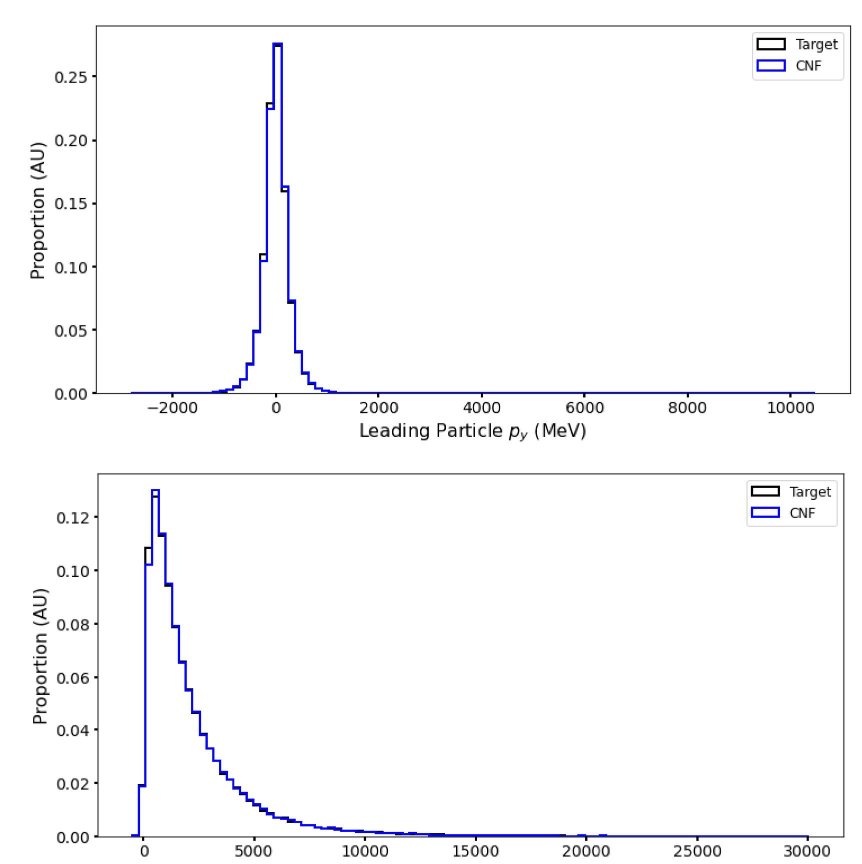


Fig 3: Predictions for the energy and p_x distributions overlaying the target distributions for the first particle generated from the event (leading particle).

The CNF model predicts 4-momenta and particle types for the leading particle very well. The predicted density distribution (blue) matches the target density distribution of the dataset (black) closely.

Results Cont.

2nd Particle

Within the 100,000 events generated by the CNF model, we examine the predictions of the density distribution for the 2nd particle in the event.

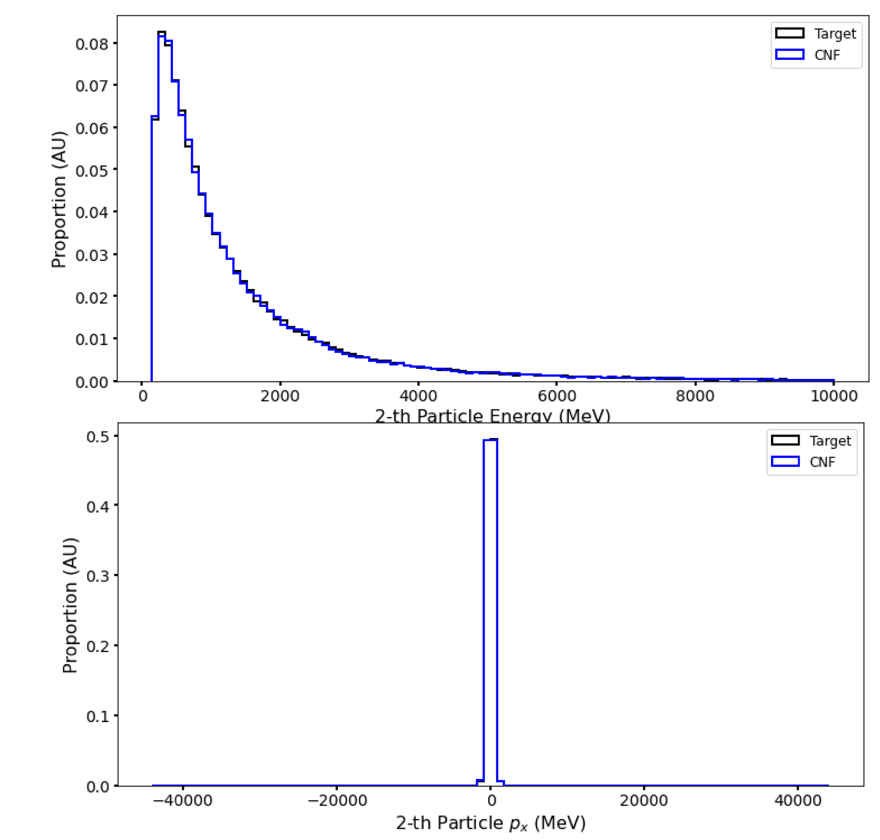


Fig 4: Predictions for the p_y and p_z momentums density distributions overlaying the target distribution for the 2nd particle in the event

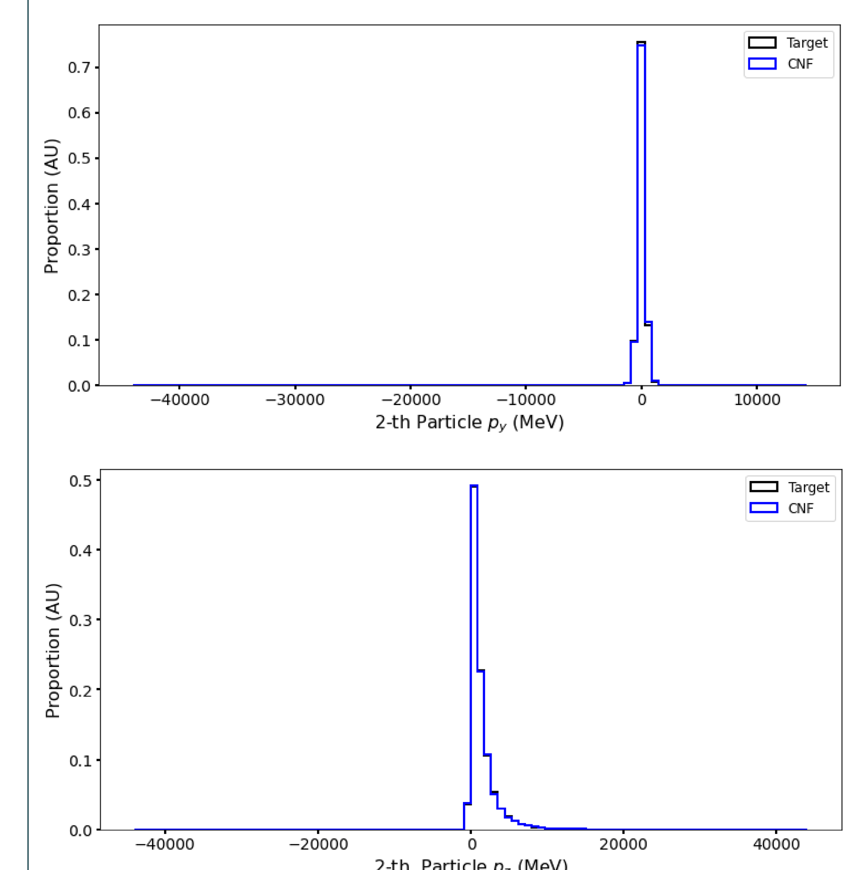
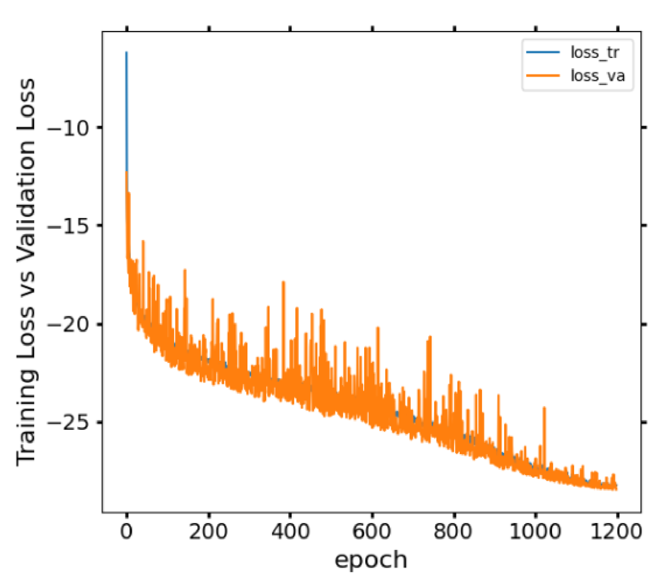


Fig 5: Predictions for the energy and p_x distributions overlaying the target distributions for the 2nd particle in event.

The model predicts the 4-momenta and particle type for the 2nd particle very well.

Training and validation loss converge together after 1200 epochs with batch size of 16384.



In addition, we see computational performance increases. GEANT4 takes 140 seconds to generate 1 M events while CNF takes 60 seconds for 1 M events

Conclusion

This work shows promise towards using conditional normalizing flows for simulating hadronic interactions. From the results, we've captured the conditional dependence for the first two particles of the event reasonably well. However more work will be needed for capturing lower-energy interactions, different interaction modes and other relevant predictions such as particle counts and particle type predictions.

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