CaloClouds III: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation

ML4Jets, Paris, France
07.11.2024

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CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE
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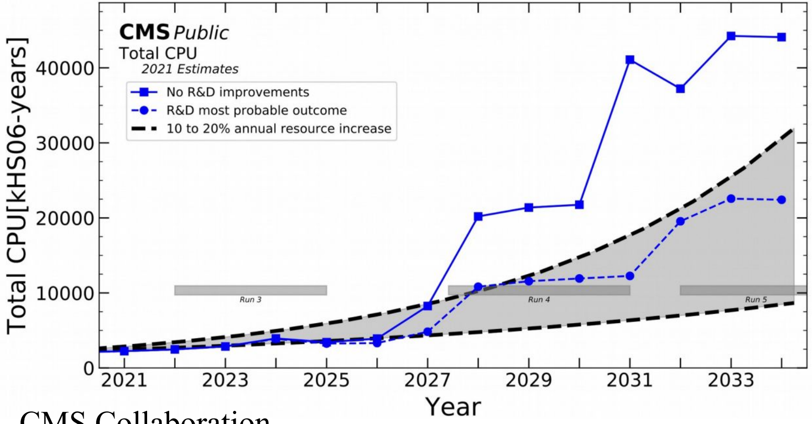
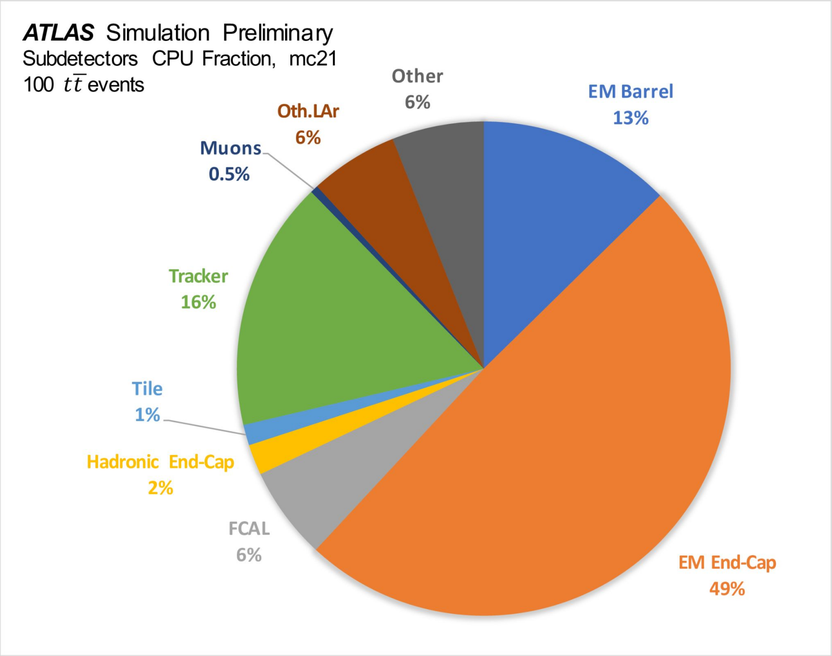
Introduction

Time-consuming Simulations



CMS Collaboration,
Offline and Computing Public Results (2021)
https://twiki.cern.ch/twiki/bin/view/CMSPublic/CMSOfflineComputingResults

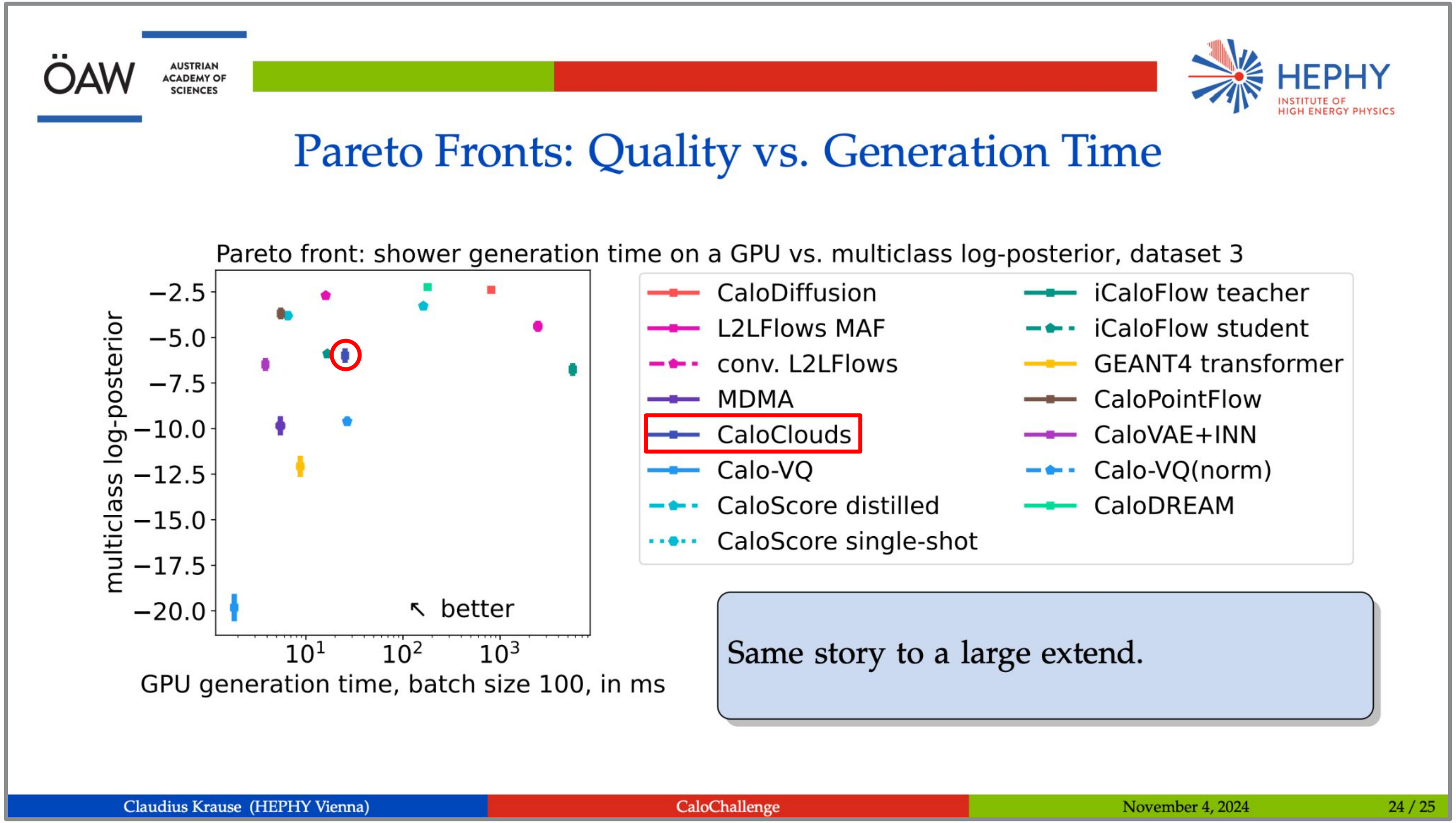


Goal: replace (or augment) most intensive part of detector simulation (calorimeters simulation) with a faster generator, based on state-of-the-art machine learning techniques

Introduction

CaloClouds II, Contributed to CaloChallange

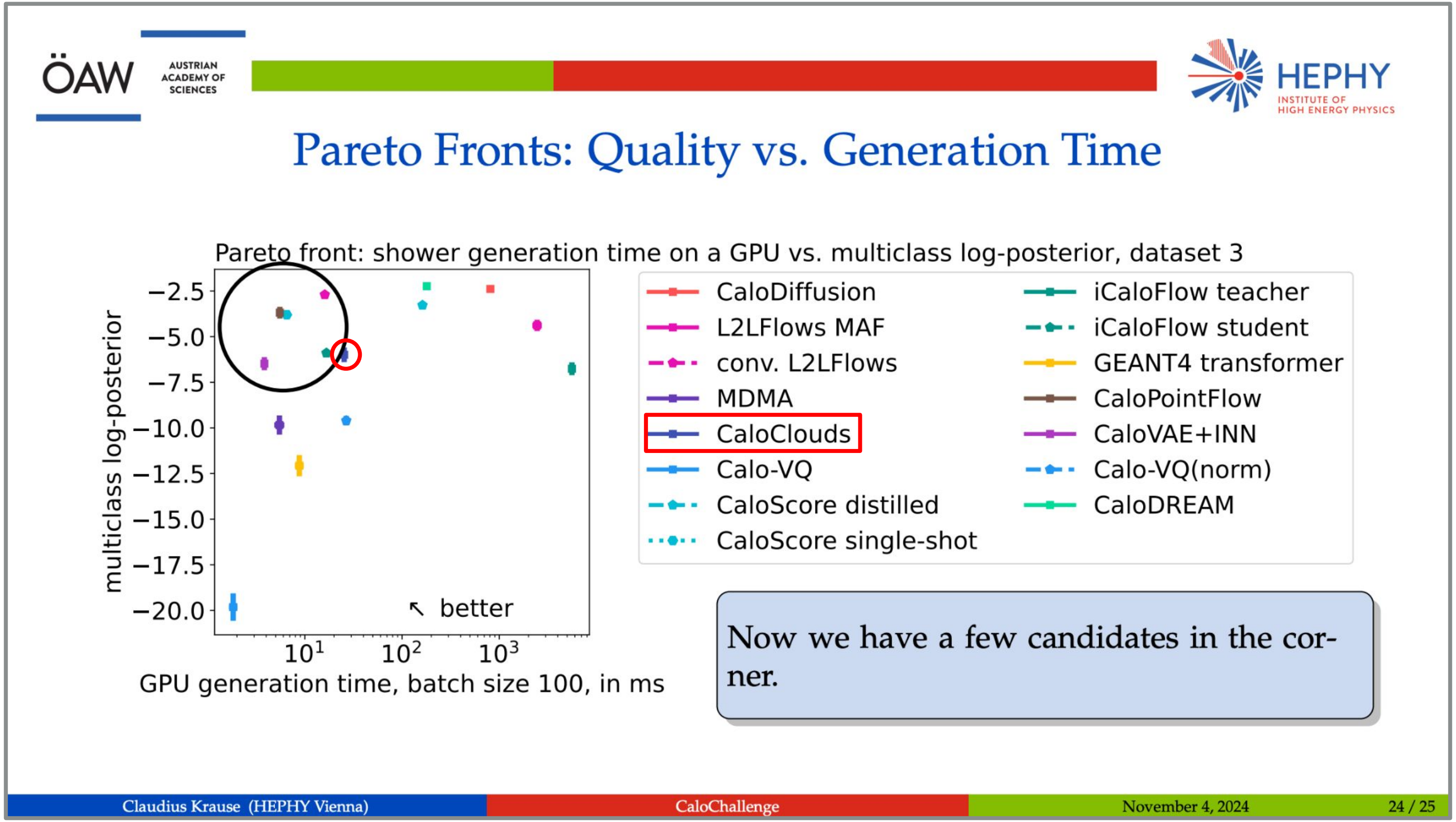
Courtesy C.Krause



Introduction

Almost Got an Invitation to Sweet Spot Club

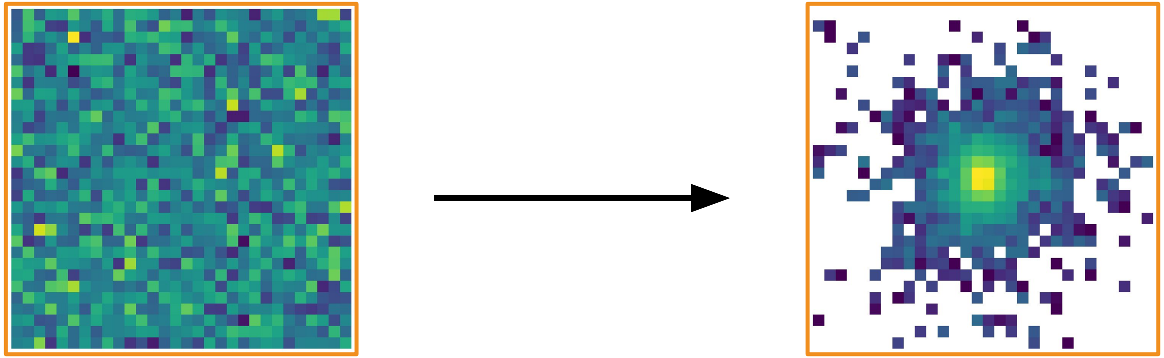
Courtesy C.Krause



Introduction

Generative Models

- A Generative Model is just a function that maps random noise to a some structure
- In most cases the structure is an **image representation** of the electromagnetic (EM) shower in the calorimeter

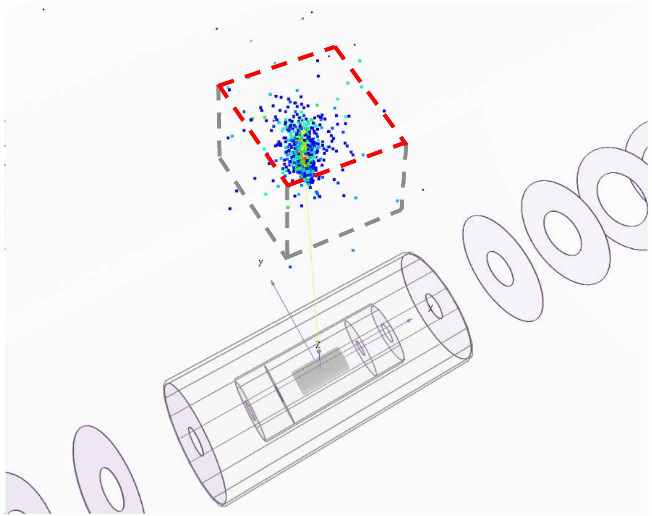


- There exist numerous generative models
  - Generative Adversarial Networks (GANs)
  - Flow-based models
  - Autoencoders (AE), e.g. BiB-AE
  - Diffusion Models (DMs)

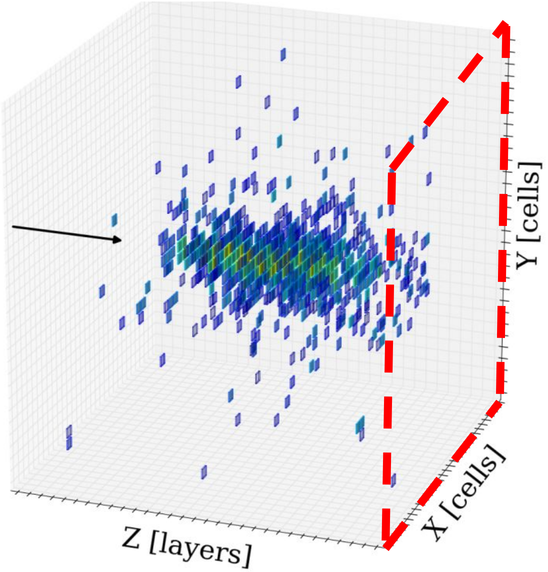
Image Representation of the EM Showers

ILD Detector

A simulated 60 GeV photon shower in the ILD detector



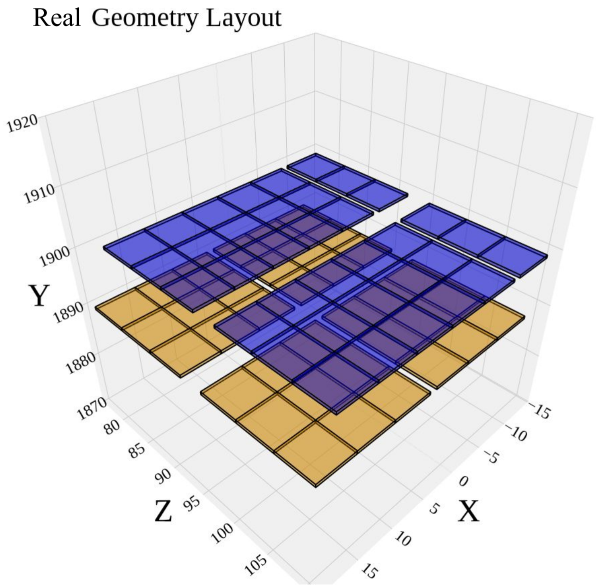
Regular grid 30x30x30

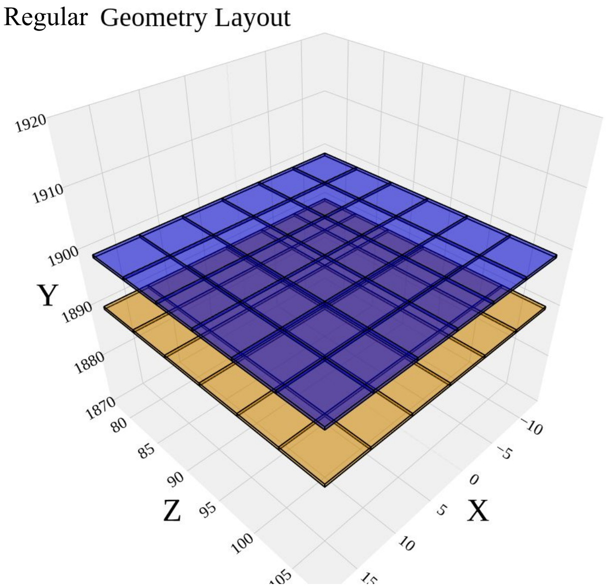


One to one mapping from detector geometry to a regular grid

Problems with Image Representation of the EM Showers

ILD Detector, ECAL Layers Structure

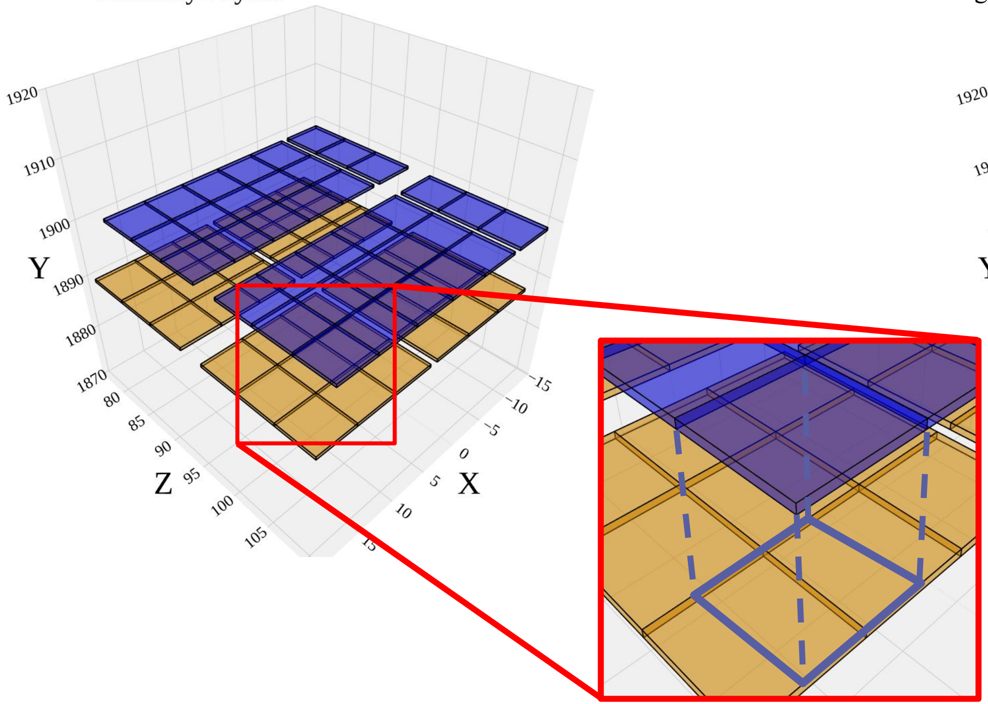




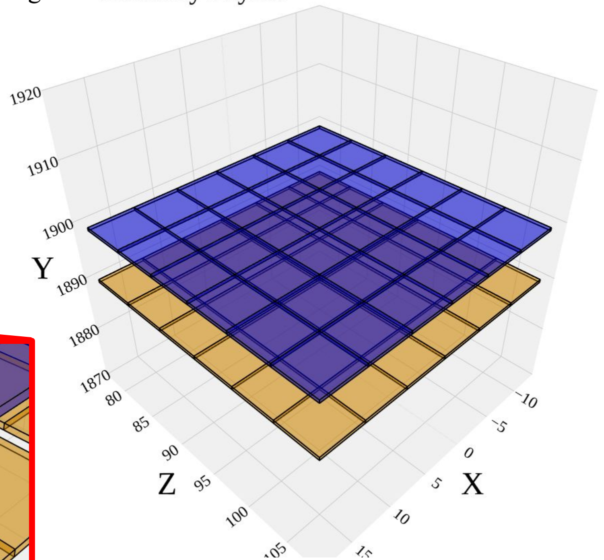
Problems with Image Representation of the EM Showers

ILD Detector, ECAL Layers Structure

Real Geometry Layout

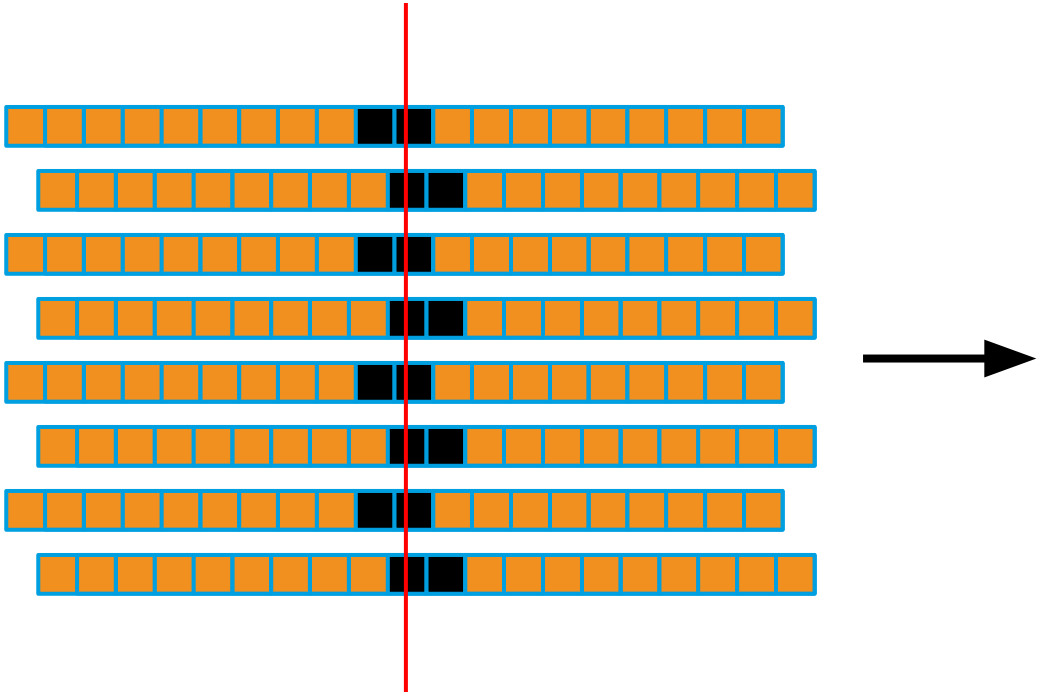


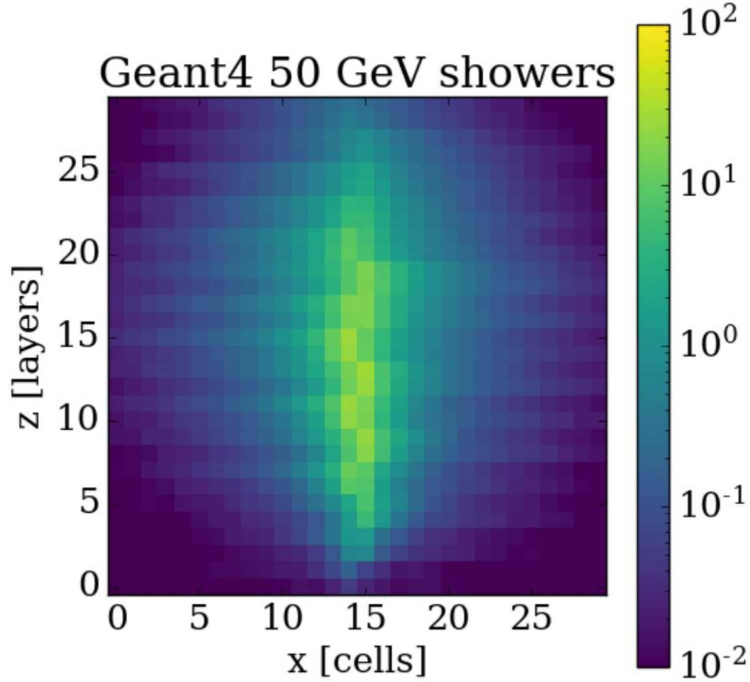
Regular Geometry Layout



Problems with Image Representation of the EM Showers

ILD Detector, ECAL Layers Structure, Staggering Effect





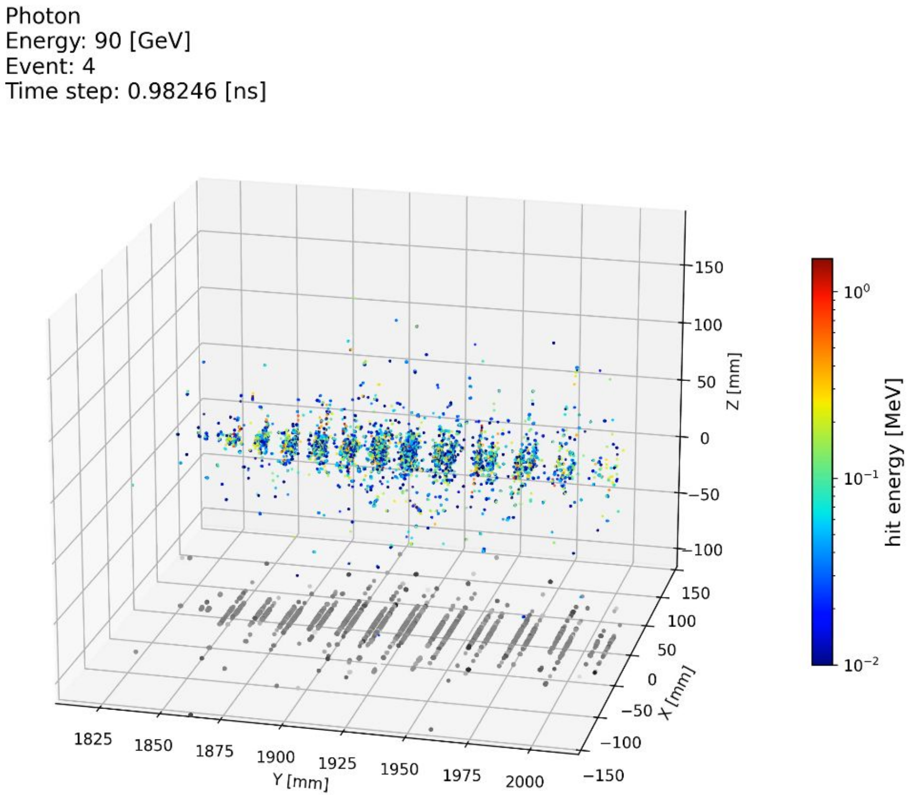
Models have to learn not only EM shower properties, but also geometry “artifacts”, like **staggering effect**

Point Cloud Representation of the EM Showers

GEANT4 Steps

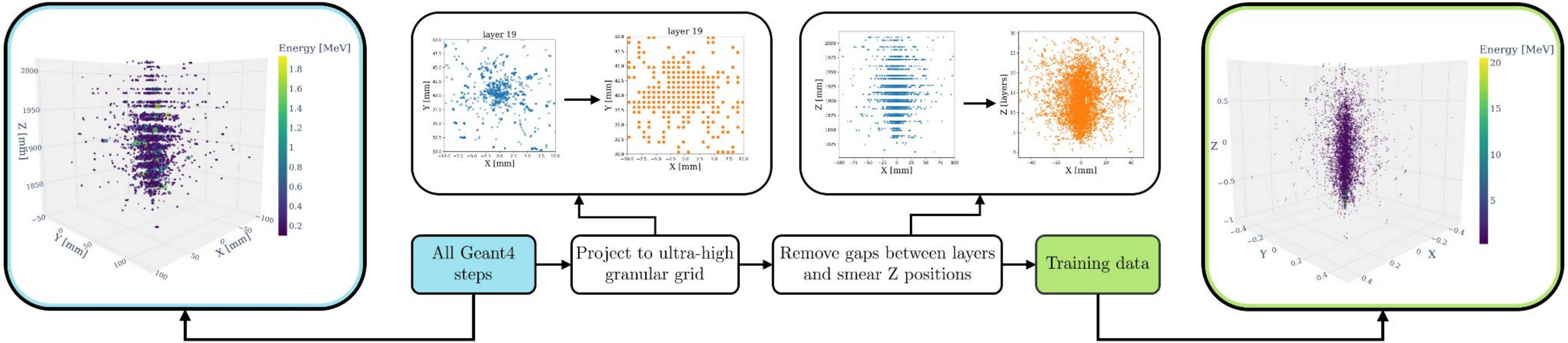
A way to overcome potential issues from irregular (realistic) cell geometry would be to use much higher granularity/resolution

- All G4 interactions, ultimate resolution
- Detached from detector layer geometry
- Too many points to generate, ~40k per shower (need pre-processing step to reduce number of spacepoints)



Point Cloud Representation of the EM Showers

Data Preprocessing

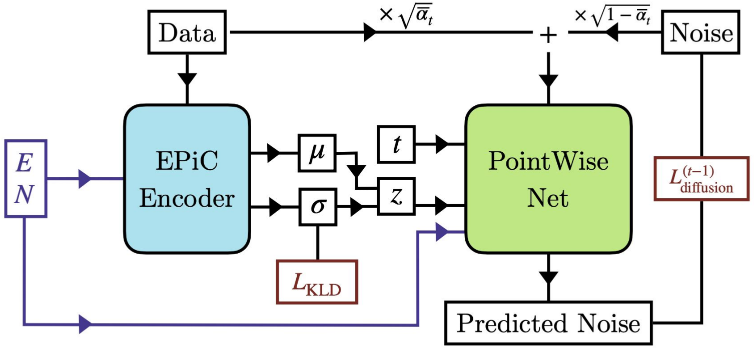


Number of points reduced to ~6k per shower, high enough resolution to move the shower in different place without harming physical properties of the shower

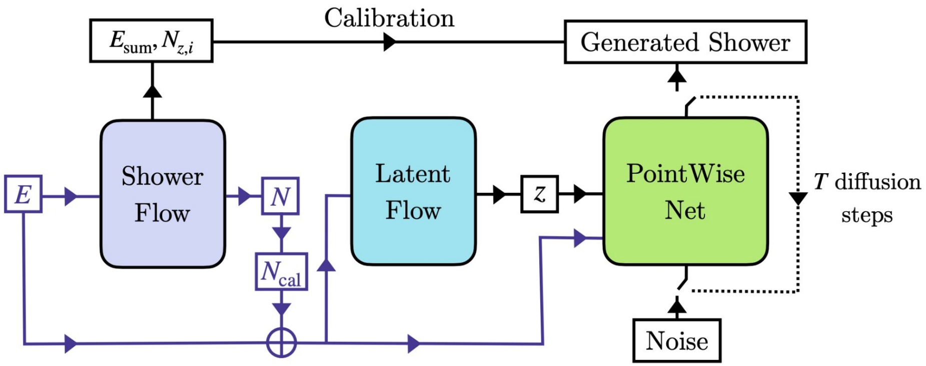
Point Cloud + Diffusion Model

CaloClouds, Model Overview

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2305.04847**



(a) Training at random time step t

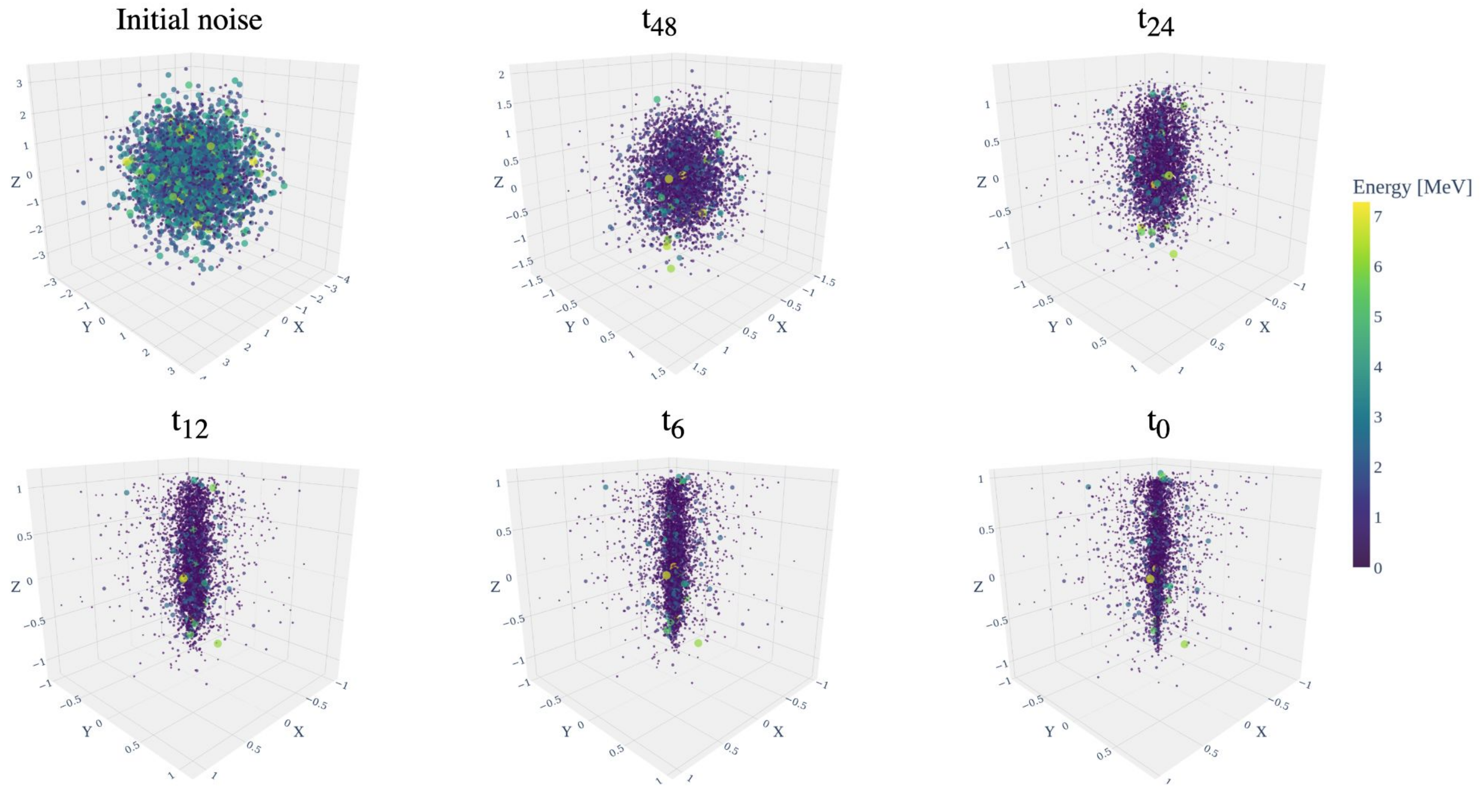


(b) Sampling with reverse diffusion through all time steps T

- GANs and VAEs convert noise from some simple distribution to a data sample
- **DMs learn to gradually denoise data starting from noise**

Point Cloud + Diffusion Model

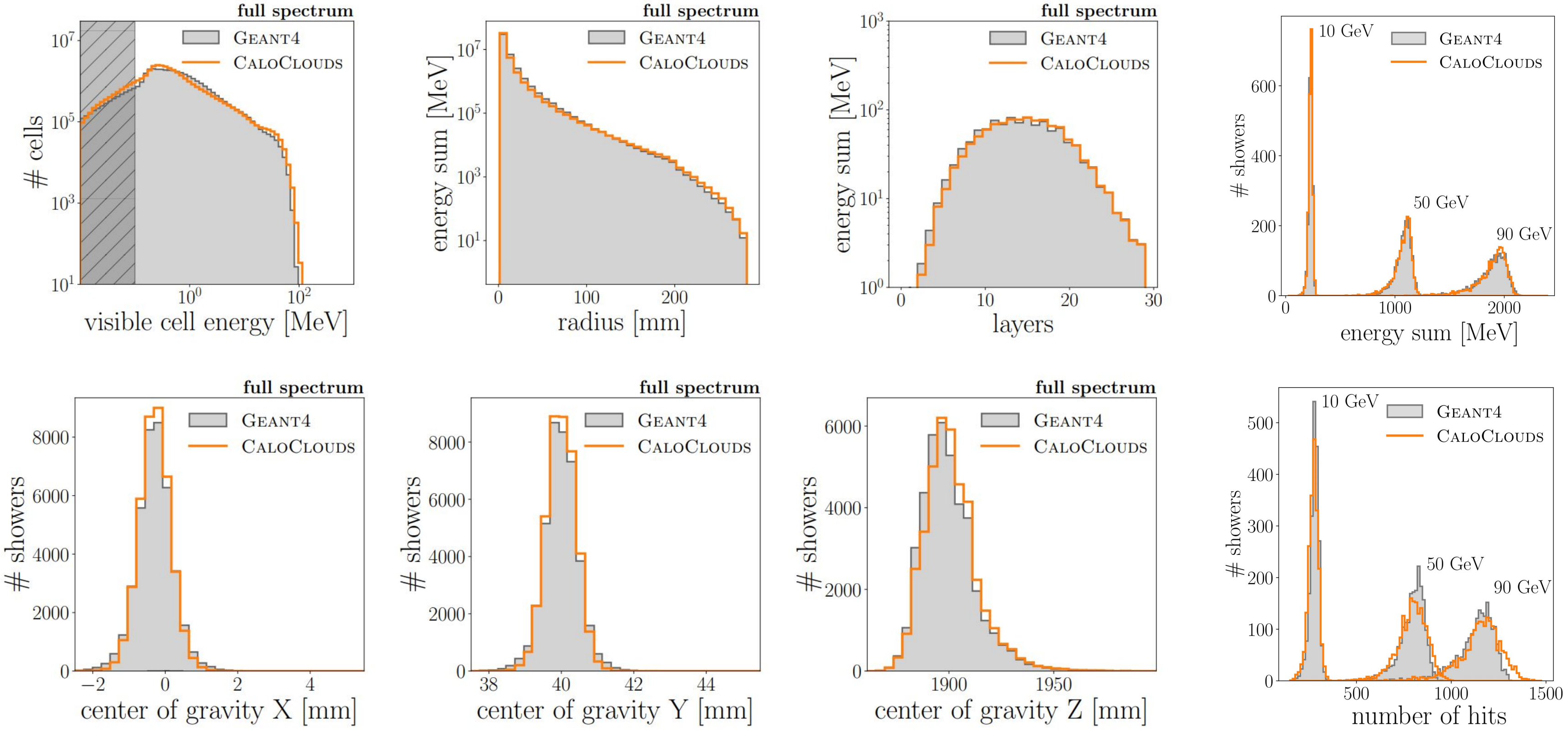
Reverse Diffusion Process



Point Cloud + Diffusion Model

Physics Observables

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2305.04847**

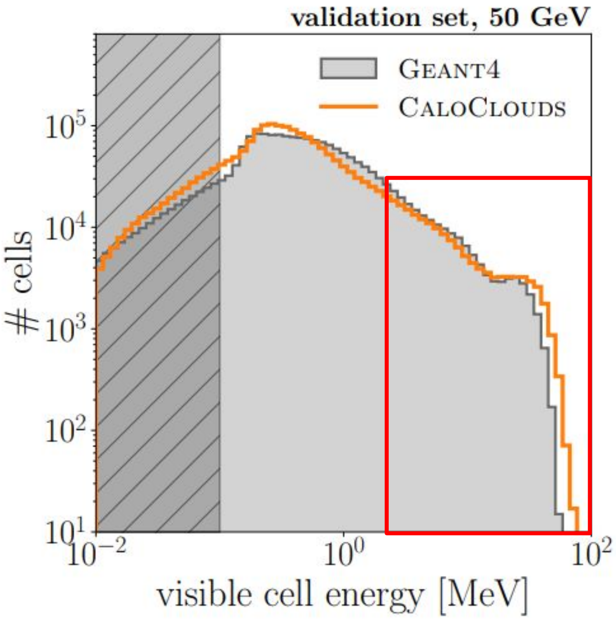


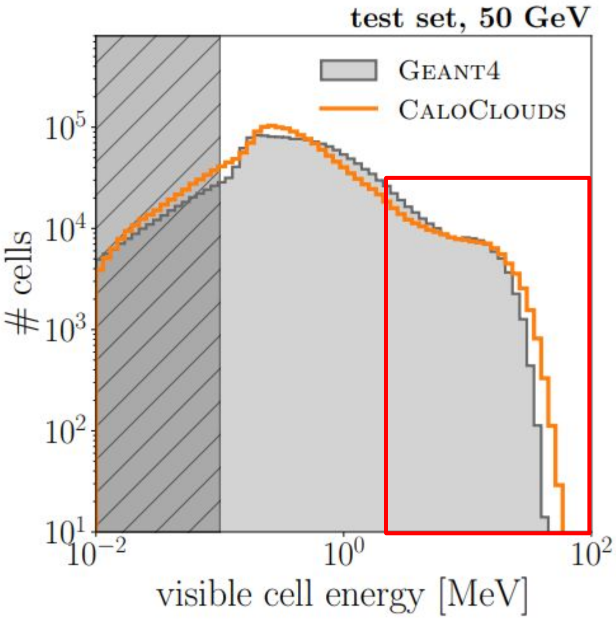
Point Cloud + Diffusion Model

Physics Observables For Different Positions

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2305.04847**

validation incident point pos.





test incident point pos.

Per-cell energy distribution for the 50 GeV validation (left) data set, created at the same position as the training data set and for a 50 GeV test (right) data set simulated at a different position with the generated point cloud translated to this position

Point Cloud + Diffusion Model

Speedup, CaloClouds I

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2305.04847**

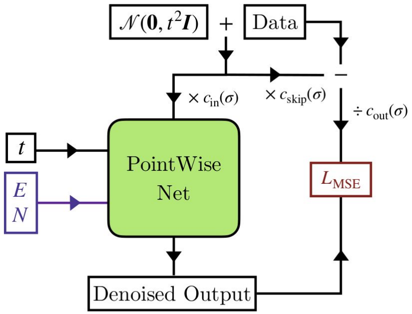
Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	4082 ± 170	$\times 1$
	CALOCLOUDS	3509 ± 220	$\times 1.2$
GPU	CALOCLOUDS	38 ± 3	$\times 107$

Not impressive inference time

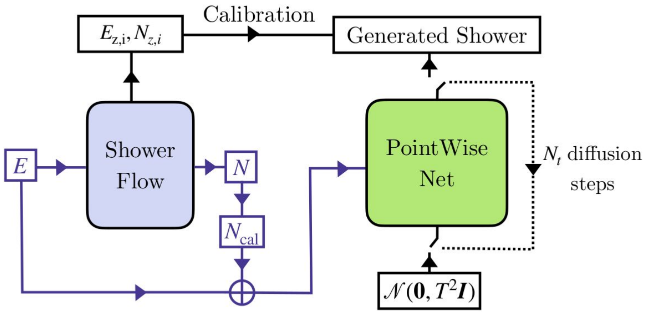
Point Cloud + Diffusion Model

CaloClouds II, Model Overview

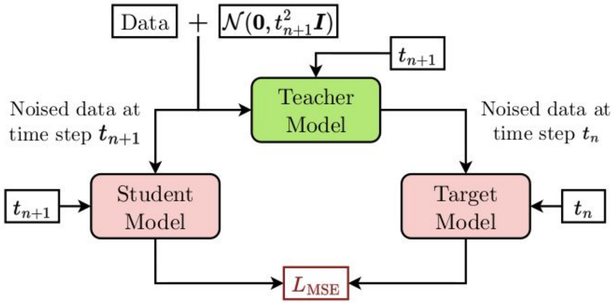
CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2309.05704**



(a) Training



(b) Sampling



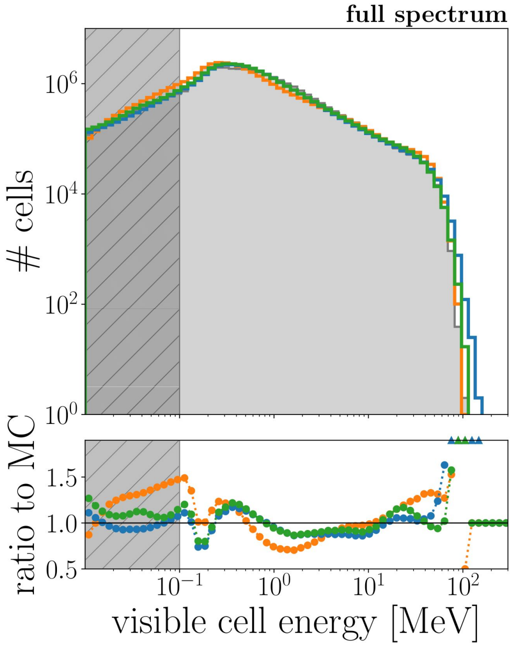
Consistency Distillation

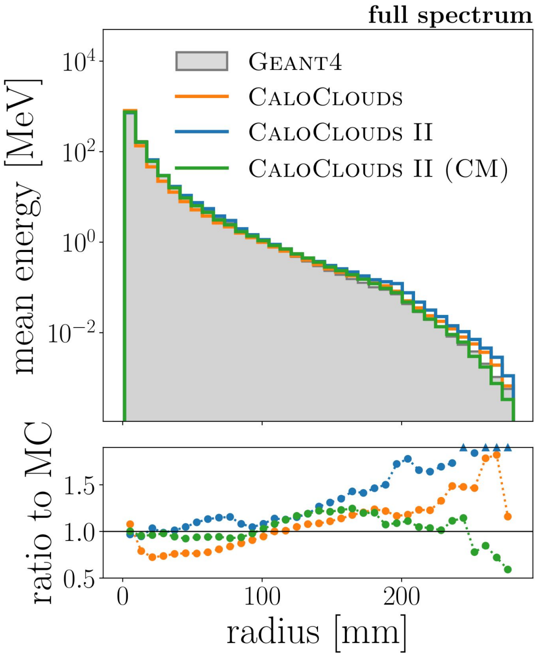
Modified version of CaloClouds + Consistency Distillation → significantly reduced inference time

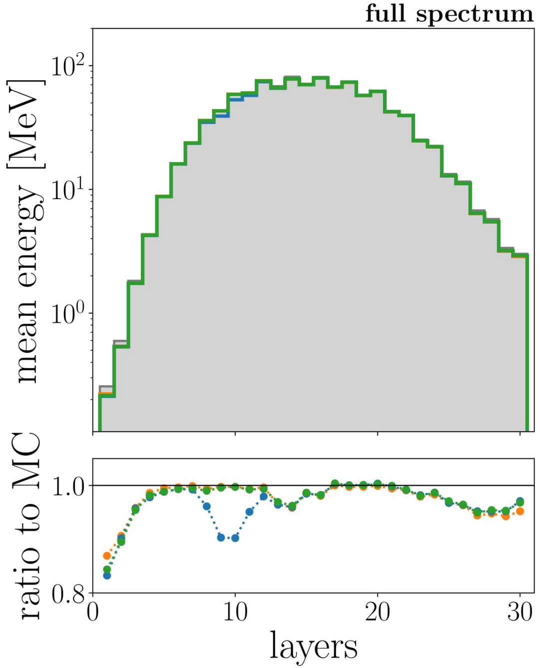
Point Cloud + Diffusion Model

Physics Observables

CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2309.05704**







Point Cloud + Diffusion Model

Speedup, CaloClouds II

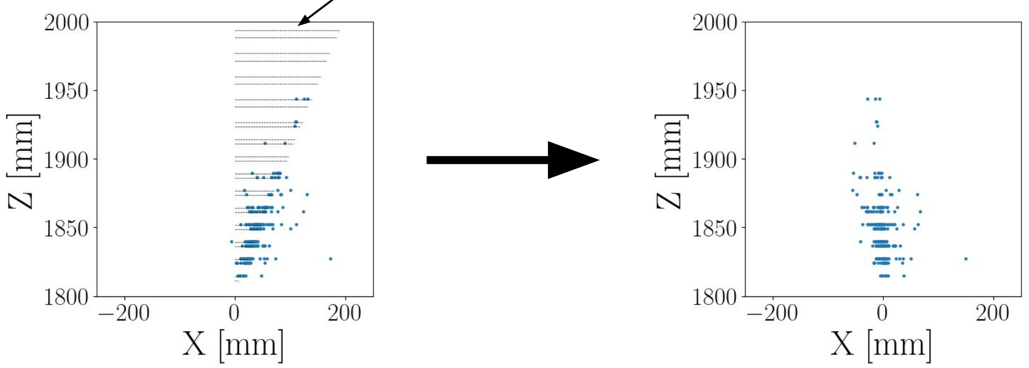
CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2309.05704**

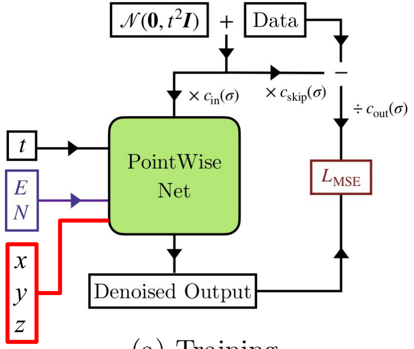
Hardware	Simulator	NFE	Batch Size	Time / Shower [ms]	Speed-up
CPU	Geant4			3914.80 ± 74.09	×1
	CaloClouds	100	1	3146.71 ± 31.66	×1.2
	CaloClouds II	25	1	651.68 ± 4.21	×6.0
	CaloClouds II (CM)	1	1	84.35 ± 0.22	×46
GPU	CaloClouds	100	64	24.91 ± 0.72	×157
	CaloClouds II	25	64	6.12 ± 0.13	×640
	CaloClouds II (CM)	1	64	2.09 ± 0.13	×1873

Point Cloud + Diffusion Model

CaloClouds III, Adding Angular Conditioning

geometrical offset





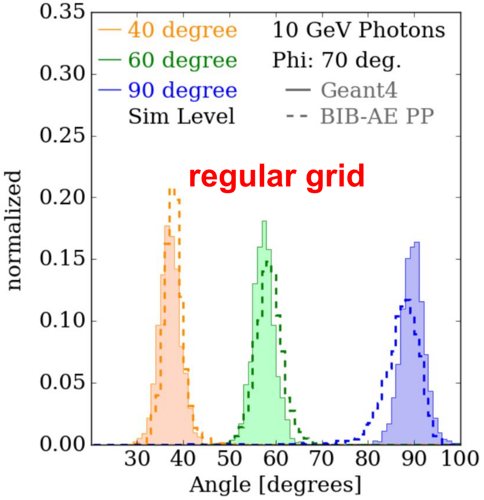
(a) Training

direction vector

Additional data preprocessing step, another conditioning vector

Point Cloud + Diffusion Model

Angle Reconstruction

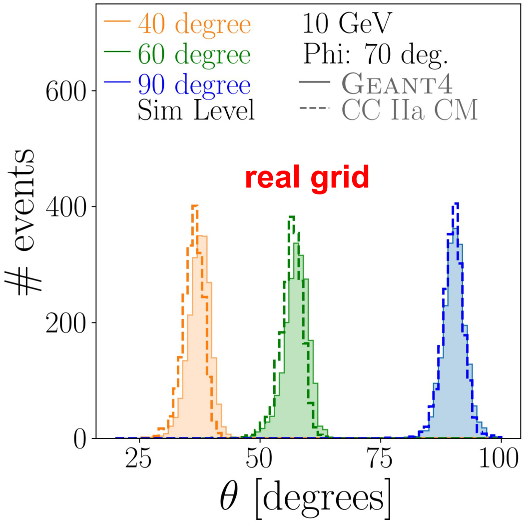


Development and Performance of a Fast Simulation Tool for Showers in High Granularity Calorimeters based on Deep Generative Models

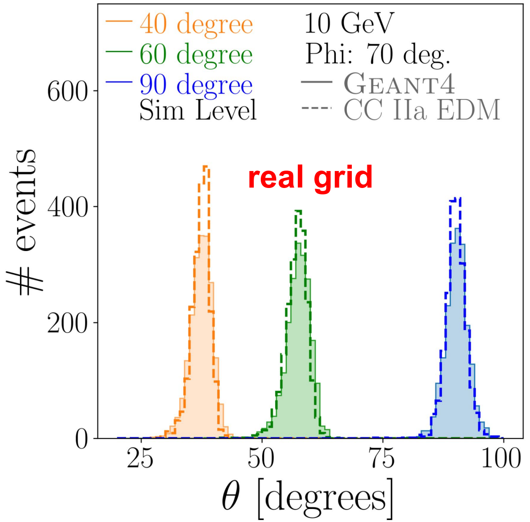
Peter McKeown (Hamburg U.), 2024

DOI: 10.3204/PUBDB-2024-01825

1 step

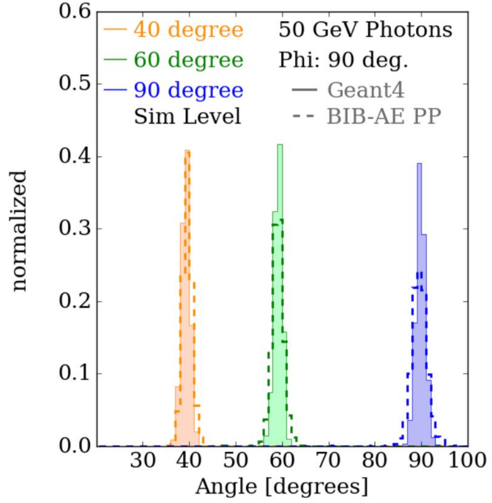


90 steps



Point Cloud + Diffusion Model

Angle Reconstruction



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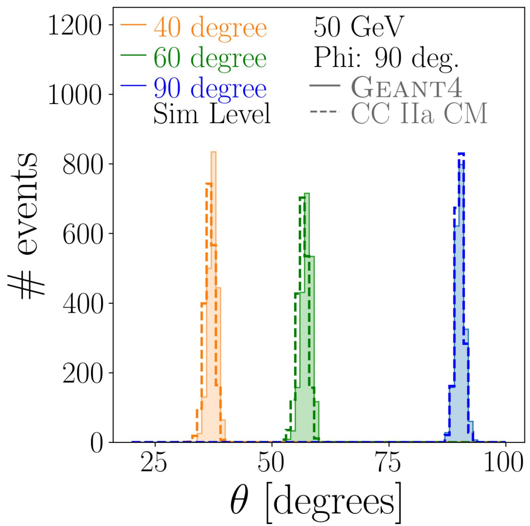
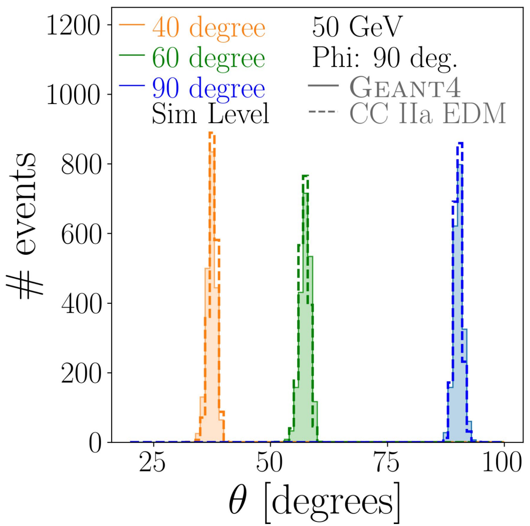
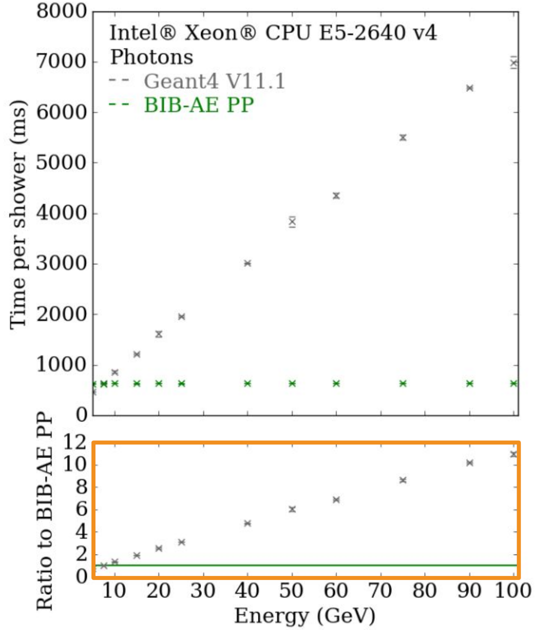


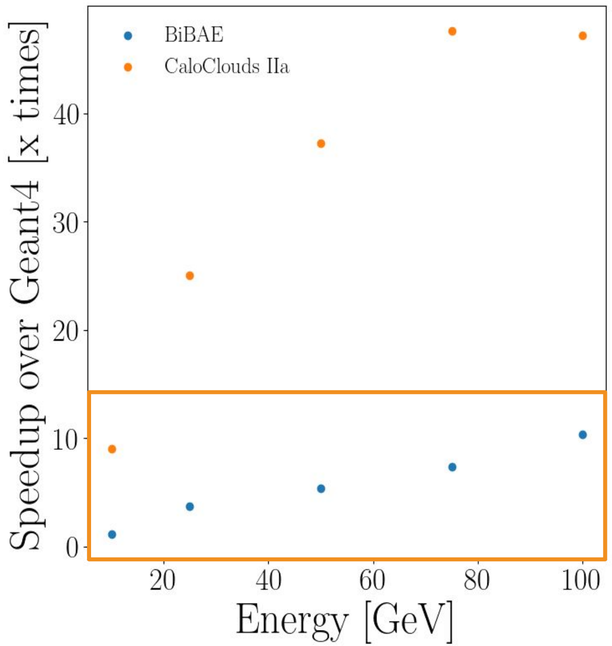
90 steps



Point Cloud + Diffusion Model

Speedup, CaloClouds III vs BiBAE





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Integration into Simulation Chain

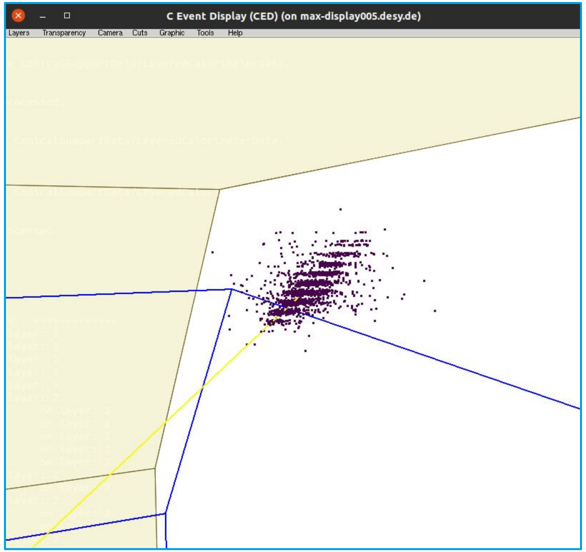
DDFastShowerML

PyTorch

Scripted fast sim model

DDFastShowerML

https://gitlab.desy.de/ilcsoft/ddfastshowerml



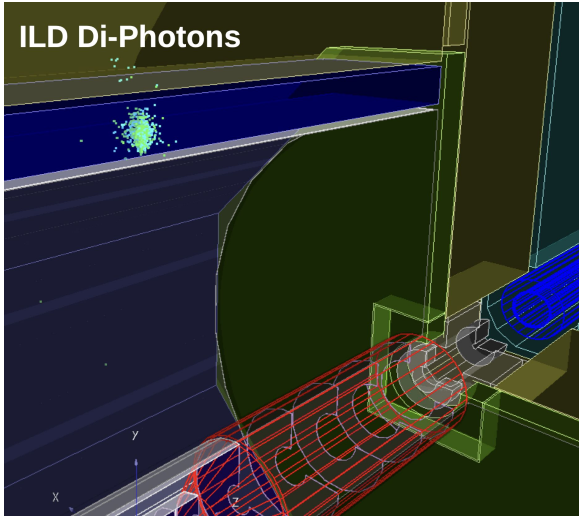
50 GeV photon shower generated with CaloClouds in the ILD ECAL

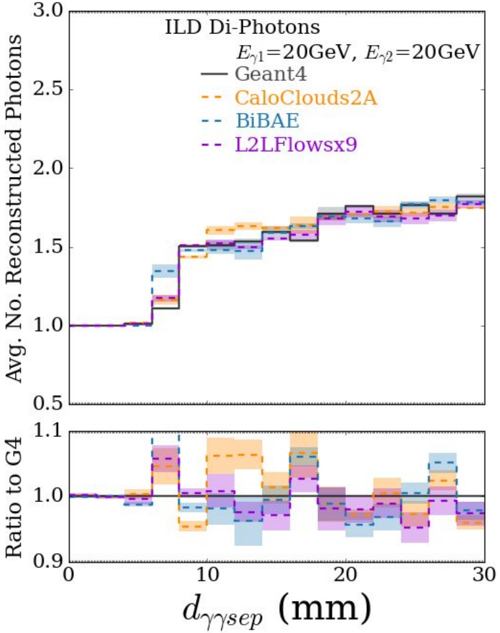
Easy to use library which can be adapted for all types of ML architectures in DD4hep

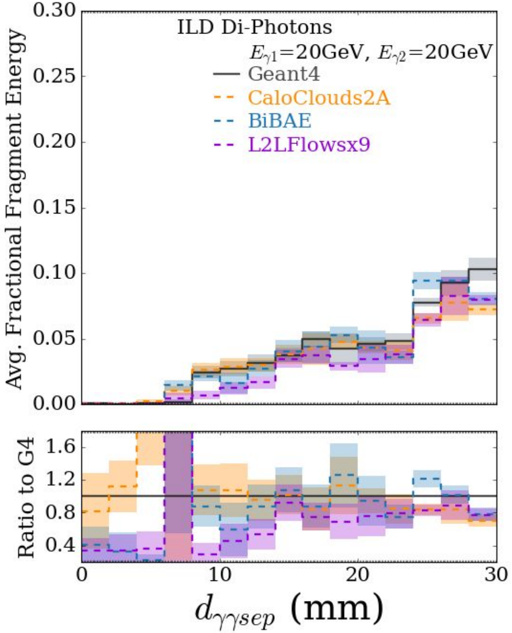
Di-Photons Reconstruction Benchmark

Two Photons Orthogonal to the Face of ILD ECAL

Courtesy P.McKeown







Di-Photon Reconstruction Benchmark provides a direct **physically relevant** quantification of model performance

Summary

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2305.04847**

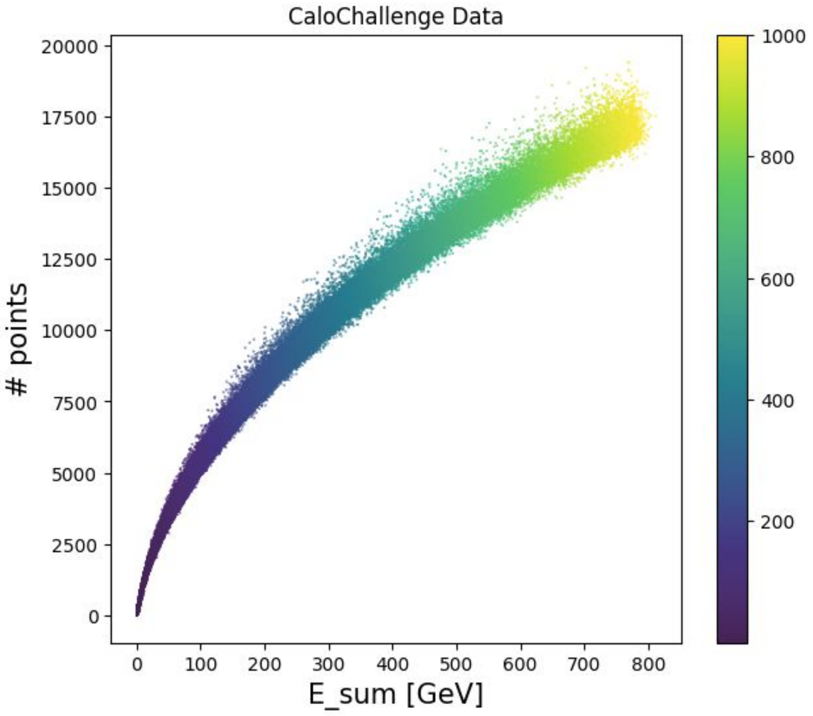
CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, AK, et al. 2023, **arXiv:2309.05704**

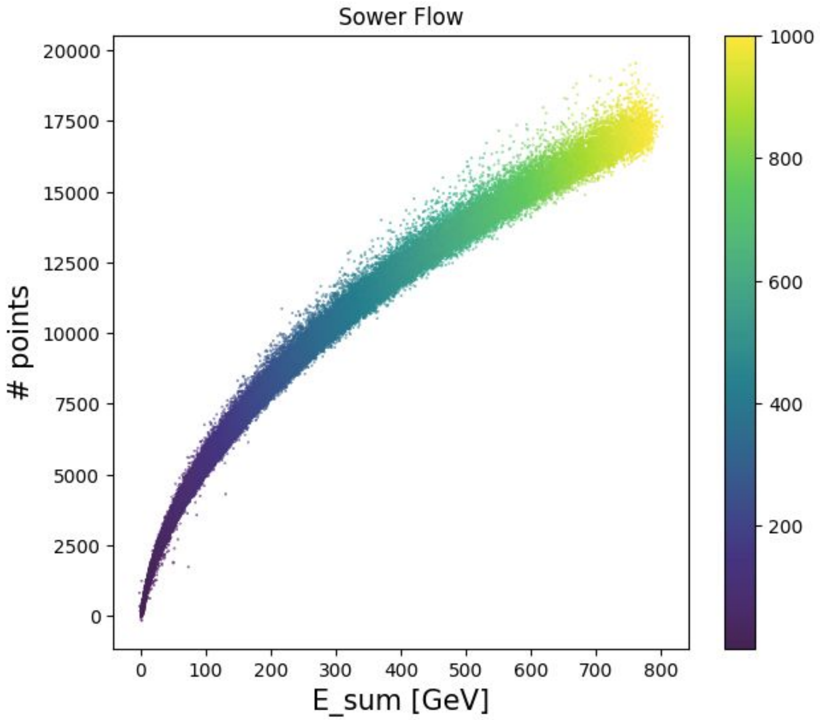
- Investigated new generative model architecture for generating EM showers in highly-granular calorimeters
- The fidelity of CaloClouds' physical properties is competitive with SOTA models (BiBAE, L2LFlows), while offering ~x6 faster inference
- Model integrated into existing software ecosystem
- Next steps: more in depth study of physics benchmarks

BACKUP SLIDES

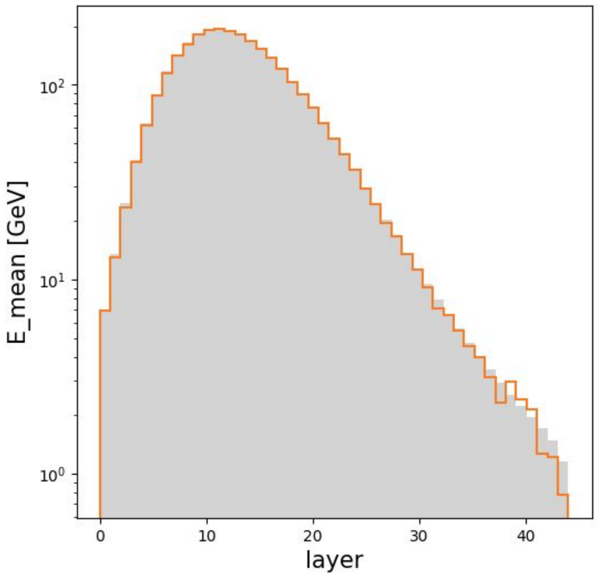
Shower Flow

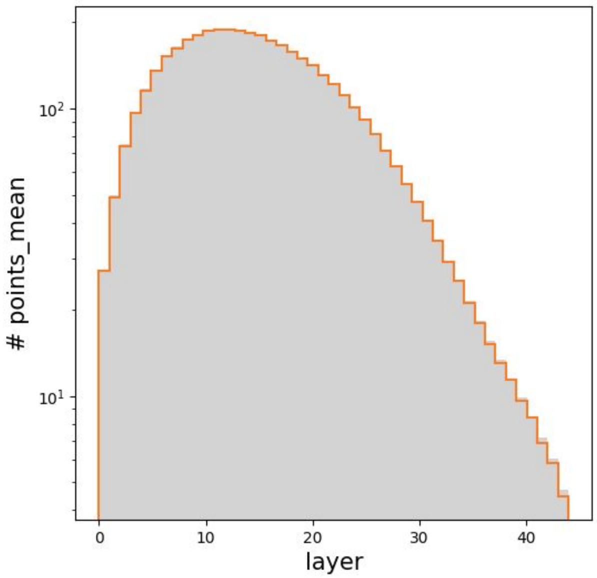
Results

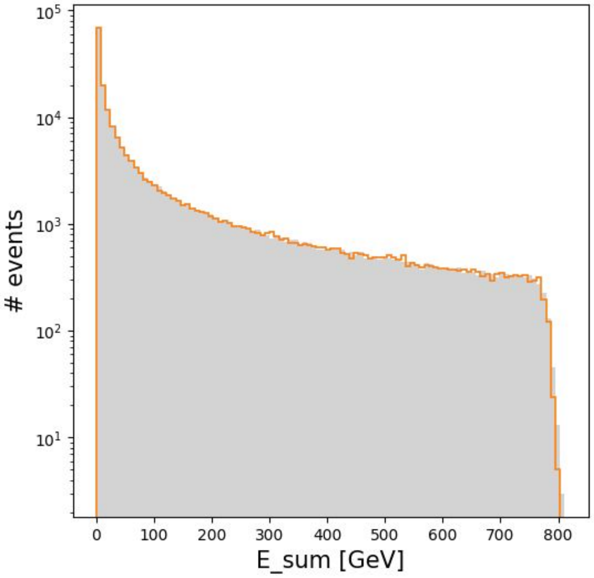




Shower Flow
Results

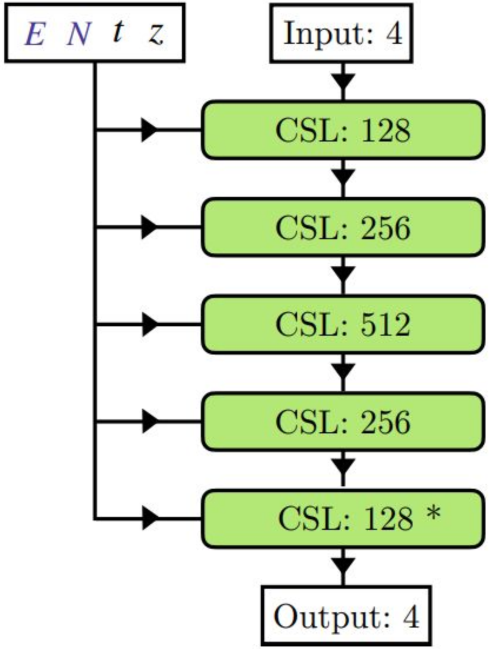




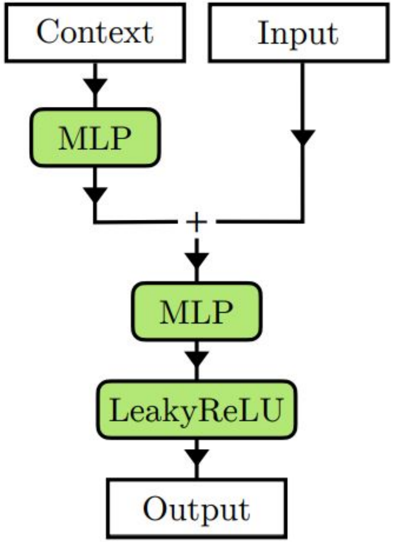


Point Cloud + Diffusion Model

PointWise Net



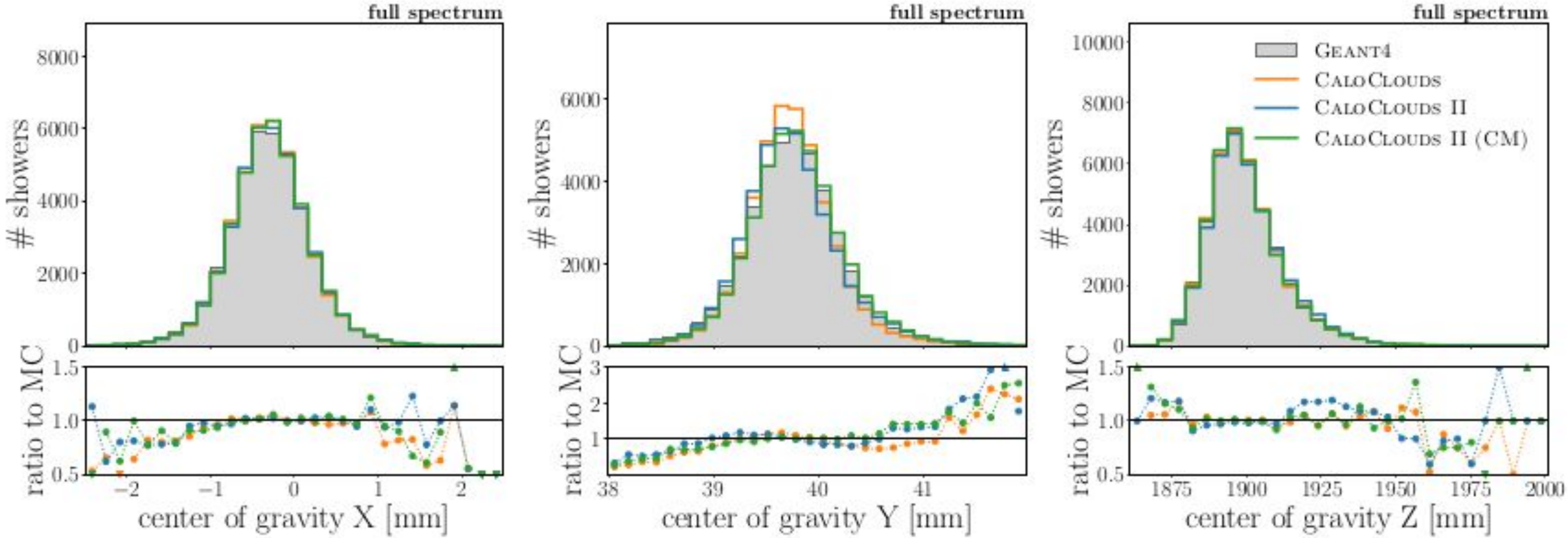
(a) PointWise Net



(b) ConcatSquash Layer (CSL)

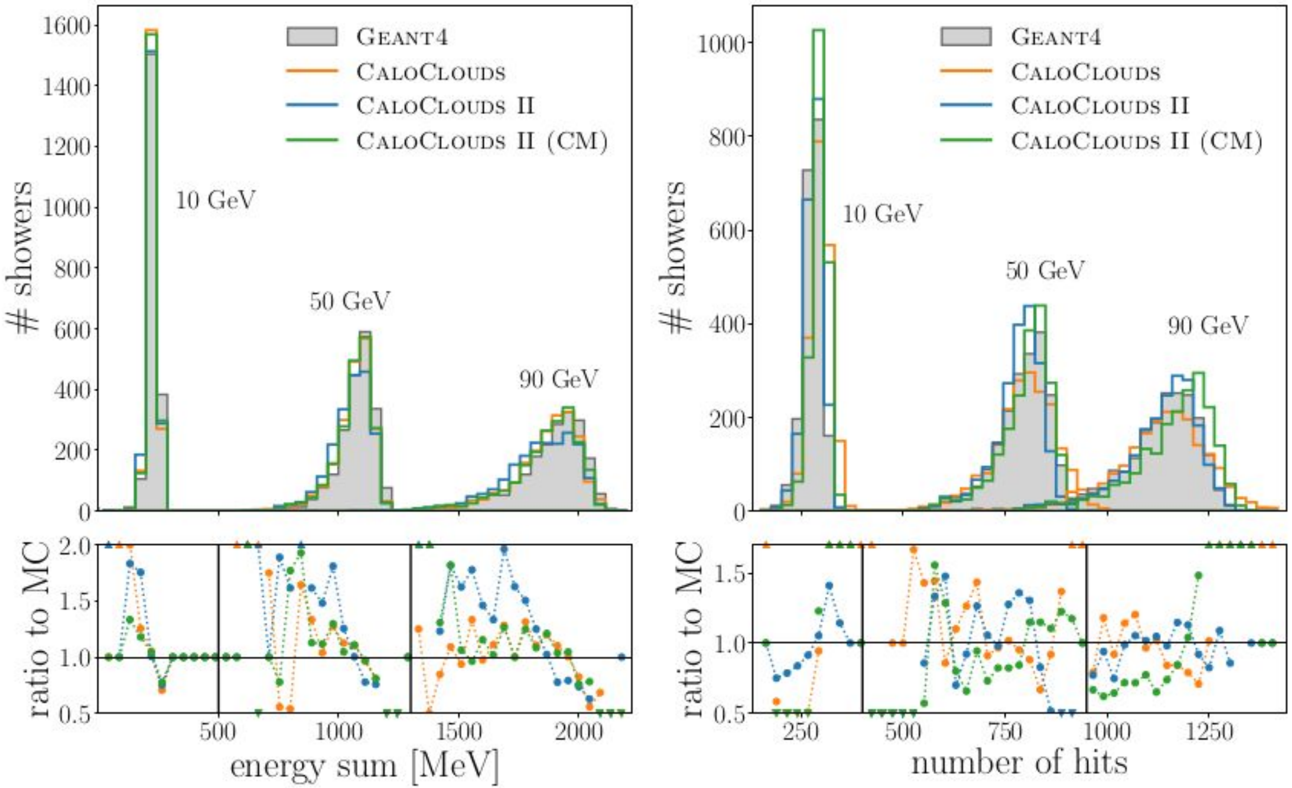
Point Cloud + Diffusion Model

Results, Position of the Center of Gravity



Point Cloud + Diffusion Model

Results, Visible Energy and the Number of Hits

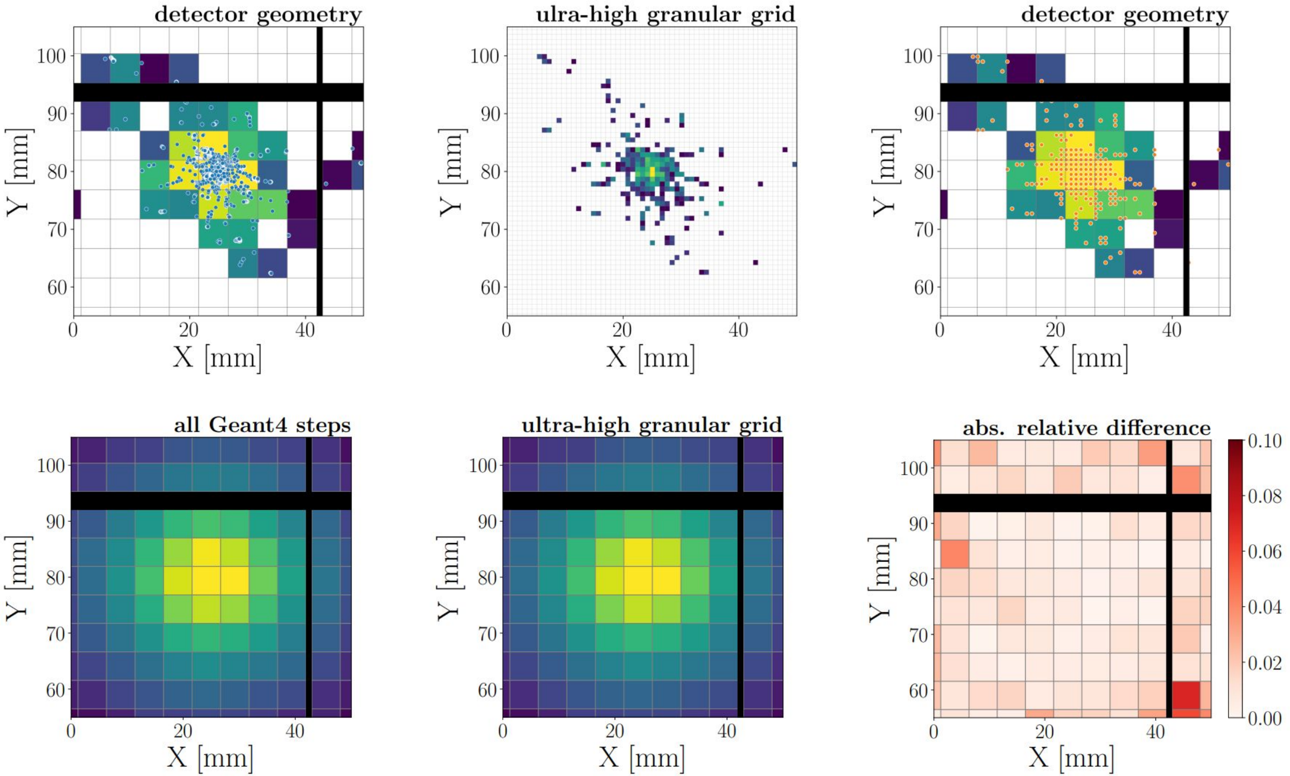


Point Cloud Representation of the EM Showers

Effects of the Pre-Clustering

Single event of 90 GeV shower in 21th layer

2k events of 90 GeV showers in 21th layer, overlay



Point Cloud Representation of the EM Showers

Effects of the Pre-Clustering