Refining Fast Simulation Using Machine Learning

Acelya Deniz Güngördü¹ ¹ Dorukhan Boncukcu¹ Kevin Pedro² Samuel Louis Bein³ Moritz Jonas Wolf⁴ Mirac Ekim Vural¹ Altan Cakir¹ on behalf of the CMS Collaboration

> 1**Stanbul Technical University** ²Fermilab ³UCLouvain

> > ⁴University of Hamburg

- **CMS** physics analysis rely on large quantities of simulated data
- **LHC Phase 2: higher luminosity, complex new** detectors, more data
- CMS experiment uses two simulation chains: 1. FullSim: Based on Geant4, high accuracy but slower 2. FastSim: Approximate techniques, faster but less accurate

Introduction

Data Sample and Method

Training sample: SUSY simplified model "T1tttt" simulated:

- 1. Gen \rightarrow FastSim + PU
- 2. Same Gen \rightarrow FullSim + PU

- A grid search system was integrated into the monitoring system.
- All models in the grid are displayed in the grouped trainings tab as a grouped training.

The aim is to establish a refined version of the FastSim data sample, which is more similar to the FullSim output, i.e., more accurate.

Matching jets using ΔR angular criterion

Network Inputs and Targets:

Input: FastSim variables $\mathbf{x}^{\text{Fast}} = 4$ DeepJet discriminators and p_T , $\vec{x} = (p_T \ b \ C \lor B \ C \lor L \ Q \lor G)^T$ Parameters: $y = p_T^{\text{GEN}}$ $_{\rm T}^{\rm GEN}, \eta^{\rm GEN},$ true hadron flavor (b, c, or light quark/gluon) $\textsf{Output:}$ Refined variables $\mathbf{x}^\text{Refined} = 4$ DeepJet discriminators and p_T $\bm{\mathrm{Target:}}$ FullSim variables $\mathbf{x}^\mathsf{Full} = 4$ DeepJet discriminators and p_T

Speed

- Comparing ensembles of jets
- To cope with independent stochasticity in both simulation chains

Given two samples from $P(X)$ and $Q(Y)$:

Training Framework

(a) Grid Search Mechanism

Figure 1. Training Framework

Conclusion

Refinement of FastSim leads to significantly improved agreement with FullSim.

Training monitoring system implemented to track progress across various configurations. Refinement of jets, electrons, photons, and muons ongoing.

References

[1] S. Bein, P. Connor, K. Pedro, P. Schleper, and M. Wolf. Refining fast simulation using machine learning. In *EPJ Web of Conferences*, volume 295, page 09032. EDP Sciences, 2024.

[2] Moritz Wolf, Lars O. Stietz, Patrick L. S. Connor, Peter Schleper, and Samuel Bein. Fast Perfekt: Regression-based refinement of fast simulation. 10 2024.

- FastSim is a rapid Monte Carlo application for detector simulation and event reconstruction, approximately 10 times faster than FullSim.
- FastSim's speed advantage comes with reduced accuracy in some observables.
- R&D: Refine FastSim output with ML
- based on methodology: Fast Perfekt[\[1\]](#page-0-0)[\[2\]](#page-0-1)

Figure 2. Network Architecture of Refinement

Primary loss: Maximum Mean Discrepancy (MMD)

$$
\widehat{\text{MMD}}(P,Q) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(x_i, x_j) + \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m k(y_i, y_j) - \frac{2}{nm} \sum_{i=1}^n \sum_{j=1}^m k(x_i, y_j)
$$

where $n = m =$ batch size = 2048 and k : Gaussian kernel (adaptive σ)

Combine loss terms via MDMM (modified differential method of multipliers):

• Allows us to account for multiple loss terms such as MSE and loss terms that enforce boundary conditions or unitarity

CMS Simulation Preliminar **CMS** Simulation Preliminary (13 TeV) (13 TeV) Distribution ㅎ 0.06 0.6 $\begin{bmatrix} 2 & 0.05 \\ 0.05 & 0 \end{bmatrix}$ 0.5 ه **FastSim Refined (Test) FastSim Refined (Test)** $\frac{1}{6}$ 0.04 ЪЪ 0.4 $\overline{2}$ 0.03 0.3

Results

(c) Correlation matrix for FullSim, FastSim, FastSim Refined

Summary table lists best models and all loss values

(f) Profiles of discrepancy from Full (mean and RMS)

FERMILAB-POSTER-24-0302-CMS-CSAID-PPD Conference on Computing in High Energy and Nuclear Physics (CHEP) 2024