Advancing Generative Modelling of Calorimeter Showers on Three Frontiers

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Abstract

Generative machine learning can be used to augment and speed-up traditional physics simulations, i.e. the simulation of elementary particles in the detector of collider experiments. Like many physics data, these calorimeter showers can either be represented as images or as permutation-invariant lists of measurements, i.e. as point clouds. We advance the generative models for calorimeter showers on three frontiers: (1) increasing the number of conditional features for precise energy- and angle-wise generation with the bounded bottleneck auto-encoder (BIB-AE), (2) improving generation fidelity using a normalizing flow model, dubbed "Layer-to-Layer-Flows" (L2LFLOWS), (3) developing a diffusion model for geometry-independent calorimeter point cloud scalable to $\mathcal{O}(1000)$ points, called CALOCLOUDS, and distilling it into a consistency model for fast single-shot sampling.

1 Introduction

Accurate simulations of physics processes are a crucial way to compare theoretical predictions with experimental results. In high-energy physics (HEP) current and future collider experiments are taking data at ever increasing rates [1, 2], while the computing budget for simulations is projected to stagnate [3, 4]. Generative machine learning can be utilized to augment and speed-up traditional physics simulations with a surrogate model leveraging recent advances in generative modelling and GPU acceleration. In various other physical sciences, such generative models are also used for e.g. generating astrophysical fields [5], molecular docking in drug design [6], and simulating inertial confinement fusion [7].

In high-energy physics considerable efforts are undertaken to develop generative models for detector simulations, such as the sensor responses to incident particles in calorimeters. These incident particles deposit energy in the calorimeter and create secondary particles leading to a measured event dubbed a calorimeter shower. Various generative modelling techniques are being explore to simulate these showers, including generative adversarial networks (GANs) [8–19], autoencoders [20–25],

Machine Learning and the Physical Sciences Workshop, NeurIPS 2023.

normalizing flows [26–33], and diffusion models [34–39]. The models are conditional generative models allowing for the targeted sampling of e.g. a specific particle energy.

The read-out sensors in calorimeters are often aligned on a (close-to) 3d grid allowing the data to be represented as 3d images with the pixel value corresponding to the measured energy. Virtually all previously used generative models used this structured image representation. However, for many events, only a small fraction of the sensors record an energy deposition, leaving many pixels empty. Such sparse images can be more efficiently represented as a point cloud with the 3d position and the energy as features. Some very recent models explore this more efficient point cloud representation to generate calorimeter showers [29, 35, 36, 39].

In our case-studies, we generate photon showers in the highly-granular eletromagnetic calorimeter (ECAL) with 30 active layers of the envisioned International Large Detector (ILD) [40]. The training datasets are simulated with GEANT4 [41], the baseline for all our comparisons. Here, we give an overview of our most recent research in advancing generative models on three major frontiers: In Sec. 2 we explore an autoencoder conditioned on multiple shower observables allowing for a more targeted sampling, in Sec. 3 we outline a flow-based generative model achieving state-of-the-art generative fidelity, and in Sec 4 we describe our diffusion-based model for large geometry-independent calorimeter point cloud generation.

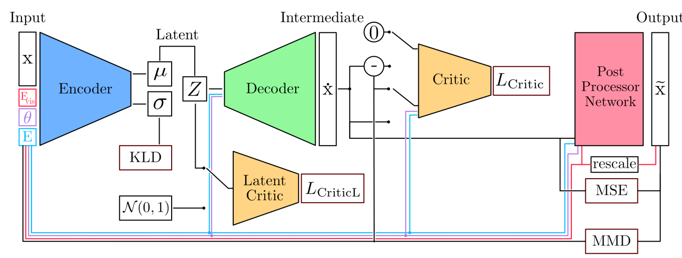

Figure 1: Overview of the BIB-AE architecture during training, including each network and its corresponding loss terms. The red, blue and lilac lines represent an input conditioning on visible energy, the incident energy, and angle of the incident particle, repectively. Figure taken from Ref. [25].

2 Conditional Flexibility: BIB-AE

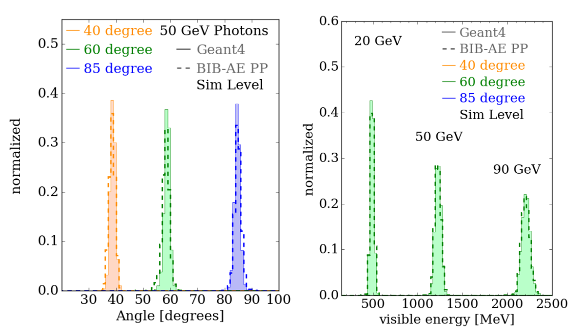

Figure 2: Left: Angular response for both GEANT4 (filled histograms), and BIB-AE generated photon showers (dashed, unfilled histograms) for 50 GeV photons and variable angles. Right: Total visible energy for 60 degree showers at various incident energies. Figures taken from Ref. [25]

The bounded information bottleneck autoencoder (BIB-AE) has previously been used to generate high fidelity photon and charged pion showers [20–22]. The BIB-AE model combines multiple submodels including a variational autoencoder (VAE) [42], two Wasserstein-GAN critics [43, 44], and a post-processor network. The sub-models consist of fully connected and convolution neural network (CNN) layers. While past iterations of the BIB-AE were only conditioned on the particle incident energy and the data used had a fixed incident angle, we expand the conditioning regime to also include a variable angle in the $y - z$ plane as well as the visible energy. To train on various energies and angles, the training dataset was created with a uniform energy distribution between 10 and 100 GeV and an angular distribution between 90 and 30 degrees. We consider a small section of the ECAL and represent the shower as a $30 \times 60 \times 30$ image. A model schema is shown in Fig. 1.

In Fig. 2 we compare the generative performance of the BIB-AE to the GEANT4 simulation. In the left figure, we sample single energy photon showers at exactly 50 GeV for the specific angles 40,

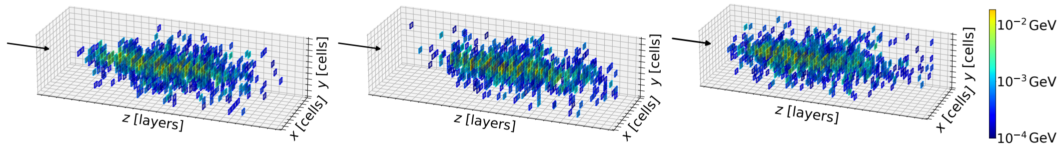

Figure 3: BIB-AE–generated shower (left), GEANT4 test shower (middle) and L2LFLOWS-generated shower (right). The black arrow indicate the fixed incident angle of the incoming photon. Figures taken from Ref. [31].

60, and 85 degrees. We show the distribution of the shower angle defined by the principle axis of a principle component analysis (PCA). In the right figure, we fix the angle at 60 degrees and sample for the energies 20, 50, and 90 GeV and show the visible energy (the sum of all pixels over a certain threshold). We see that for all fixed angle and energy combinations, the generated showers agree well with GEANT4. A more detailed analysis of the physics performance can be found in Ref. [25]. We conclude that the BIB-AE model is able to produce high fidelity conditional samples. Further conditioning, i.e. on the $x - z$ angle, is under investigation.

3 Generative Fidelity: L2LFlows

Normalizing flows (NFs) are achieving state-of-the-art generative fidelity on low- and high-granular calorimeter showers [26–33]. We have advanced the previously introduced CaloFlow model [27, 28, 30] — originally introduced for a three layer calorimeter — and applied it to higher granular photon showers represented as $30 \times 10 \times 10$ voxelized images. For these photon showers a uniform incident energy distribution, but fixed angle is used. This "Layer-to-Layer-Flows" (L2LFLOWS) model uses a two-step strategy for shower generation: First, we use a lightweight NF to generated the total visible energy in each calorimeter layer. Second, 30 separate NFs are trained with each NF generating the shower response in one specific layer. Each of these NFs is conditioned on the voxel energies and the total energies of the preceding five layers — with an intermediate embedding network to reduce the conditioning dimensionality. This split into 30 NFs is done to keep the memory consumption of L2LFLOWS in check since the masked autoregressive flows (MAFs) [45] used compute the Jacobian determinant efficiently, but scale with the input dimensionality. Overall L2LFLOWS is conditioned on the incident particle energy.

We compare the L2LFLOWS generated showers to BIB-AE generated showers and the GEANT4 "truth". Fig. 3 shows a 3d image visualisation of single 50 GeV showers. Empty voxels are the result of a low energy cut at 10^{-4} GeV since below this threshold the sensor response is indistinguishable from noise. Both generated showers align visually with the GEANT4 shower. Figure 4 shows the voxel energy distibution for the full 10-100 GeV incident energy spectrum (left) and for single energy showers the number of non-zero voxels (hits above the threshold) (right). Overall both models agree well with GEANT4, but L2LFLOWS achieves higher generative fidelity than the BIB-AE. Further details can be found in Ref. [31].

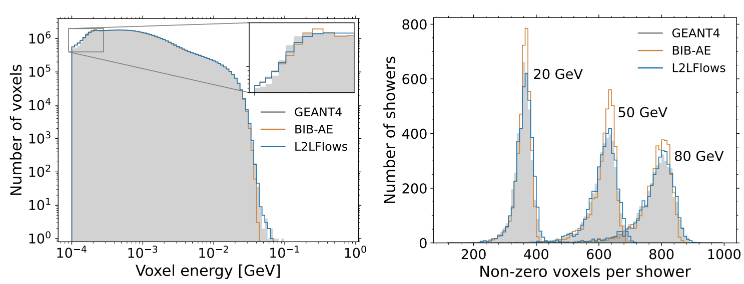

Figure 4: Left: Distribution of voxel energies with shower incident energies uniformly distributed between 10 and 100 GeV. Right: Number of voxels above threshold for single energy 20, 50, and 80 GeV photons. Figures taken from Ref. [31].

4 Scalability & Speed: CaloClouds

CaloClouds [35] is the first model introduced for calorimeter showers as high-cardinality point clouds with $\mathcal{O}(1000)$ points. It consists of multiple sub-models, including two NFs (one for conditioning and calibrating shower observables, one for the latent space), an encoder (based on equivariant point cloud (EPIC) layers [46]), and a diffusion model based on Refs. [47, 48] using 100 denosing steps. We further introduce the enhanced CaloClouds II model [39], which drops the latent NF and encoder and implements the advanced diffusion regime of Ref. [49], allowing for sampling with 25 model passes. Finally, we distill this model into CaloClouds II (CM), a consistency model (CM) [50] allowing for single shot generation without loss in fidelity. The diffusion model architecture uses weight sharing among all points, hence it samples all points independently and identically distributed (i.i.d.) with respect to the global conditioning. Due to the computational efficiency of CaloClouds and the linear scaling of the computing cost with the point cloud size, the models can be applied to point clouds with a higher granularity than the actual physical sensors. This way, the models become largely cell geometry-independent, and showers can be projected into any part of the detector (except changing its depth) with minimal artifacts. We generated such a dataset with Geant4 using photon showers with energies between 10 and 90 GeV. The dataset contains point clouds with up to 6,000 points per shower — noticeably higher than the number of cell hits ($< 1,500$).

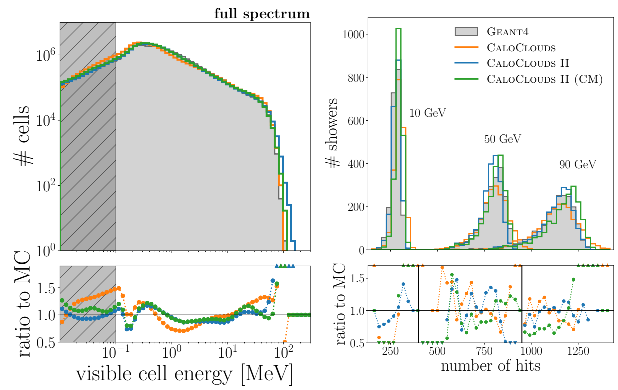

Figure 5: Left: Histogram of the cell energies. Right: Number of hits distributions for single energies at 10, 50, and 90 GeV. The bottom panel provides the ratio to Geant4. Figures taken from Ref. [39].

We compare the generative fidelity of the CaloClouds variants to Geant4 with various cell-level and shower-level observables after projecting the point cloud to the real ILD ECAL geometry with 30 layers each containing 30×30 cells. Fig. 5 shows the cell energy distribution for the full energy spectrum and the number of hits (non-zero cells) for single energy showers. Overall, both CaloClouds II models improve upon CaloClouds and reach a high fidelity compared to Geant4.

Table 1: Comparison of the computational performance of CaloClouds, CaloClouds II, and CaloClouds II (CM) to the baseline Geant4 simulator on a single CPU core. The number of function evaluations (NFE) indicate the number of diffusion model passes. Table adapted from Ref. [39].

Simulator	NFE	Time / Shower [ms]	Speed-up
Geant4		3914.80 ± 74.09	$\times 1$
CaloClouds	100	3146.71 ± 31.66	$\times 1.2$
CaloClouds II	25	651.68 ± 4.21	$\times 6.0$
CaloClouds II (CM)	1	84.35 ± 0.22	$\times 46$

In Tab. 1 we benchmark the speed-up of the CaloClouds models over the Geant4 simulation. For a fair comparison the performance is compared on the same single CPU core, as Geant4 does not support GPUs, and CPUs are cheaper and more widely available. Using consistency distillation, the CaloClouds II (CM) model is able to generate photon showers $46\times$ faster than Geant4. A comparison to the BIB-AE and L2LFlows models is not performed as the data structures are too different to allow for a fair comparison. More details on the CaloClouds models can be found in Refs. [35, 39].

5 Conclusion

We have shown recent advances on three different frontiers in the generative modelling of calorimeter showers. Eventually we envision a model that combines all three: flexible conditional sampling, high fidelity, and computational efficiency. For the already established models, further fidelity and timing studies with common benchmark metrics datasets with the same dimensionalities should be performed. A valuable comparison is currently undertaken in form of the *Fast Calorimeter Challenge* [51]. Beyond photon showers, we plan to explore the generative modelling of hadronic showers, which are more challenging to model due to their more complex shower topology. For CALOCLOUDS this will likely necessitate a more complex model architecture taking inter-point correlations during sampling into account, e.g. by using linearly scalable EPiC layers [46] introduced for particle jet modelling. Finally, ongoing efforts are made to include the generative models as a drop-in replacement for parts the full GEANT4 simulation pipeline.

Acknowledgments and Disclosure of Funding

We are thankful for the support of the Deutsche Forschungsgemeinschaft under Germany's Excellence Strategy — EXC 2121 Quantum Universe — 390833306 making the in-person presentation at the NeurIPS 2023 ML4PS workshop possible.

This research was supported in part through the Maxwell computational resources operated at Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany. This project has received funding from the European Union's Horizon 2020 Research and Innovation programme under Grant Agreement No 101004761. We acknowledge support via the KISS consortium (05D23GU4, 13D22CH5) funded by the German Federal Ministry of Education and Research BMBF in the ErUM-Data action plan. EB is partially funded by a scholarship from the Friedrich Naumann Foundation for Freedom. The work of CK and DS was supported by DOE grant DOE-SC0010008. CK would like to thank the Baden-Württemberg-Stiftung for support through the program *Internationale Spitzenforschung*, project *Uncertainties — Teaching AI its Limits* (BWST_IF2020-010). AK has received support from the Helmholtz Initiative and Networking Fund's initiative for refugees as a refugee of the war in Ukraine.

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