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Novel Approaches for Fast Simulation in HEP using Diffusion and Graph-to-Graph Translation

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The simulation of particle physics data is a fundamental but computationally intensive ingredient for physics analysis at the Large Hadron Collider. In traditional fast simulation schemes, a surrogate calorimeter model is the basis for a set of reconstructed particles. We demonstrate the feasibility of generating the reconstructed objects in one step, replacing both the calorimeter simulation and reconstruction step. Our previous model that employed slot attention achieved promising results on a simplified synthetic dataset. In this work, we propose two novel approaches to improve this task and evaluate them on a more realistic dataset. In the first approach, we augment the slot-attention mechanism with a state-of-the-art diffusion model, where we start with a noisy graph and perform gradual noise reduction by solving Stochastic Differential Equations with gradient approximation and obtain the reconstructed particles. The second approach incorporates iterative graph refinement, where we directly transform the set of truth particles into the set of reconstructed particles. These approaches are able to go beyond our previous baseline performance in terms of both accuracy and resolution of the predicted particle properties.

Brainstorming idea [title]

Enhancing the set generation by physics-based models

Brainstorming idea [abstract]

Set generation is a useful application of ML in HEP for fast jet and reconstructed particles generation. The output sets are generated based on initial particles or events. However, current set generation models are not explicitly considering physical constraints and features relevant to correctly model the detector effects. The following questions arise: what available models can we use for this task? How can we incorporate physics knowledge to achieve our goal? Beyond these, can we think of new set-based loss functions tailor-made to achieve good accuracy in modeling detector resolutions and efficiencies?

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