ZDC Simulation with ML

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2025/2/10

* Date: Feb 10 (Monday), 2025

* Time: 11:00-12:00 AM at Taiwan (GMT+8)

* Zoom link:

https://cern.zoom.us/j/66342263280?pwd=DBemHUOnO6QIiQyU5y2WbeaEaBGcyT.1

CaloChallenge 2022: A Community Challenge for Fast Calorimeter Simulation
https://arxiv.org/abs/2410.21611

Table 1: Models submitted to the CaloChallange.

Approach	Model	Code	Dataset $1-\gamma$	Dataset $1-\pi$	Dataset 2	Dataset 3	Section
GAN	`CaloShowerGAN` [21]	[22]	✓	✓			3.1
	`MDMA` [23, 24]	[25]			✓	✓	3.2
	`BoloGAN` [26]	[27]	✓	✓			3.3
	`DeepTree` [28, 29]	[30]			✓		3.4
NF	`L2LFlows` [31, 32]	[33]			✓	✓	4.1
	`CaloFlow` [34, 35]	[36, 37]	✓	✓	✓	✓	4.2
	`CaloINN` [38]	[39]	✓	✓	✓		4.3
	`SuperCalo` [40]	[41]			✓		4.4
	`CaloPointFlow` [42]	[43]			✓	✓	4.5
Diffusion	`CaloDiffusion` [44]	[45]	✓	✓	✓	✓	5.1
	`CaloClouds` [46, 47]	[48, 49]				✓	5.2
	`CaloScore` [50, 51]	[52, 53]	✓		✓	✓	5.3
	`CaloGraph` [54]	[55]	✓	✓			5.4
	`CaloDiT` [56]	[57]			✓		5.5
VAE	`Calo-VQ` [58]	[59]	✓	✓	✓	✓	6.1
	`CaloMan` [60]	[61]	✓	✓			6.2
	`DNNCaloSim` [62, 63]	[64]		✓			6.3
	`Geant4-Transformer` [65]	[66]				✓	6.4
	`CaloVAE+INN` [38]	[39]	✓	✓	✓	✓	6.5
	`CaloLatent` [67]	[68]			✓		6.6
CFM	`CaloDREAM` [69]	[70]			✓	✓	7.1
	`CaloForest` [71]	[72]	✓	✓			7.2

Metrics (Sec. 8)

1. High-level Features (Histograms)
2. Pearson Correlation Coefficient (PCC)
3. Classifier-based Metrics
4. Computer Science-inspired Metrics
5. Manifold-based Metrics
6. Generation Timings
7. Memory Requirements

8.4. Computer Science-inspired Metrics

- **Fr´echet Inception distance (FID)**: to extract salient high-level features of real and generated images via the activations of the penultimate layer of a high-performing inception classifier, and then compare them using the Fr´echet, or 2-Wasserstein, distance between Gaussian fits to the two sets of features. This metric has been shown to be highly sensitive to the quality and diversity of generated images and has been extended as well to evaluate jet simulations using the ParticleNet classifier.

8.4. Computer Science-inspired Metrics

- **Fréchet Inception distance (FID)**
- Fréchet physics distance (FPD)
- Kernel physics distance (KPD)
- Kernel Inception distance (KID)

FID from ChatGPT

The **Fréchet Inception Distance (FID)** is a metric used to evaluate the quality of generated images by comparing their statistical similarity to real images. It is commonly used in generative model research, especially for GANs (Generative Adversarial Networks).

How FID Works

FID calculates the distance between feature representations of real and generated images extracted from a deep neural network, typically **Inception-v3**. The steps are:

1. Pass both real and generated images through a pre-trained **Inception-v3** network.
2. Extract features from an intermediate layer.
3. Model the feature distributions as **multivariate Gaussians**.
4. Compute the **Fréchet distance** (a.k.a. Wasserstein-2 distance) between the two Gaussians:

$$\text{FID} = ||\mu_r - \mu_g||^2 + \text{Tr}(\Sigma_r + \Sigma_g - 2(\Sigma_r\Sigma_g)^{1/2})$$

- μ_r, Σ_r → Mean and covariance of real images.
- μ_g, Σ_g → Mean and covariance of generated images.
- **Tr** → Trace of a matrix.

Why is FID Important?

- **Lower FID** indicates better quality and diversity of generated images.
- **More robust** than Inception Score (IS) as it captures both the quality and variety.
- **Sensitive to mode collapse** (where a generator produces limited variations).

Computer Science-inspired Metrics

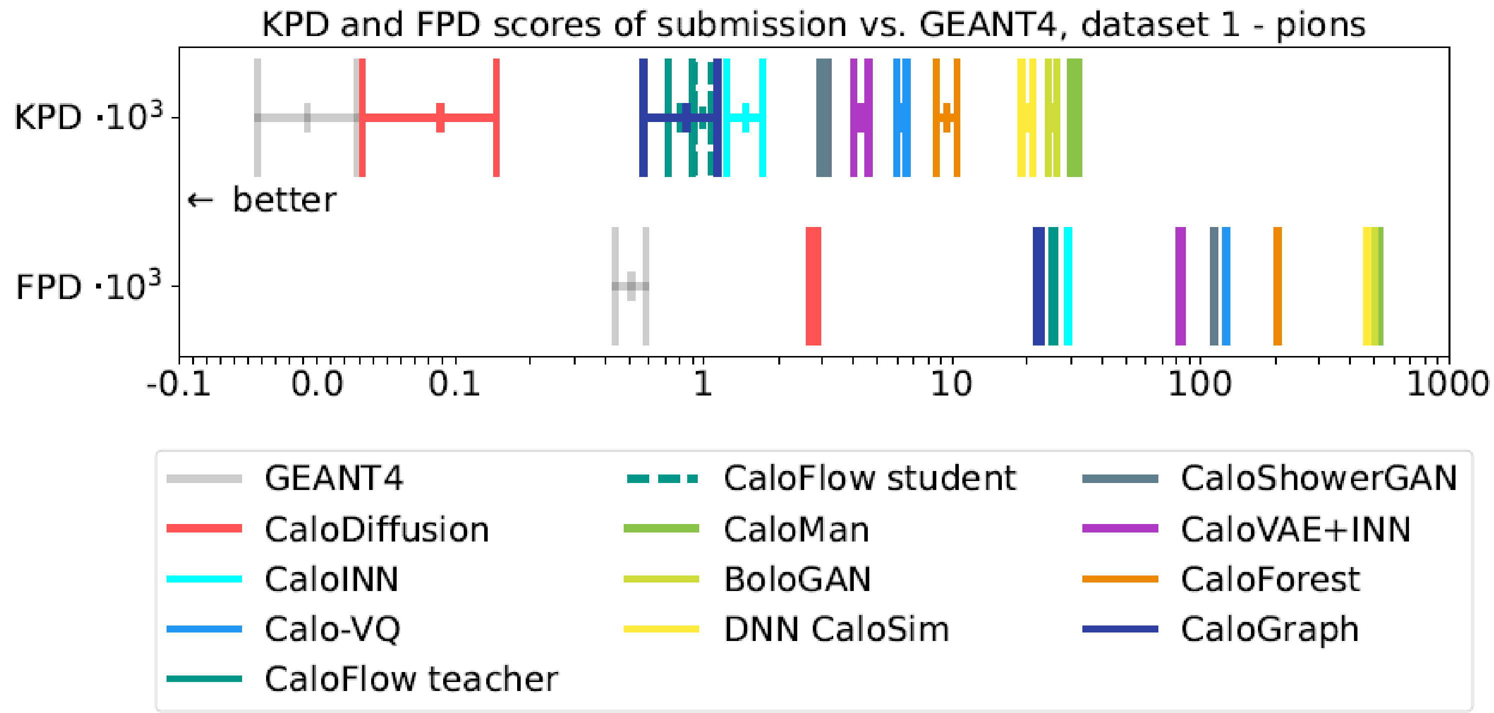

Figure 53: KPD and FPD for evaluating GEANT4 vs. submission of ds 1 – π^+. For the precise numbers, see Table C9.

8.5. Manifold-based Metrics

Manifold-Based Metrics in Generative Models

Manifold-based metrics are evaluation techniques used in generative models (such as GANs, VAEs, and diffusion models) to assess the quality and diversity of generated samples. These metrics rely on the idea that real data and generated data lie on a **lower-dimensional manifold** in a high-dimensional feature space, rather than being uniformly distributed in the entire space.

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1. What is a Manifold in This Context?

A **manifold** is a lower-dimensional structure embedded in a higher-dimensional space. In image generation, natural images occupy only a small subset of the high-dimensional pixel space. Manifold-based metrics assume that high-quality generated images should closely follow the manifold of real images.

8.5. Manifold-based Metrics

2. Key Manifold-Based Metrics

(a) Precision and Recall for Distributions

- **Precision**: Measures how well the generated samples match the real data manifold (quality).
- **Recall**: Measures how much of the real data manifold is covered by generated samples (diversity).
- These are often computed by estimating local neighborhoods in feature space.

(b) Coverage and Density

- **Coverage**: Measures the fraction of real data points whose local neighborhood contains at least one generated sample.
- **Density**: Measures the average number of generated samples in the local neighborhood of each real sample.
- Useful for understanding both **mode collapse** and **overfitting**.

(c) Geometry Score

- Compares the topological features (e.g., connected components, loops) of real and generated data manifolds using **persistent homology** (a technique from algebraic topology).
- Provides insight into whether generated images truly capture the underlying structure of real images.

Manifold-based Metrics

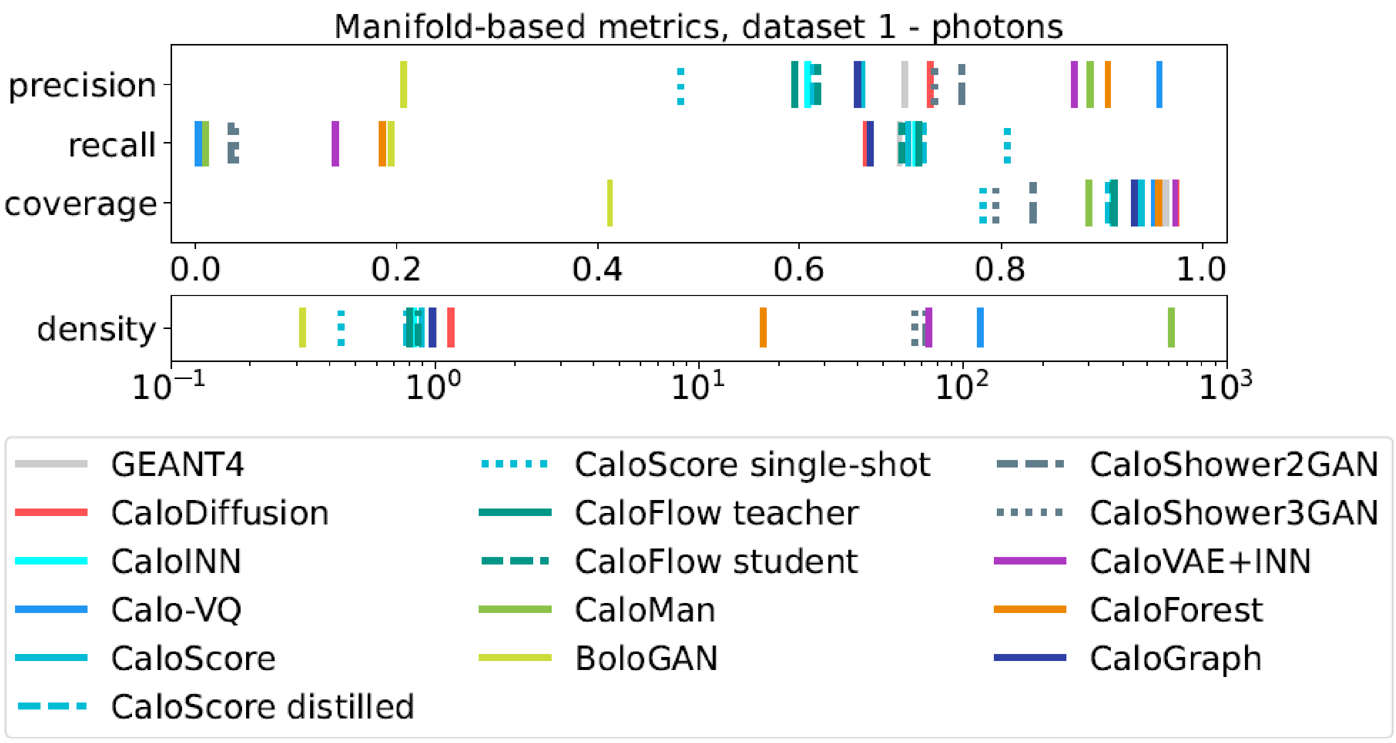

Figure 42: Precision, density, recall, and coverage for ds 1 – γ submissions. For the precise numbers, see Table C4.

8.6. Generation Timings

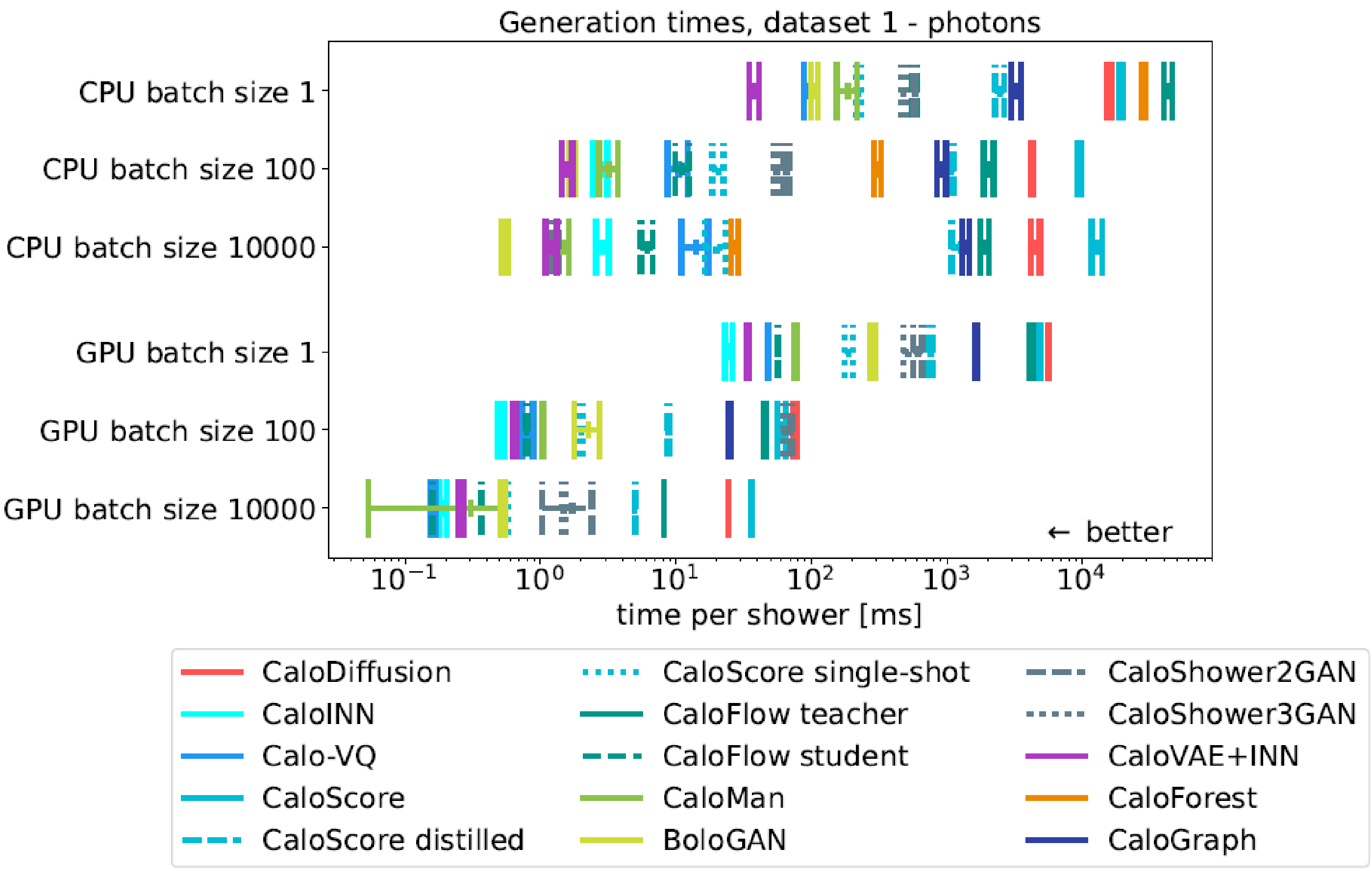

Figure 44: Timing of ds 1 – γ submissions on CPU and GPU architectures. Not all submissions are shown everywhere due to memory and other constraints. More details are in table C6 and table C7.

8.7. Memory Requirements

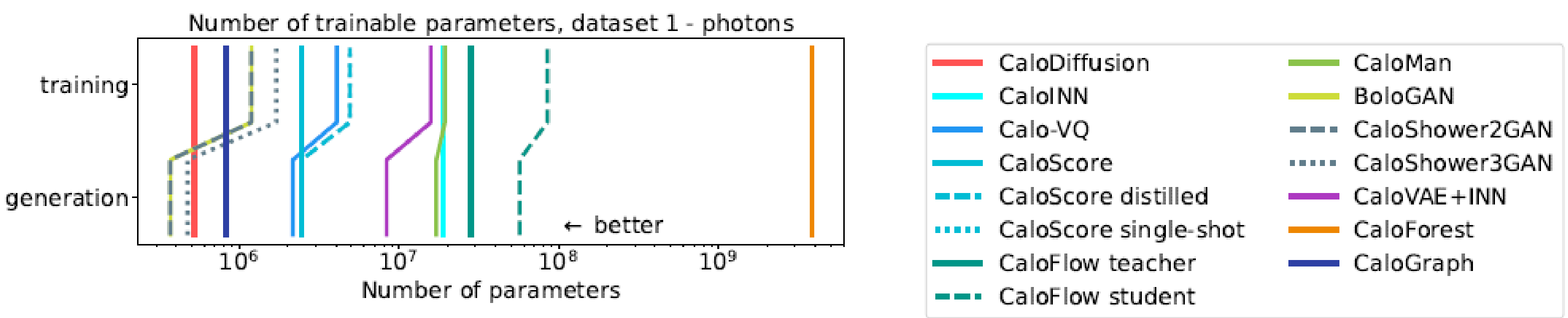

Figure 43: Number of trainable parameters for training and generation of ds $1-\gamma$ submissions. For the precise numbers, see Table C5.