EUROPEAN AI FOR
FUNDAMENTAL PHYSICS
CONFERENCE
EuCAIFCon 2025

Contribution ID: **118** Type: **Poster + Flashtalk**

Differentiable modeling for calorimeter simulation using diffusion models

The design of calorimeters presents a complex challenge due to the large number of design parameters and the stochastic nature of physical processes involved. In high-dimensional optimization, gradient information is essential for efficient design. While first-principle based simulations like GEANT4 are widely used, their stochastic nature makes them non-differentiable, posing challenges in gradient-based optimization. To address this, we propose a machine learning-based approach where we train a conditional diffusion denoising probabilistic model (CDDPM) as a differentiable surrogate for these simulations. The CDDPM not only predicts particle showers based on different particle types and incoming energy levels but also conditions on different detector design variables. Furthermore, we explore post-training adaptation techniques, such as adapter-based fine-tuning, to efficiently specialize the model for new calorimeter conditions without requiring full retraining. This allows for flexible optimization across different calorimeter configurations while maintaining computational efficiency. We evaluate the predictive accuracy of the model and assess its gradient output to demonstrate its potential for the future detectors design and optimization.

AI keywords

machine learning; diffusion model; gradient-based optimization

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Track Classification: Simulations & Generative Models