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Generative Models for Fast Simulation of Electromagnetic and Hadronic Showers in Highly Granular Calorimeters

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While simulation is a crucial cornerstone of modern high energy physics, it places a heavy burden on the available computing resources. These computing pressures are expected to become a major bottleneck for the upcoming high luminosity phase of the LHC and for future colliders, motivating a concerted effort to develop computationally efficient solutions. Methods based on generative machine learning models hold promise to alleviate the computational strain produced by simulation, while providing the physical accuracy required of a surrogate simulator.

This contribution provides an overview of a growing body of work focused on simulating showers in highly granular calorimeters, which is making significant strides towards realising fast simulation tools based on deep generative models. Progress on the simulation of both electromagnetic and hadronic showers will be reported, with a focus on the high degree of physical fidelity achieved. Additional steps taken to address the challenges faced when broadening the scope of these simulators, such as those posed by multi-parameter conditioning, will also be discussed.

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1. Introduction

The ability to precisely simulate particle interactions with complex detector systems lies at the heart of analysis in high energy physics. Traditionally, simulation toolkits such as Geant4 [1] have relied on the use of Monte-Carlo methods. While such methods can produce high quality simulators they are slow, with the strain they place on the available computing resources expected to become prohibitive for upcoming experiments [2]. Initiated by Ref. [3], a path to potentially speed up the simulation of calorimeter showers through the use of generative models, typically the most intensive part of a detector simulation, is emerging.

In this work, we address the simulation of particle showers in highly granular calorimeters with surrogate simulators based on generative models. Building on initial work that developed several models with the ability to provide a good description of several key differential distributions for photon showers [4] [5], we report on progress in two important directions. In the first instance, we review recent work which demonstrated high fidelity simulation of hadron showers in a highly granularity calorimeter, based on Ref. [6]. In the second instance, we show progress on the ability to condition these simulation tools on multiple parameters- a crucial step towards being able to simulate an entire calorimeter subsystem.

2. Datasets

Our studies focus on the International Large Detector (ILD) [7], a next generation particle detector proposed for the International Linear Collider (ILC). The detector features highly granular sampling calorimeters optimized for particle flow reconstruction. The Si-W electromagnetic calorimeter (ECAL) consists of 30 active silicon layers in a tungsten absorber stack, with the silicon layers featuring sensors of size 5×5 mm^2. To create the dataset described in Section 5, cells containing energy deposits were projected into a regular grid containing $x \times y \times z = 30 \times 60 \times 30$ cells with each cell in the shower image corresponding to exactly one sensor. Photons were fired into a fixed point on the face of the ECAL barrel with energy varying uniformly in the range $10 - 100$ Gev simultaneously with the polar angle, which was varied uniformly in the range $30 - 90$ degrees with constant azimuthal angle. In total, 500k such showers were used to create the training dataset. Additionally, 9 test datasets, each consisting of 1900 showers produced by photons at fixed combinations of incident energies of {20, 50, 90} GeV and polar angles of {40, 60, 85} degrees, were created to check the model performance across the phase space.

The Analogue Hadronic Calorimeter (AHCAL) of the ILD consists of 48 layers, with active scintillator tiles of size 3×3 cm^2 individually read out by Silicon Photomultipliers (SiPMs), in a stack of stainless steel absorber plates. To create the dataset described in Section 4, the ECAL was removed from the geometry and a 3.5 T axial magnetic field applied. The sensors were projected into a regular grid, consisting of $x \times y \times z = 25 \times 25 \times 48$ cells. Charged pions (π^+) were fired under an approximately constant angle into an almost constant position on the calorimeter face. The energy of the incident pions was varied uniformly in the range $10 - 100$ GeV, with punch-through particles which traversed the calorimeter without showering being removed. The data set was split into 500k showers used for training, and 49k for a test set. Additionally, single energy samples of 8k showers were produced for incident particle energies in 10 GeV steps between 20 and 90 GeV.

Both datasets were simulated using GEANT4 [1] vesion 10.4 with the QGSP_BERT physics list, as well as a detailed and realistic detector model of ILD implemented in DD4HEP [8].

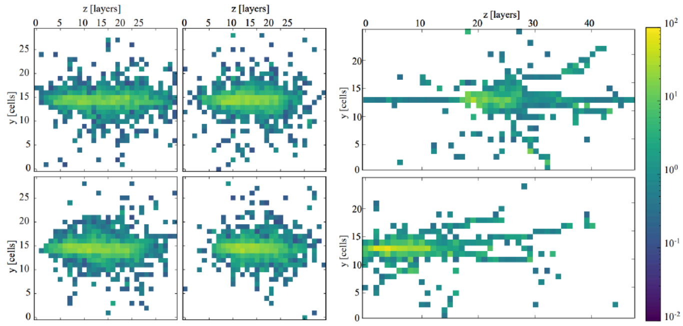

Figure 1: Left: four example 2D projections of photon showers. Right: two examples of pion showers. On average the pion showers exhibit significantly more varied topologies. Figure taken from [6].

Figure 1 shows examples of photon showers (left) compared to pion showers (right), created by incident particles at the same energy. Pion showers can be seen to display much larger event-to-event fluctuations and significantly more complex topologies. In both cases, the high granularity of the calorimeters pose significant challenges for a generative model based simulator.

3. Generative Models

Generative models aim to learn the underlying distribution of a given set of training data, in a manner that permits later sampling and thereby the generation of new data samples. All models considered here were built in PYTORCH [9].

The first generative model considered in these studies is a rather lightweight Wasserstein Generative Adversarial Network (WGAN) [10]. It uses the Wasserstein-1 distance as a loss function, which can be expressed as

$$\mathcal{L}_{WGAN} = \sup_{f \in \mathrm{Lip}_1} \{\mathbb{E}[f(x)] - \mathbb{E}[f(\tilde{x})]\}. \tag{1}$$

The supremum runs over all 1-Lipschitz functions f, and is approximated by a Critic network C during the adversarial training, which estimates the Wasserstein distance between real and generated images. A constrainer network [11] is incorporated into the architecture to aid the performance of the energy conditioning in the setup.

The second generative model is a significantly more complicated Bounded Information Bottleneck Autoencoder (BIB-AE), first proposed in [12], that unifies features present in many popular GAN and VAE architectures. At its core, it is an autoencoder which maps shower images to a lower dimensional latent space and back. A number of secondary components aid either the regularisation of the latent space, or the reconstruction of images from the latent space. To ensure regularisation of the latent space, a Kullback-Leibler divergence ($\mathcal{L}_{KLD}$) term is combined with a Maximum Mean Discrepancy ($\mathcal{L}_{MMD}$) term and a Wasserstein GAN-like critic ($\mathcal{L}_{Critic_L}$). A separate dual purpose Wasserstein GAN-like critic ($\mathcal{L}_{Critic}$) simultaneously judges whether showers look realistic and facilitates reconstruction from the latent space. The individual loss terms are then combined with independent weights from hyperparameters β_i

$$\mathcal{L}_{BIBA-AE} = \beta_{KLD} \cdot \mathcal{L}_{KLD} + \beta_{MMD} \cdot \mathcal{L}_{MMD} + \beta_{Critic_L} \cdot \mathcal{L}_{Critic_L} + \beta_{Critic} \cdot \mathcal{L}_{Critic}. \tag{2}$$

After the training of the main architecture, a dedicated post-processor network is trained with the intention of improving the cell energy spectrum, as well as refining the energy conditioning. This stage of the training primarily relies on a number of loss terms using either a Mean Squared Error (MSE) or Sorted Kernel Maximum Mean Discrepancy ($SK - MMD$) [4]. Further details on the architectures and their specific implementations can be found in Ref. [6].

4. Hadron Shower Simulation

Ref. [6] studied the ability of the BIB-AE and WGAN models described in Section 3 to reproduce statistical distributions of physically relevant observables at the simulation level, as well as performing an initial investigation into performance after interfacing with a state-of-the-art Particle Flow reconstruction algorithm. Here, we highlight some salient distributions at the simulation level, refering the reader to that work for a thorough treatment and discussion of performance after reconstruction.

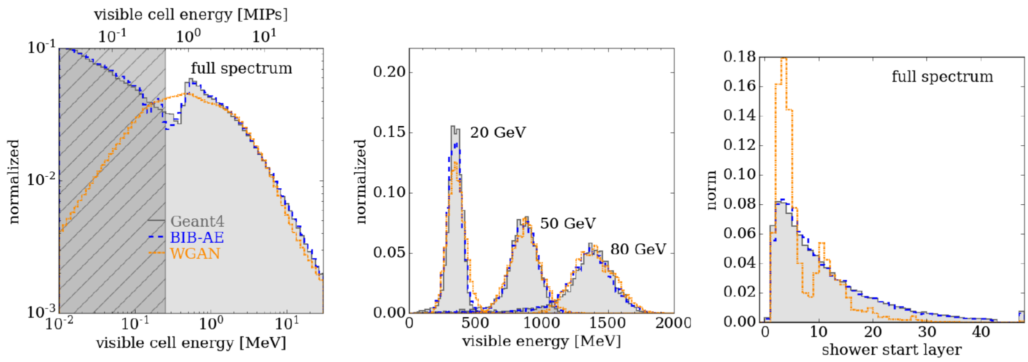

Figure 2: Exemplary distributions comparing physics quantities between GEANT4 and the different generative models for charged pion showers. Left: Cell energy spectrum in MeV on the bottom axis, and in multiples of the expected energy deposit of a minimum ionizing particle (MIP) on the top axis. The greyed out area indicates the 0.5 MIP cutoff. Middle: the total visible energy deposited in the calorimeter. Right: the layer in which showers start. The left and right plots are for showers generated with uniform energies in the 10-100 GeV range. Plots from Ref. [6].

Some key results from the study can be seen in Figure 2. The GEANT4 distributions are shown in the grey, filled distributions, while the generative model results are shown by the dashed lines- the BIB-AE in blue, and the WGAN in orange. Cells with an energy of less than half the most probable energy deposition of a minimal ionizing particle (MIP), which is 0.25 MeV for this calorimeter, are mapped to zero. This region lies below the noise floor of a typical detector, indicated by the hatched region of the cell energy distribution shown in the left plot. The key feature in this distribution is the distinct peak that occurs at 1 MIP. This feature is well described by the BIB-AE architecture, but is not captured by the WGAN, inline with previous work [4]. The central distribution shows the total visible energy deposited in the calorimeter, which is well described by both the BIB-AE and the WGAN. The rightmost plot shows the distribution of the layers in which showers start, which the BIB-AE is able to reproduce well in contrast to the WGAN, which produces a significant excess of early starting showers. The models reached a relative speed-up of up to 3-4 orders of magnitude [6].

5. Multi-parameter Conditioning for Photon Shower Simulation

In ongoing work, the BIB-AE model described in Section 3 has been adapted to permit conditioning of the model on the incident angle of photons as well as their energy. The main challenge for the model stems from the significantly expanded phase space that has to be covered, which is created as a result of simultaneously varying the two conditioning parameters. To benchmark the physics performance of the model, showers are generated with the fixed energy and angle combinations spread across the phase space described in Section 2. Exemplary distributions are shown in Figure 3. The GEANT4 distributions are again shown in the filled distributions, while the BIB-AE distributions are shown with a dashed line. The distributions are colour coded according to the incident angle to which they pertain- 40 degree showers in orange, 60 degree showers in green and 85 degree showers in blue. A cut at half a MIP is again applied, which in this case lies at 0.1 MeV. The leftmost plot and the central plot show distributions that are strongly correlated with the incident angle and energy of the incident photon, and therefore provide a strong indication of the conditional performance of the model. The reconstructed angular response for 20 GeV photons in the left plot is found from a principal component analysis applied to the shower, while in the central plot the visible energy response for 40 degree showers is shown for incident energies of 20, 50 and 90 GeV. The good agreement between generated showers and the corresponding GEANT4 distributions indicates a strong performance from the model in terms of angular and energy conditioning. The rightmost plot shows the cell energy distribution for 90 GeV, 60 degree photons, with the region below half a MIP again lying in the grey hatched region. The rise in the cell energy distribution that is now somewhat smeared by the incident angle is still well described by the model, indicating that the post-processor network can be conditioned on multiple parameters and still provide a good description of this distribution.

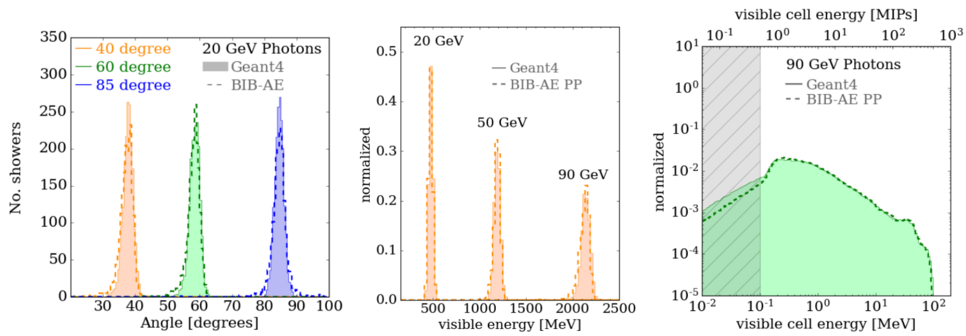

Figure 3: Exemplary distributions comparing physics quantities between GEANT4 and BIB-AE for angled photons. Left: angular response for 20 GeV photons. Middle: total visible energy deposited in the calorimeter for 40 degree photons. Right: cell energy spectrum for 90 GeV, 60 degree photons.

6. Conclusions

Generative models are promising options for producing significantly faster simulation tools. We have demonstrated that these models possess the capability to simulate hadron showers in highly granular calorimeters, as well as generalising to multi-parameter conditioning setups. Although significant progress has been made, there is still some way to go for a full realisation of such tools- including integration into existing frameworks and tackling complex and irregular detector geometries.

Acknowledgments

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References

[1] S. Agostinelli et al., *Geant4—a simulation toolkit*, *Nucl. Instrum. Meth. A* **506** (2003) 250 .

[2] HEP Software Foundation collaboration, *A Roadmap for HEP Software and Computing R&D for the 2020s*, *Comput. Softw. Big Sci.* **3** (2019) 7 [1712.06982].

[3] M. Paganini, L. de Oliveira and B. Nachman, *Accelerating Science with Generative Adversarial Networks: An Application to 3D Particle Showers in Multilayer Calorimeters*, *Phys. Rev. Lett.* **120** (2018) 042003 [1705.02355].

[4] E. Buhmann et al., *Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed*, *Comput. Softw. Big Sci.* **5** (2021) 13 [2005.05334].

[5] E. Buhmann et al., *Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network*, *EPJ Web Conf.* **251** (2021) 03003 [2102.12491].

[6] E. Buhmann et al., *Hadrons, Better, Faster, Stronger*, *Mach. Learn. Sci. Tech.* **3** (2022) 025014 [2112.09709].

[7] ILD collaboration, *International Large Detector: Interim Design Report*, 2003.01116.

[8] M. Frank, F. Gaede, C. Grefe and P. Mato, *DD4hep: A Detector Description Toolkit for High Energy Physics Experiments*, *J. Phys. Conf. Ser.* **513** (2014) 022010.

[9] A. Paszke et al., *PyTorch: An Imperative Style, High-Performance Deep Learning Library*, *Adv. Neural Inf. Process. Syst. 32* (2019) 8024 [1912.01703].

[10] M. Arjovsky, S. Chintala and L. Bottou, *Wasserstein GAN*, 1701.07875.

[11] M. Erdmann, J. Glombitza and T. Quast, *Precise simulation of electromagnetic calorimeter showers using a Wasserstein Generative Adversarial Network*, *Comput. Softw. Big Sci.* **3** (2019) 4 [1807.01954].

[12] S. Voloshynovskiy, M. Kondah, S. Rezaeifar, O. Taran, T. Holotyak and D.J. Rezende, *Information bottleneck through variational glasses*, 1912.00830.