Quantum GAN-Based Fast Calorimeter Simulation

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Outline

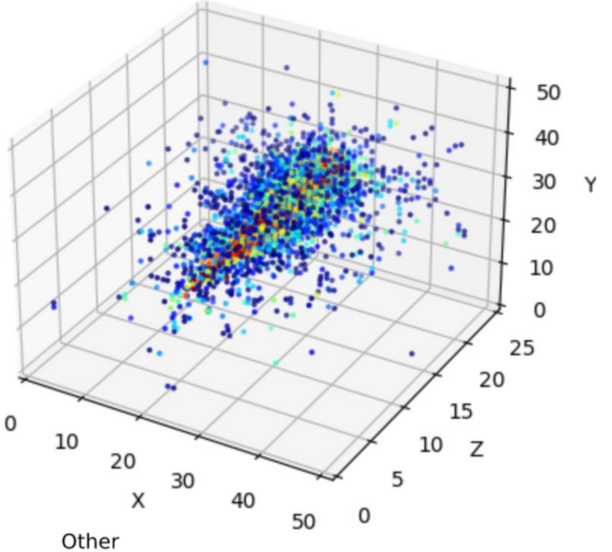
- Motivation
- Quantum GAN
- Methods
- Training Result
- DiT-based fast simulation method
- Summary

Motivation

Calorimeter Simulation

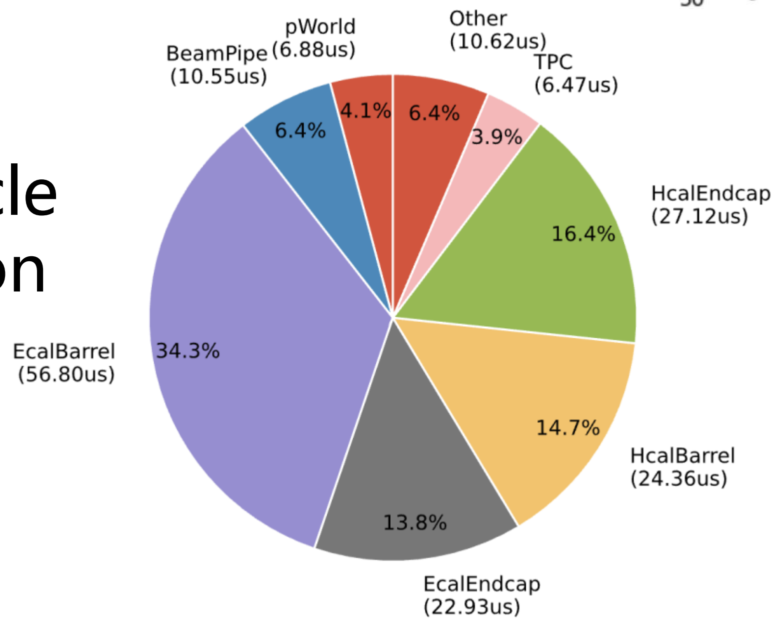
- Modeling of high-energy particles inducing cascade showers and depositing energy in the calorimeter
- Shower spatial distribution & energy deposition pattern

  → particle identification & energy measurement



Geant4: Monte Carlo (MC) Method

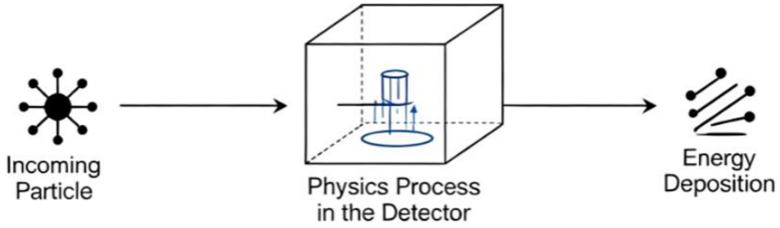
- MC method: step-by-step tracking of particle generation, transport, and energy deposition
- Accurate results, complex geometry
- Enormous computational cost

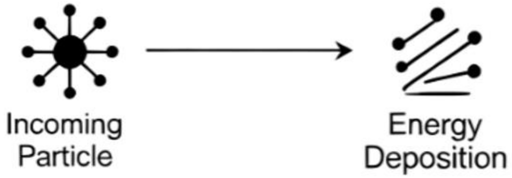


Motivation

❖ Fast Calorimeter Simulation

- Incoming particle → energy deposition
- Methods: Parametric models、GAN、DiT. . .



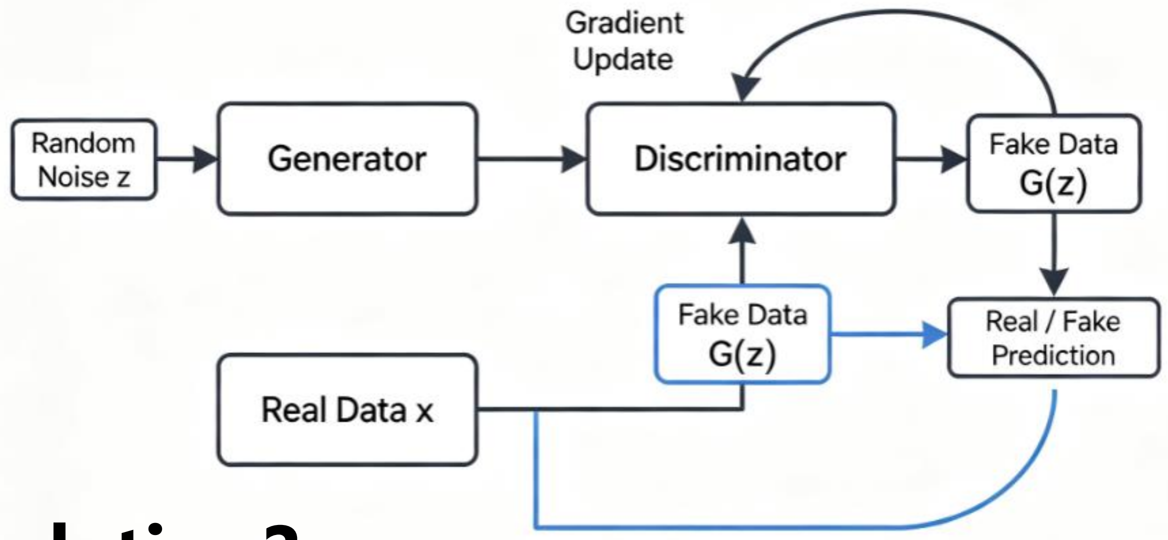


❖ Why Quantum Machine Learning (ML)?

- GANs proven: similar accuracy, orders-of-magnitude speedup
- Quantum ML: superposition & entanglement → exponentially larger representational space
- Can quantum ML match Geant4 fidelity at even lower computational cost?

Quantum GAN

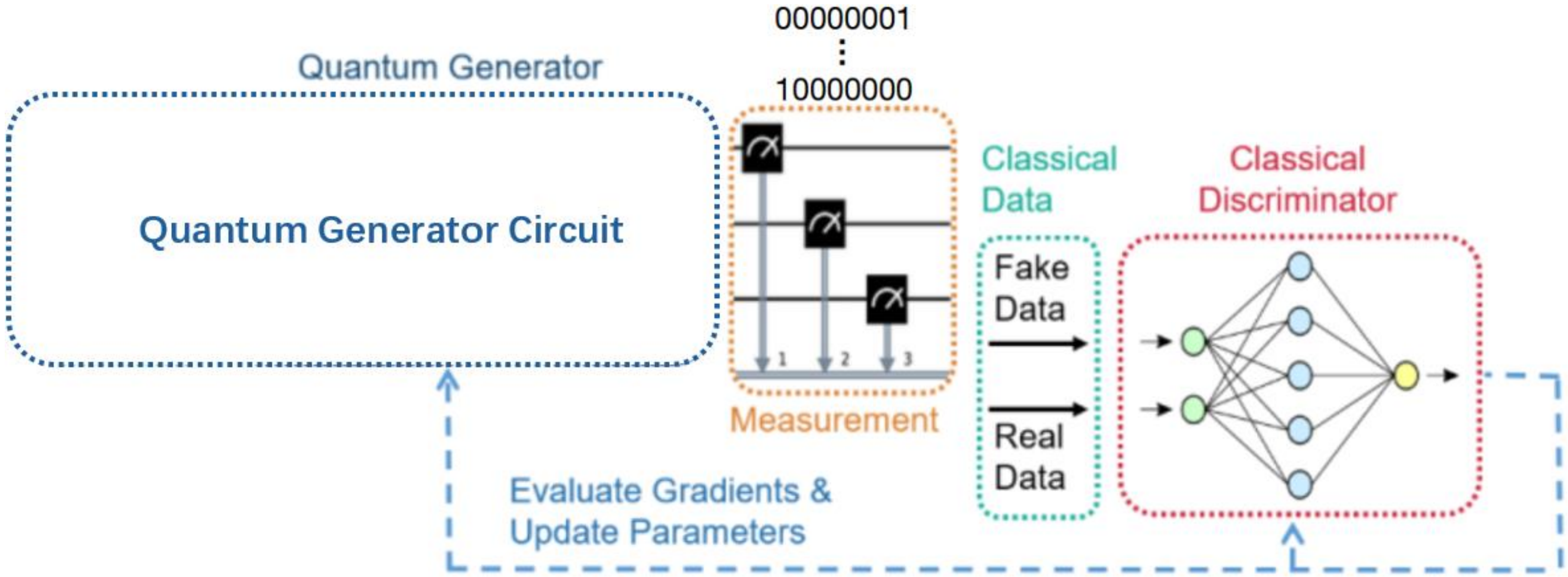
- **Generative Adversarial Network (GAN):** GAN is a deep learning framework where two neural networks compete to learn and generate realistic new data
  - **Generator:** creates fake data to fool the discriminator
  - **Discriminator:** learns to tell real data from fake



- **Why GAN for calorimeter simulation?**
  - Learns complex distributions through adversarial competition
  - No need for explicit physical modeling

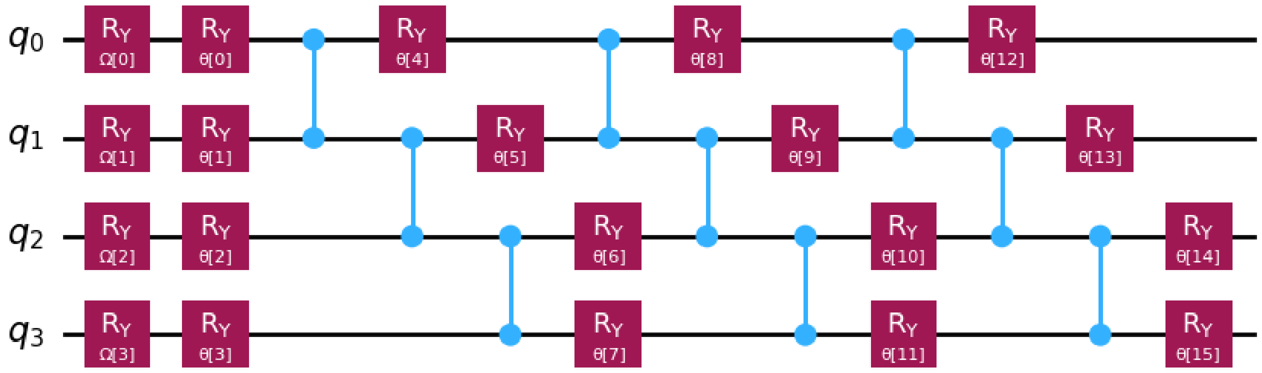
Quantum GAN

- **NISQ (Noisy Intermediate-Scale Quantum)-Era Constraints**
  - Limited qubits, high error rates, short coherence times
  - Full quantum GANs impractical → Hybrid approach necessary
- **Hybrid Architecture:** quantum generator + classical discriminator



Quantum GAN

- **Parameterized Quantum Circuit:** 4 qubits
  - Statevector simulation cost ∝ 2^n → exponential in qubit count



- **Two-part circuit structure**
  - Feature Map: encodes classical noise into quantum state

    single-qubit RY rotations per qubit
  - Ansatz: trainable variational circuit

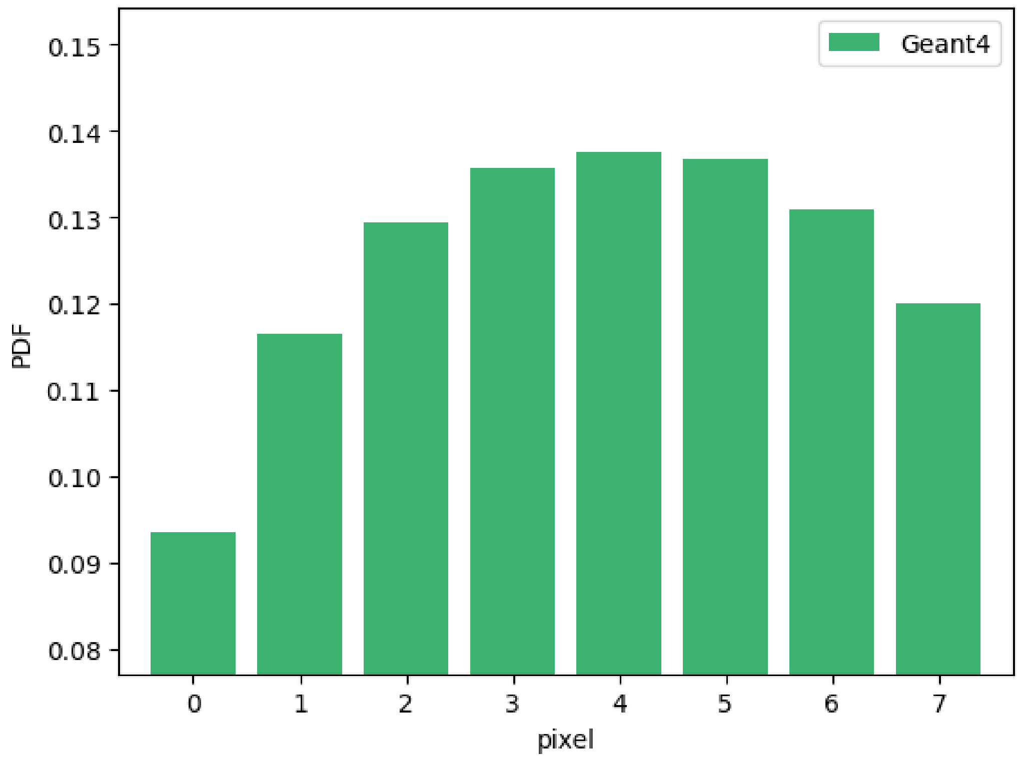
    RY rotation gates + CZ entangling gates

Methods

❖ Data Reduction

- Raw data: CLIC Calorimeter Electron showers at Fixed Angle by Geant4, 3D voxel grid
- Shower develops primarily along z (depth) → Average over all x and y voxels at each z-layer
- 25 original z-layers compressed into 8 representative layers:

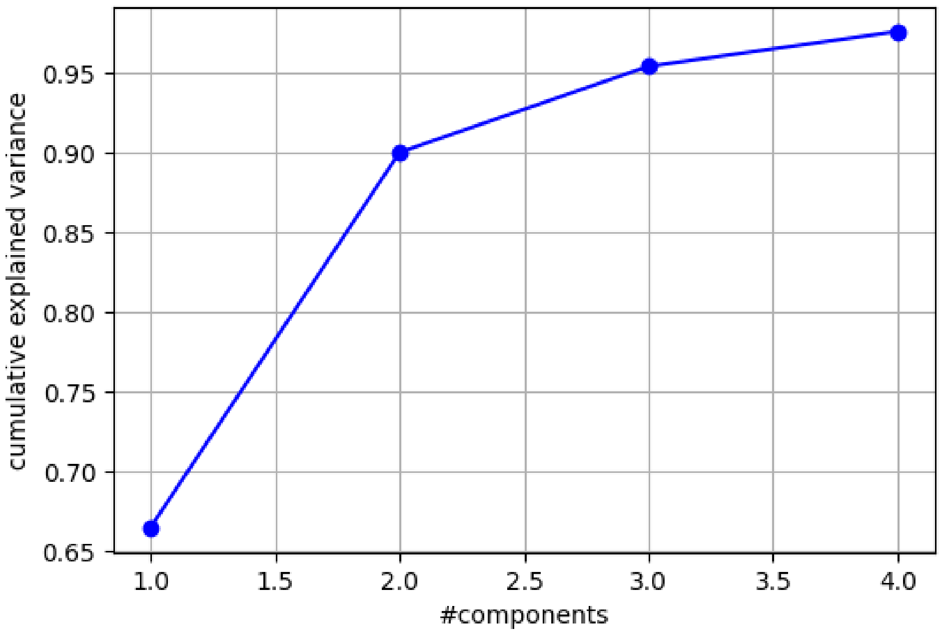
z-direction binning → 8 pixels

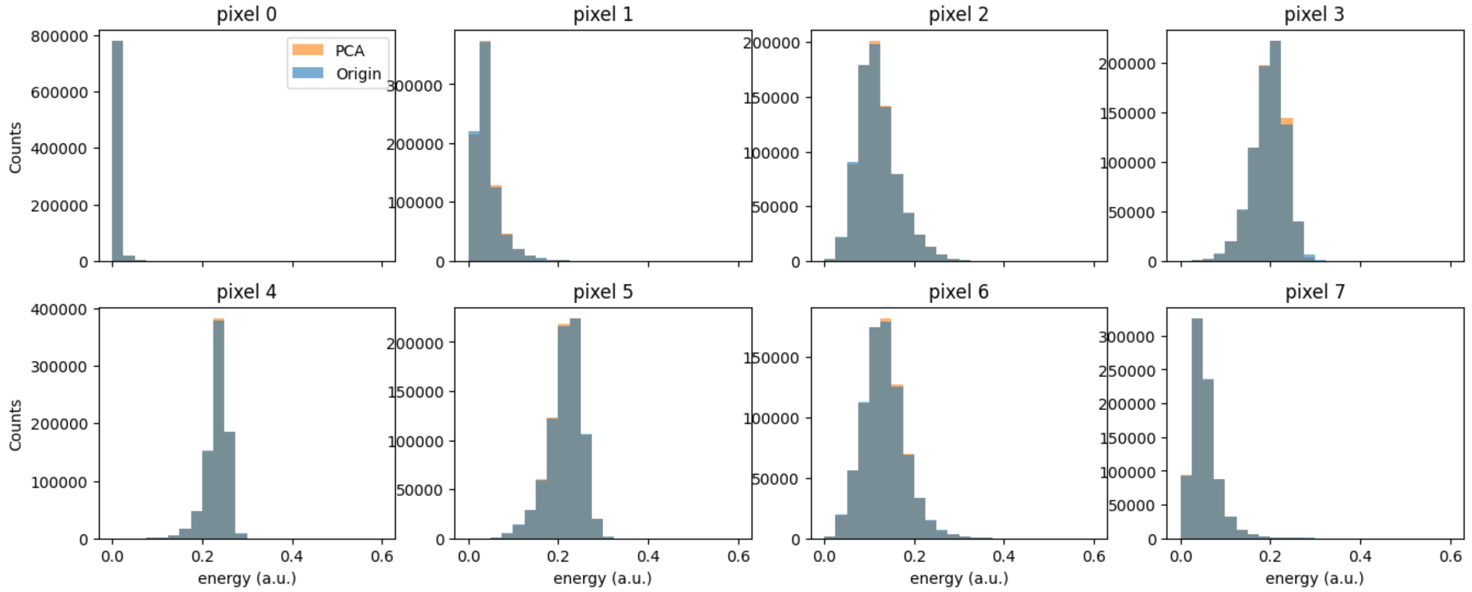


Methods

❖ Principal Component Analysis (PCA)

- Linear dimensionality reduction methods, Computes eigenvectors of the covariance matrix of the 8 pixels
- 4 components retain dominant shower shape information





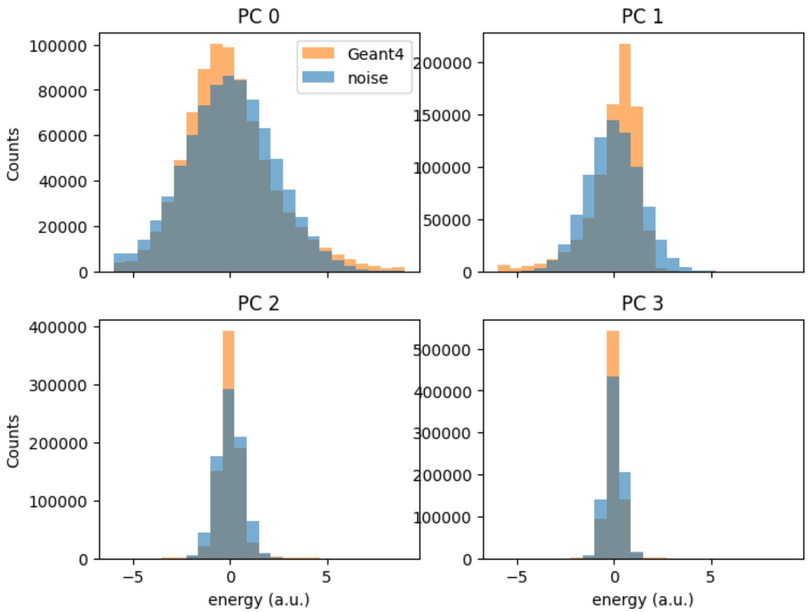
Methods

❖ Training Strategy

- Data encoding: Energy → Bloch sphere angle

  E_i → linear transform → Angle ∈ [0, π] → θ_i

- Gaussian noise prior in θ-space: Noise drawn as $\theta \sim \mathcal{N}(\mu\_pixel, \sigma\_pixel)$, feeds into the Feature Map as input



- Loss function: Wasserstein GAN & Gradient penalty (WGAN-GP)

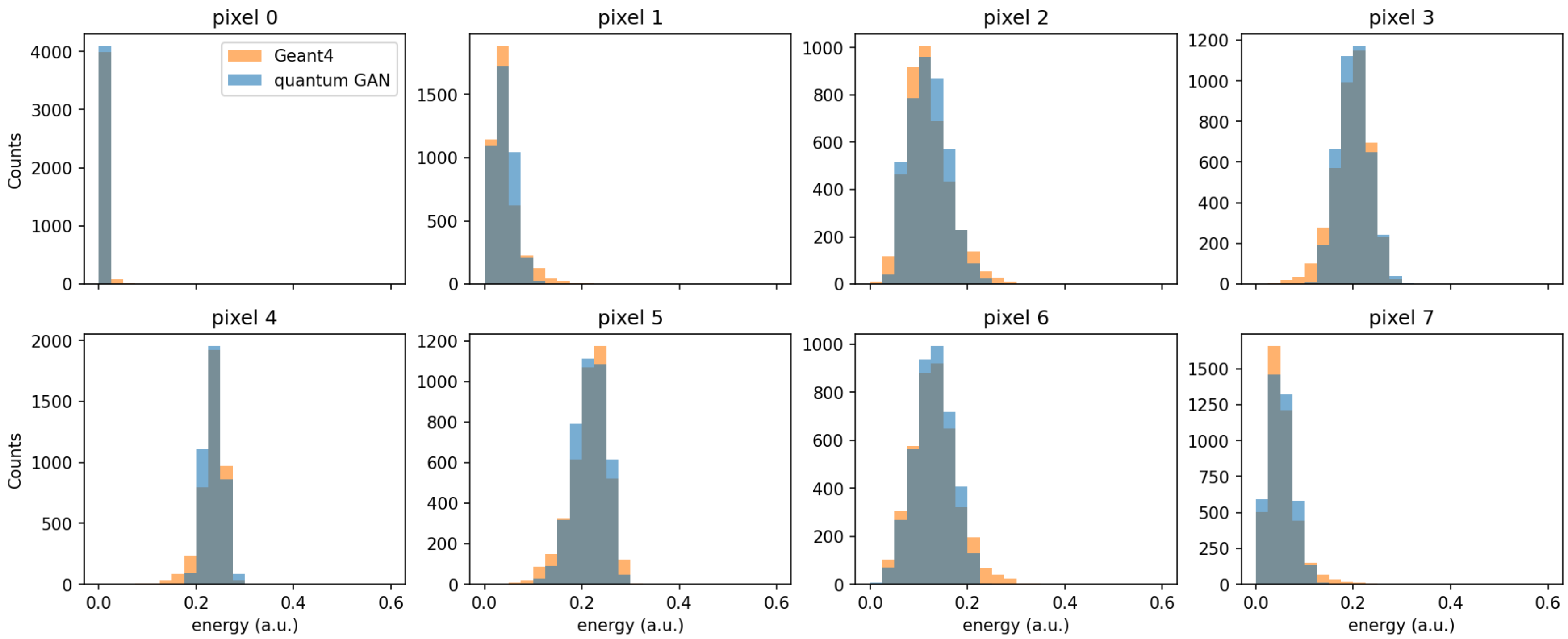
  $L\_D = E[D(G(z))] - E[D(x)] + \lambda \cdot GP, \quad L\_G = -E[D(G(z))], \quad \lambda = 10$

- Training configuration: lr_gen = 0.008, lr_disc = 0.001,

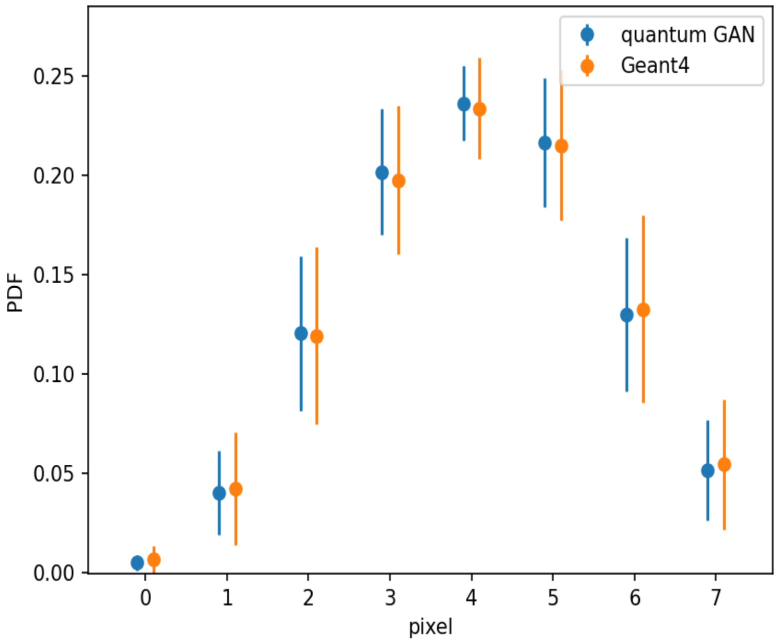
  γ (lr decay) = 0.995/epoch, disc:gen = 10:1

Training Result

❖ Quantum GAN vs Geant4 Shower Distributions



Per-Pixel Distribution

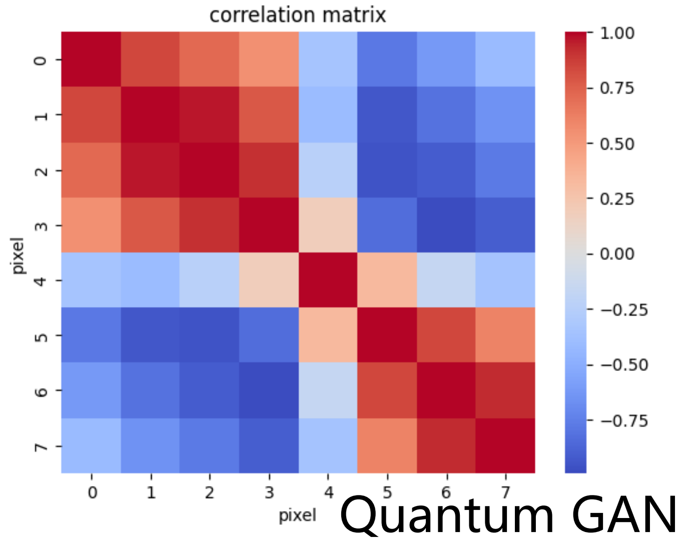


Average Pixel Distribution

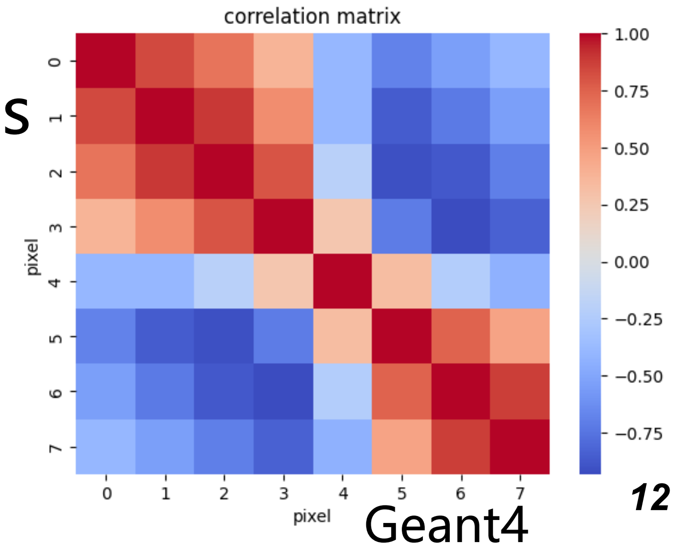
Training Result

- **Correlation Structure**
  - Visually consistent patterns
    → GAN captures inter-pixel shower correlations
- **Parameter Efficiency**
  - Quantum GAN generator: 16 parameters
  - Classical generator: typically thousands to millions
  - Expressivity comes from superposition and entanglement, not parameter volume

pixel correlation matrices



Quantum GAN



Geant4

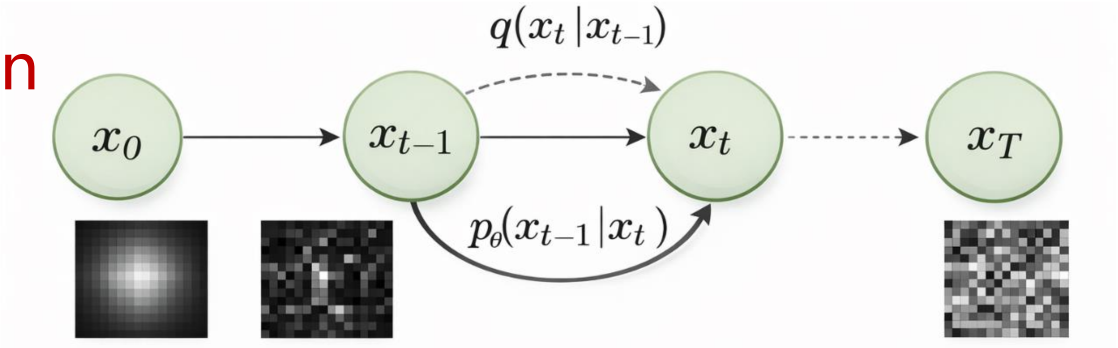
Diffusion Transformer (DiT)

❖ Forward diffusion process

- Starting from original data x_0, Gaussian noise is gradually added in steps to produce a sequence

$$x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_T$$

where x_T approaches an isotropic Gaussian distribution as T.



❖ Reverse diffusion process

- The model learns a parameterized denoising distribution

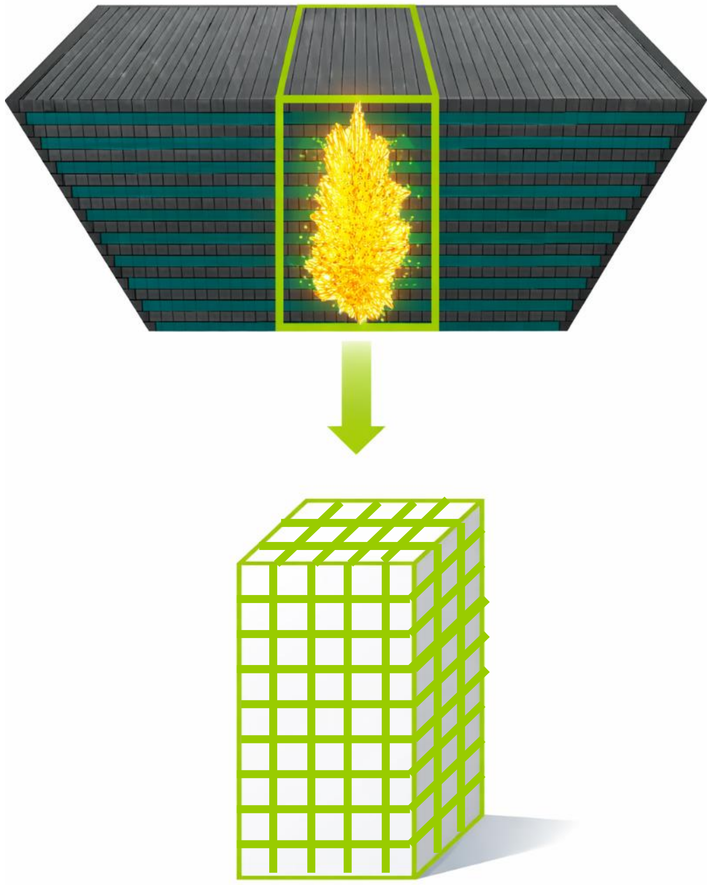
$$p_\theta(x_{t-1} \mid x_t)$$

which predicts how to iteratively remove noise from x_t to recover x_{t-1} effectively reversing the forward process.

DiT: Dataset

Data Preprocess

- Geant4 photon simulations based on CEPC Ref-TDR geometry.
- Segmented with DD4hep into a $15 \times 15 \times 18$ voxel grid ($15\ mm$ cube size).
- Log-transformed and normalized voxel energies.

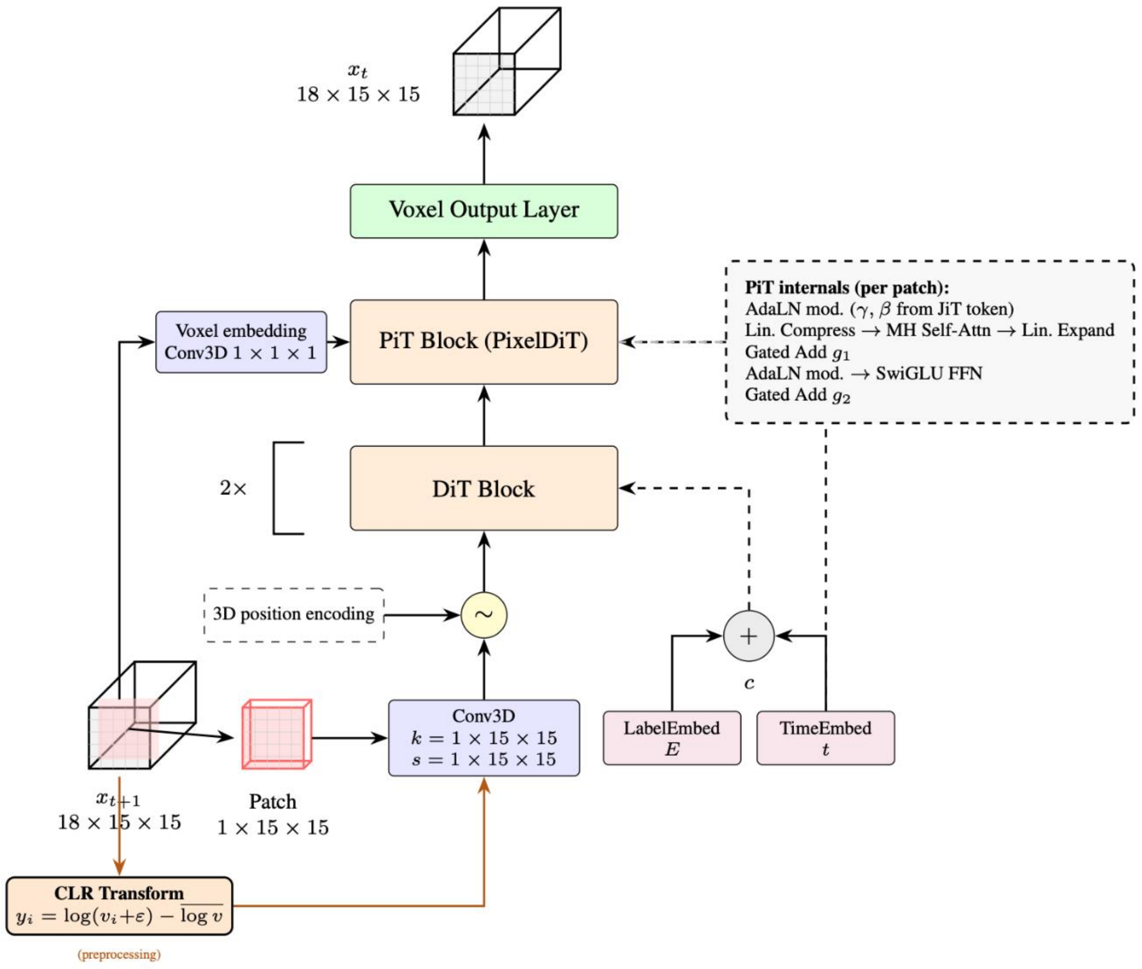


Area of interest selected as dataset

DiT: Model Architecture

❖ VoDiT4CAL Architecture:

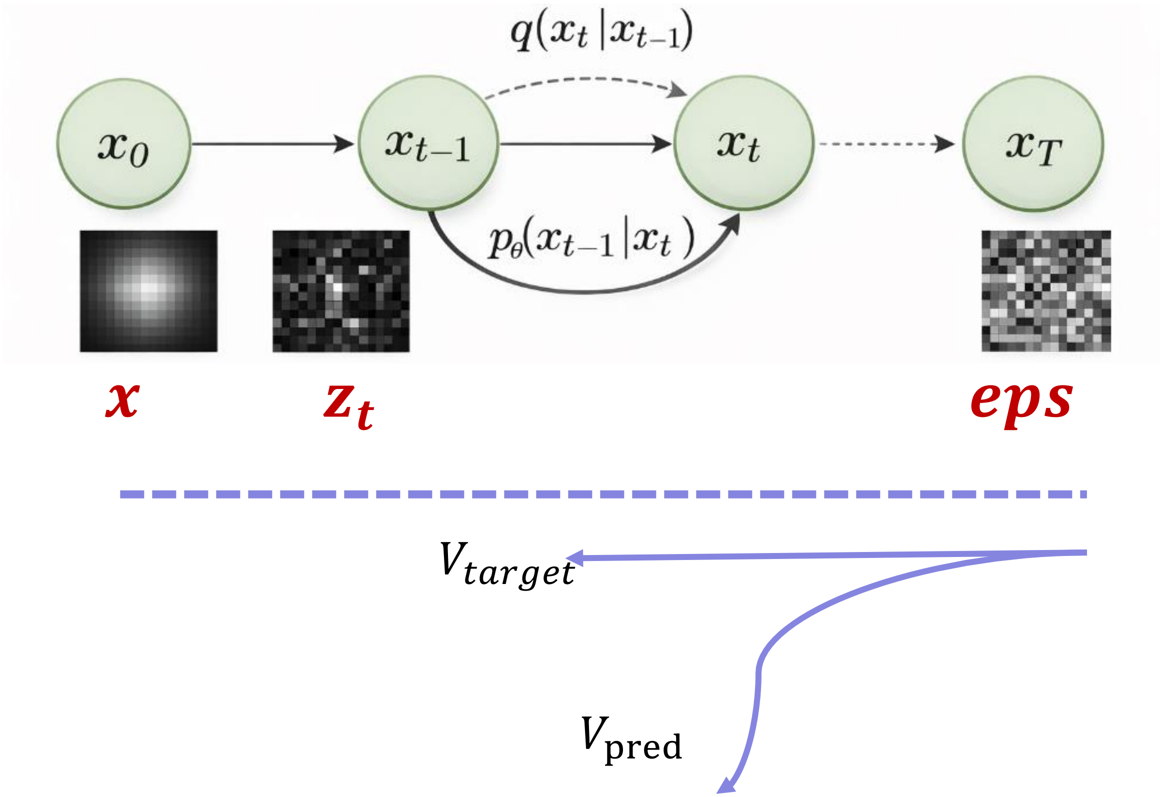
- **DiT Blocks:** Transformer self-attention blocks exchange information across tokens globally.
- **PiT Blocks**: Transformer self-attention blocks exchange information within each token across voxels.
- **Voxel Output**: The final token representations are mapped back to energy space to produce voxel-level predictions.



DiT: Training

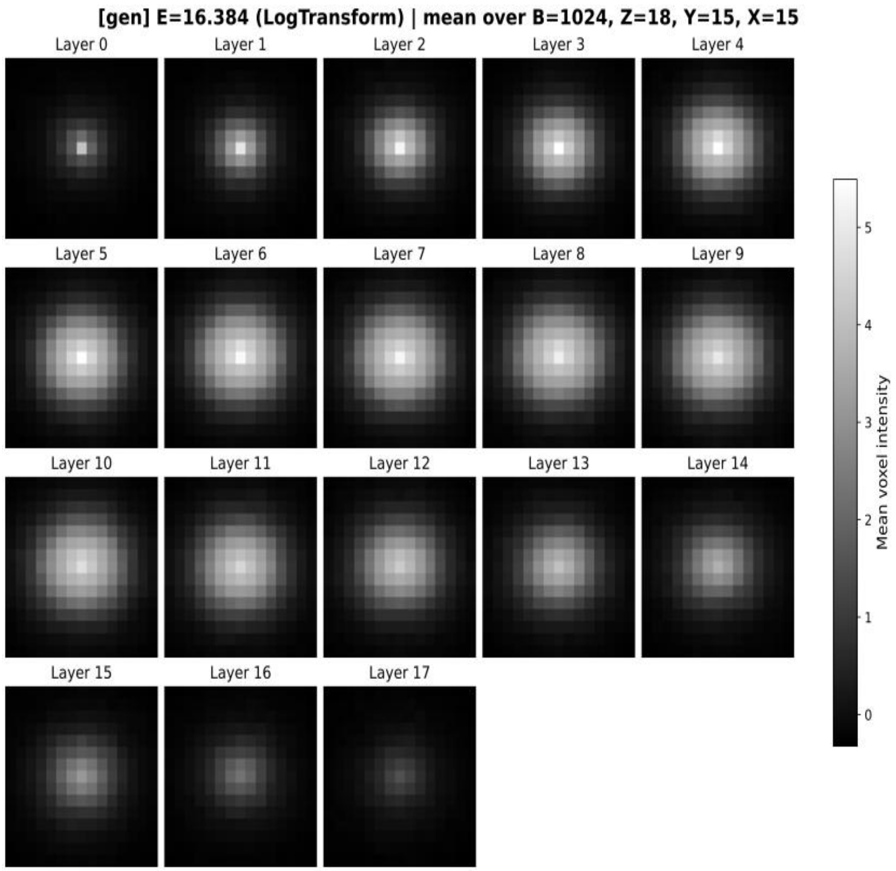
❖ Training:

- **PyTorch** provides tensor computation and automatic differentiation, while **PyTorch Lightning** offers a high-level training framework.
- **Training Time:** The total effective training time is **3h23m19s** on a single RTX 5090 GPU.

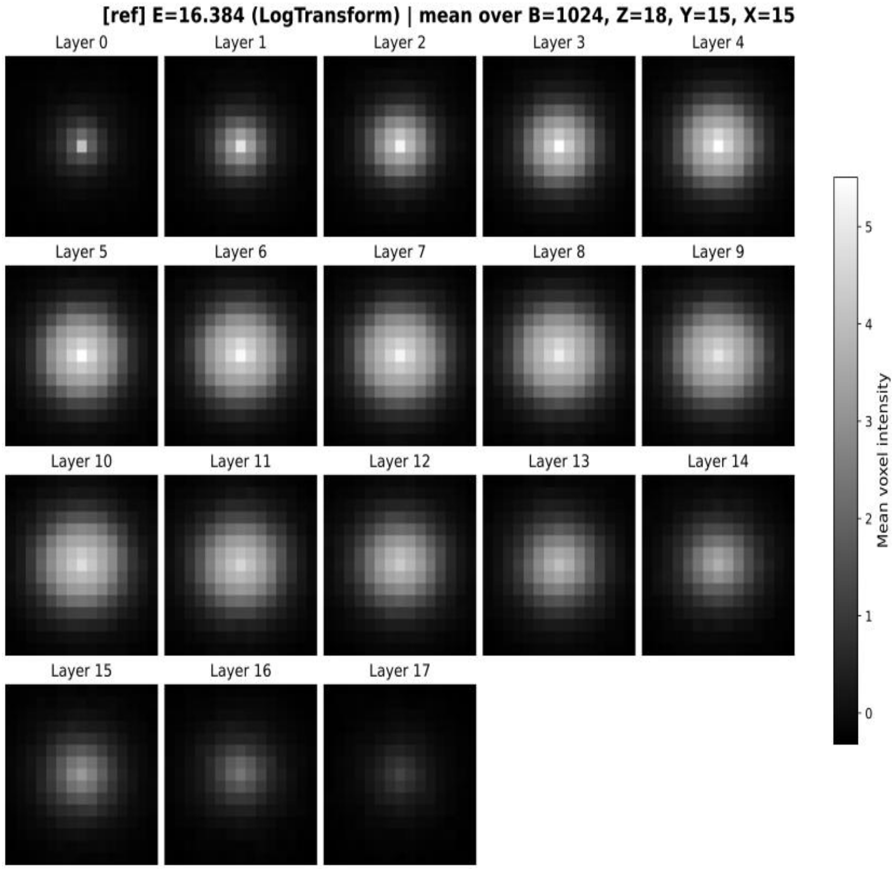


DiT: Result

- Generate photon shower at **16 GeV** for example



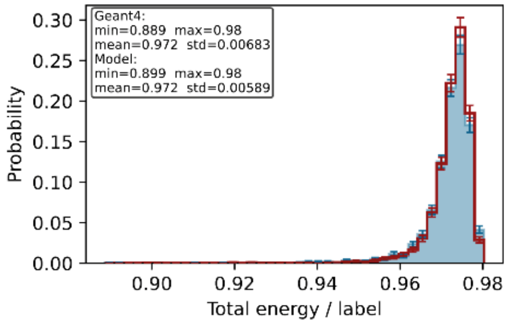
GEANT4

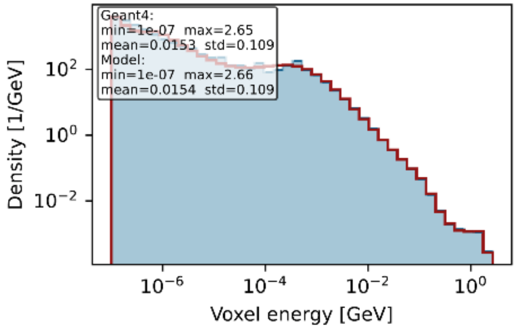


MODEL

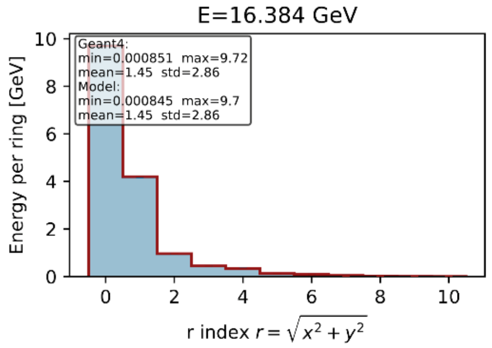
DiT: Generation Quality

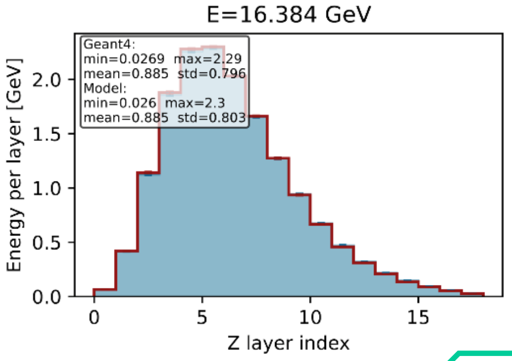
❖ Overview



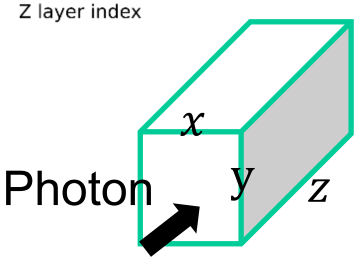


❖ Geometry

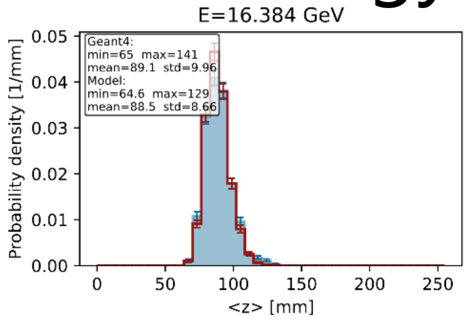


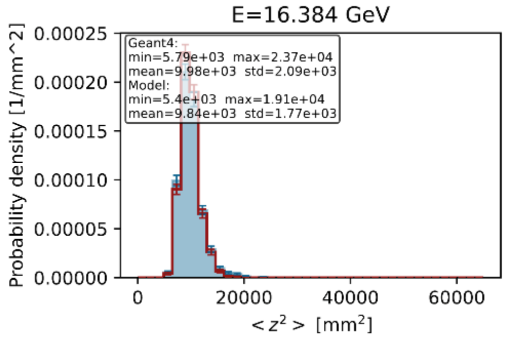


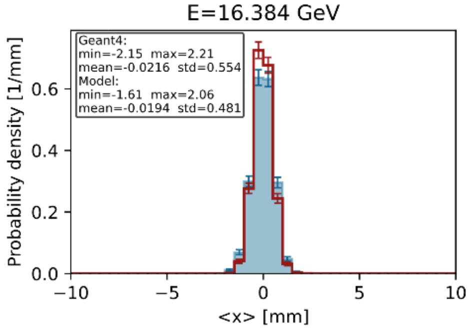
- Red line: Geant4
- Bule block: Model

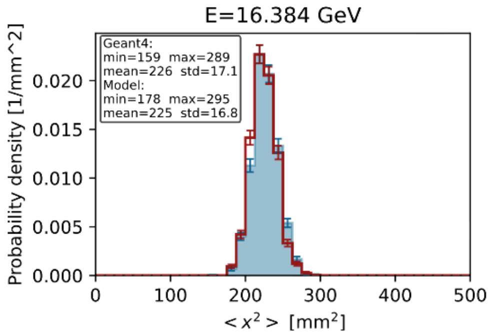


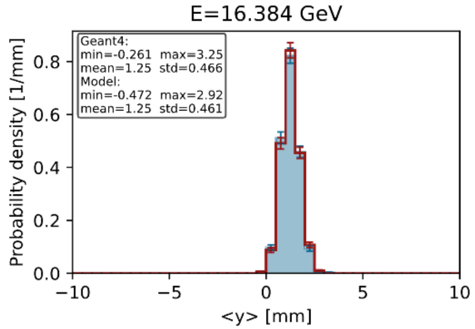
❖ ZXY energy center

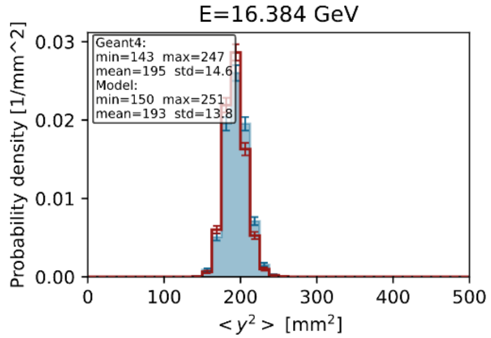






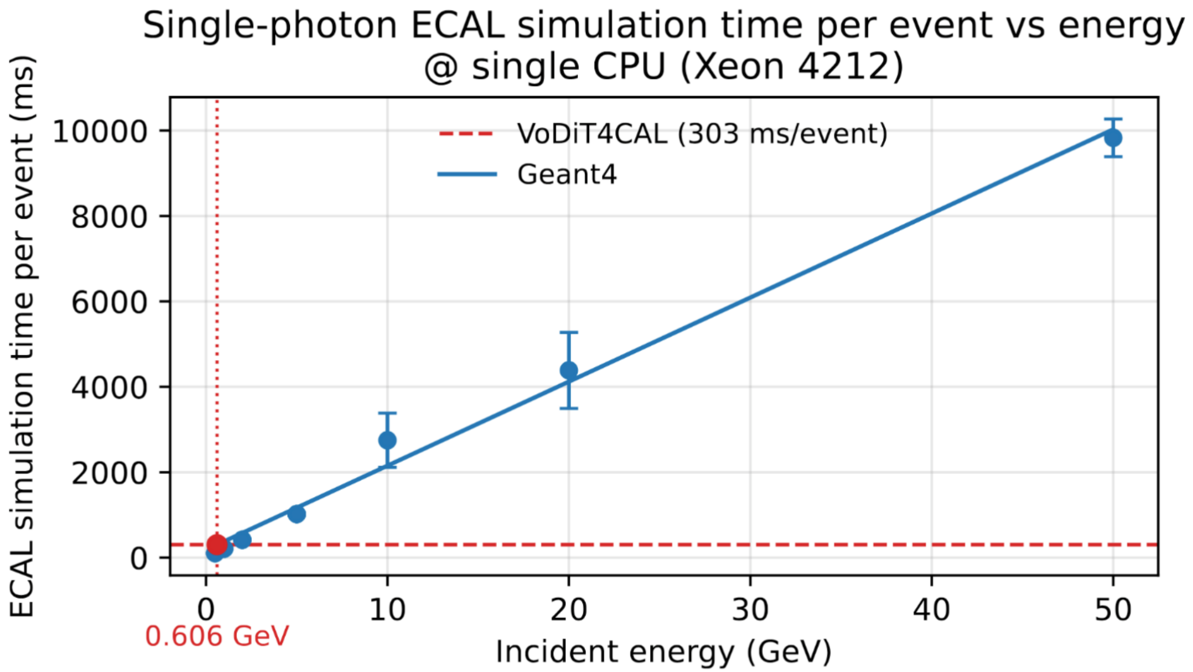






DiT: Generation Speed

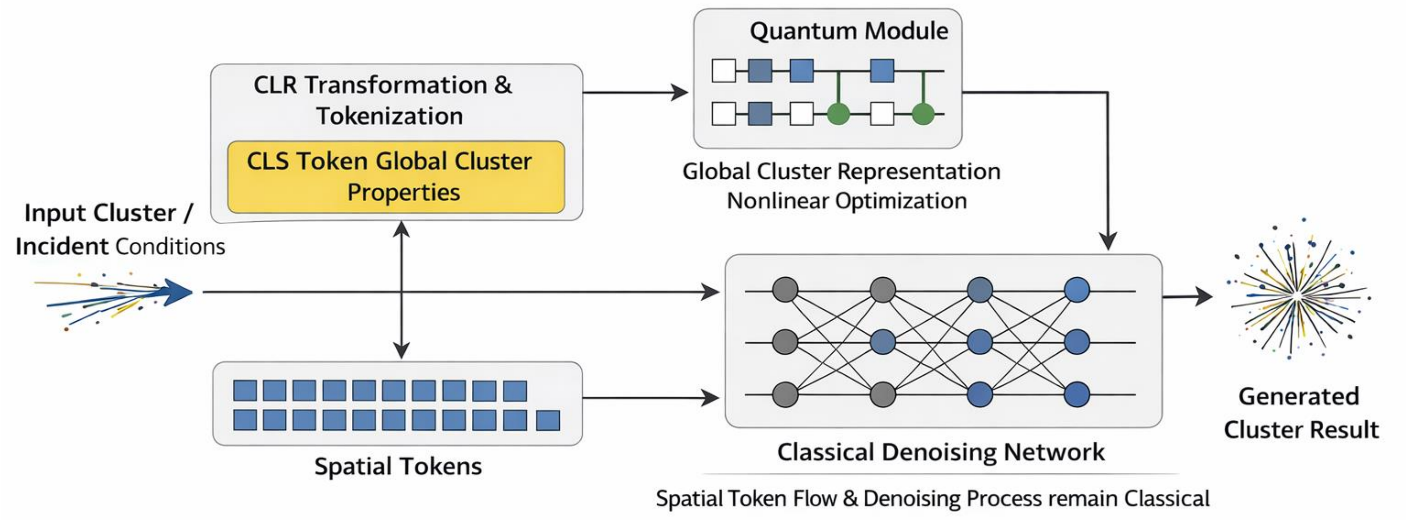
- Benchmark:
  - GPU (Nvidia RTX 8000): **3.19 ms /event**
  - CPU (Xeon 4214, single thread): **303.45 ms /event**
  - Geant4: generation time $T \sim E$ with particle energy E



DiT: Quantum Motivation

- Our classical results have already shown that **DiT offers stronger stability, generation quality, and scalability than GAN.**
- the natural next question is: under the same diffusion/Transformer framework, **quantum modules can further improve global modeling?**
- **Early studies on quantum diffusion already suggest that this direction is promising**, providing initial evidence that Quantum-enhanced DiT are worth exploring beyond Quantum GAN.

DiT Future Plan: Quantum-enhanced DiT



- Current DiT model uses **CLR transform**; a dedicated **Class token** captures global shower properties.
- The quantum module operates **exclusively on the Class token**, performing nonlinear renormalization of the global shower representation.
- Spatial token flow and backbone denoising remain **fully classical** — minimizing quantum overhead while preserving generation fidelity
- Class and spatial tokens are **jointly trained end-to-end**, enabling the quantum module to meaningfully influence the denoising process

Summary

❖ Quantum GAN

- Successfully learns the 1D Geant4 shower distributions
- Hybrid quantum-classical architecture + WGAN-GP training is viable
- Add realistic noise models & Deploy on real quantum hardware

❖ DiT

- Learned the 3D calorimeter simulation with high fidelity to Geant4
- Achieved fast generation speed
- Extend toward a Quantum-enhanced DiT

Thank you for your listening !