Generative Modeling for Fast Simulation of Highly Granular Calorimeters in HEP

KISS Annual Meeting 2024, Hamburg

E. Buhmann[2], T. Buss[2], S. Diefenbacher[3], E. Eren[1], F. Gaede[1], G. Kasieczka[2], W. Korcari[2], **A. Korol**[1*], K. Krüger[1], M. Mozzanica[2], P. McKeown[1], L. Valente[2]

[1] Deutsches Elektronen-Synchrotron, DESY
[2] University of Hamburg, UHH
[3] Lawrence Berkeley National Laboratory, LBNL
*anatolii.korol@desy.de

CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE
HELMHOLTZ

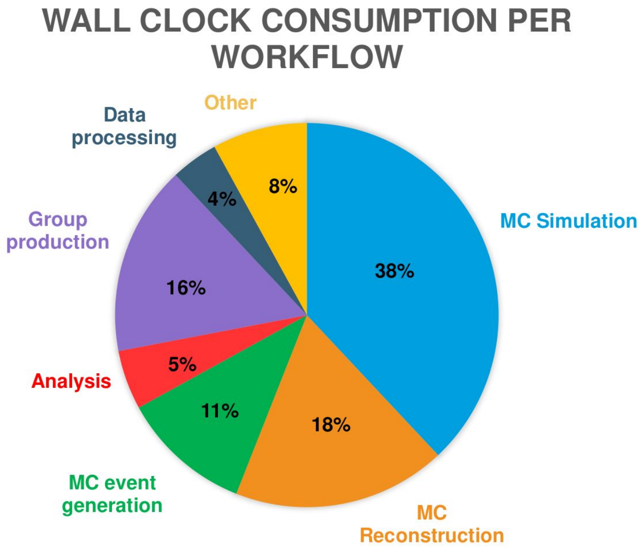
KISS

AIDA innova

Introduction

Time-consuming Simulations

- The most computationally expensive step in the simulation pipeline of a typical HEP experiment is **MC Simulation**
    - Calorimeters most intensive part of detector simulation



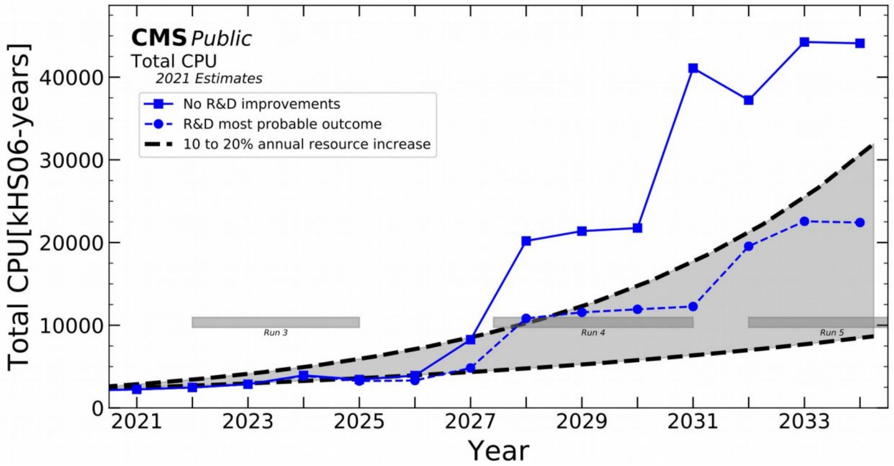
D. Costanzo, J. Catmore, ATLAS Computing update, LHCC meeting , 2019

Introduction

Time-consuming Simulations

- Projected computing resources required far outstrip what will be available
  - E.g High Luminosity LHC (HL-LHC)
- Future lepton colliders also benefit from much faster MC

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



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

Introduction

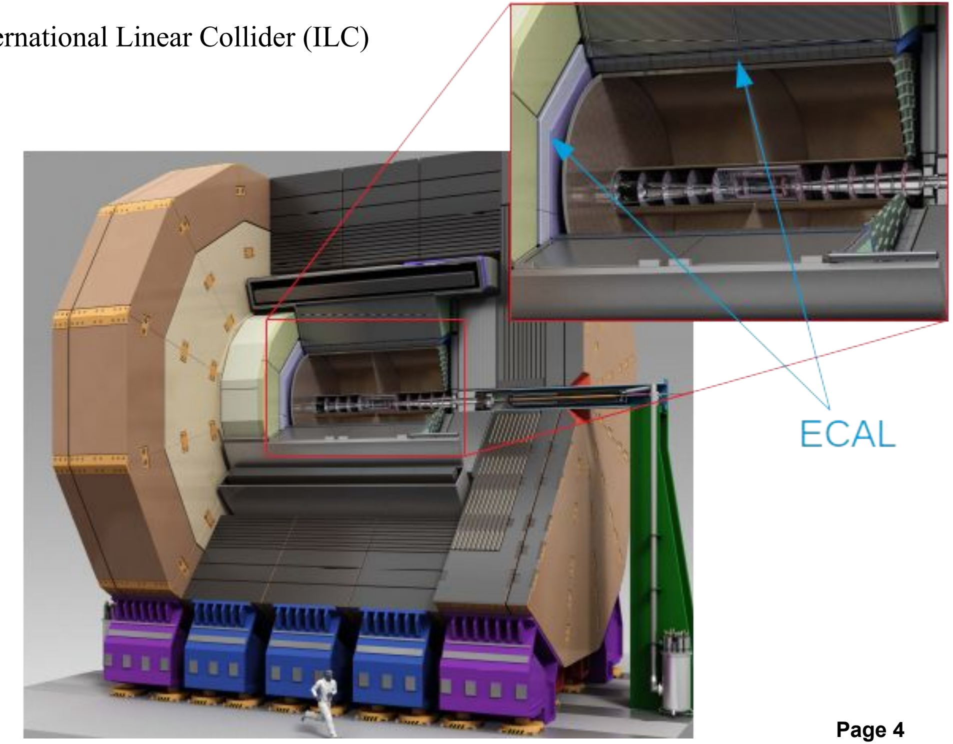
Highly Granular Calorimeters for Future Experiments

- Widely planned for future experiments: e.g. HL-LHC, e+e- Higgs Factories

- Case Study: International Large Detector (ILD) concept for the International Linear Collider (ILC)

- Optimized for Particle Flow
  - Reconstruct each individual particle in subdetector
  - Obtain optimal detector resolution

- High granularity calorimeters:
  - ECAL: Si-W - 5mm x 5mm
  - HCAL: Sci-Fe - 30mm x 30 mm



Introduction

Highly Granular Calorimeters for Future Experiments

- Widely planned for future experiments: e.g. HL-LHC, e+e- Higgs Factories

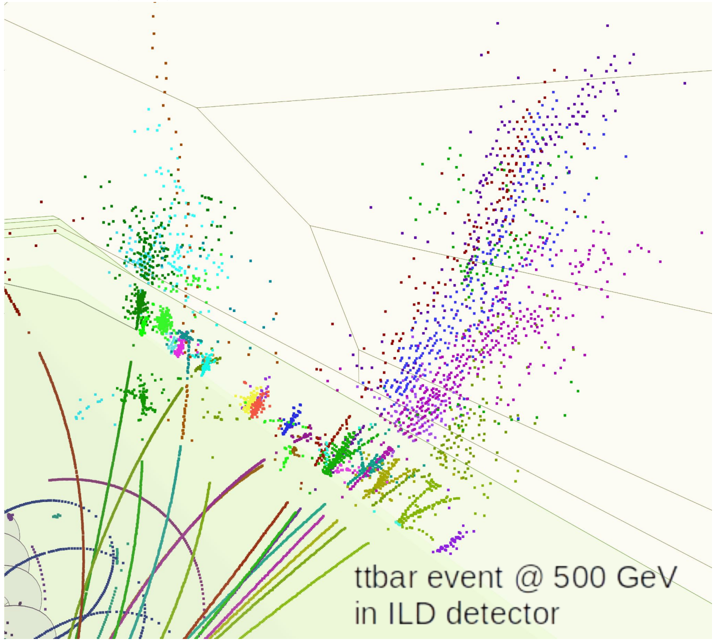
- Case Study: International Large Detector (ILD) concept for the International Linear Collider (ILC)

- Optimized for Particle Flow
  - Reconstruct each individual particle in subdetector
  - Obtain optimal detector resolution

- High granularity calorimeters:
  - ECAL: Si-W - 5mm x 5mm - ~ 80 million channels
  - HCAL: Sci-Fe - 30mm x 30 mm - ~ 8 million channels

c.f. a few cm2 for ATLAS/CMS ECAL (before High Lumi)

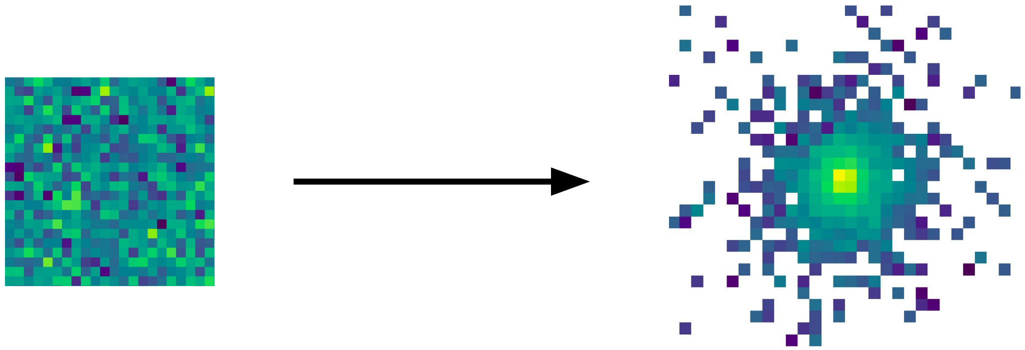
High granularity ⟶ **Need for high fidelity simulation**



Introduction

Generative Models

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

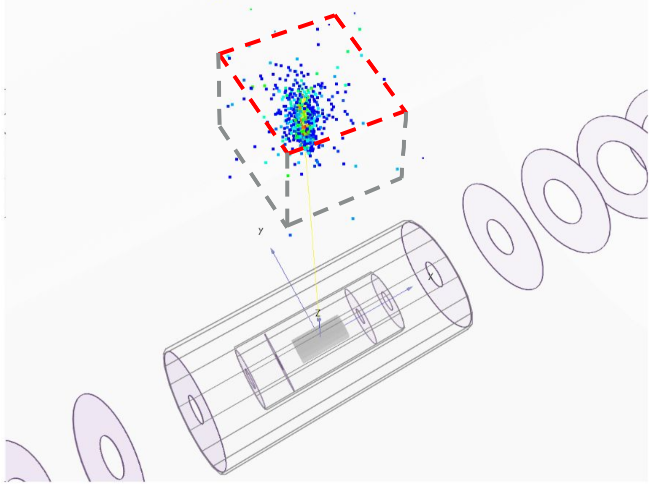


- There exist numerous generative models
    - Generative Adversarial Networks (GANs)
    - Flow-based models
    - Autoencoders (AE), e.g. BiB-AE
    - Diffuison Models (DMs)

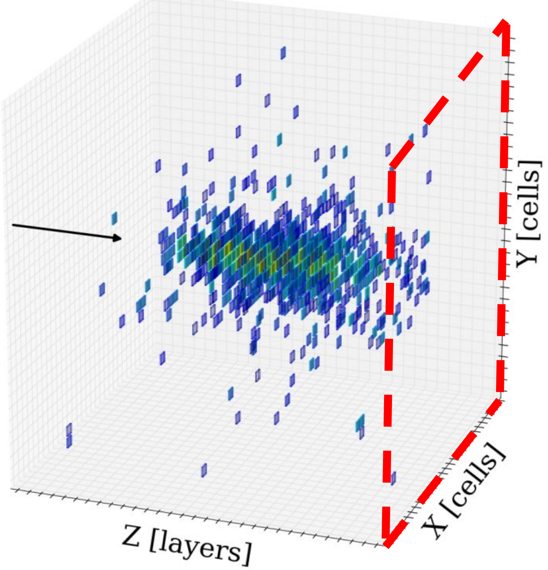
Image Representation of the EM Showers

ILD Detector

A simulated 60 GeV photon shower in the ILD detector



Regular grid 30x30x30

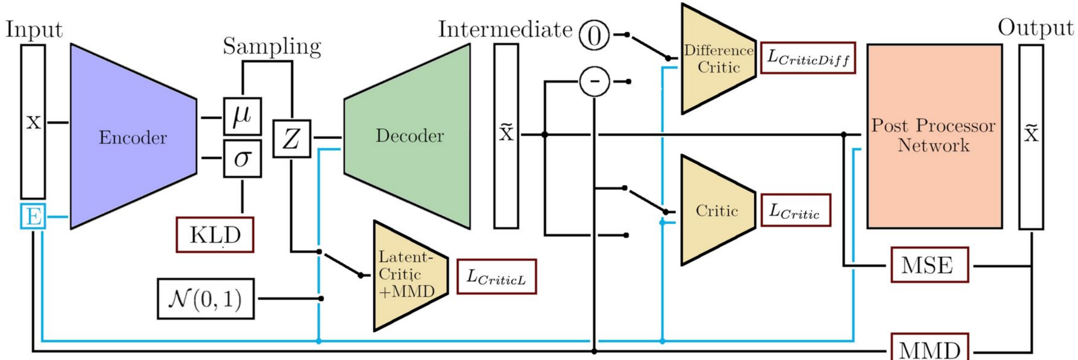


One to one mapping from detector geometry to a regular grid

Progress on 3D Regular Grid

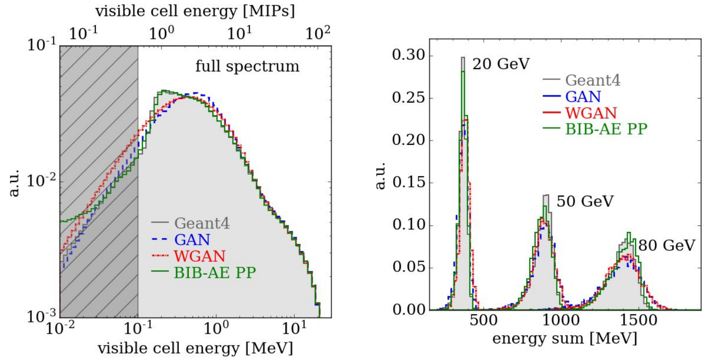
Photons and Pions

- Achieved **high fidelity** generation of **photon** and **pion** showers with **BIB-AE** architecture (and post processing)
- 90 deg impact angle, fixed position in calorimeter
- Fixed regular 3D grid geometry (O(10-100k) voxels)

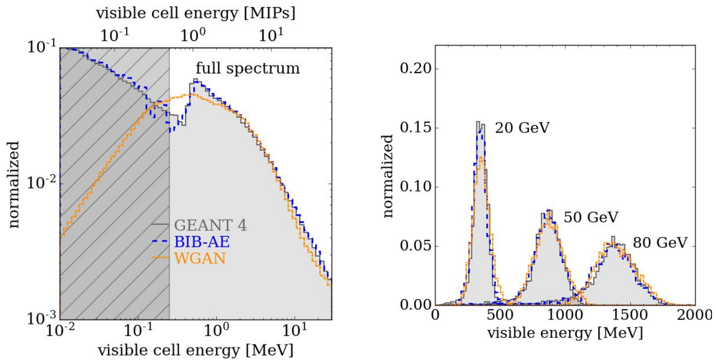


BIB-AE: Bounded Information Bottleneck Autoencoder

as well as comparison to GAN and WGAN …



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

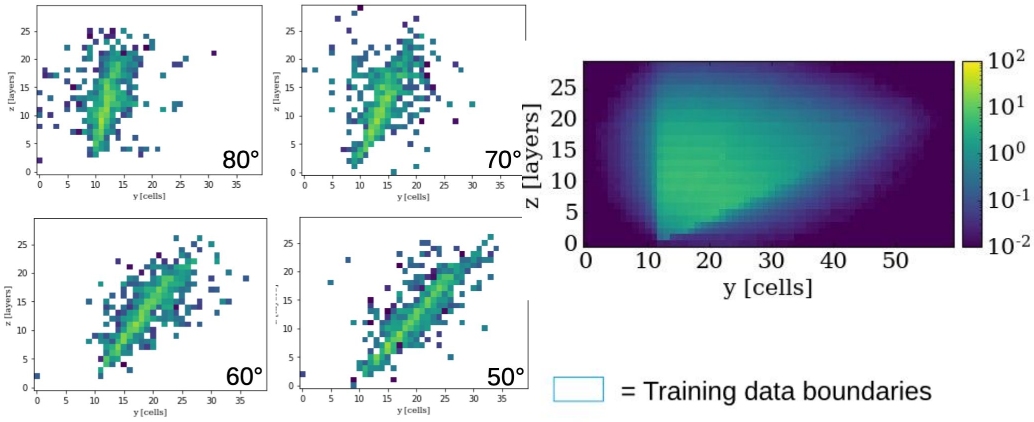


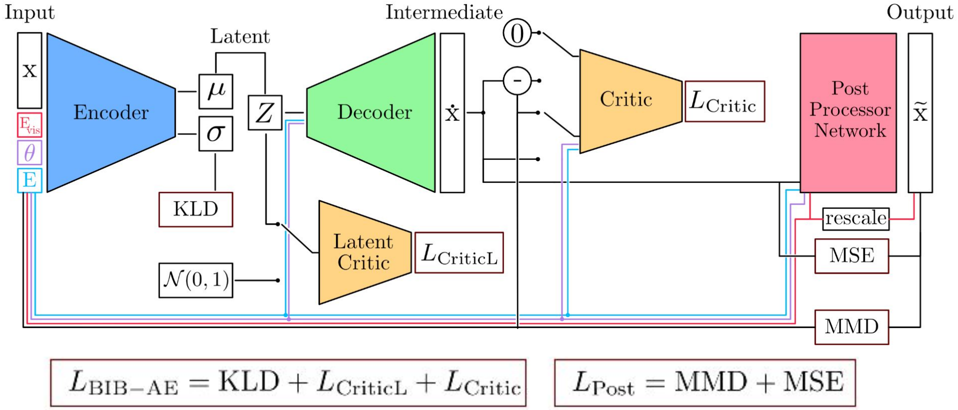
Hadrons, Better, Faster, Stronger
Buhmann, et al., **arXiv:2112.09709**, MLST 3 2, 025014 (2022)

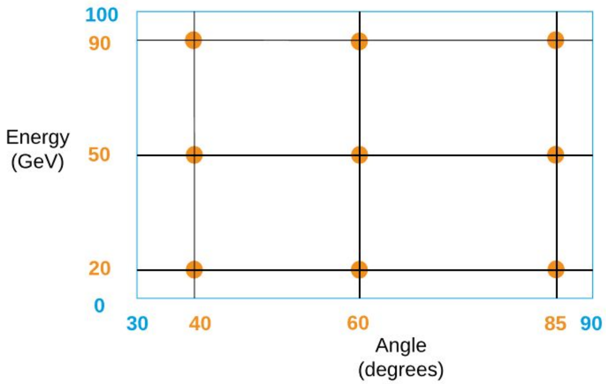
Progress on 3D Regular Grid

Energy and Angular Conditioning

- Photons incident at fixed position
- Extend BIB-AE architecture
- **Vary incident energy and polar angle**
  - Large training sample - 500k showers
  - Uniform in [10-100 GeV, 30-90 deg]
  - Test/validation samples at dedicated energies and angles



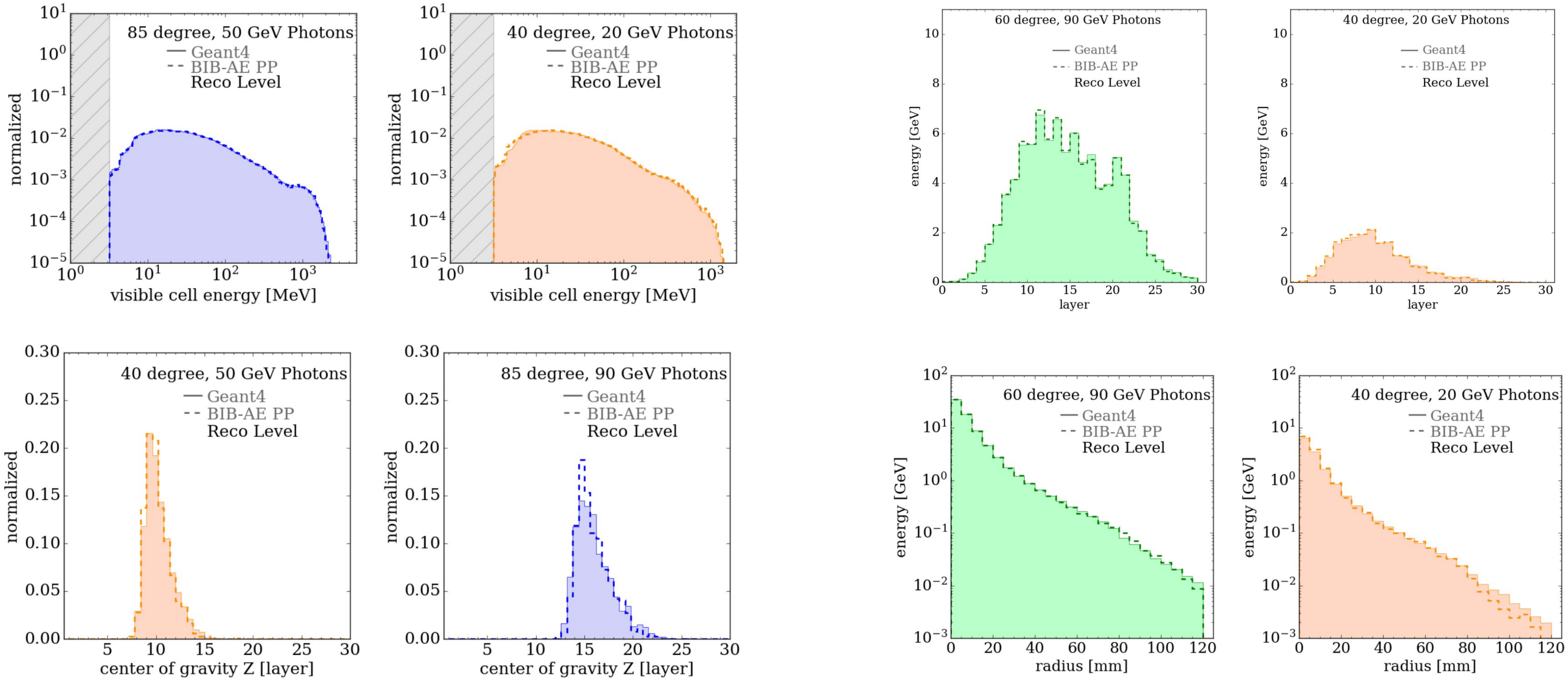




Progress on 3D Regular Grid

Energy and Angular Conditioning, Performance After Reconstruction

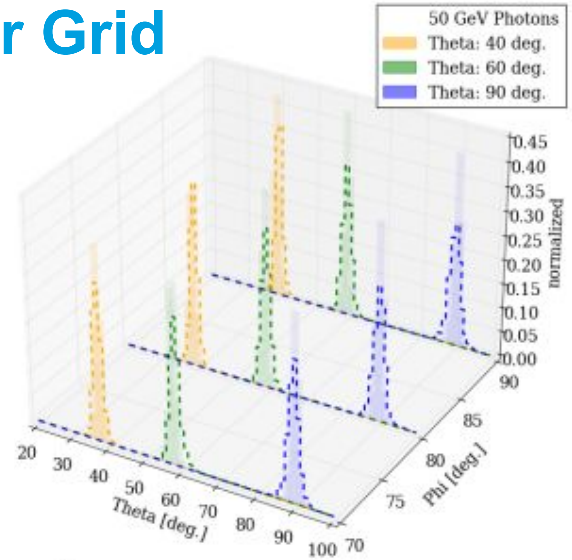
New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, et al., 2023 MLST in press
DOI 10.1088/2632-2153/acefa9, **arXiv: 2303.18150**

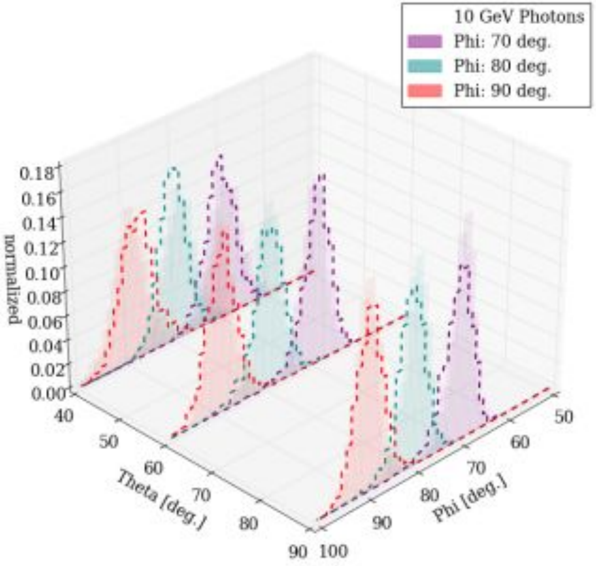


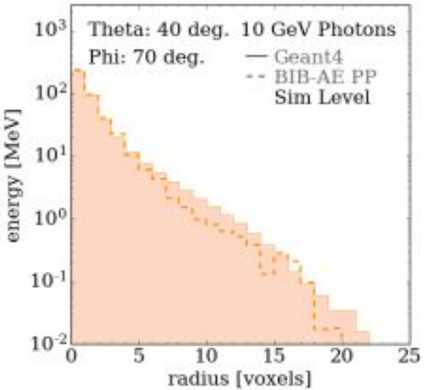
Progress on 3D Regular Grid

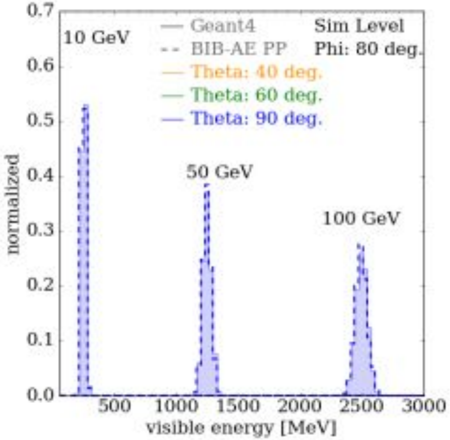
Adding Another Angle

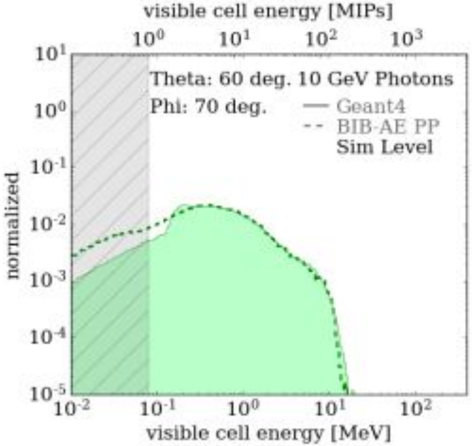
- Need to condition on **energy, theta and phi** for full application
- **Extending phase space** can be challenging





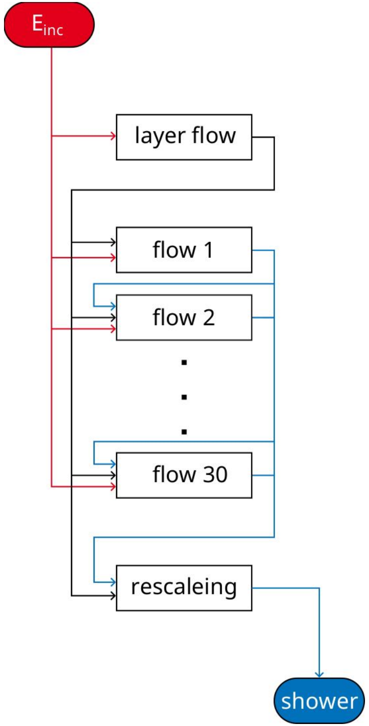


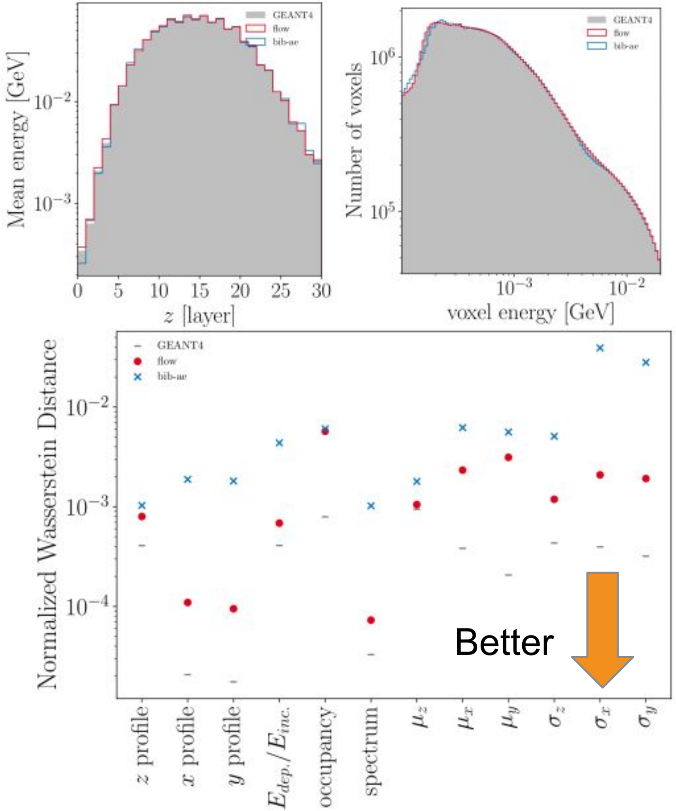




Progress on 3D Regular Grid

Layer-to-Layer Normalising Flow Model





[1] **Fast and accurate simulations of calorimeter showers with normalizing flows**,
Krause & Shih., **Phys. Rev. D 107, 113003**

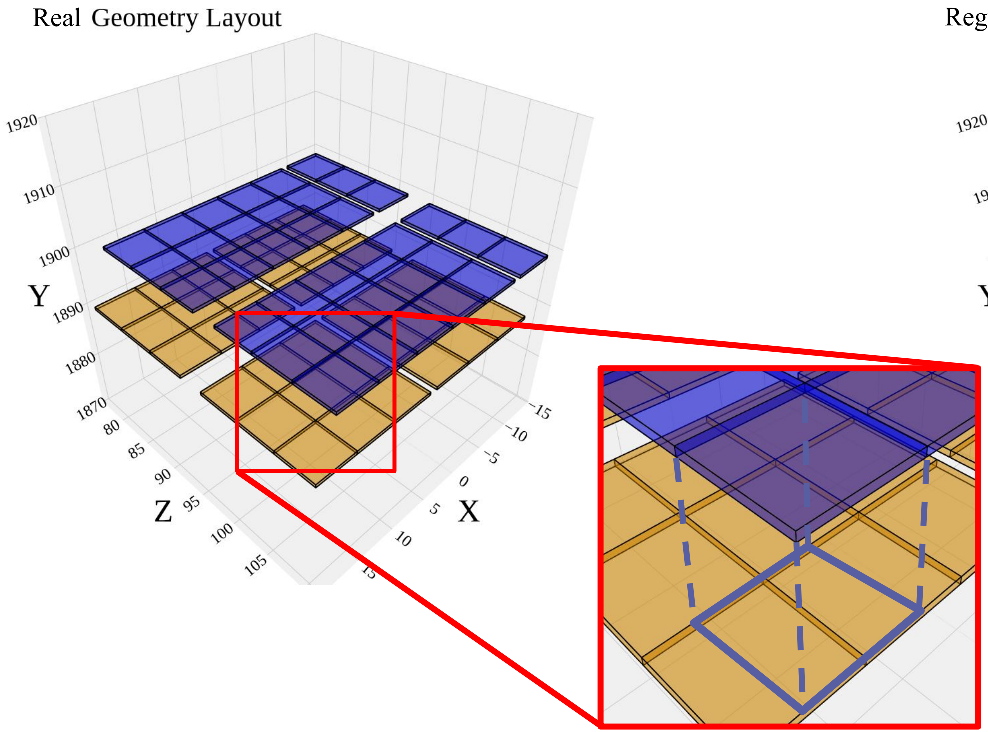
[2] **L2LFlows: Generating High-Fidelity 3D Calorimeter Images**,
Diefenbacher et al., **arXiv:2302.11594**

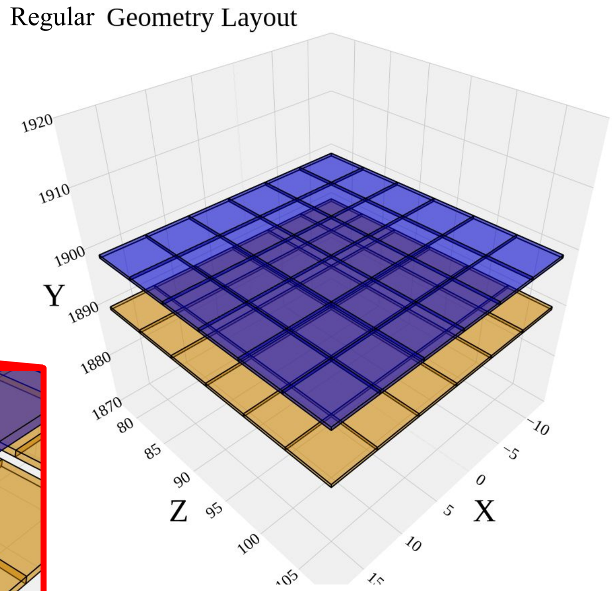
Convolutional L2LFlows: Generating Accurate Showers in Highly Granular Calorimeters Using Convolutional Normalizing Flows,
Buss et al., **coming soon on arXiv…**

- Fully **invertible model**
- Learns to **sequentially** produce shower shape in each layer
- Extends previous work [1,2] to scale to full shower
- **Superior** simulation-level **performance** vs a BIB-AE across a range of observables
- More work required to achieve competitive simulation speed

Problems with Image Representation of the EM Showers

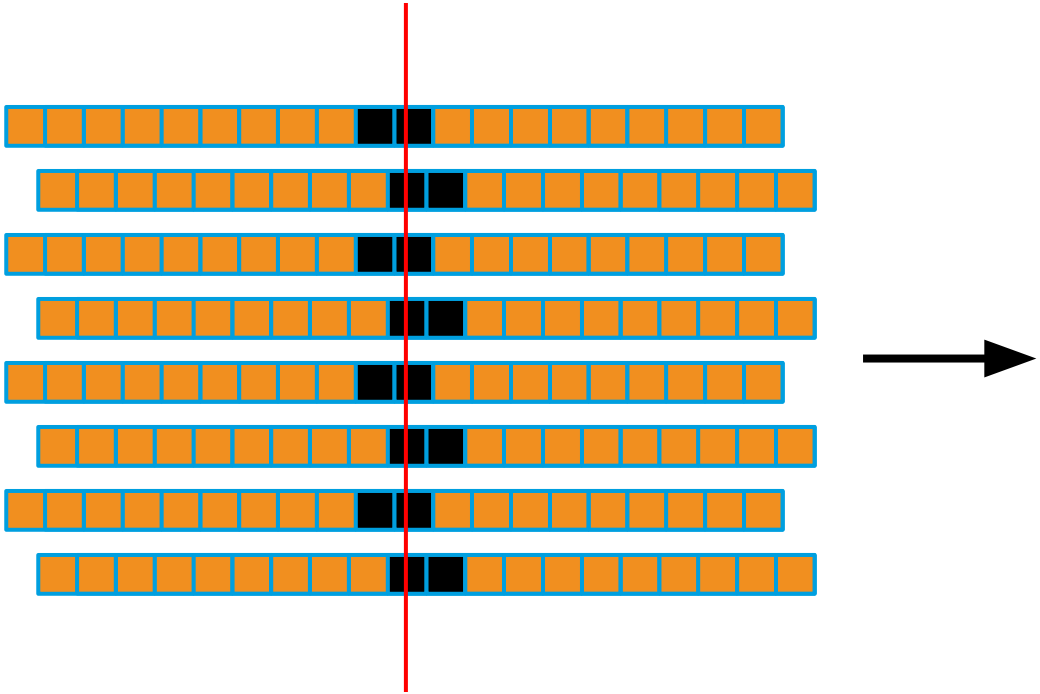
ILD Detector, ECAL Layers Structure

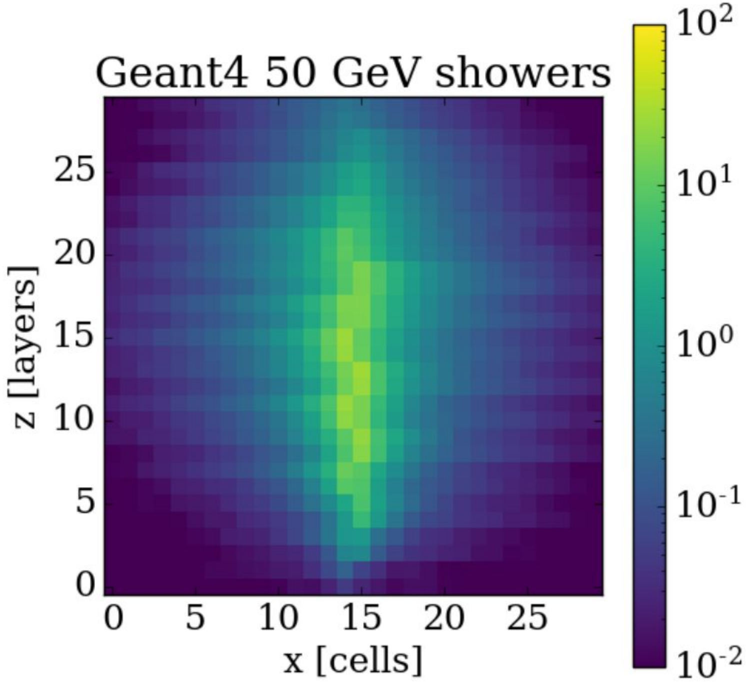




Problems with Image Representation of the EM Showers

ILD Detector, ECAL Layers Structure, Staggering Effect





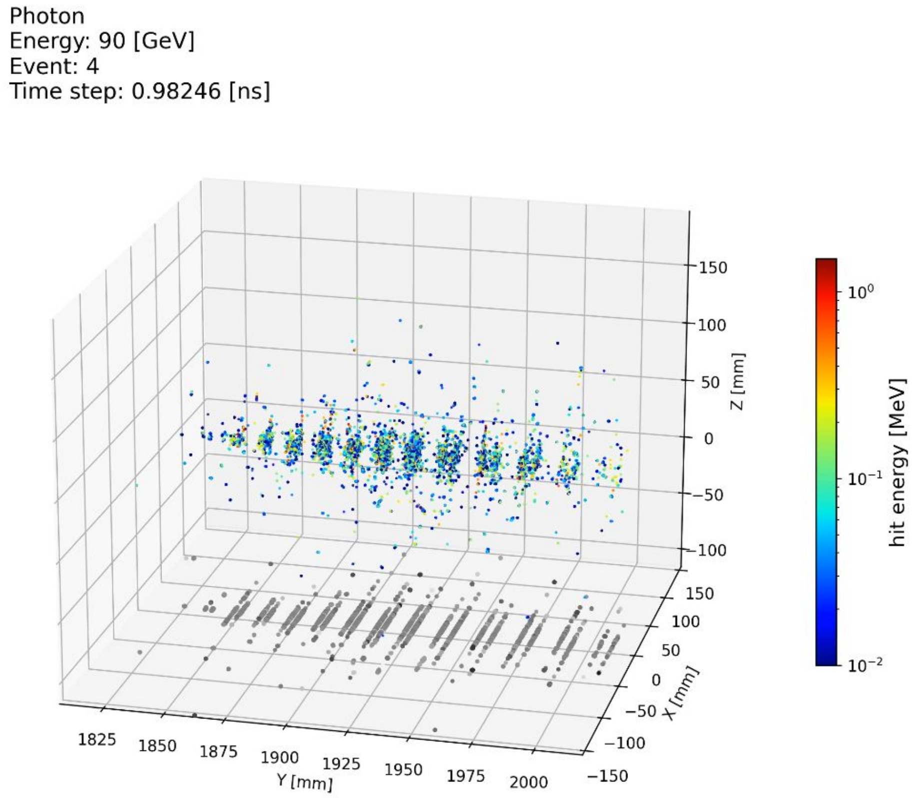
Models have to learn not only EM shower properties, but also geometry “artifacts”, like **staggering effect**

Point Cloud Representation of the EM Showers

GEANT4 Steps

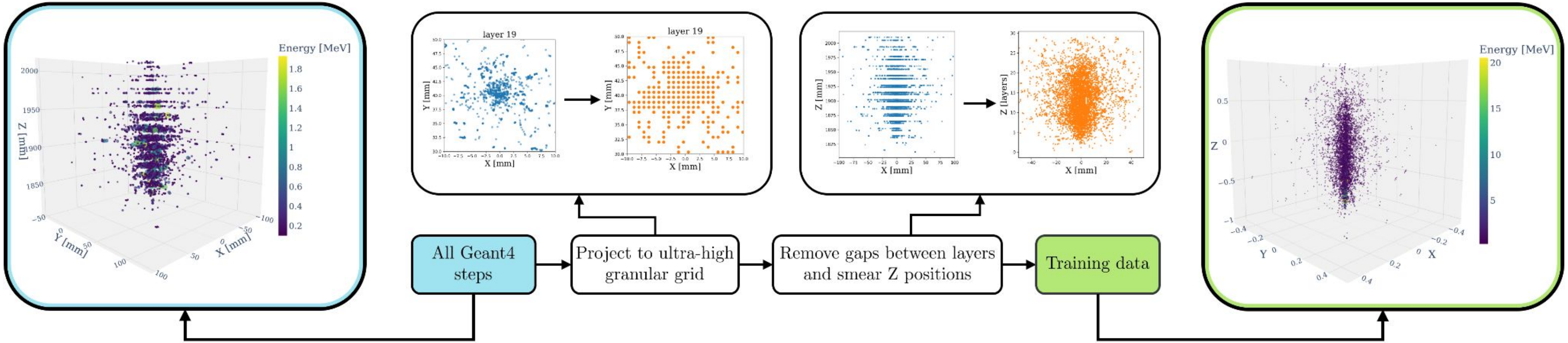
A way to overcome potential issues from irregular (realistic) cell geometry would be to use much higher granularity/resolution

- 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

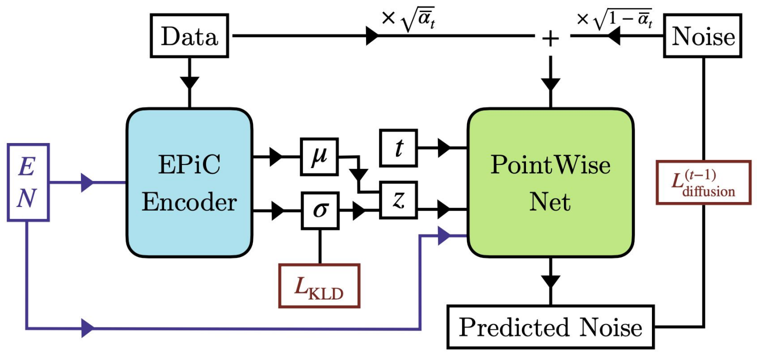


Number of points reduced to ~6k per shower, high enough resolution to move the shower in different place without harming physical properties of the shower

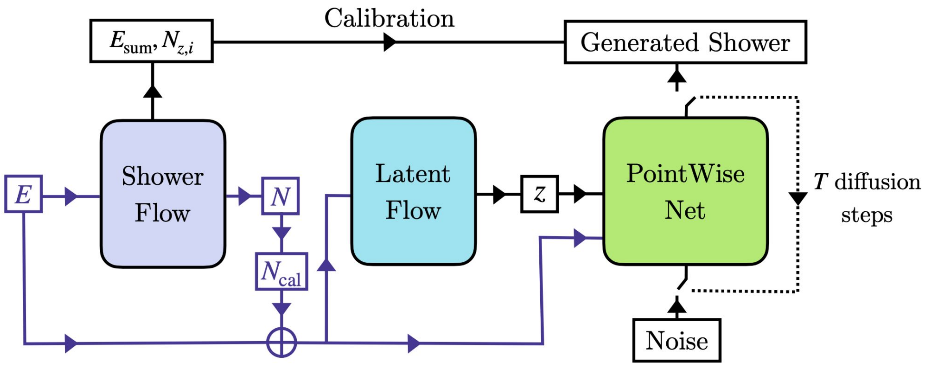
Point Cloud + Diffusion Model

CaloClouds, Model Overview

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



(a) Training at random time step t

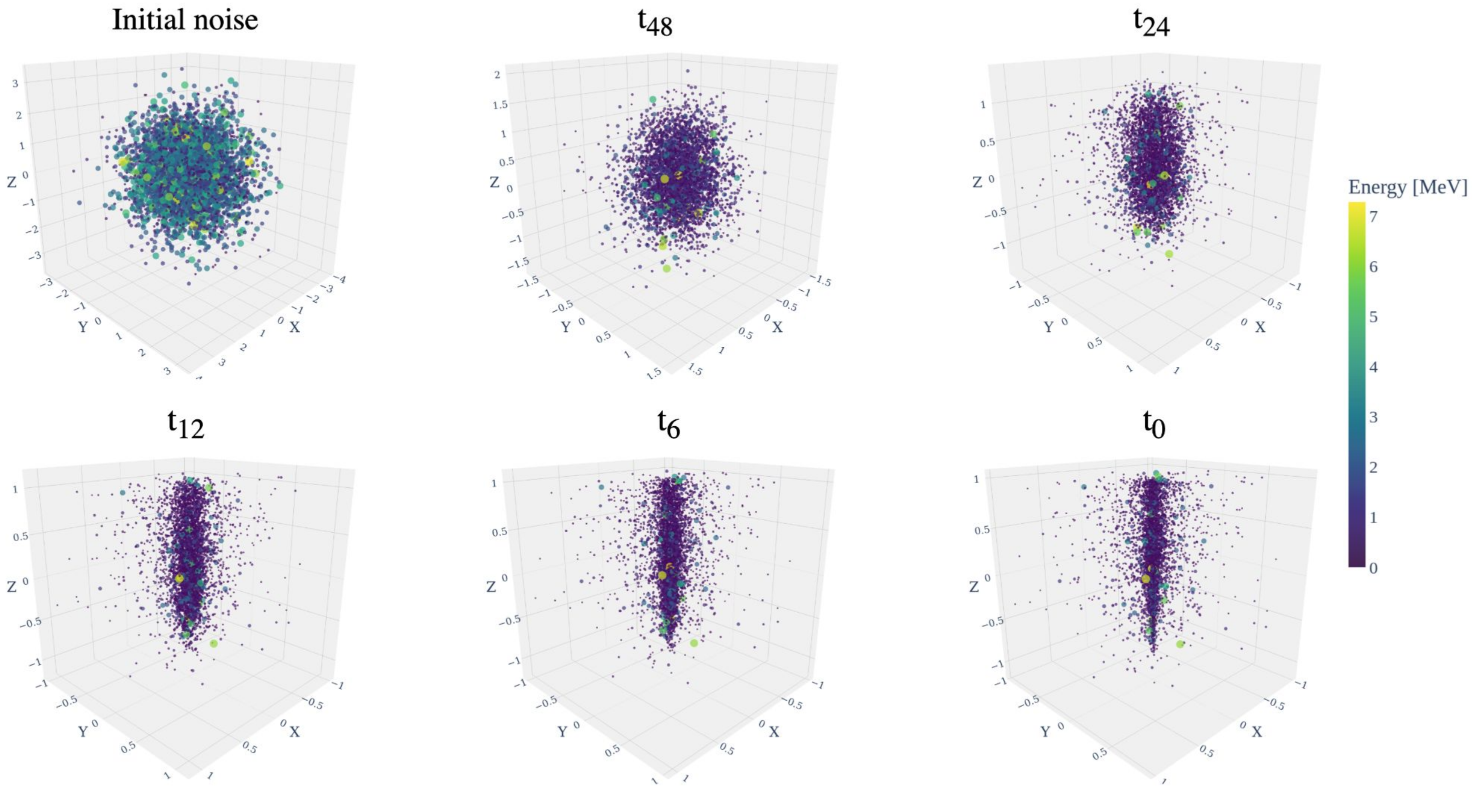


(b) Sampling with reverse diffusion through all time steps T

- 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

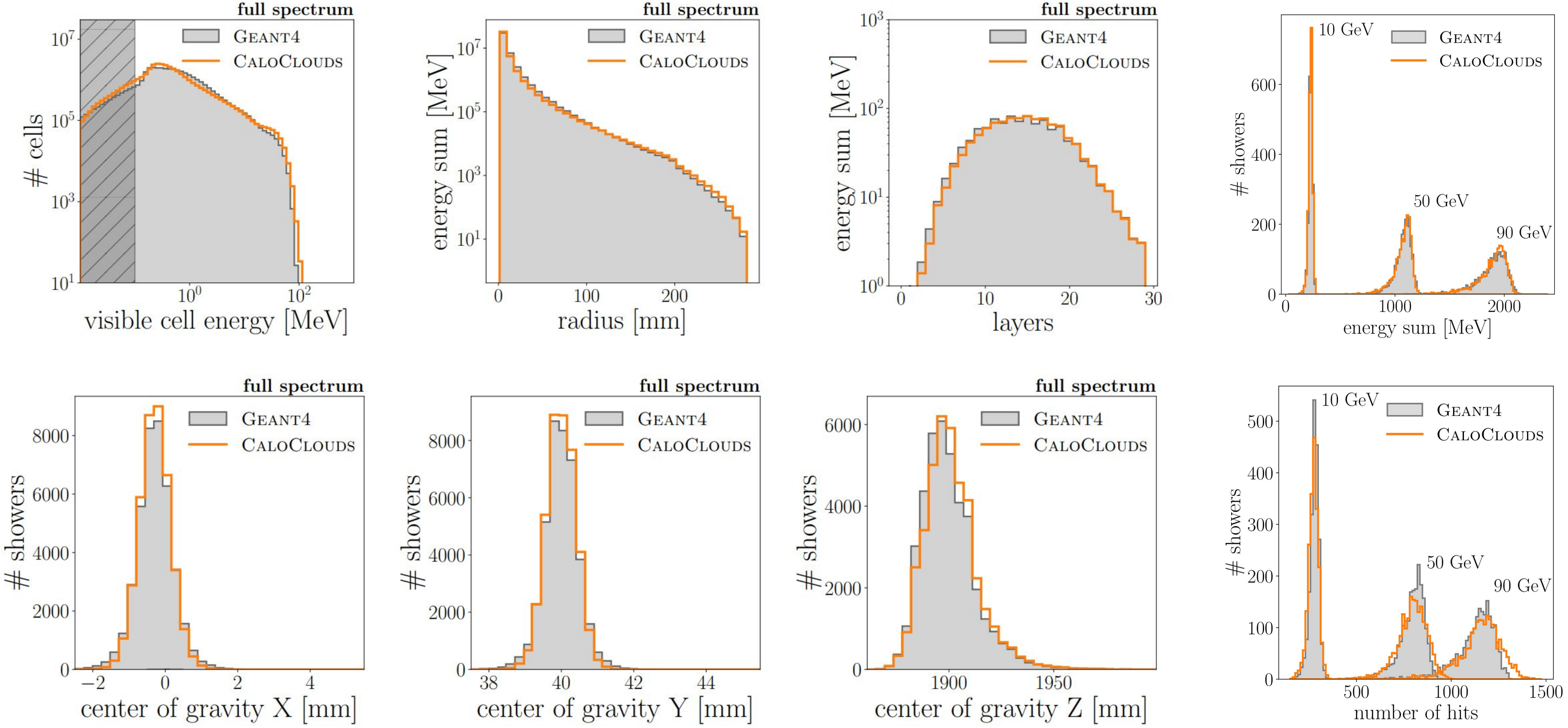
Reverse Diffusion Process



Point Cloud + Diffusion Model

Results

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

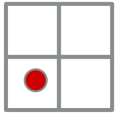


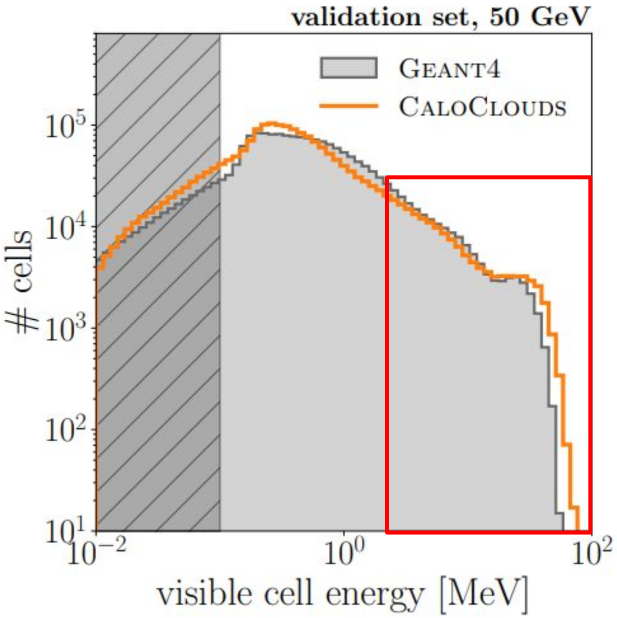
Point Cloud + Diffusion Model

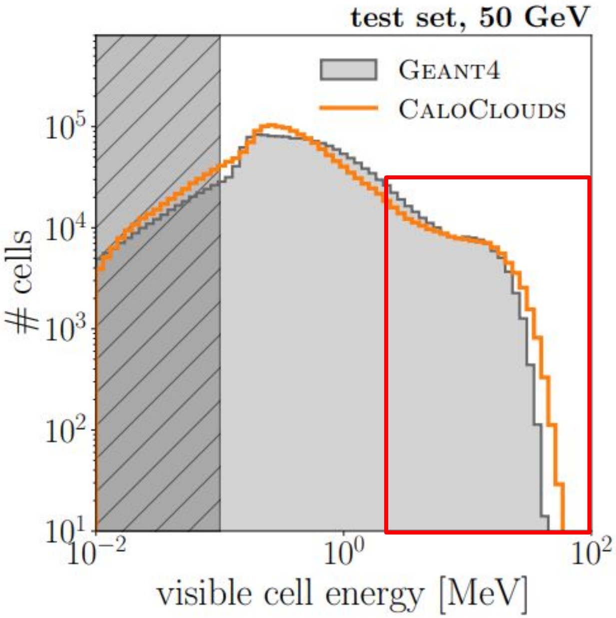
Results

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

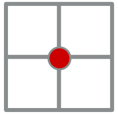
validation incident point pos.







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

Results

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

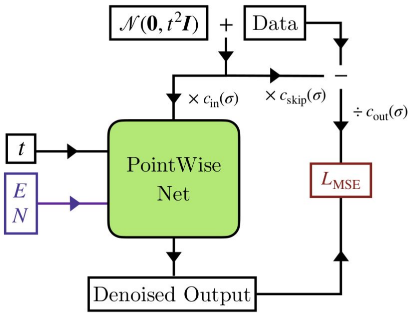
Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	4082 ± 170	$\times 1$
	CALOCLOUDS	3509 ± 220	$\times 1.2$
GPU	CALOCLOUDS	38 ± 3	$\times 107$

Not impressive inference time

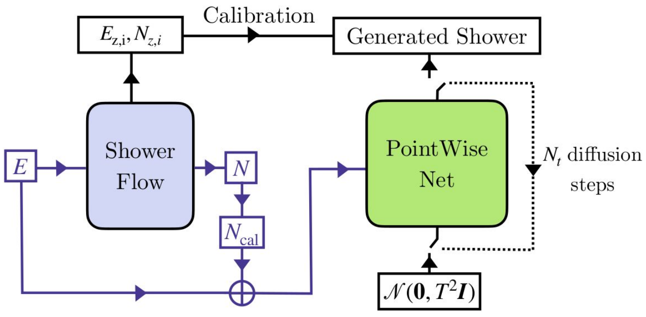
Point Cloud + Diffusion Model

CaloClouds II, Model Overview

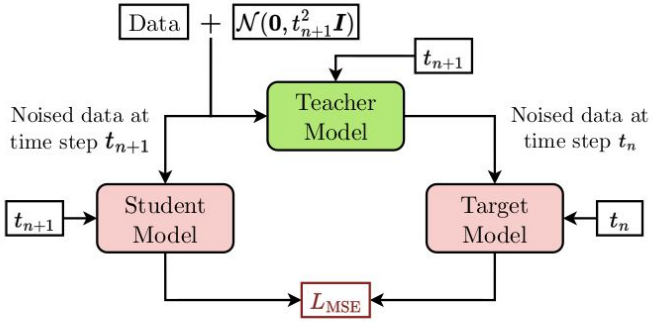
CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, et al. 2023, **arXiv:2309.05704**



(a) Training



(b) Sampling



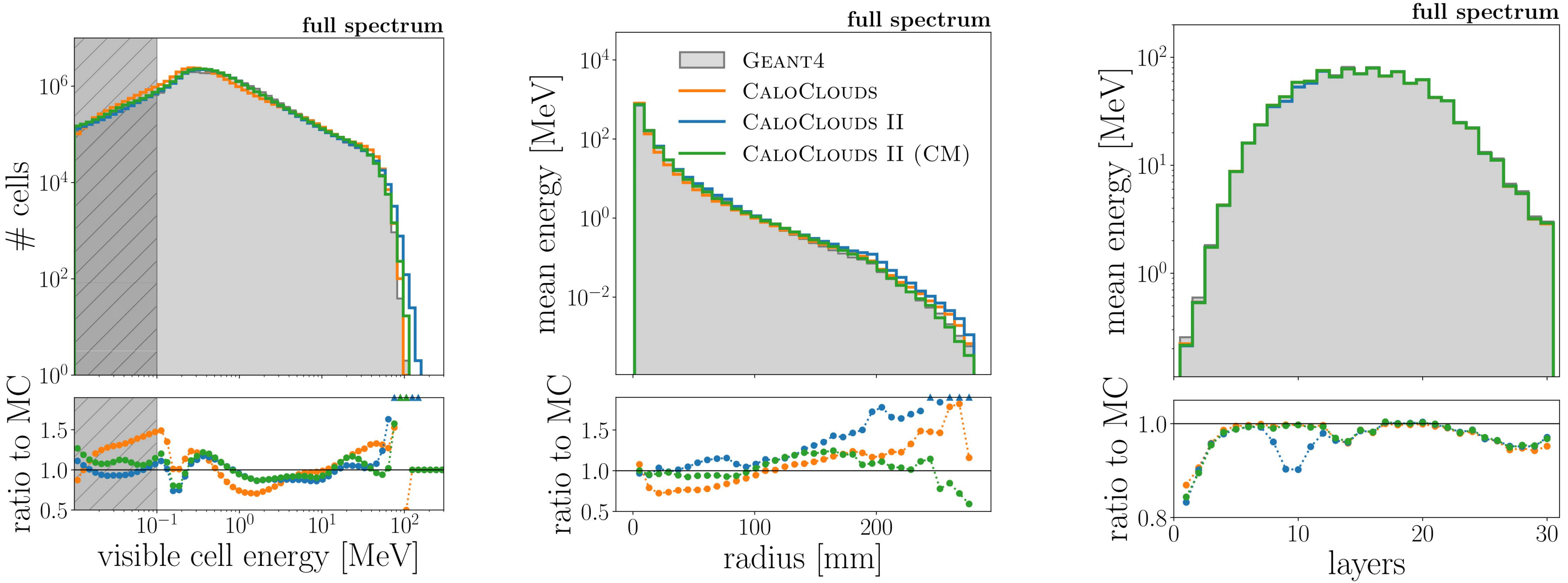
Consistency Distillation

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

Point Cloud + Diffusion Model

Results

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



Point Cloud + Diffusion Model

Results

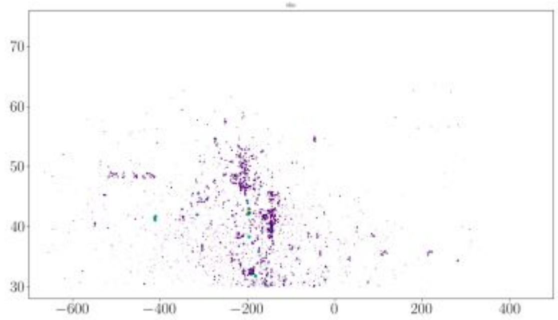
CaloClouds II: Ultra-Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, et al. 2023, **arXiv:2309.05704**

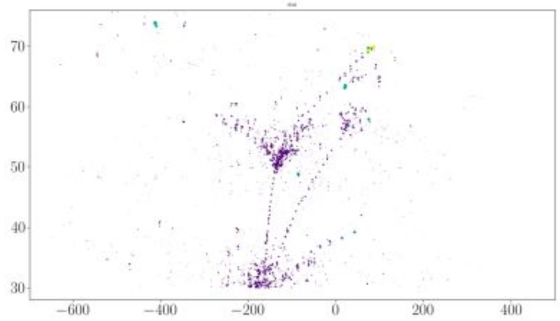
Hardware	Simulator	NFE	Batch Size	Time / Shower [ms]	Speed-up
CPU	GEANT4			3914.80 ± 74.09	$\times 1$
	CALOCLOUDS	100	1	3146.71 ± 31.66	$\times 1.2$
	CALOCLOUDS II	25	1	651.68 ± 4.21	$\times 6.0$
	CALOCLOUDS II (CM)	1	1	84.35 ± 0.22	$\times 46$
GPU	CALOCLOUDS	100	64	24.91 ± 0.72	$\times 157$
	CALOCLOUDS II	25	64	6.12 ± 0.13	$\times 640$
	CALOCLOUDS II (CM)	1	64	2.09 ± 0.13	$\times 1873$

Point Cloud + Diffusion Model

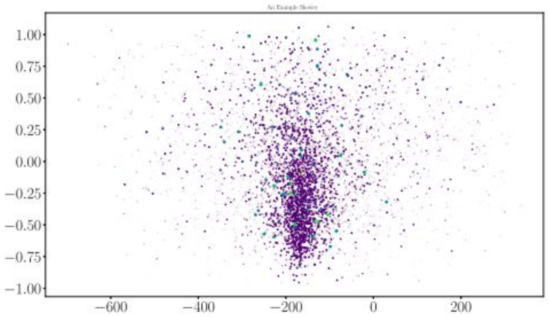
Development of Point Cloud Model for Pions

Geant 4 examples
Pi+ @ 50 GeV

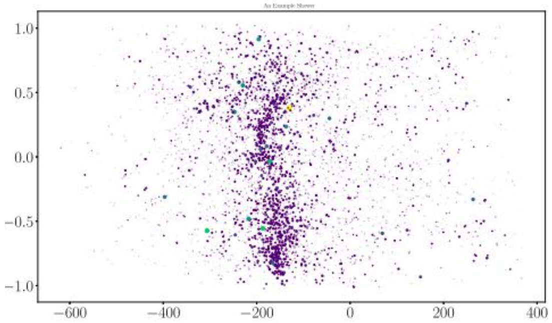




CaloClouds2



CaloClouds2 with Attention



Summary

BiB-AE Family

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

New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, et al., 2023 MLST in press **DOI 10.1088/2632-2153/acefa9**, **arXiv: 2303.18150**

Hadrons, Better, Faster, Stronger Buhmann, et al., **arXiv:2112.09709**, MLST 3 2, 025014 (2022)

High Fidelity / **High speed** / **Challenging to Scale** / **Challenging to Integrate**

CaloClouds Family

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

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

Fair Fidelity / **High speed** / **Easy to Scale** / **Layer Geometry Independent** / **Straightforward to Integrate**

Flows Family

Convolutional L2LFlows: Generating Accurate Showers in Highly Granular Calorimeters Using Convolutional Normalizing Flows, Buss et al., **coming soon on arXiv…**

L2LFlows: Generating High-Fidelity 3D Calorimeter Images, Diefenbacher et al., **arXiv:2302.11594**

Ultimate Fidelity / **Fair speed** / **Challenging to Scale** / **Layer Geometry Independent** / **Straightforward to Integrate**

BACKUP SLIDES

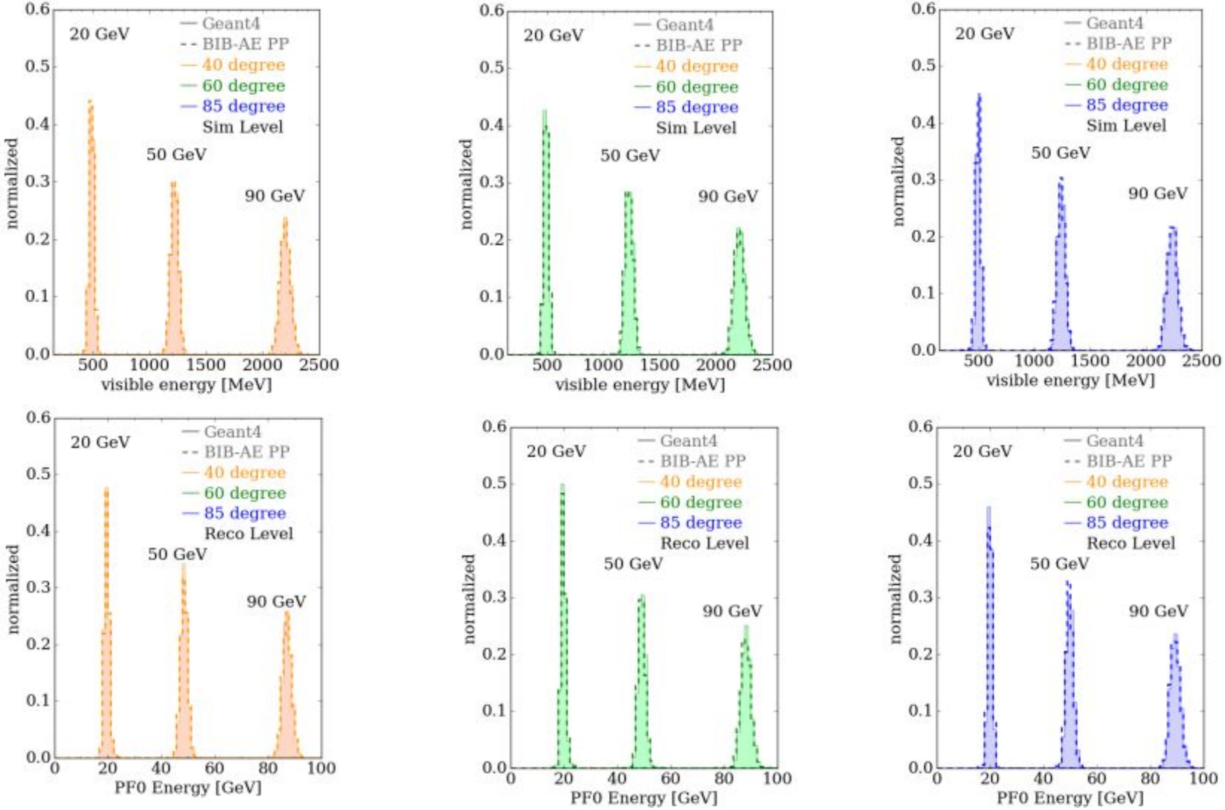
New Angles

Energy Conditioning Performance

New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, et al. 2023 MLST in press
DOI 10.1088/2632-2153/acefa9, **arXiv: 2303.18150**

- **Sim** level visible energy

- **Rec** level calibrated energy
  - After full PandoraPFA reco

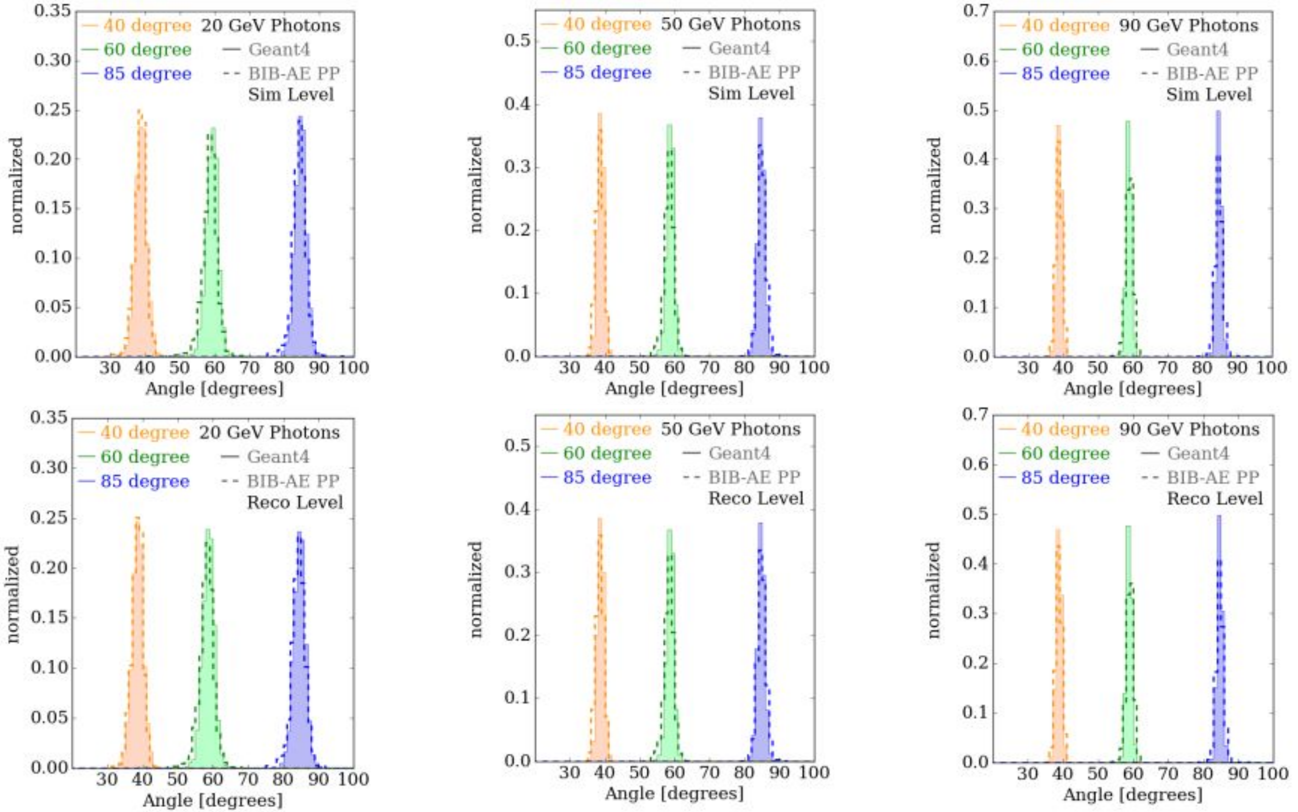


New Angles

Angular Conditioning Performance

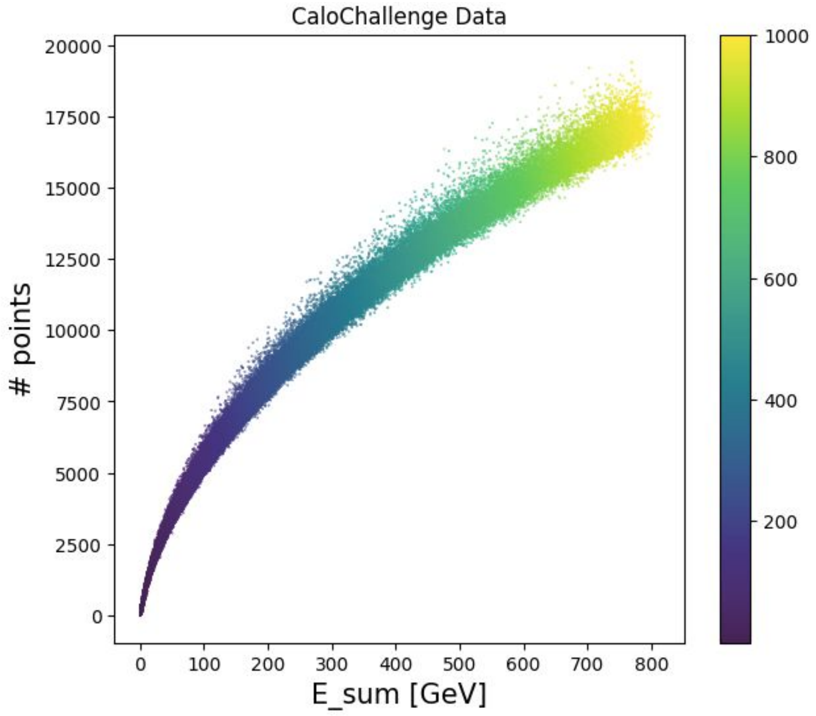
New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, et al. 2023 MLST in press
DOI 10.1088/2632-2153/acefa9, **arXiv: 2303.18150**

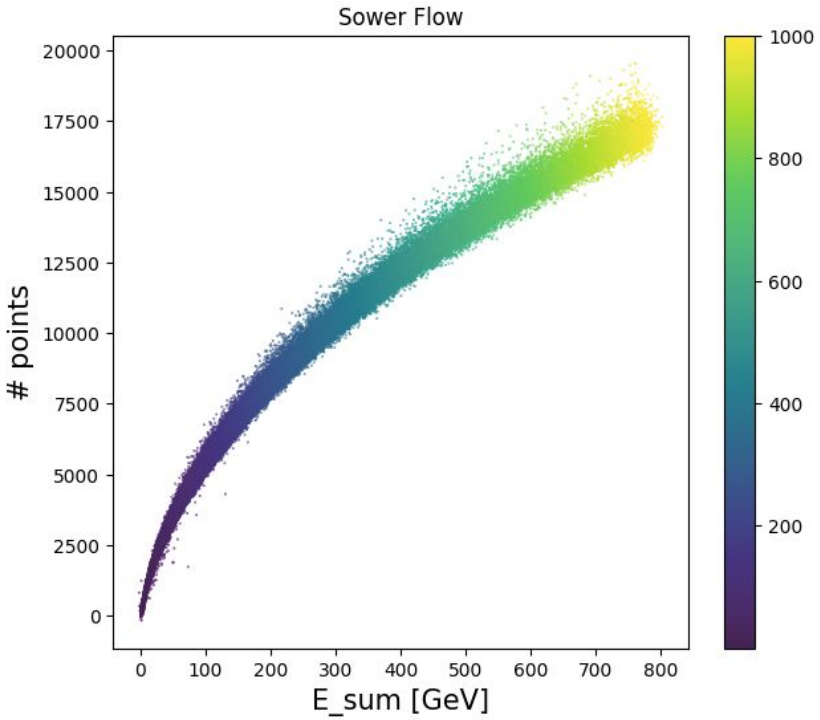
- **Sim** level angle reconstruction
- **Rec** level angle reconstruction
  - After full reconstruction with PandoraPFA



Shower Flow

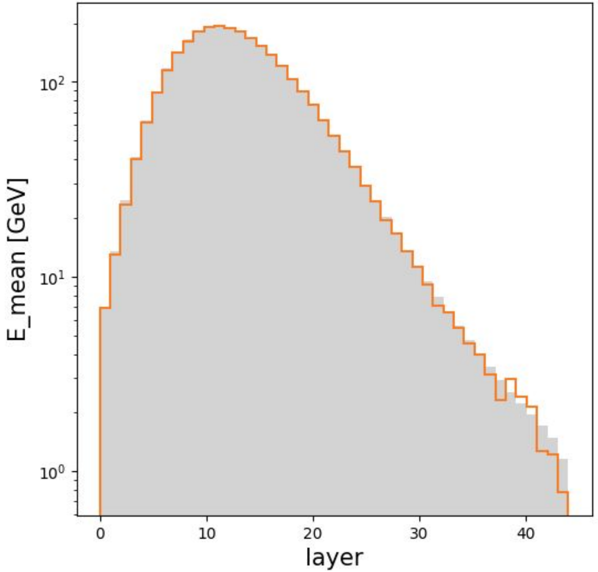
Results

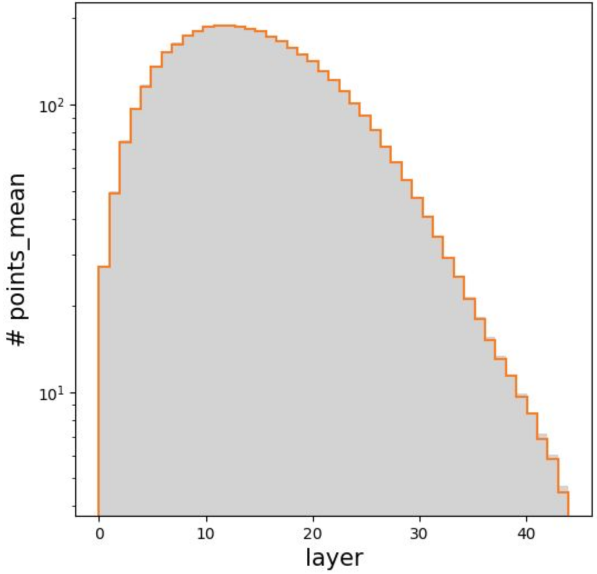


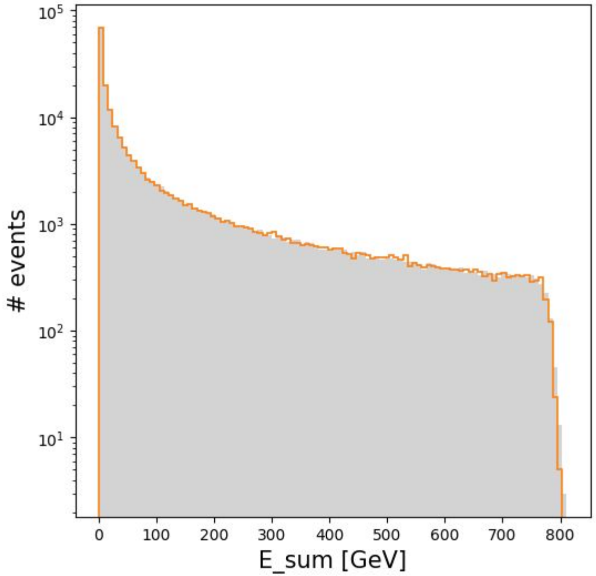


Shower Flow

Results

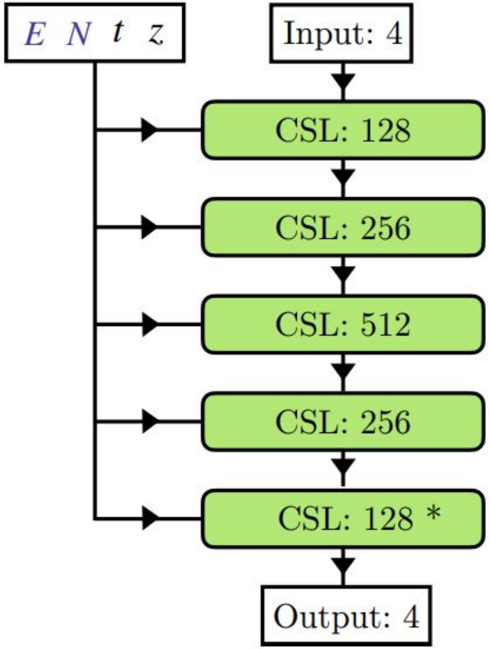




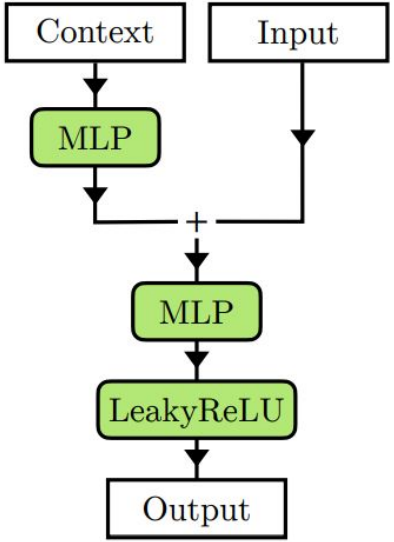


Point Cloud + Diffusion Model

PointWise Net



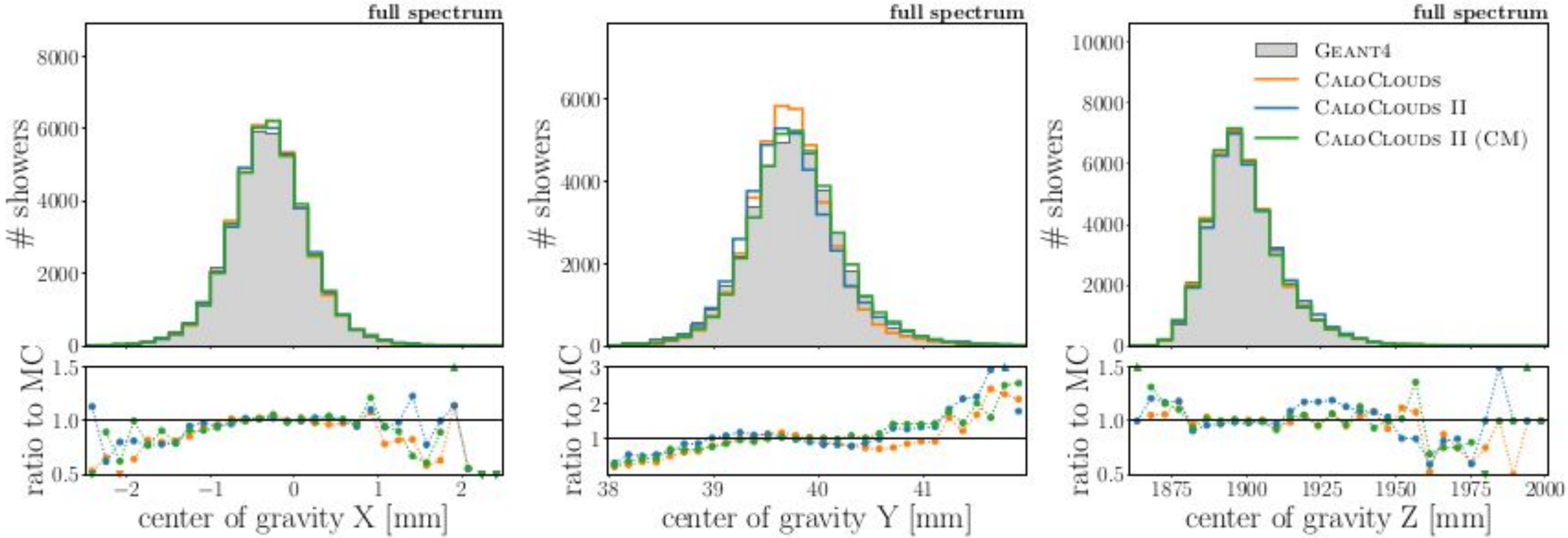
(a) PointWise Net



(b) ConcatSquash Layer (CSL)

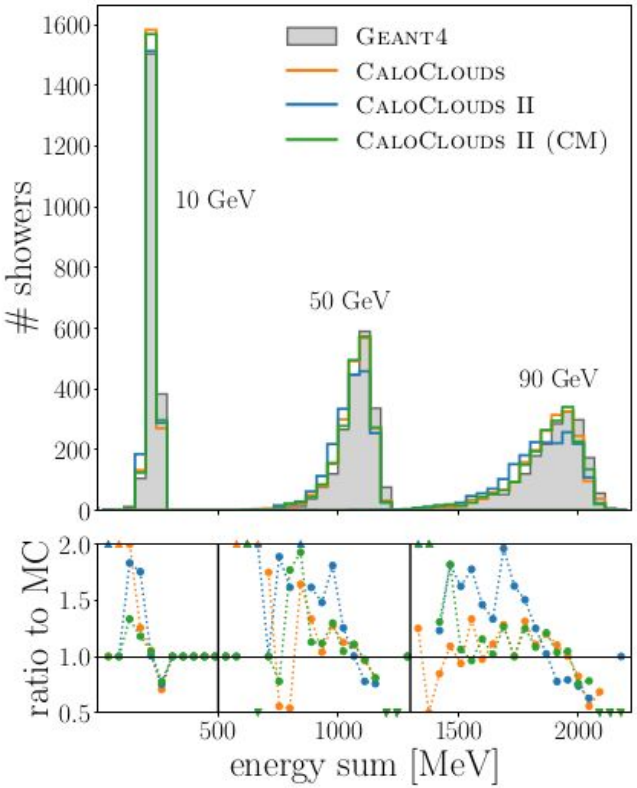
Point Cloud + Diffusion Model

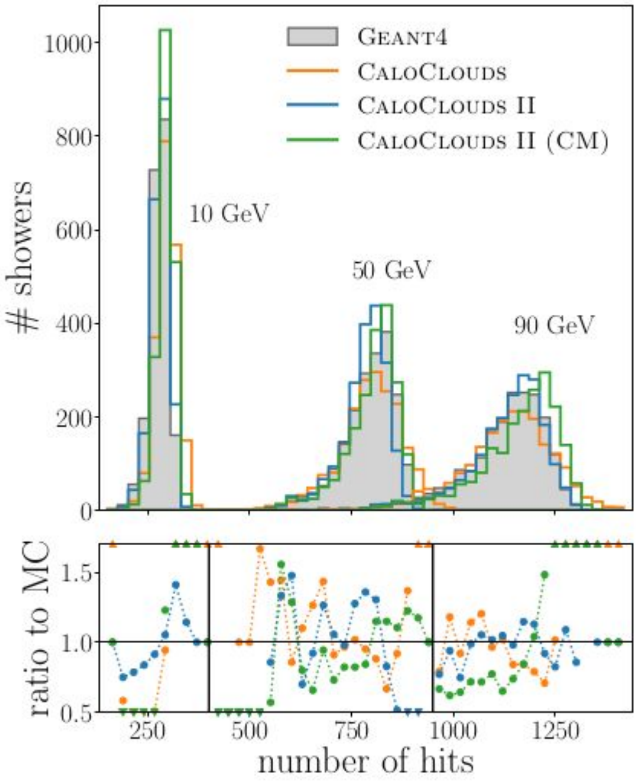
Results, Position of the Center of Gravity



Point Cloud + Diffusion Model

Results, Visible Energy and the Number of Hits

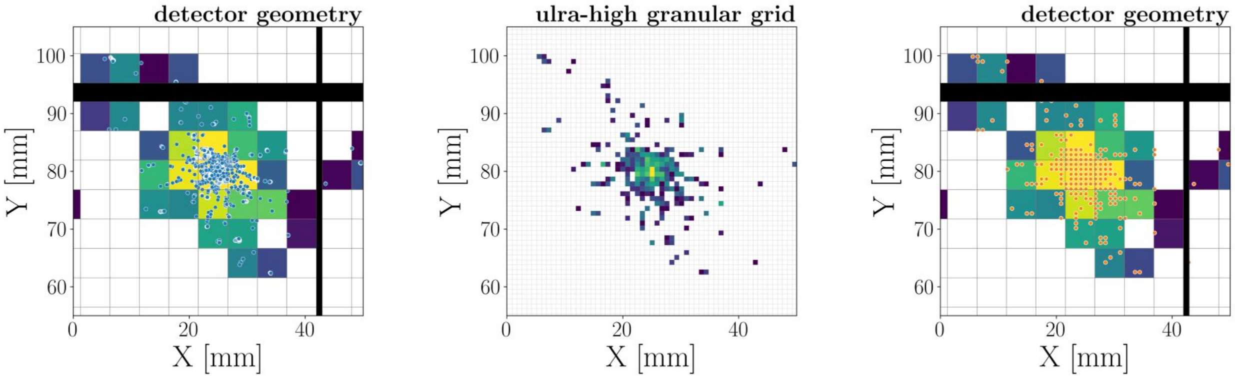




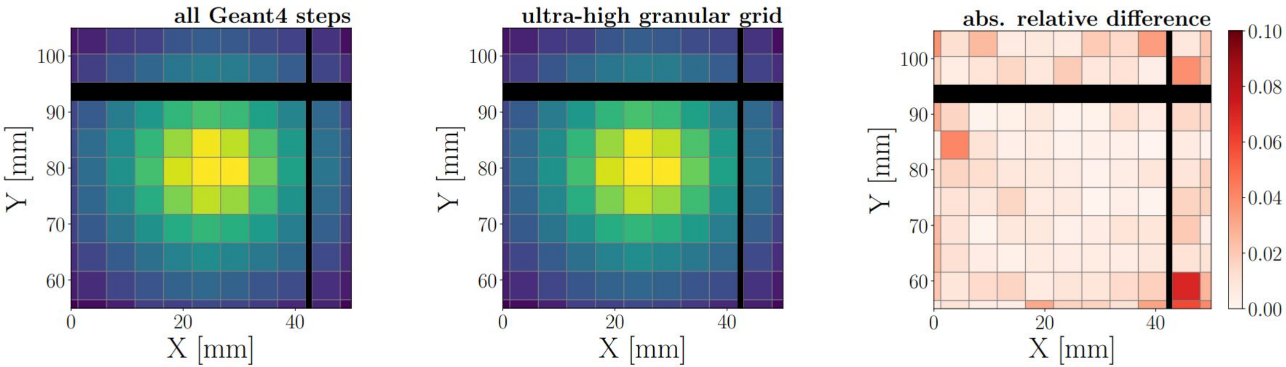
Point Cloud Representation of the EM Showers

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