Generative Models for Fast Simulation of Electromagnetic and Hadronic Showers in Highly Granular Calorimeters

CHEP 2023, Norfolk, USA-VA

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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

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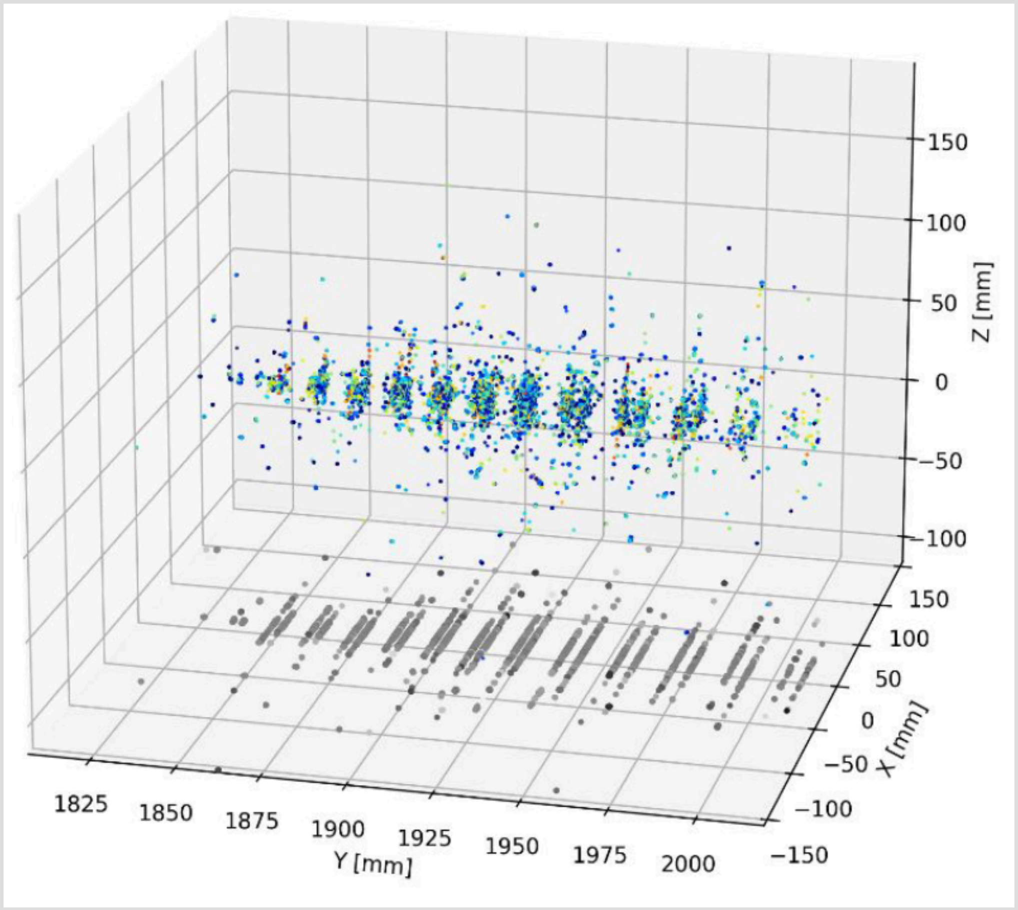
AIDA innova

Outline

- Introduction
- Previous Work
- Hadron Generation and Reconstruction
- Angular and Energy Conditioning
- CaloCloud - diffusion model
- Summary and Outlook



Introduction

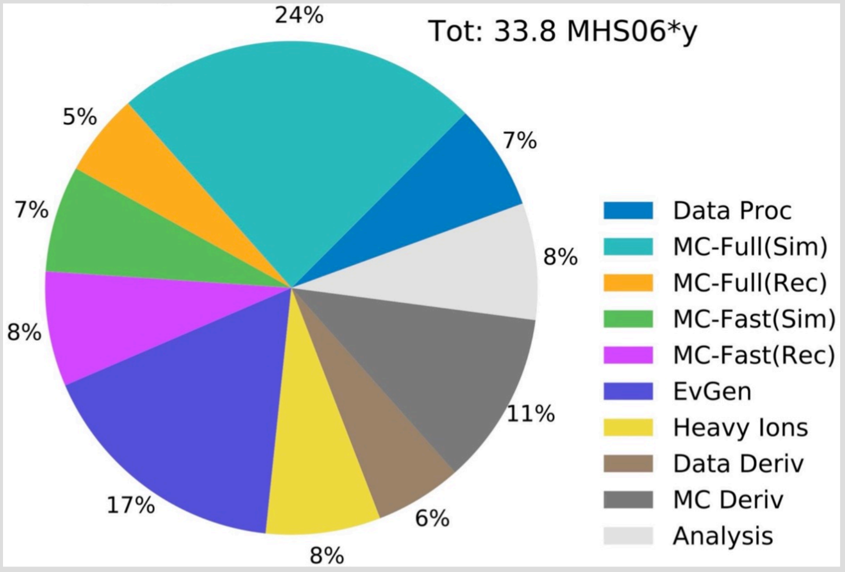
High Fidelity Shower Simulation with ML

- calorimeter shower (full) simulation is computationally very expensive -> need for fast simulation

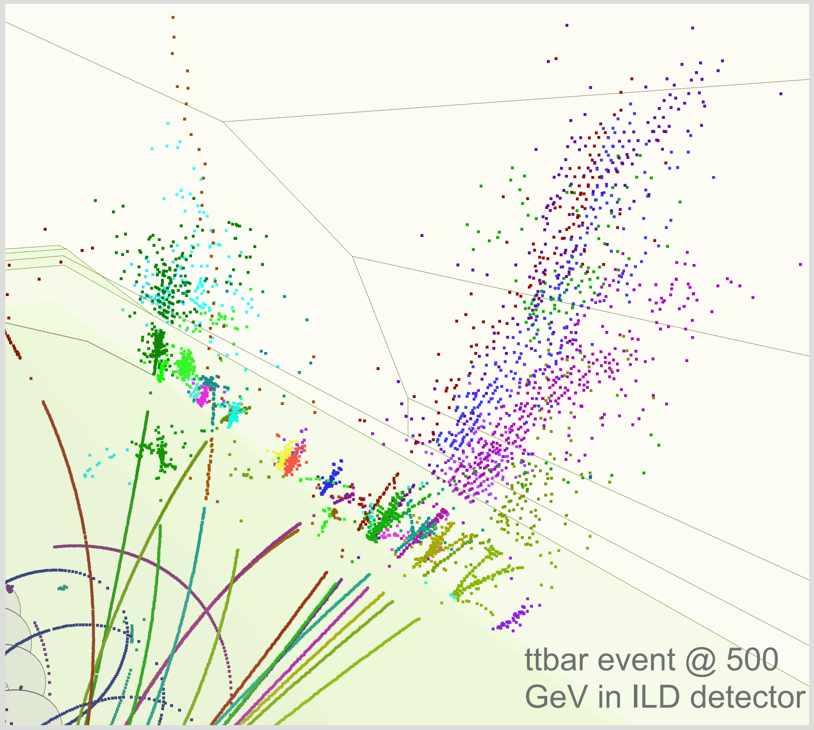
- **generative ML models** offer prospect of **high fidelity** simulation at significant **speed up:**
  - more sustainable computing

- DESY-UHH group addressing this issue by investigating generative ML architectures in context of **ILD** detector:
  - high granularity sandwich calorimeters:

    - **ECal**: Si-W - 5mm x 5mm
    - **HCal**: Sci-Fe - 30mm x 30 mm



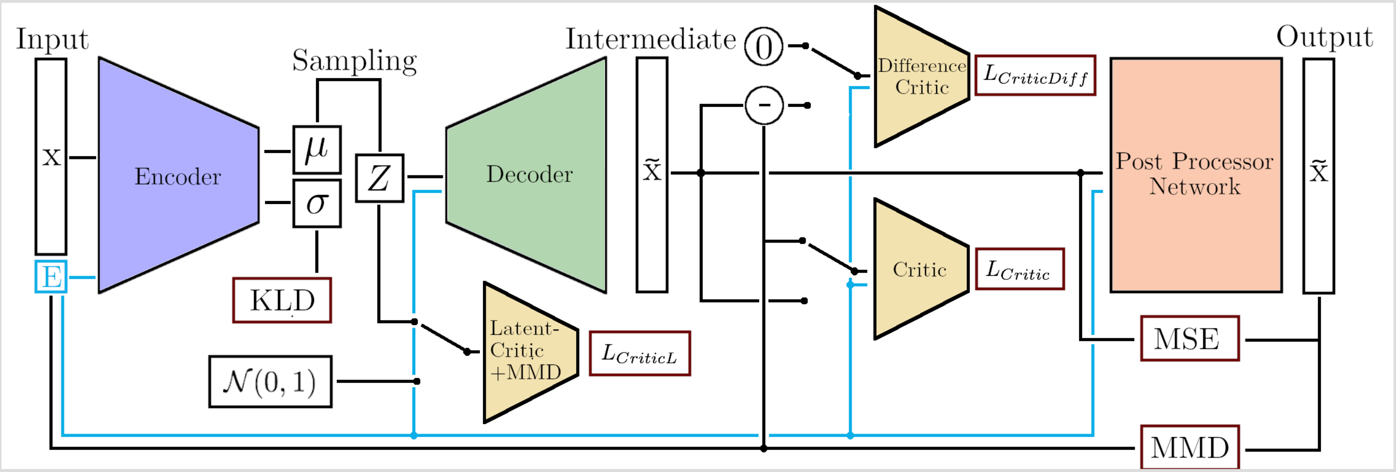
ATLAS Software and Computing HL-LHC Roadmap, CERN-LHCC-2022-005



Previous Work

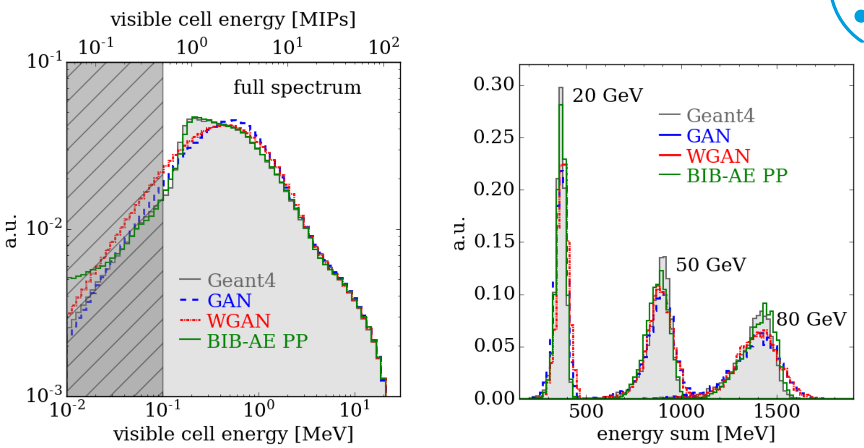
presented at vCHEP 2021

- 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)



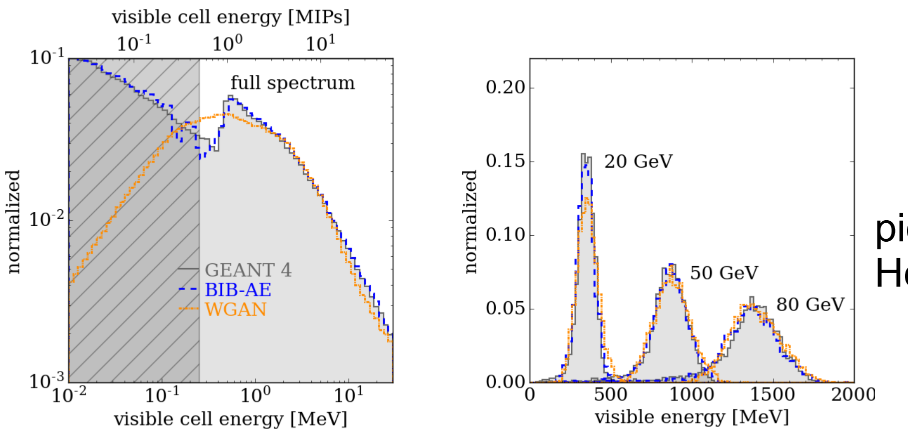
BIB-AE: Bounded Information Bottleneck Auto-Encoder

also comparison to GAN and WGAN …



photons
Ecal

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



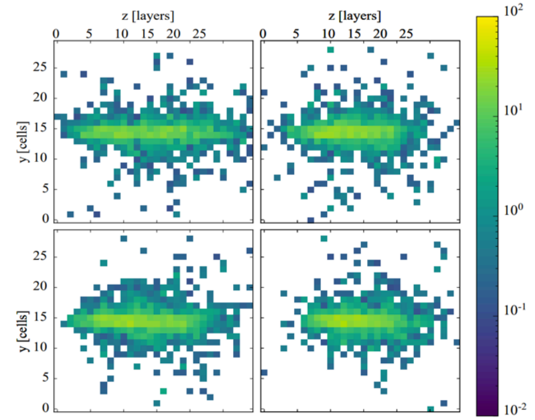
pions
Hcal

Hadrons, Better, Faster, Stronger
E. Buhmann, S. Diefenbacher, E. Eren, F. Gaede et al,
Published in: Mach.Learn.Sci.Tech. 3 (2022) 2, 025014,
arXiv:2112.09709

Our work plan

towards application in realistic detector simulation (of ILD)

From Photons to Pions

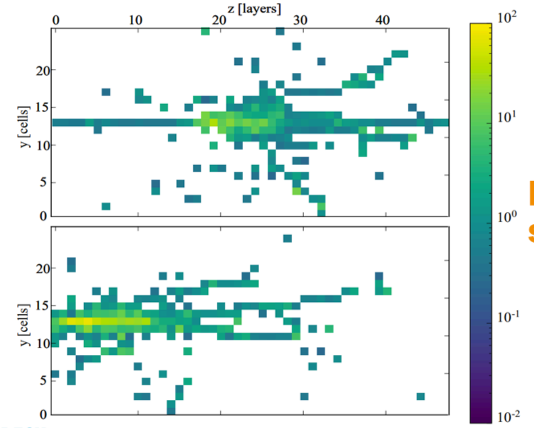


Photon showers

- Predominantly governed by EM interactions
- Compact structure

↓

Relatively easy to generalise



Pion showers

- Hadronic and EM interactions
- Complex structure
- Large event-to-event fluctuations

↓

Hard to learn

	Energy	Angles θ, ϕ	ECAL +HCAL	Reco
Photon showers	✓	+	N/A	+
Pion showers	✓	X	X	+

✓ = Achieved   X = Yet to be done   + = Addressed here

- for **realistic application** need to address several next steps:
  - **angular conditioning**
  - performance after **reconstruction**
  - …
- continue to investigate other promising **ML architectures**

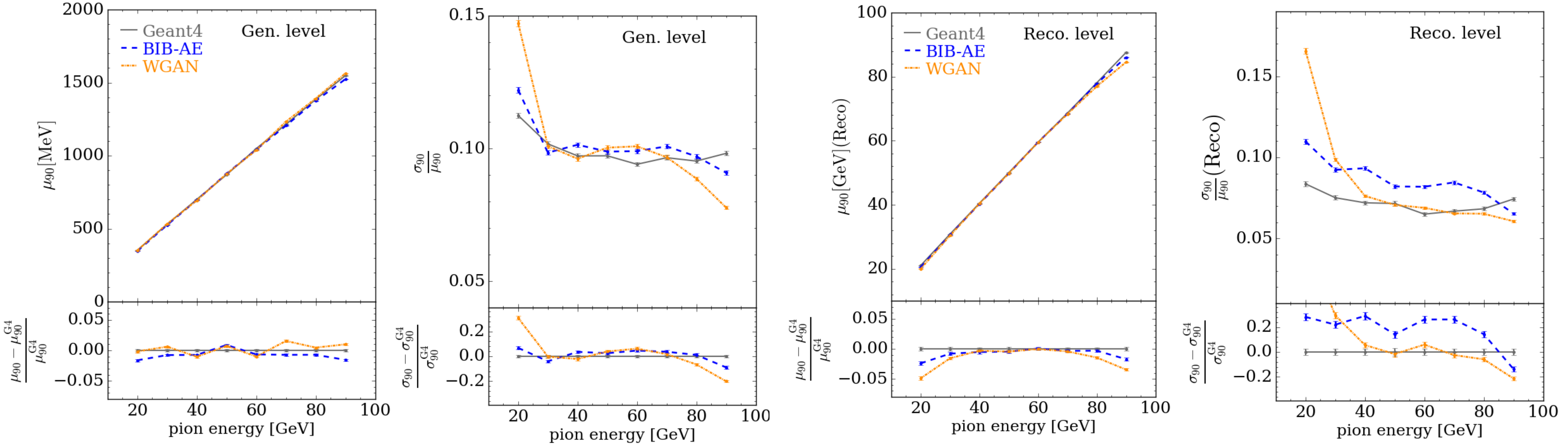
-> this talk

see also:
T.Buss: "Generating Accurate Showers in Highly Granular Calorimeters Using Normalizing Flows"
track 9, May 11, 2023, 2:15 PM

Benchmarking of Generative Fast Simulation

Need to apply full reconstruction

single pion showers in ILD Sci-W HCal

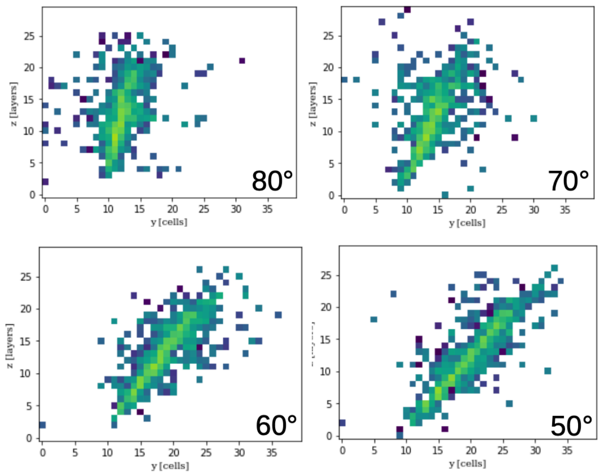


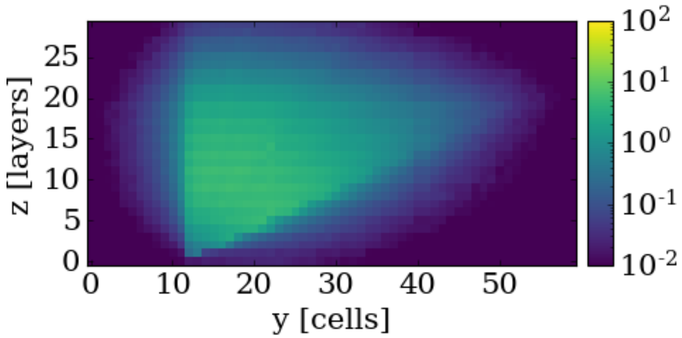
- most important quantities for calorimeter performance: **linearity** and **resolution**
  - comparison with Geant4 after **generation/simulation** and after **full reconstruction** with PandoraPFA
- achieve reasonably good performance for both - yet WGAN better models resolution after reconstruction ! further tuning need for realistic application ….

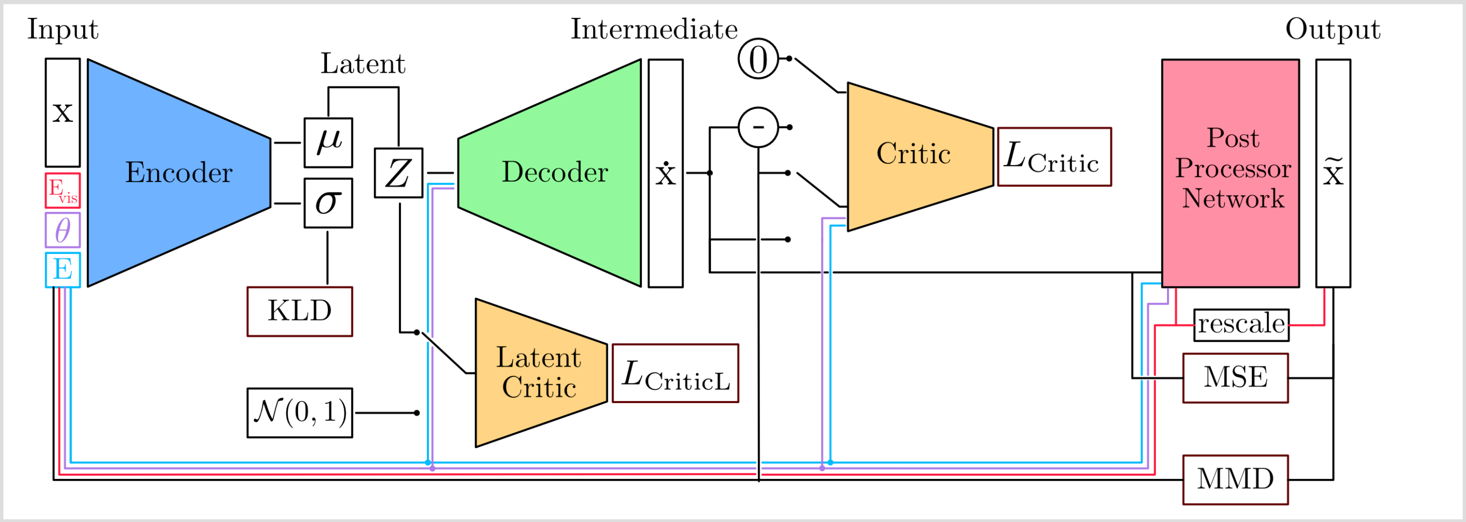
Energy and Angular Conditioning

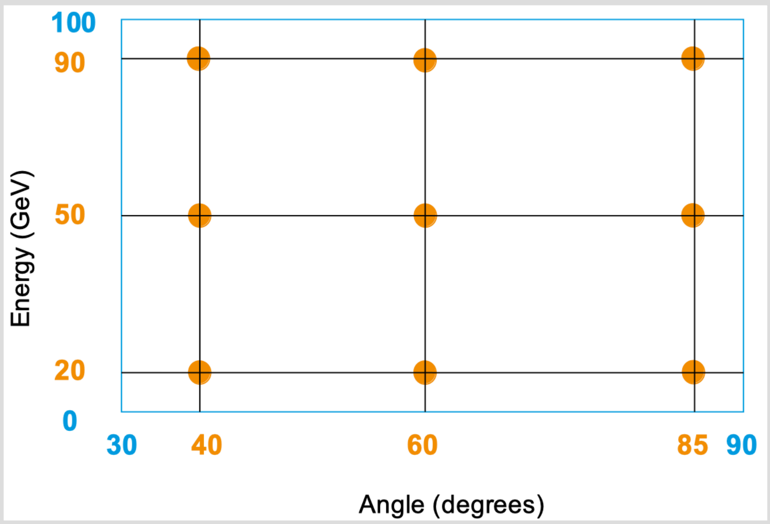
for photon showers in ILD ECal

- extend **BIB-AE-**PP architecture to condition on
- **incident energy and polar angle**
  - large training sample - 500 k showers
    - uniform in [10-100 GeV, 30-90 deg]
  - test/validation samples at dedicated energies and angles









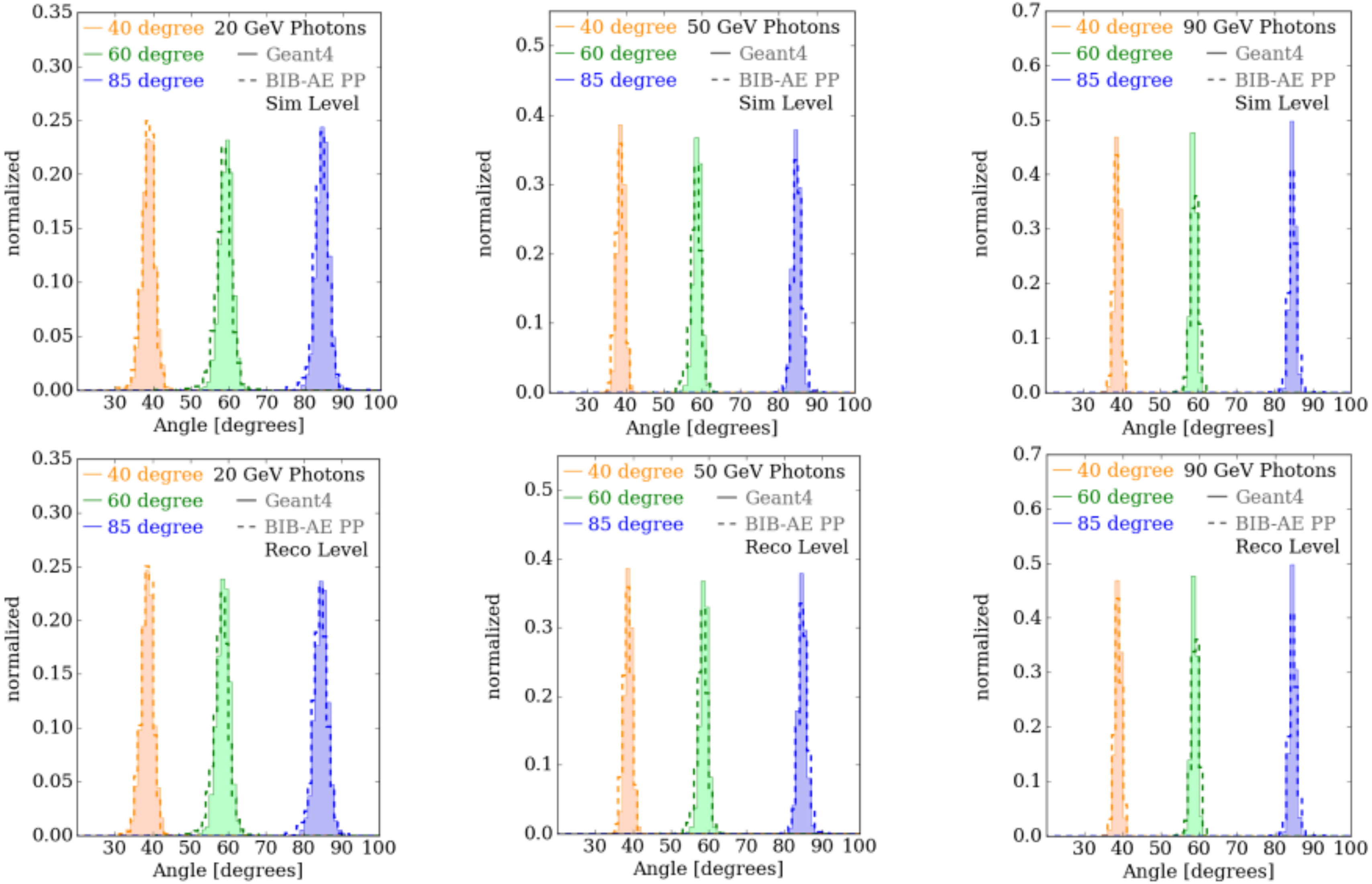
training and validation samples - 30x60x30 grid

Energy and Angular Conditioning

for photon showers in ILD ECal - angles

New Angles on Fast Calorimeter Shower Simulation,
S.Diefenbacher, P.McKeown et al
arXiv: 2303.18150, submitted to MLST

- **sim** level PCA angle reconstruction
- **rec** level PCA angle reconstruction
  - after full PandoraPFA reco

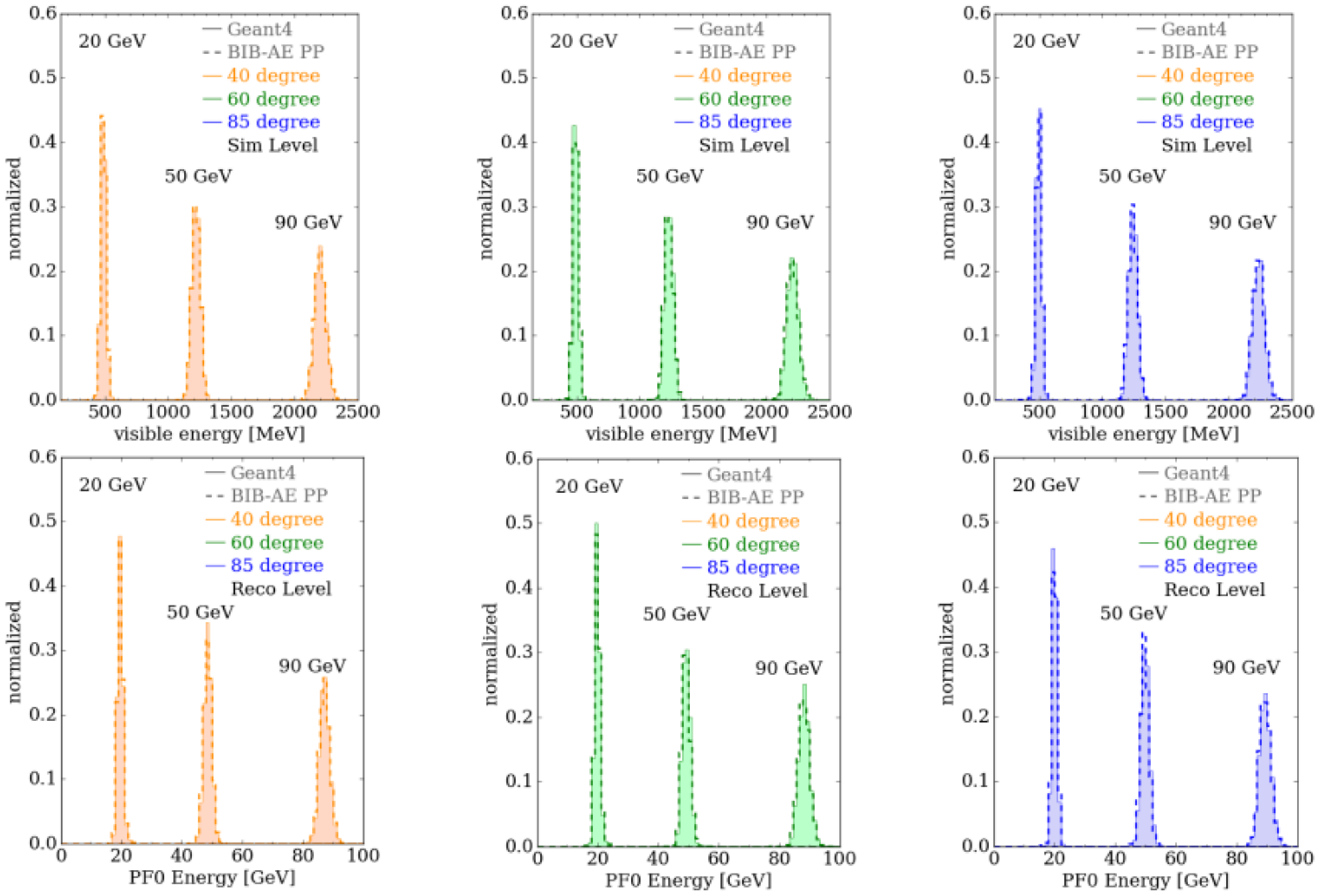


Energy and Angular Conditioning

for photon showers in ILD ECal - energies

New Angles on Fast Calorimeter Shower Simulation,
S.Diefenbacher, P.McKeown et al
arXiv: 2303.18150, submitted to MLST

- **sim** level **visible** energy
- **rec** level **calibrated** energy
  - after full PandoraPFA reco



Energy and Angular Conditioning

example distributions after full reconstruction

New Angles on Fast Calorimeter Shower Simulation,
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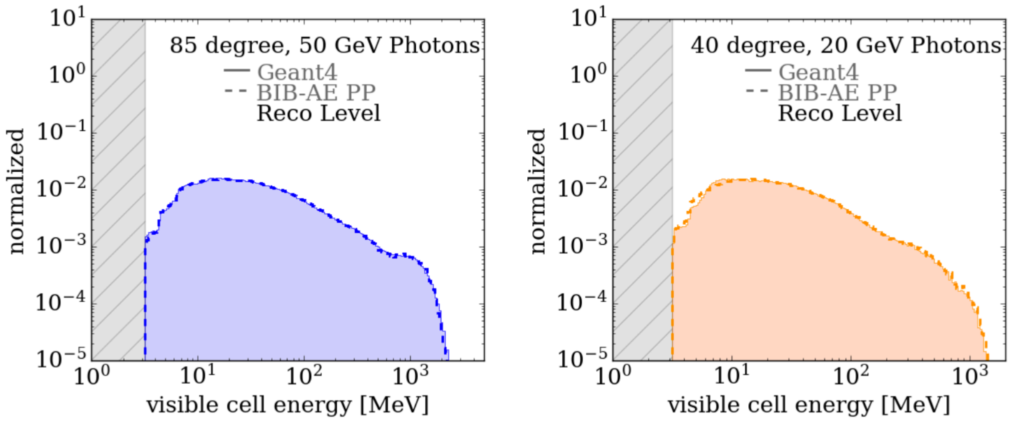
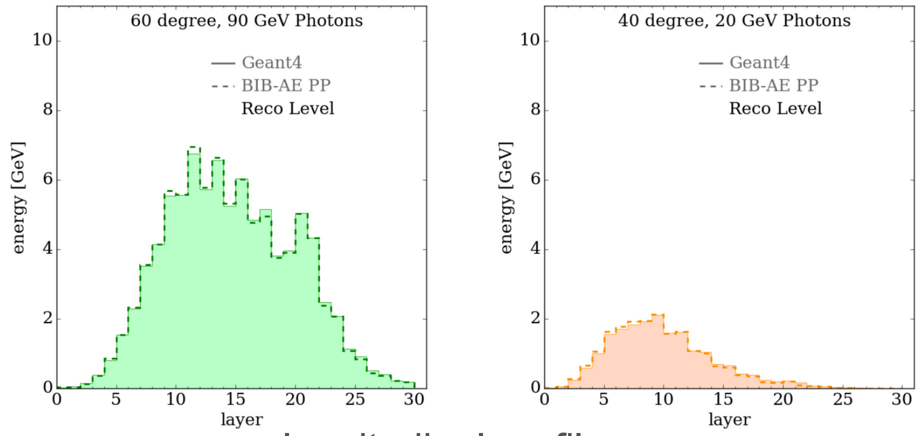
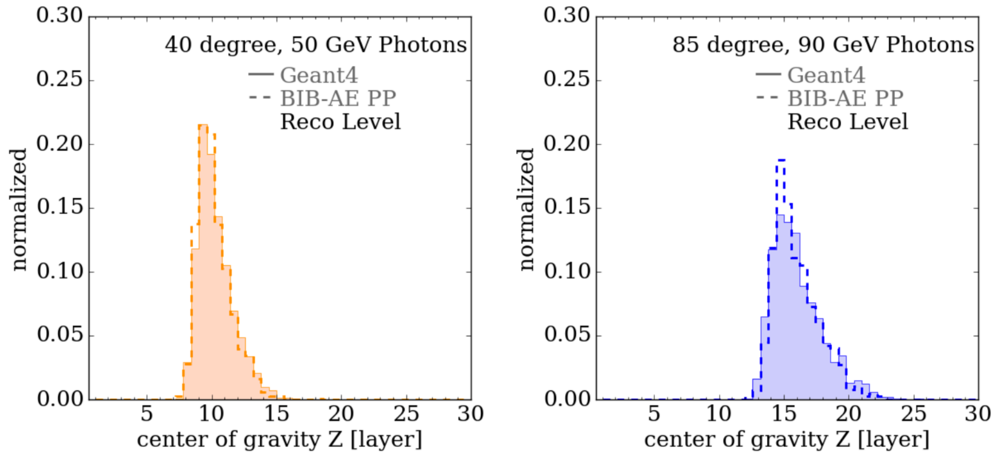


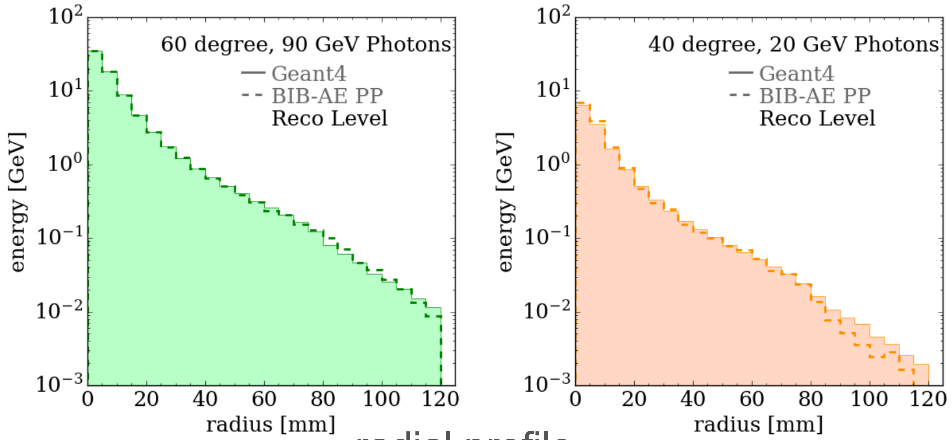
hit energy spectrum



longitudinal profile



centre of gravity in z



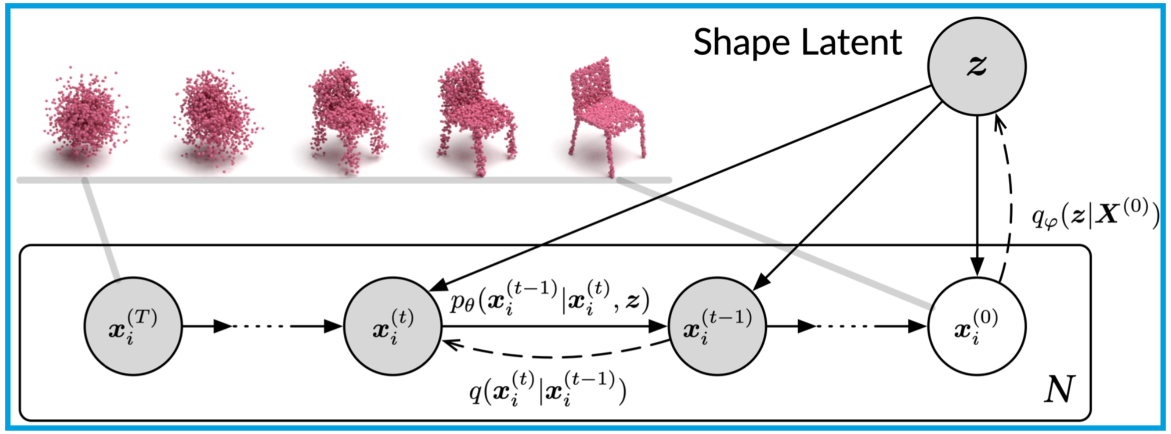
radial profile

best (left) and worst (right) test point - based on JSD -> excellent physics fidelity

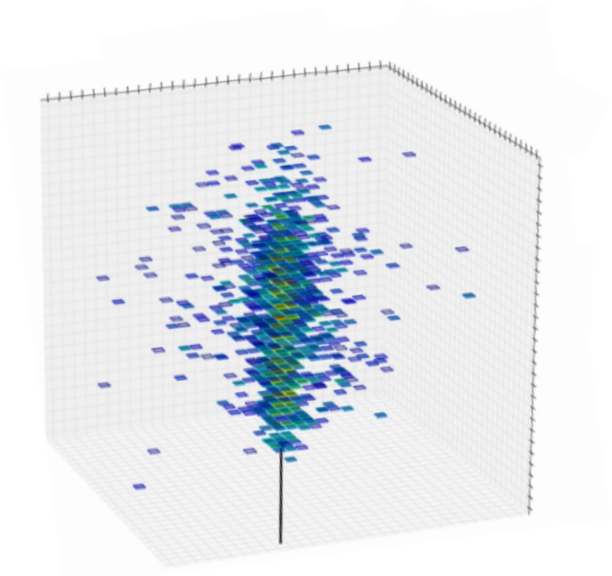
CaloCloud diffusion model

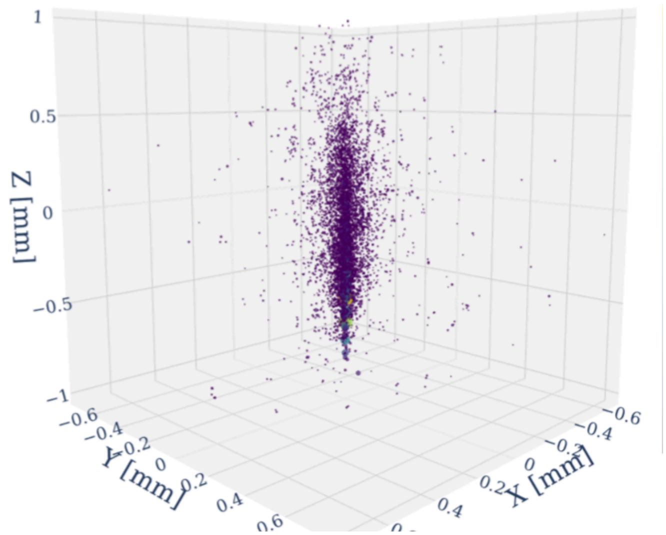
from regular grids to point clouds

S.Luo, W.Hu: Diffusion Probabilistic Models for 3D Point Cloud Generation, arXiv:2103.01458



- regular grid models like WGAN or BIB-AE show very high physics fidelity - yet they have two problems:
  - low occupancy -> lots of superfluous compute
  - projecting energy back into realistic detector cells causes artefacts
- are point clouds a “way out” ?

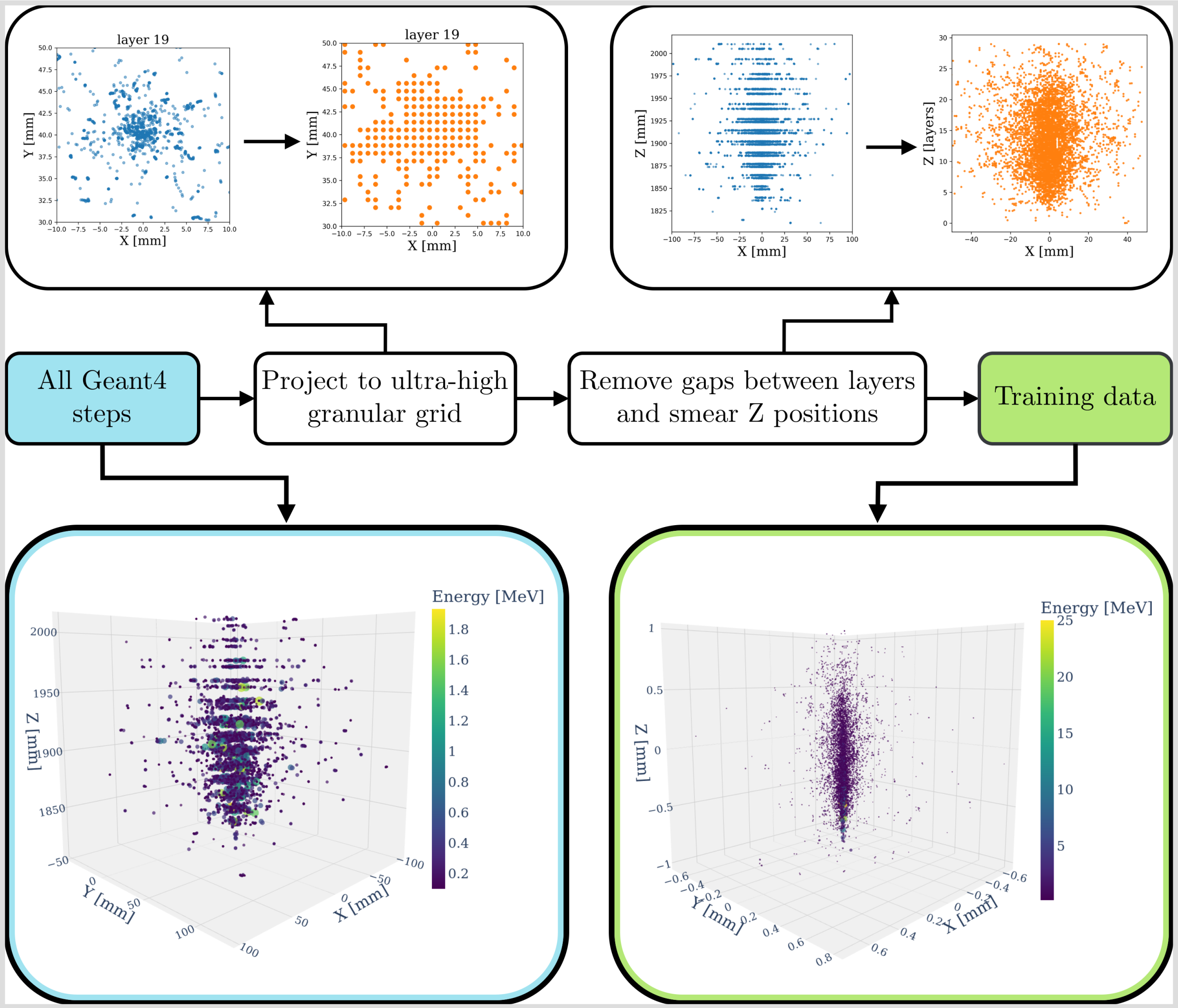




- recently many publications using point clouds and diffusion models
- can we adapt this to our HEP calorimeter use case - using much higher granularity provided by individual Geant4 steps ?

CaloCloud diffusion model

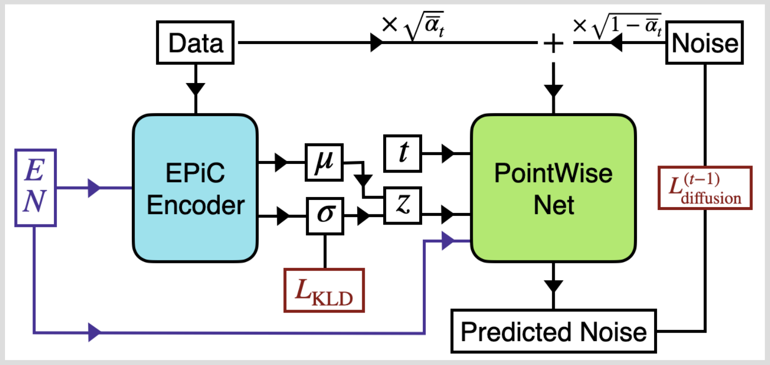
preprocessing for training data

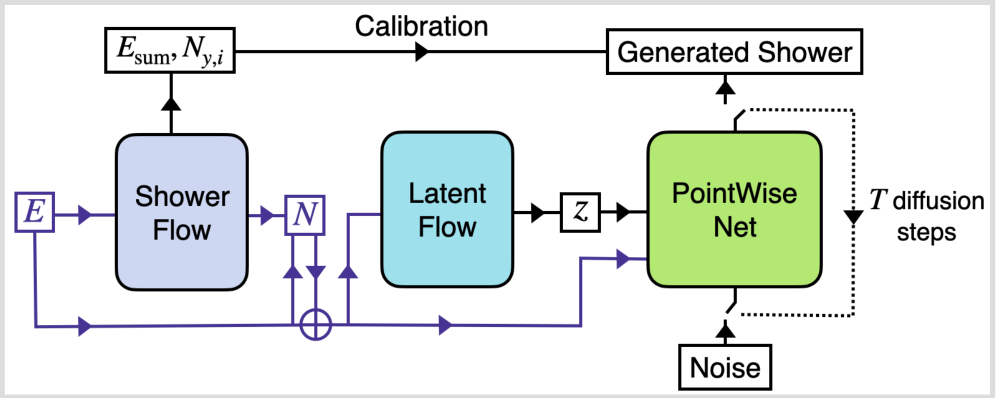


- using all Geant4 steps directly turns out to be prohibitive wrt. compute time
  - 40k Geant4 steps at 90 GeV
- apply preprocessing step:
  - project Geant4 steps into ultra-high granularity grid 36 times more granular than ILD Ecal
    - reduction by factor ~7:
    - up to **6000 space points**
- use again photon sample in ILD Ecal
  - 10-100 GeV, 90 deg impact

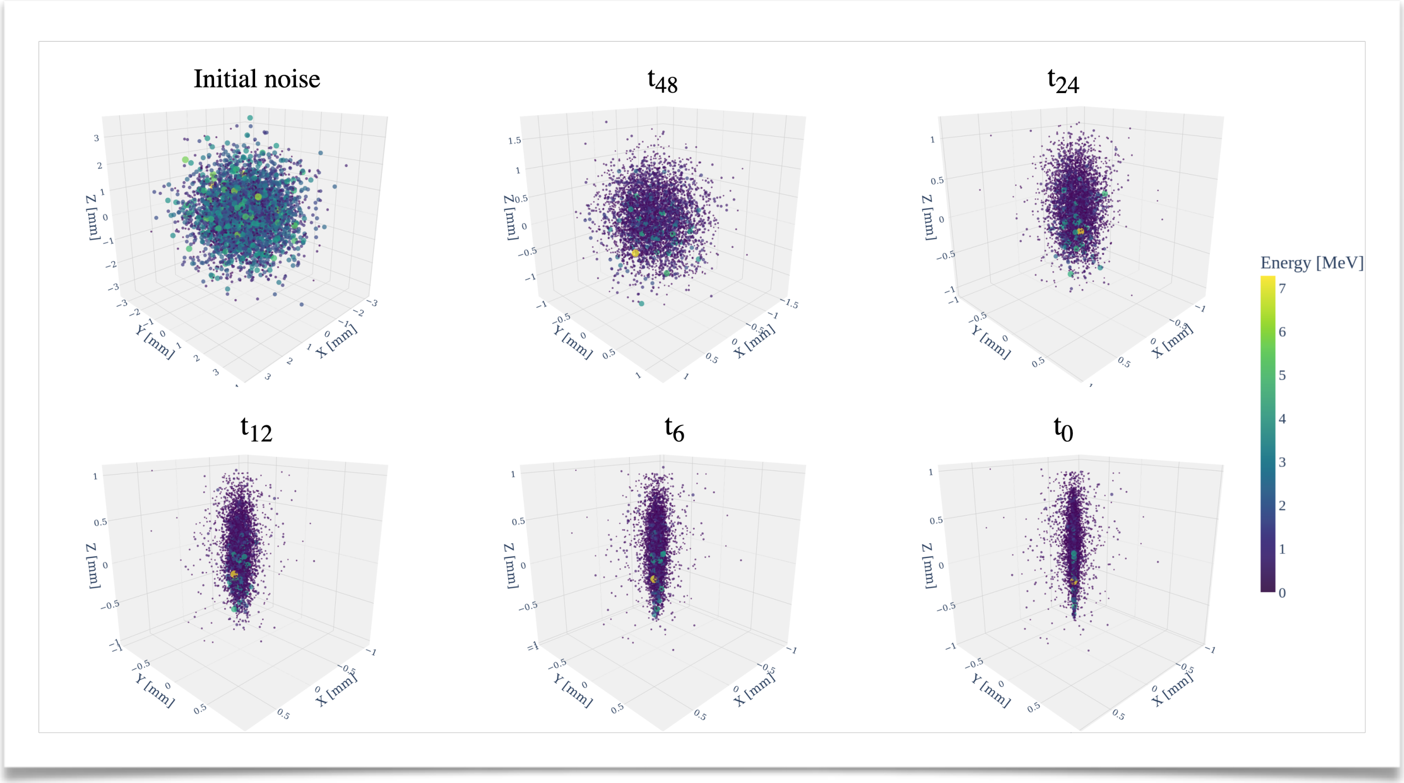
CaloCloud diffusion model

model architecture



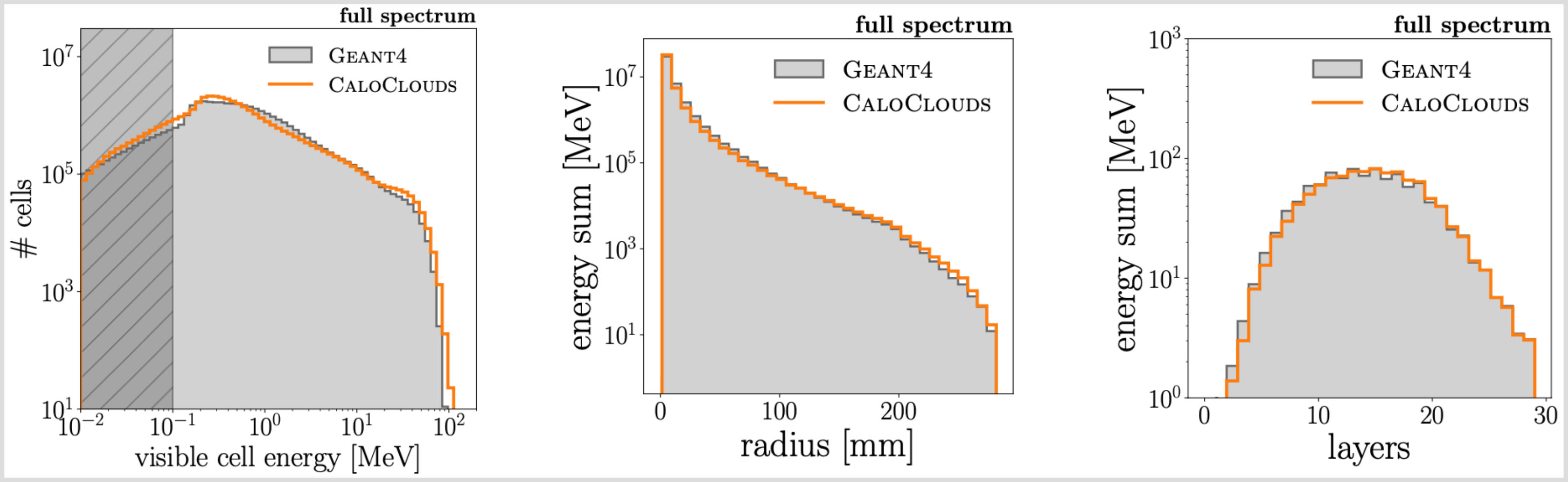


- training of PointWise Net with EPiC Encoder (e-Print: 2301.08128)
- inference uses two additional flows for number of space points, calibration and latent space



CaloCloud diffusion model

performance



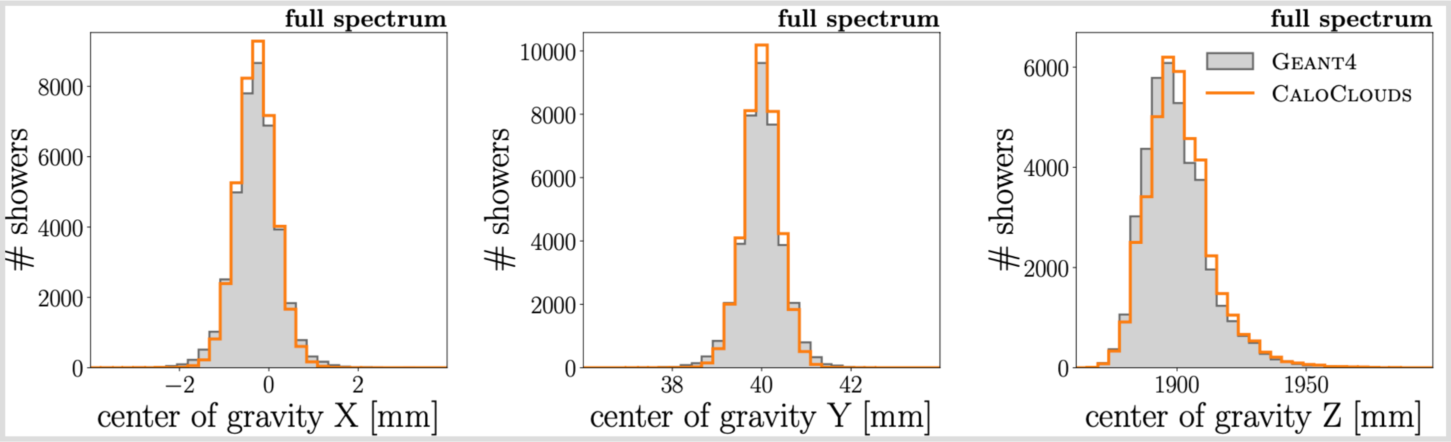
- observe overall very good physics fidelity on photon sample

- first successful application of diffusion models to (high granular) calorimeter simulation using point clouds

preprint will be available soon…

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

improvement of timing
focus of future work



Summary and Outlook

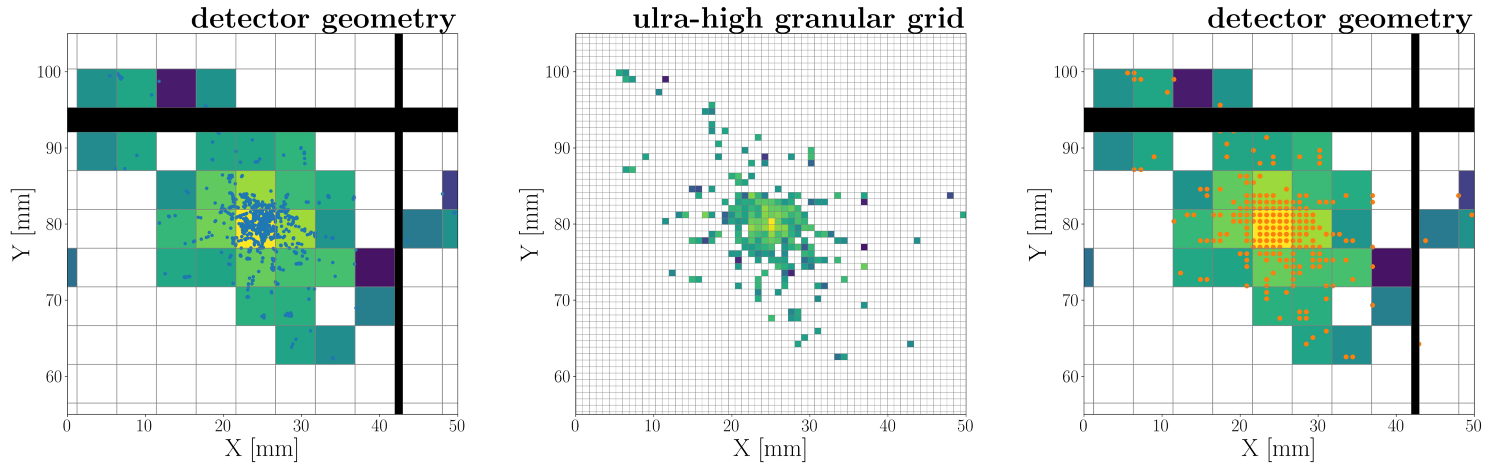
- great progress in work towards applying generative ML in full physics simulation of ILD
- using **BIB-AE** with fixed 3d grid data layout:
  - first **generation of pion showers** in high granular calorimeter incl. full **reconstruction** with PandoraPFA
  - **energy and angular conditioning** for EM showers with high fidelity incl. full **reconstruction** with PandoraPFA
- **CaloCloud**: first application of **diffusion** model for EM shower generation in highly granular calorimeter using ultra-high granularity point clouds - up to **6000** space points

- Outlook:
  - continue to improve models wrt. performance and speed and extend functionality
    - include ML models in full ddsim/DDG4 simulation and study w/ physics benchmarks
    - investigate methods to speed up CaloCloud diffusion model
    - …

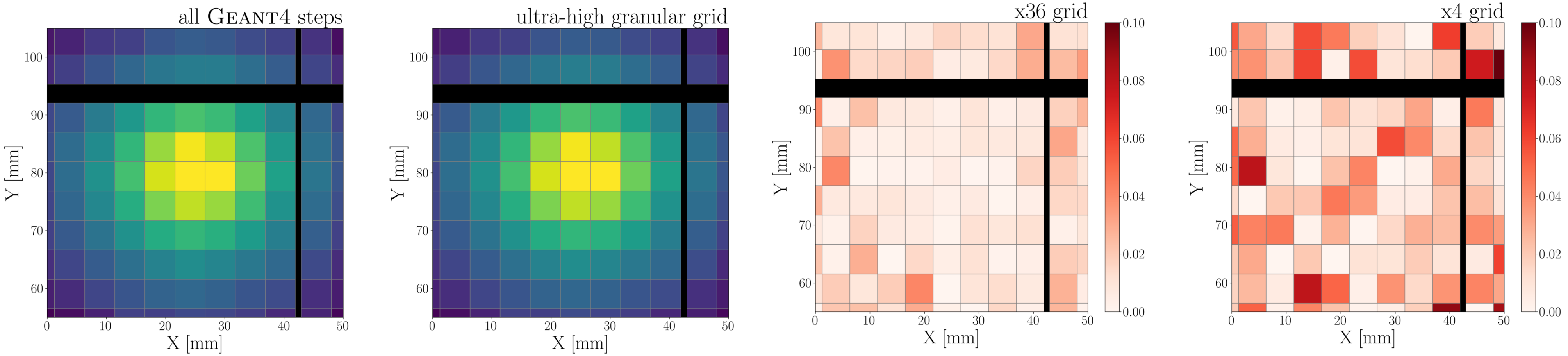
Additional Material

Effects of pre-clustering to ultra-high granularity

in CaloCloud



example:
Geant4 90 Gev shower in layer 21
with full round-trip pre-clustering and back-projection



overlay of 2k Geant4 90 Gev showers in layer 21
with full round-trip pre-clustering and back-projection

relative difference per cell
< 2% in core of shower

relative difference with
lower granularity

Timing of generative ML Methods

Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	2684 ± 125	$\times 1$
	WGAN	47.923 ± 0.089	$\times 56$
	BIB-AE	350.824 ± 0.574	$\times 8$
GPU	WGAN	0.264 ± 0.002	$\times 10167$
	BIB-AE	2.051 ± 0.005	$\times 1309$

BIB-AE/WGAN, pion showers 10-90 GeV uniform

Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	4417 ± 83	$\times 1$
	BIB-AE	362 ± 2	$\times 12$
GPU	BIB-AE	4.32 ± 0.09	$\times 1022$

BIB-AE, photon showers 10-90 GeV - 30-90 deg uniform

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

CaloCloud, photon showers 10-90 GeV uniform