Generative Models for Particle Shower Simulation in Fundamental Physics

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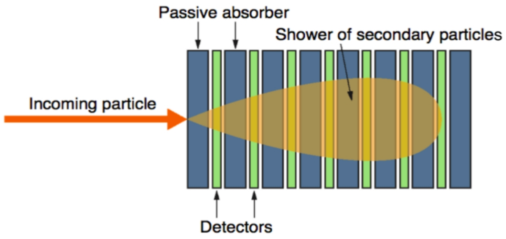
DESY.

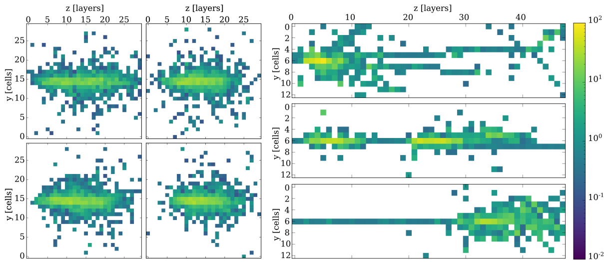
Introduction

- Investigate laws of nature at the scale of 10^{-18} meters by the interaction of elementary particles at collider experiments:
  - Use simulations of the occurring processes via Monte Carlo (MC) event generators
- However, MC based simulations are computationally **costly**
  - Dominated by *calorimeter* simulations (energy measurements)
  - Becoming more complex due to highly granular calorimeters
  - Hence potential bottleneck for future experiments



Training Data

- Simulate chains of particles, so-called *showers,* initiated by incoming primary particles.
- Consider two different types of particles:
  - Photons (1 million training examples) – incident on the electromagnetic calorimeter
  - Charged pions (0.5 million training examples) – incident on the hadronic calorimeter



Cell Layout: 30 x 30 x 30 (Photon showers)

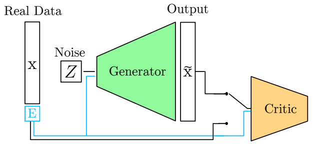
Cell Layout: 48 x 13 x 13 (Pion showers)

Generative Models

We train and evaluate three generative models in this study: Generative Adversarial Network (GAN), GAN optimizing a Wasserstein loss (WGAN), and Bounded-Information Botteleneck Autoencoders (BIB-AE)

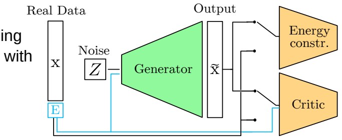
GAN

- First generative architecture used for simulating showers in particle physics
- Apply mini-batch discrimination
- Trained and evaluated on photon showers



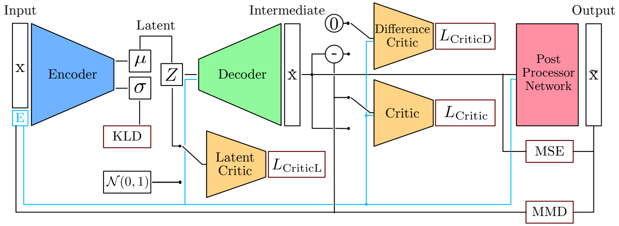
WGAN

- Alternative to classical GAN training:
  - Helps improve the stability of the training
  - Use Wasserstein-1 distance as a loss with gradient penalty
- Second network to constrain energy
- Latent optimization method (LO) [1] is employed for pion showers



BIB-AE and Post-Processor

- Unifies features of GANs and Autoencoders [2]
- WGAN-like critics evaluate the quality of reconstructed images
- Latent regularization is improved by an additional critic and a Maximum Mean Discrepancy (MMD) term
- Additional Post-Processor network [3], trained in a second step, is used to improved per-pixel energies
- Sampling from encoded latent space via multi-dimensional Kernel Density Estimation (KDE) [4]



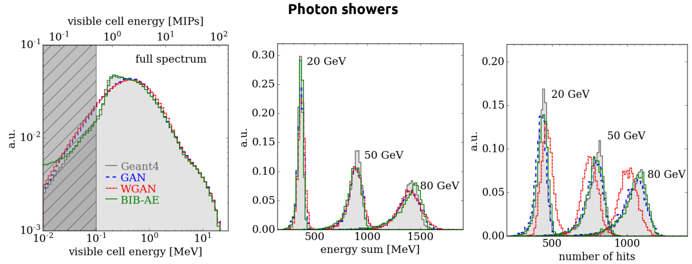
$$L_{\mathrm{BIB-AE}} = \mathrm{KLD} + L_{\mathrm{CriticL}} + L_{\mathrm{Critic}} + L_{\mathrm{CriticD}}$$

$$L_{\mathrm{Post}} = \mathrm{MMD} + \mathrm{MSE}$$

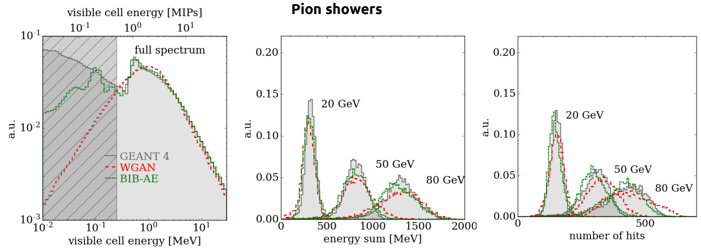
Results

- Differential distributions of physics quantities between ground truth (GEANT4) and the different generative models
  - The energy contained in a single pixel (visible cell energy)
  - Total energy sum over all pixels in a shower
  - The number of non-zero pixels (number of hits)
  - First to achieve this level of precision in differential distributions for high-resolution detector

Photon showers



Pion showers



Computational Performance

Our major goal is to speed-up the sampling process:
- We observe speed-ups of up to three orders of magnitude

Hardware	Simulator	Photons time/shower [ms]	Photons speed-up	Pions time/shower [ms]	Pions speed-up
CPU	GEANT4	4082 ± 170	×1	2684 ± 125	×1
	WGAN	61.44 ± 0.03	×66	195.67 ± 0.56	×14
	BIB-AE	95.98 ± 0.08	×43	36.05 ± 0.82	×74
GPU	WGAN	3.93 ± 0.03	×1039	2.695 ± 0.004	×996
	BIB-AE	1.60 ± 0.03	×2551	1.101 ± 0.004	×2438

References

[1] arXiv:1905.06723
[2] arXiv:1912.00830
[3] arXiv:2005.05334
[4] arXiv:2102.12491

GitHub