First Physics Benchmark for ML Generated Photon Showers in the ILD ECAL

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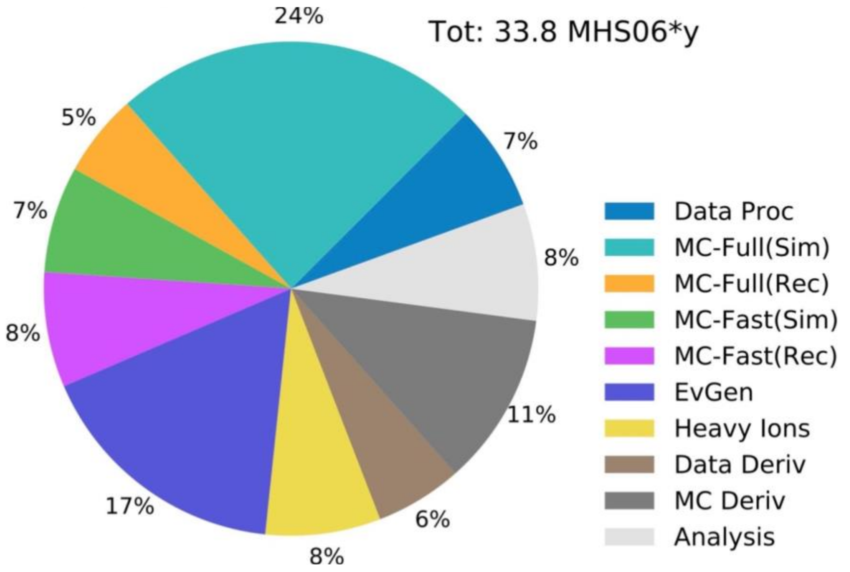
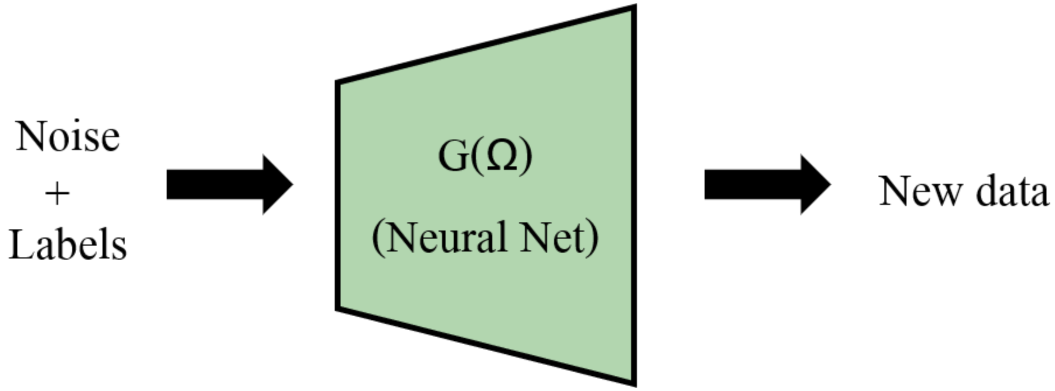
Introduction

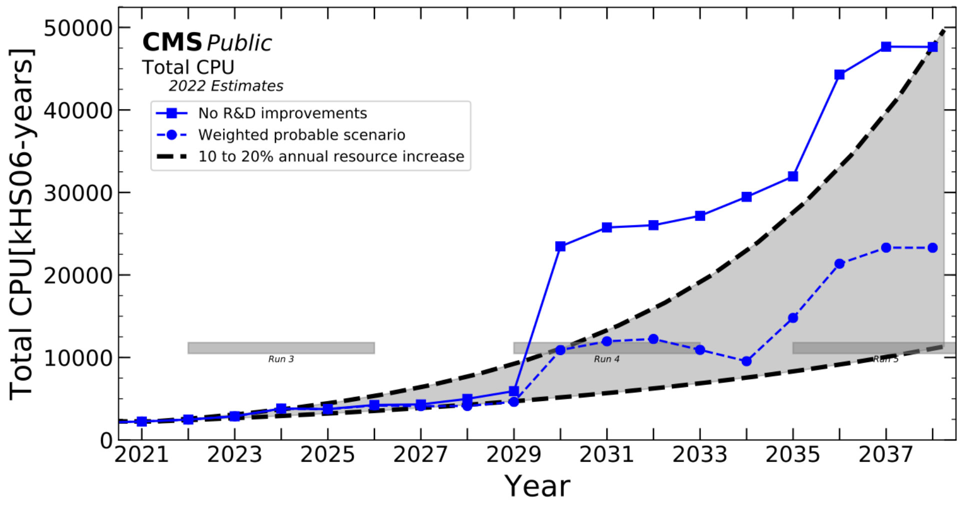
- **Full MC simulation (Geant4)** is computationally **expensive**
  - Calorimeters most intensive part of detector simulation



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

- **Generative models** potentially offer **high fidelity** simulation with significant **speed up:**
  - More sustainable computing 





CMS Collaboration, Offline and Computing Public Results (2022), https://twiki.cern.ch/twiki/bin/view/CMSPublic/CMSOfflineComputingResults

Highly Granular Calorimeters for Future Experiments

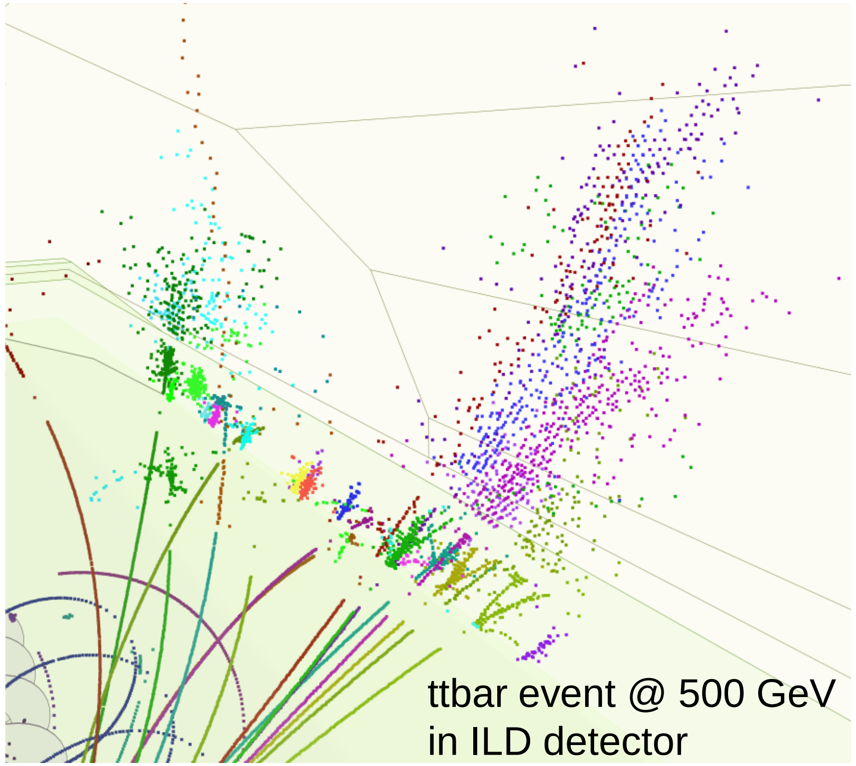
- Widely planned for future experiments: e.g. HL-LHC, e+e- Higgs Factories

- 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 cm^2 for ATLAS/CMS ECAL (before High Lumi)



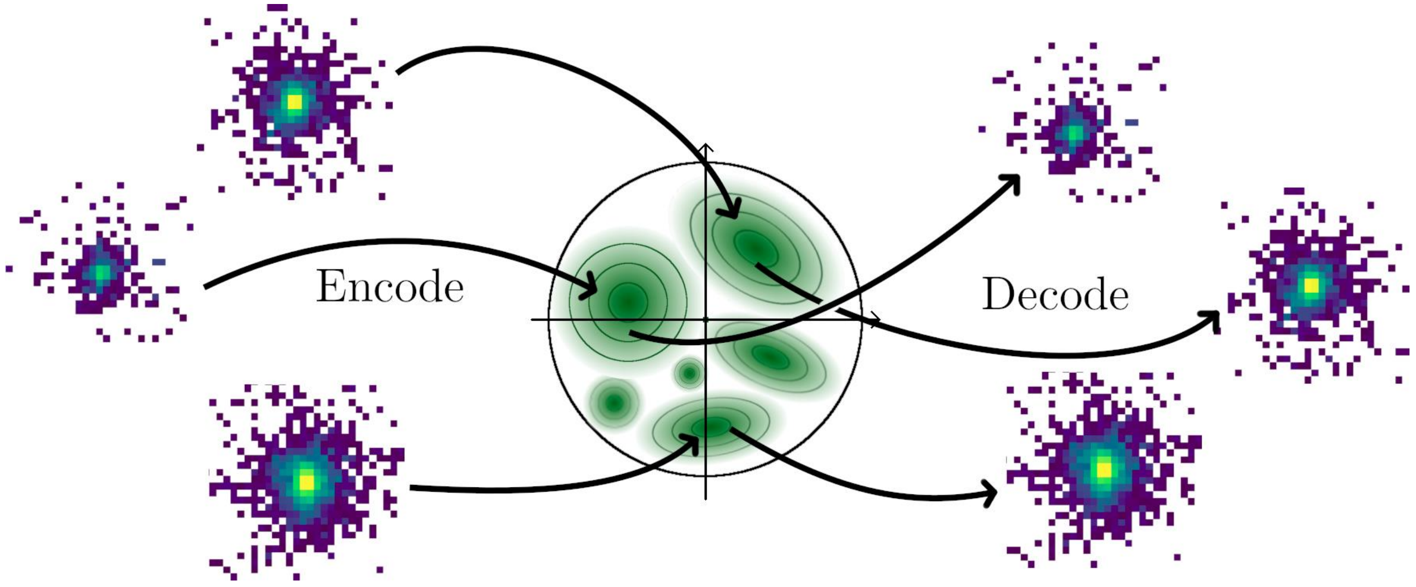
ttbar event @ 500 GeV in ILD detector

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

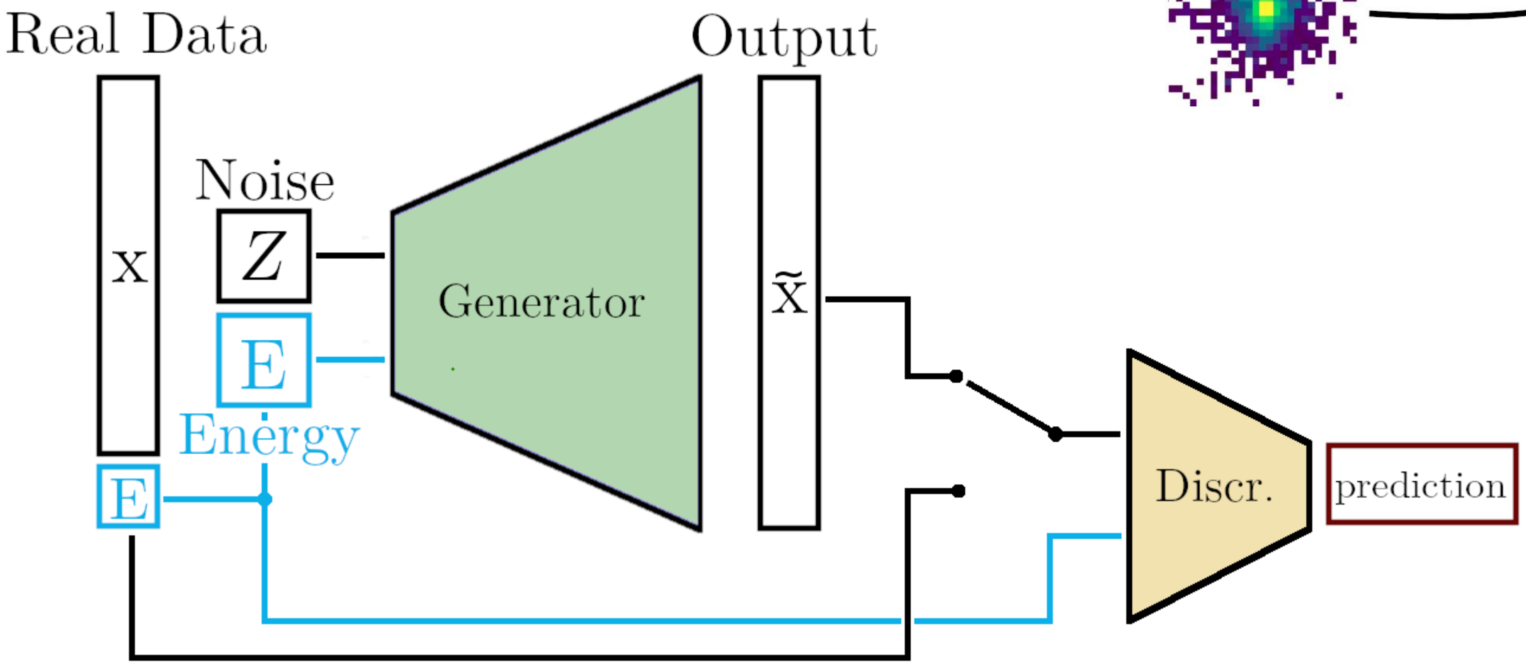
Common Generative Models

- **VAE[1]: Encoder-decoder structure**
- **GAN[2]: Adversarial feedback from discriminator**

Variational Autoencoder (**VAE**)



Generative Adversarial Network (**GAN**)

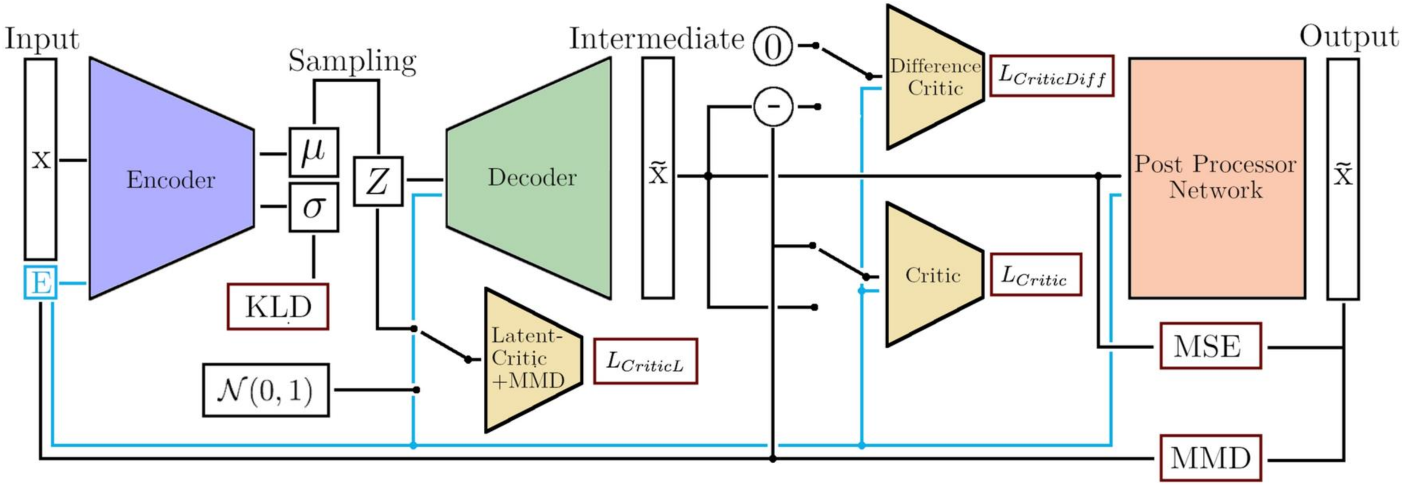


[1]D.P. Kingma, M. Welling. Auto-encoding Variational Bayes (2014), arXiv:1312.6114

[2]Goodfellow et. al., Generative Adversarial Nets (2014), arXiv:1406.2661

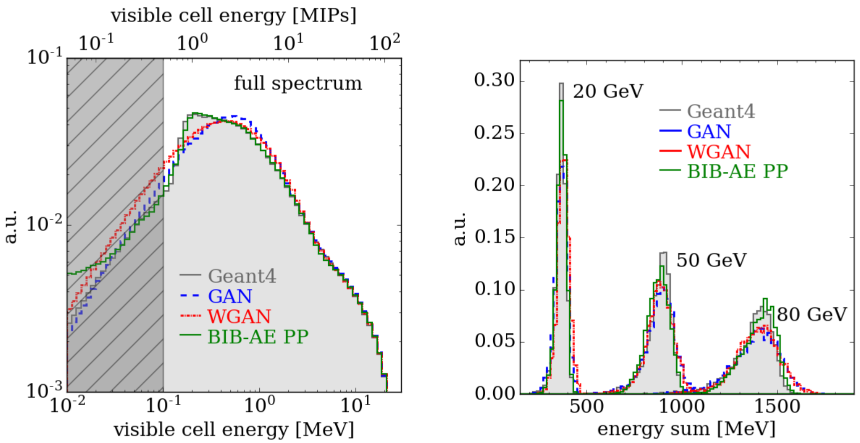
Initial Progress: Photons and Pions

- 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)



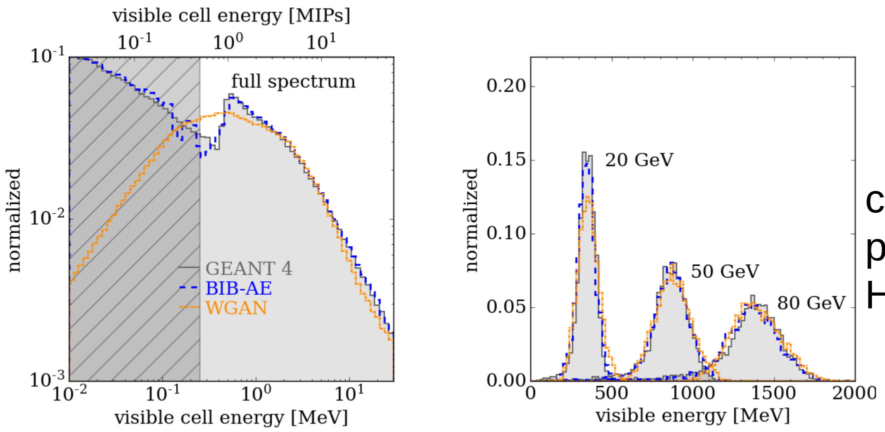
BIB-AE: Bounded Information Bottleneck Auto-Encoder

as well as comparison to GAN and WGAN …



photons ECAL

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)

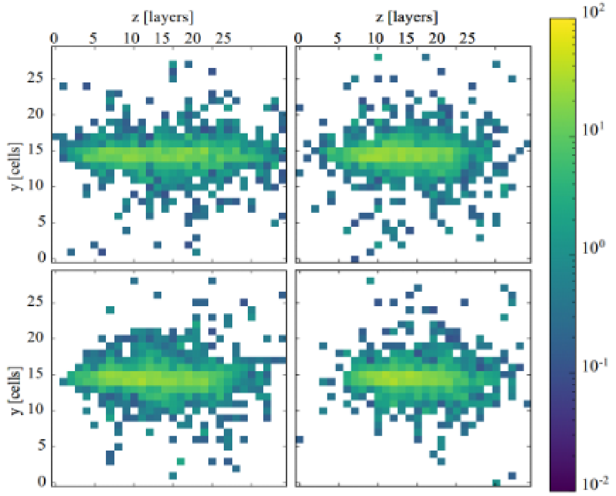


charged pions HCAL

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

Towards An Application In Realistic Detector Simulation

From Photons to Pions

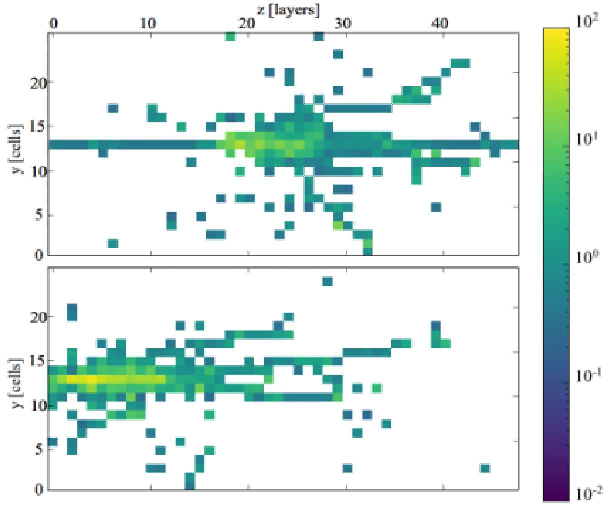


Photon showers

- 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	ECAL +HCAL	Reco
Photon showers	✓	+	N/A	+
Pion showers	✓	X	X	—

✓ = Achieved X = Yet to be done

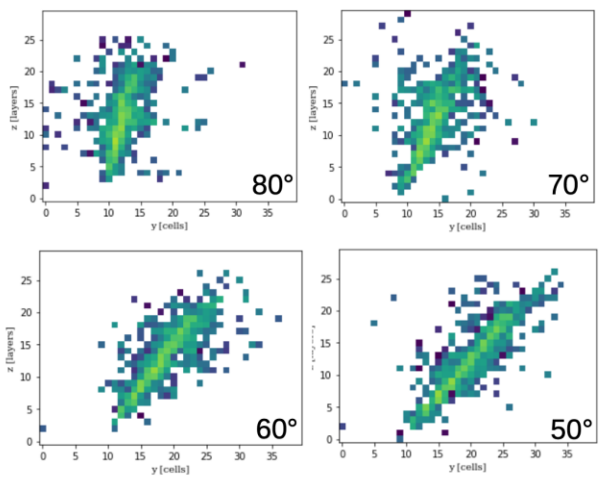
— = Partially Addressed + = Addressed here

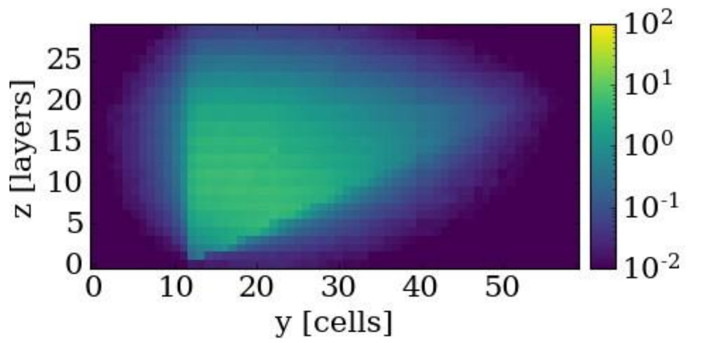
For **realistic application** also need:

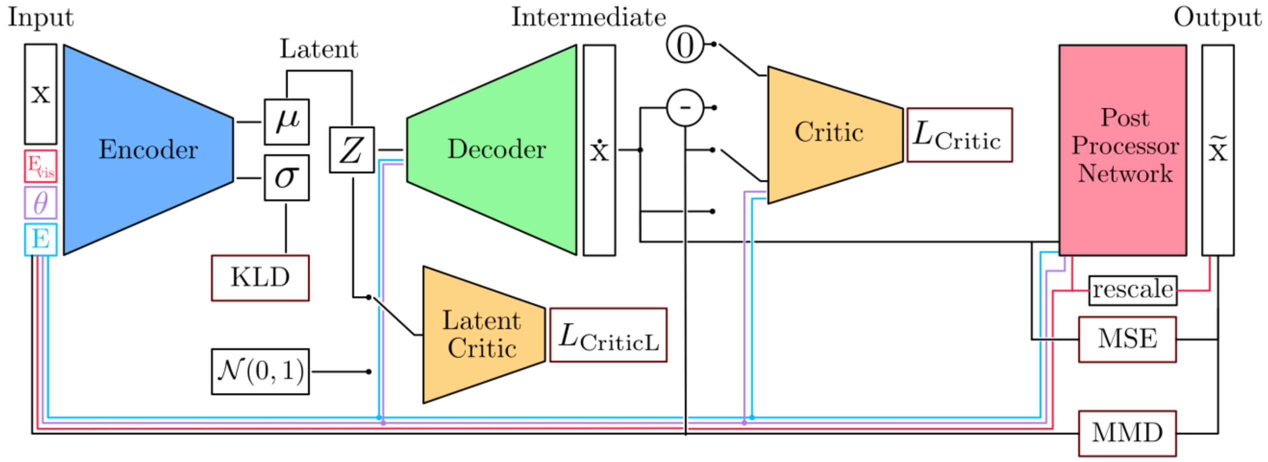
- **Angular conditioning**
- High performance after **reconstruction**
- **Integration** into existing software frameworks
- …

Previously: Energy and Single Angle Conditioning

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

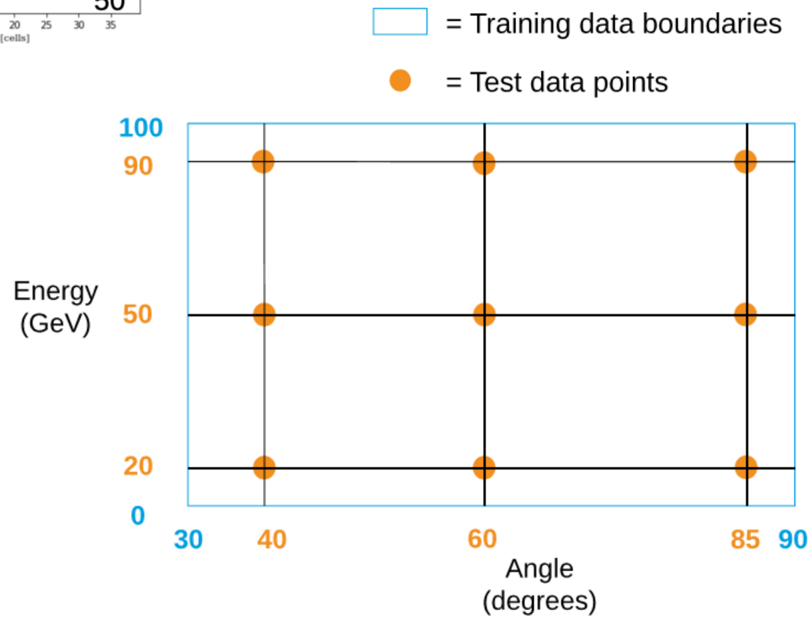






$$L_{BIB-AE} = KLD + L_{CriticL} + L_{Critic}$$

$$L_{Post} = MMD + MSE$$



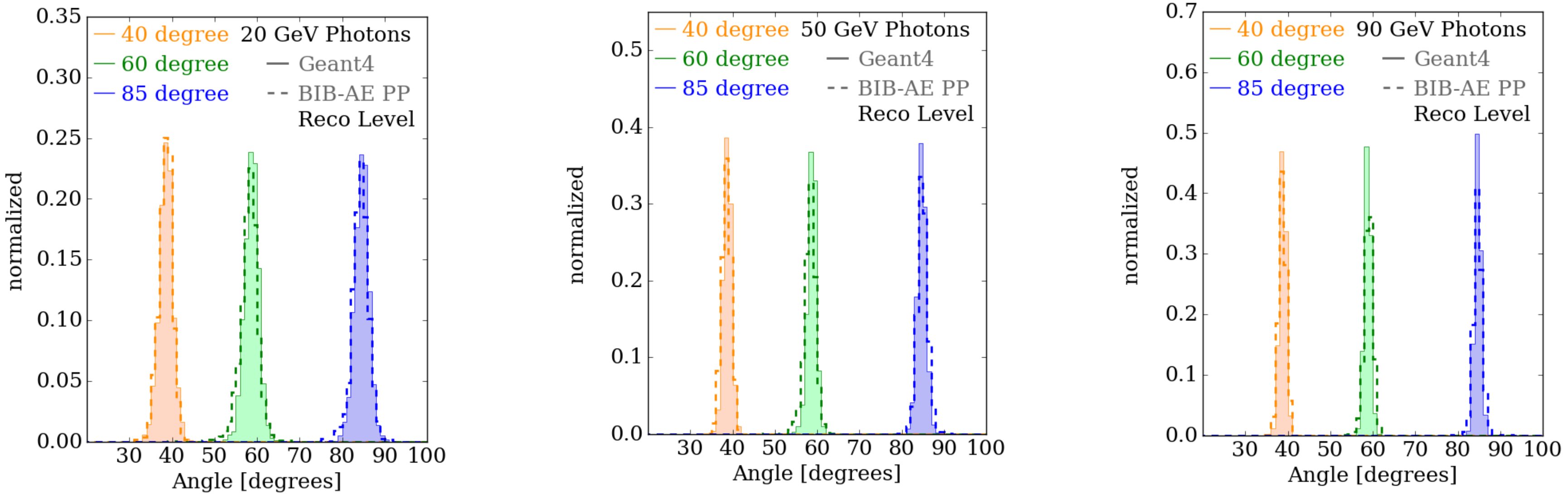
Training and validation samples - 30x60x30 grid

Previously: Conditioning Performance

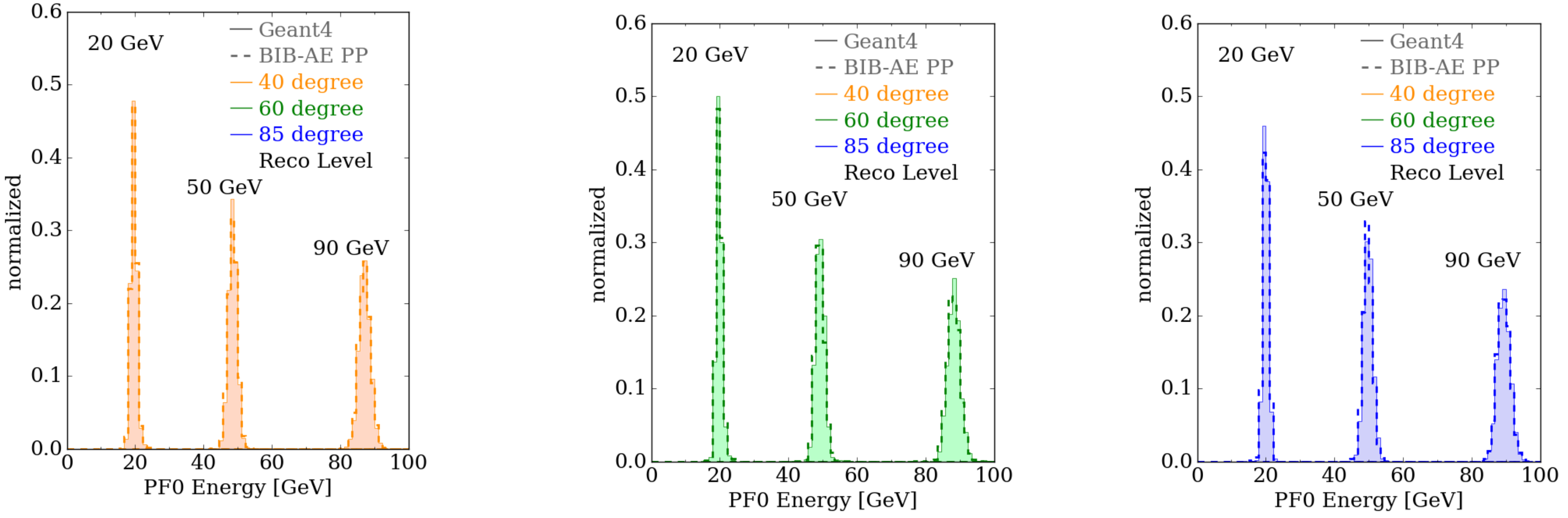
New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, P.M. et al. 2023 MLST 4 035044
DOI 10.1088/2632-2153/acefa9, arXiv: 2303.18150

- After full PandoraPFA reco

- **Rec** level **angle** reconstruction

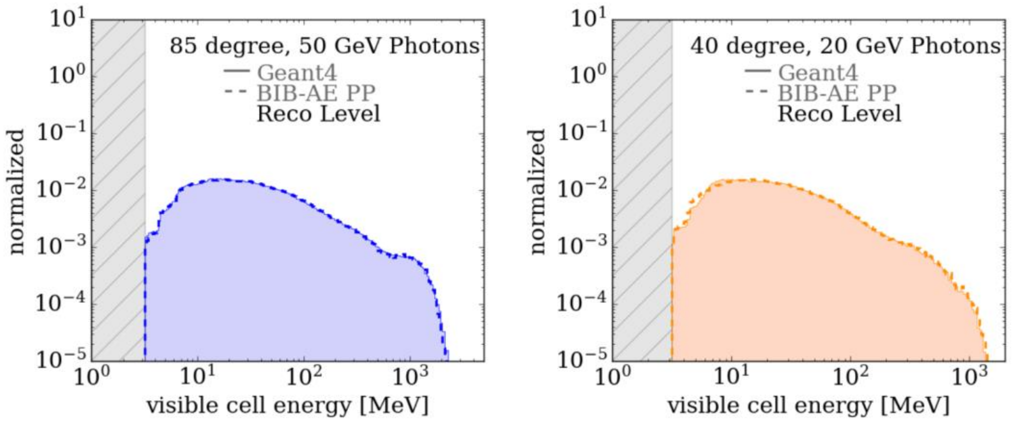


- **Rec** level **calibrated energy**

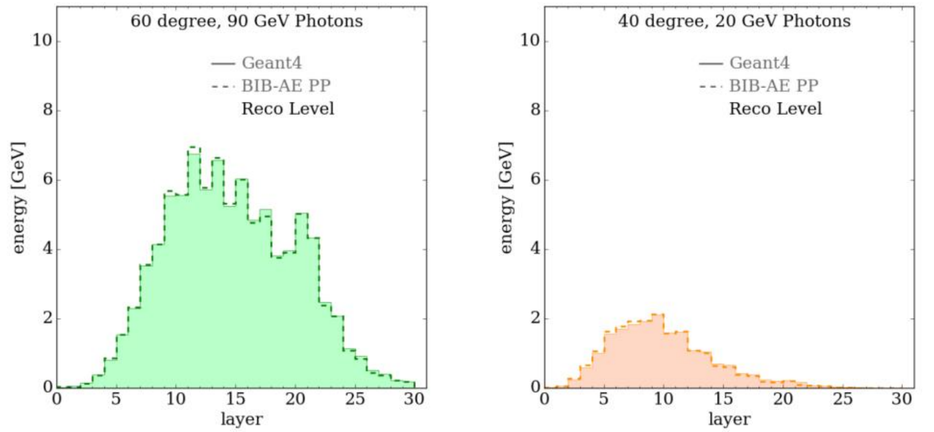


Previously: Performance After Reconstruction

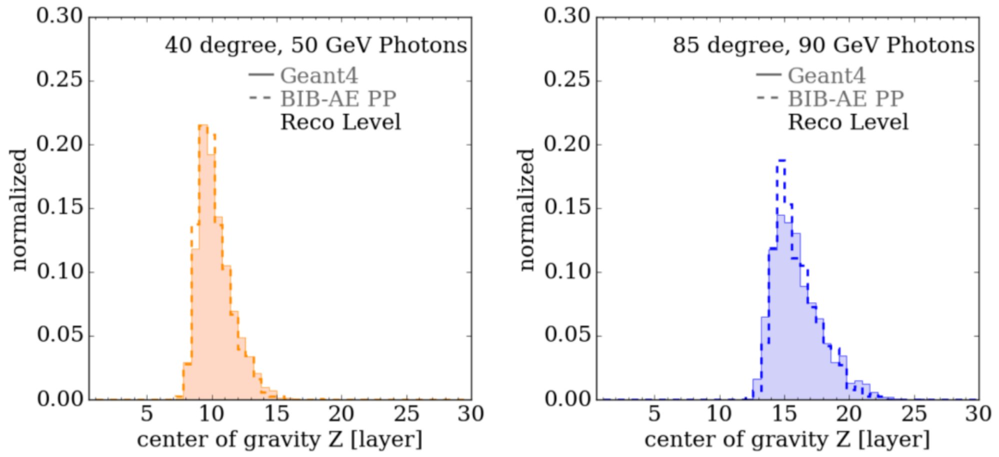
New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, P.M. et al. 2023 MLST 4 035044
DOI 10.1088/2632-2153/acefa9, arXiv: 2303.18150



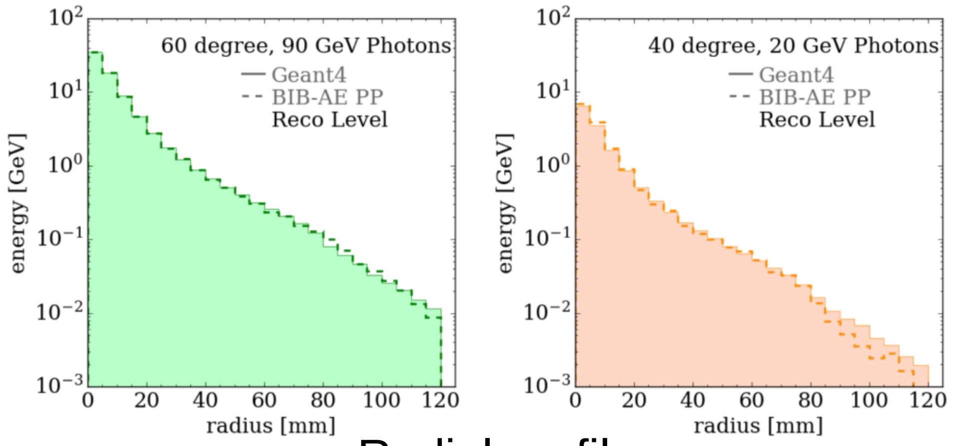
Hit energy spectrum



Longitudinal profile



Centre of gravity in z



Radial profile

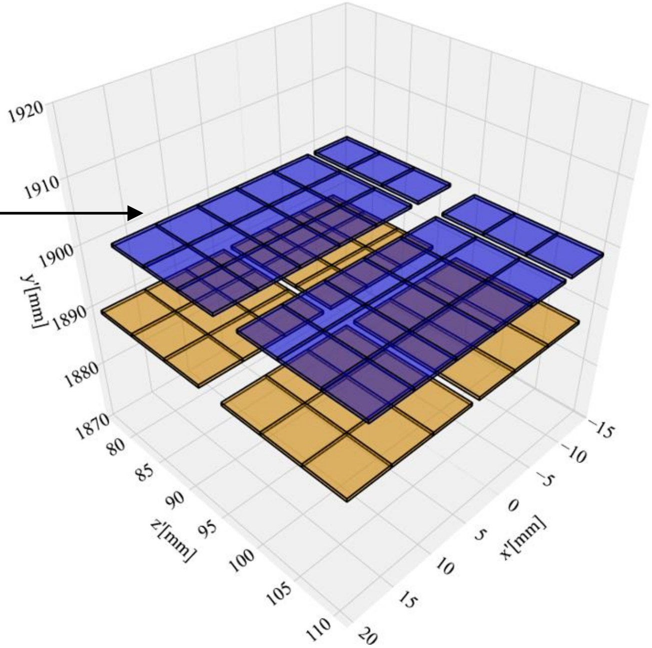
Best (left) and worst (right) test point → **Excellent** physics fidelity

Two Angle Training Data – Regular ECAL

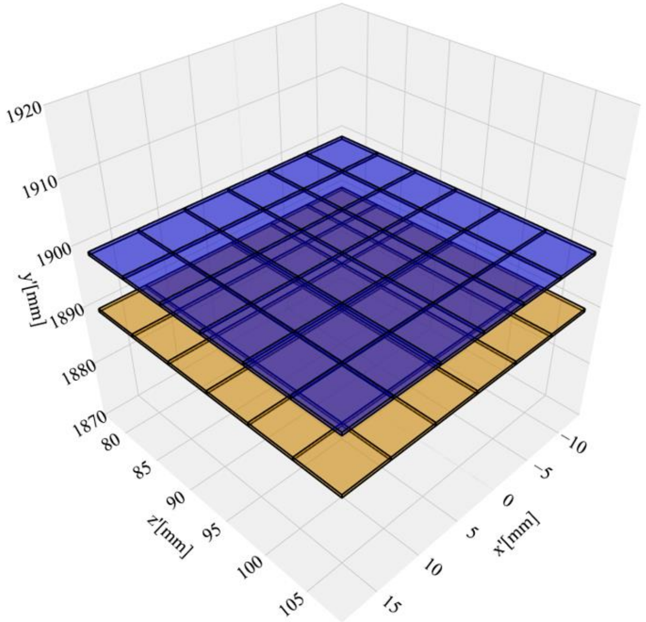
- Create ILD ECAL with **regular** structure for **training**
- Exactly the **same layer wise** material **composition**
- **Purely sensitive** material in active layers (remove dead material)

- **No projection** to from irregular to regular grid
- **All energy** deposited in active layers recorded
- During **simulation with realistic detector geometry**, hits in dead material are dropped by Geant4

Staggering present in real ILD ECAL due to irregular structure



Real ILD ECAL



Regular ILD ECAL

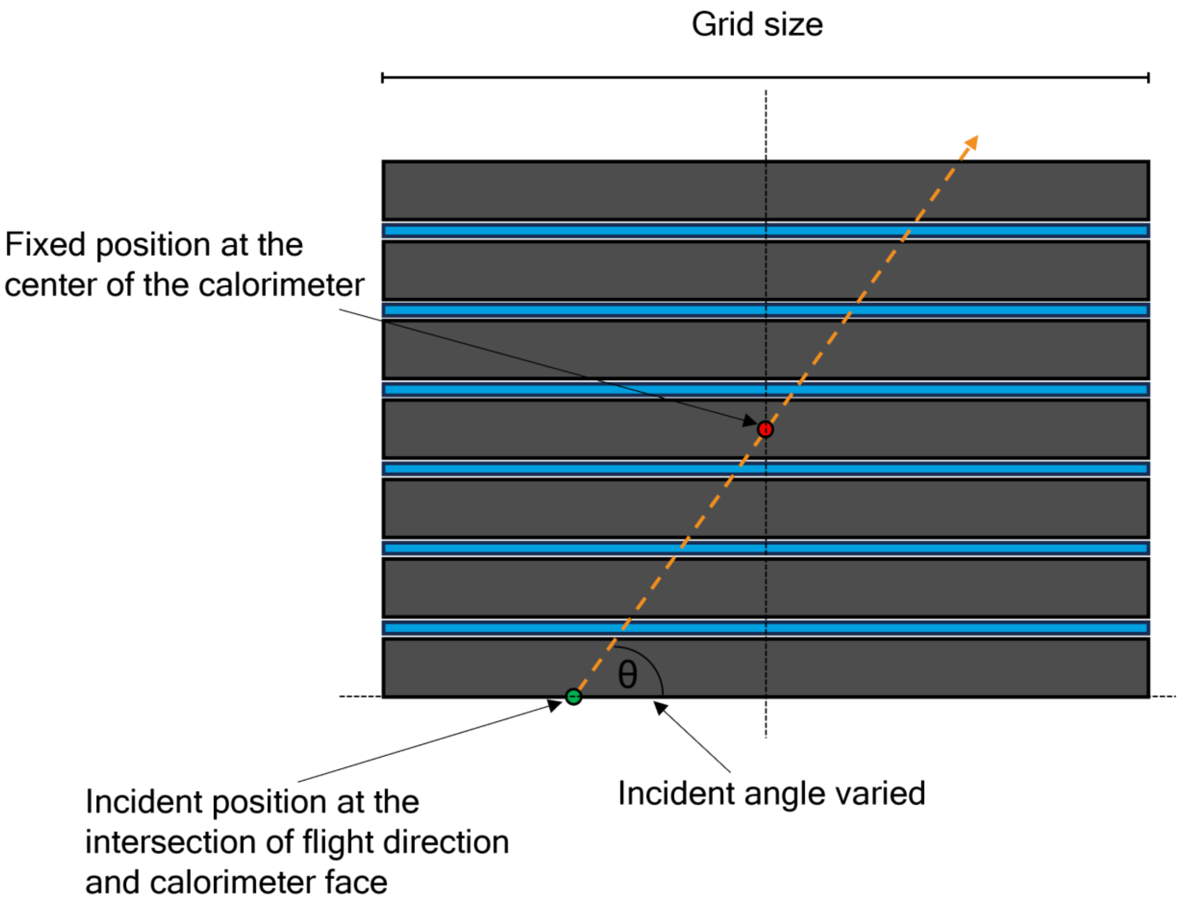
Two Angle Training Data

- Vary angles to **minimise box size**, but retain information about **incident position**

- Used Geant4 version **10.4**

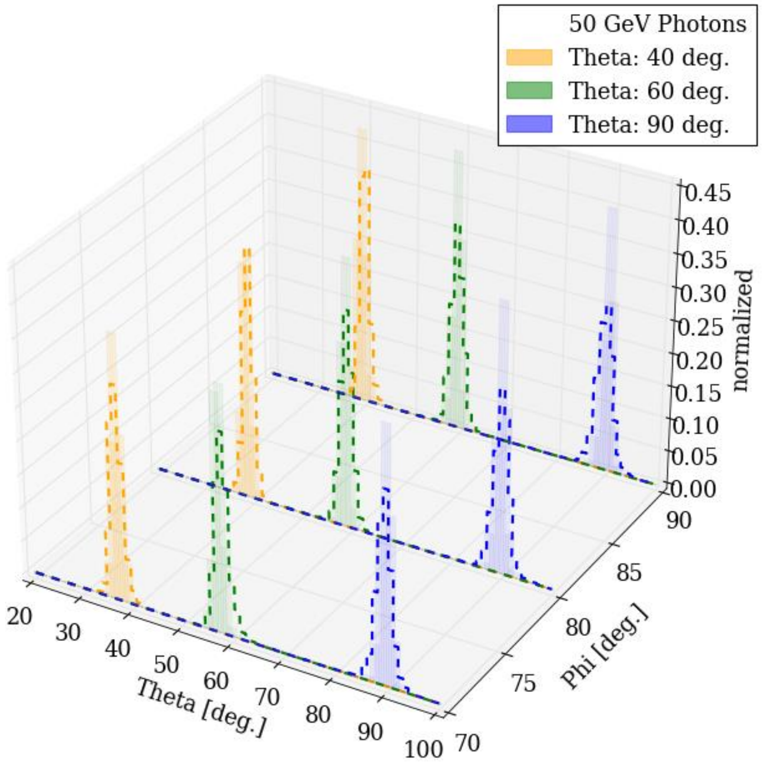
- Training: vary **energy** and **two angles** simultaneously:
  - Energy: 5-126 GeV
  - Theta: 30-95 degrees
  - Phi: 65-95 degrees

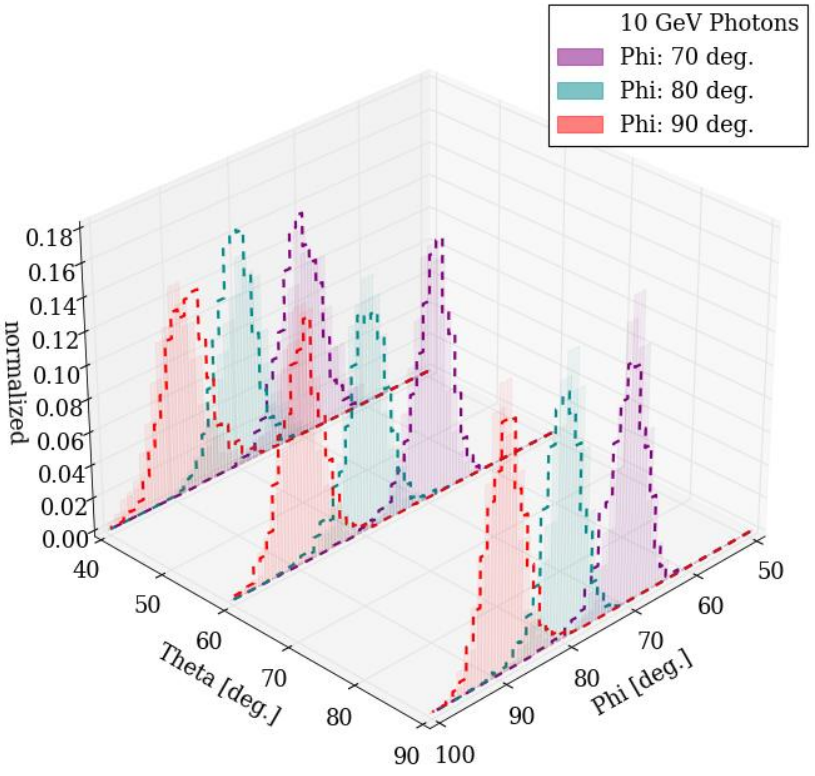
- Test **7** calorimetric **observables** at **27 fixed points**:
  - E: 10, 50, 100 GeV
  - Theta: 40, 60, 90 deg.
  - Phi: 70, 80, 90 deg.

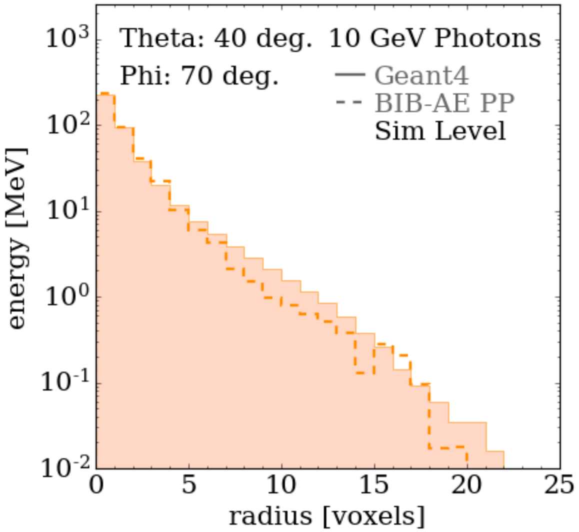


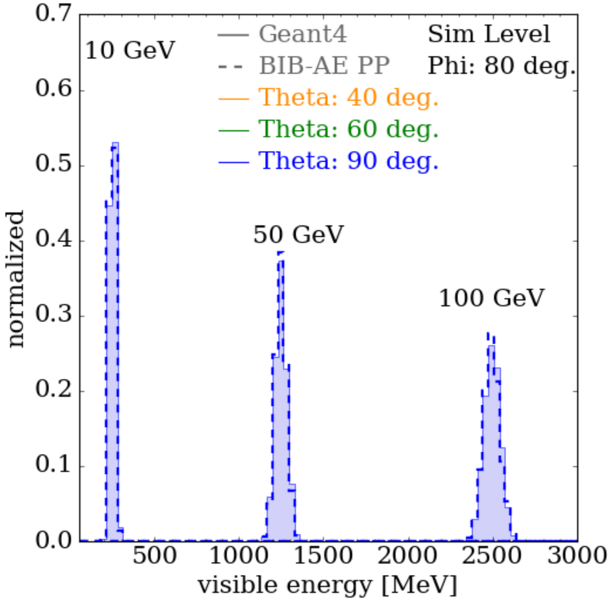
Adding Another Angle

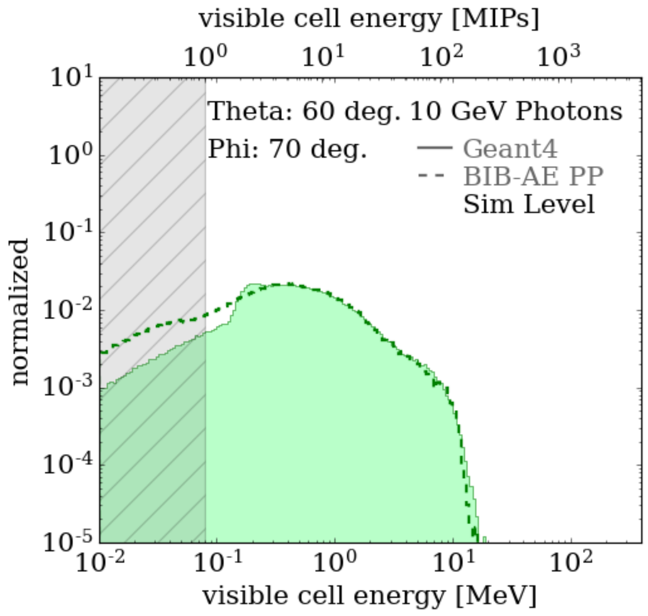
- Need to condition on **energy, theta and phi** for full application
- **Extending phase space** can be challenging



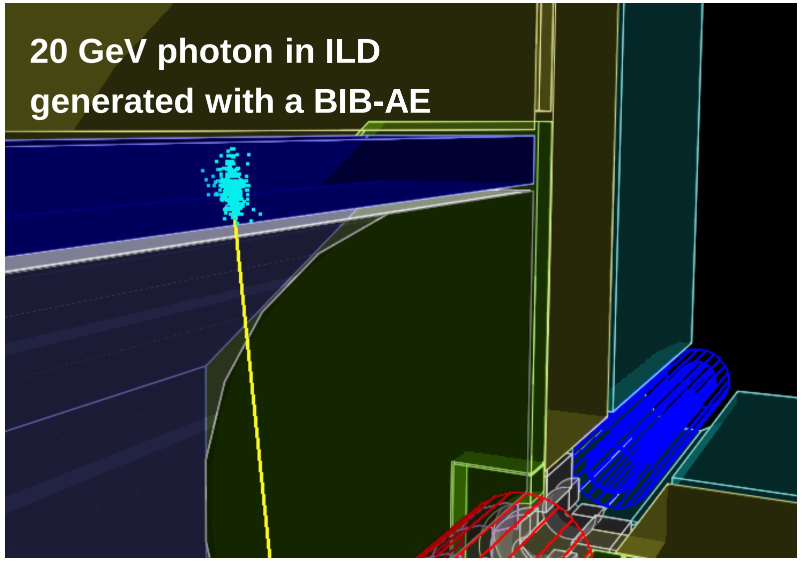








Integration into the Full Simulation Chain



- Prototype library for running ML-based fast sim models: ***DDFastShowerML***
  https://gitlab.desy.de/ilcsoft/ddfastshowerml
  - Use fast sim hooks in DDG4/Geant4
  - Use realistic, detailed detector models
  - Currently only supports CPU
  - Development ongoing

Necessary update to Geant4 version **11.1**!

Trigger
- Fast Sim trigger
  - e.g. particle type, energy, geometry

Model
- Model-specific implementation of ML architecture
  - e.g. BIB-AE, Flow, Diffusion model

- Aim to have an easy to use library which can be adapted for all types of ML architectures in DD4hep

Inference
- Concrete inference in C++
  - ONNX, LibTorch etc…

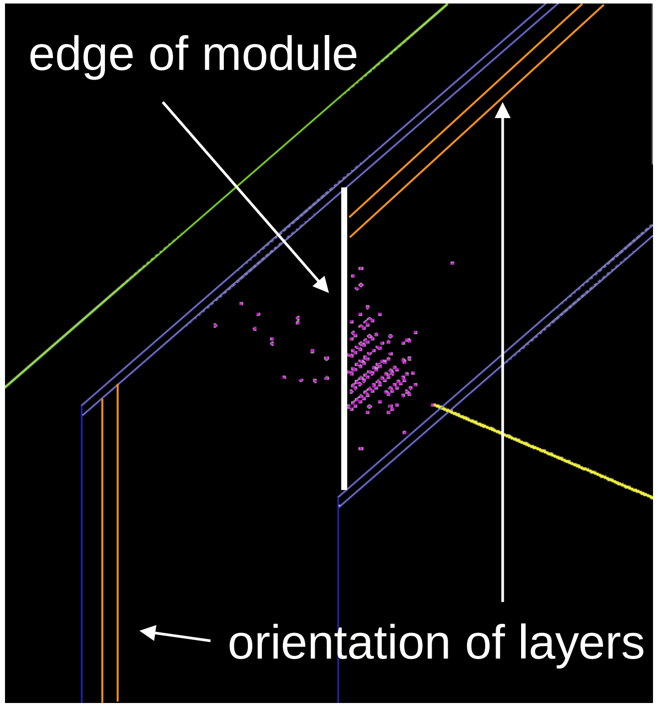
Geometry
- Concrete placement in detector geometry
  - Endcap, barrel etc…

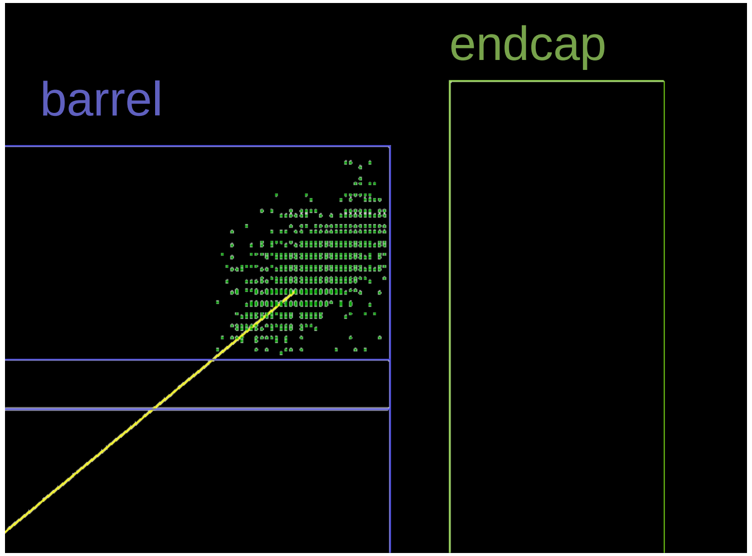
- **Essential** step to be able to study performance of model with **full physics benchmarks**

BIB-AE Integration Into Realistic Geometry

- **BIB-AE** model with full conditioning now **integrated** into ILD detector simulation chain
- **Seamless integration** with full MC simulation in Geant4

- **Exclude regions** of detector where model cannot be applied to geometry
  - **Corners** of octagonal barrel
    - Exclude **8 degree** window (in phi) for each corner
  - **Transition** between barrel and endcap
    - Exclude **7 degree** window (in theta) for each barrel/endcap transition



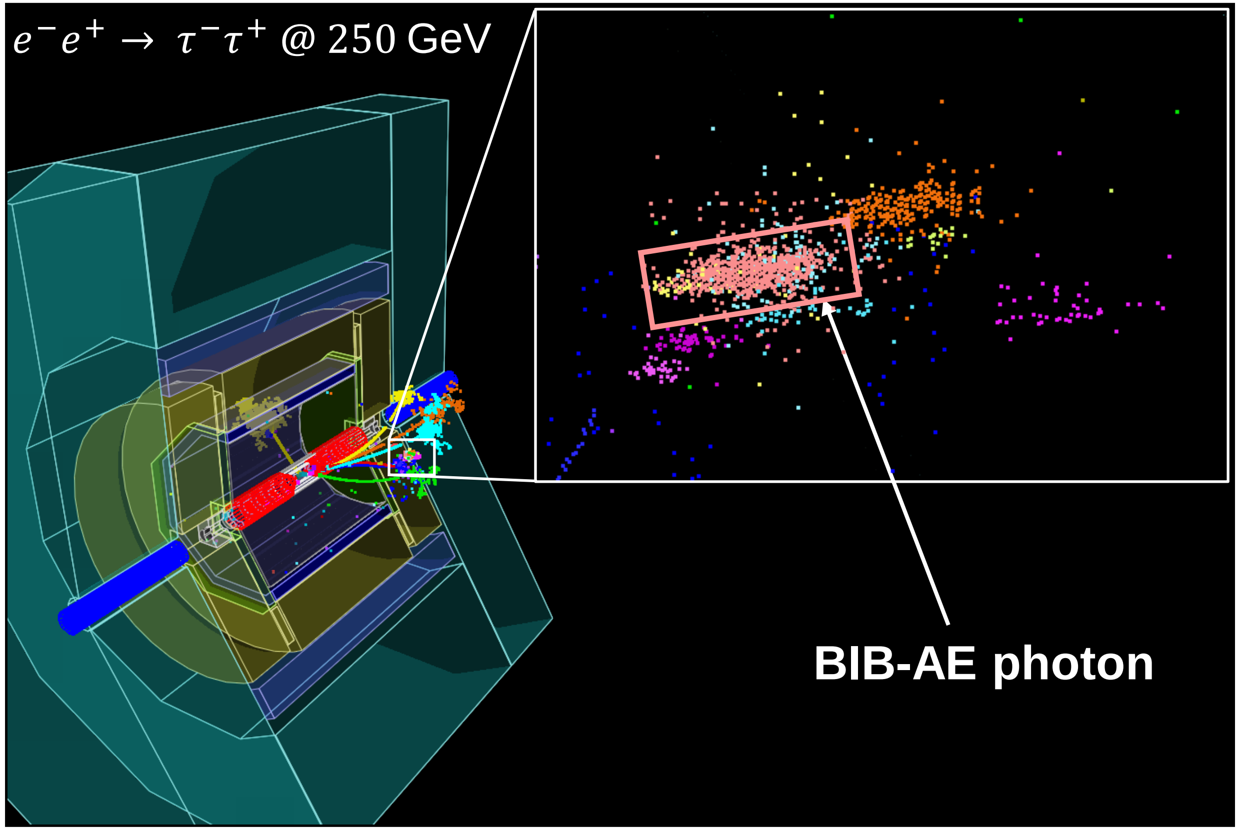


Hadronic Tau Decays as a First Benchmark

- Now possible to run ML model in **full physics simulation**

- Tau branching fractions:
  - ~17.8% $\tau \rightarrow e\bar{\nu}_e\nu_\tau$
  - ~17.4% $\tau \rightarrow \mu\bar{\nu}_\mu\nu_\tau$
  - ~**64.8% hadronic decays**

- Hadronic decay modes often involve $\boldsymbol{\pi^0}$**s** (di-photon)
  - Classic benchmark of ECAL performance



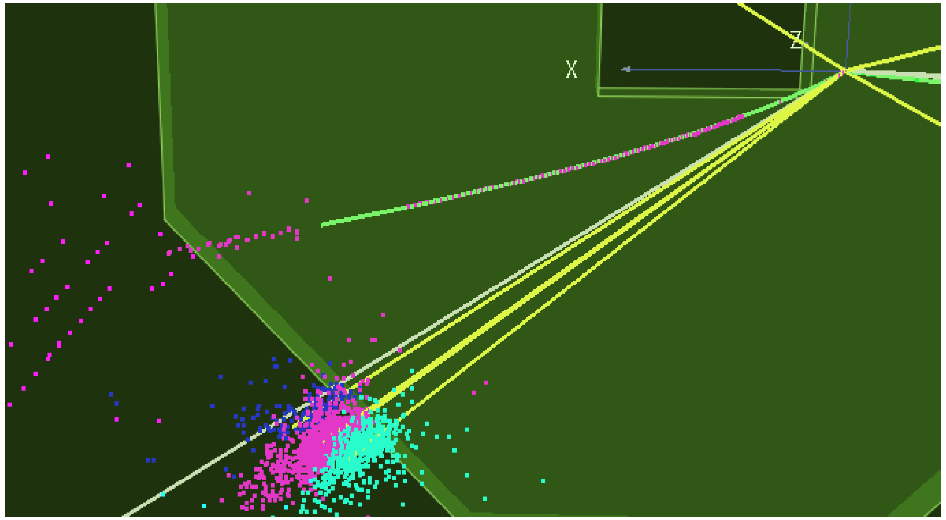
Benchmark on Photons From Pi0 decays in Tau Pair Samples

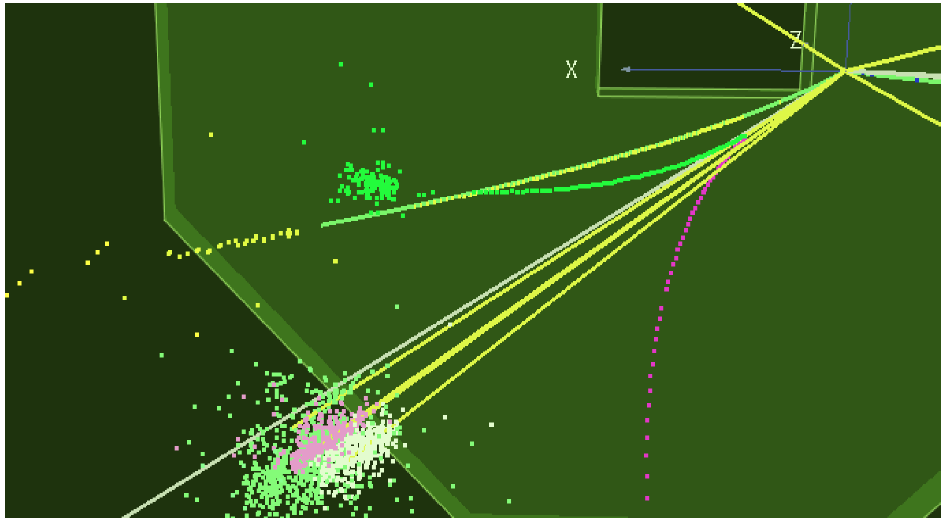
- Use generator files for **2f_leptonic_eL_pR** from 2020 production
  - Select events with **E>10 GeV** for **both** γs from a π^0 (from a τ)

- Simulate 9,000 $e^-e^+ \rightarrow \tau^-\tau^+$ @ 250 GeV
  - Sample 1+2: Full Geant4 (**Version 10.4** and **Version 11.1**)
  - Sample 3: Use **BIB-AE** for $\boldsymbol{e^{+/-}}$ and $\boldsymbol{\gamma}$ incident on calorimeter with E>10 GeV (+ passing geo trigger)
  - Exactly the **same events from generator** in both cases
  - 3 runs with **different random seeds** for uncertainties

- Apply **full standard reconstruction** in both cases

Reconstruction performance depends on what happens in Geant4 (both full G4)



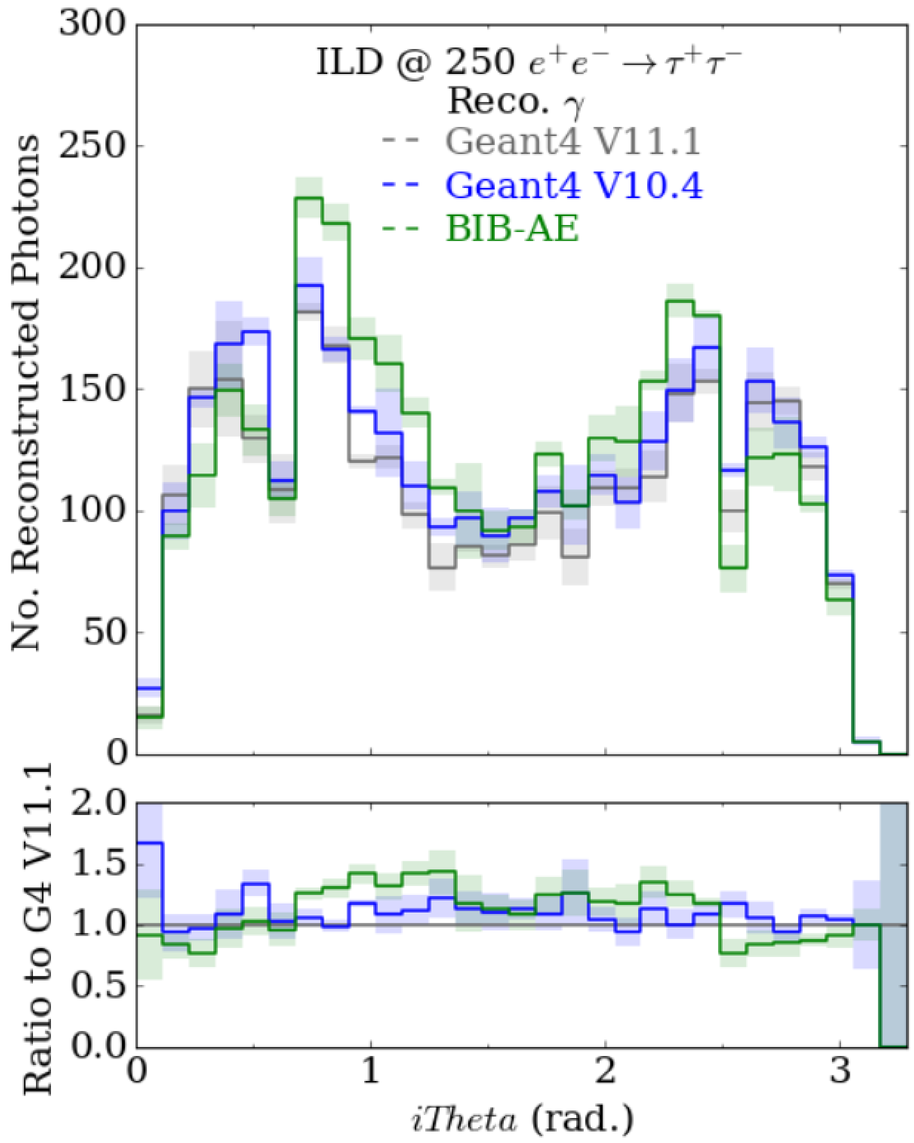


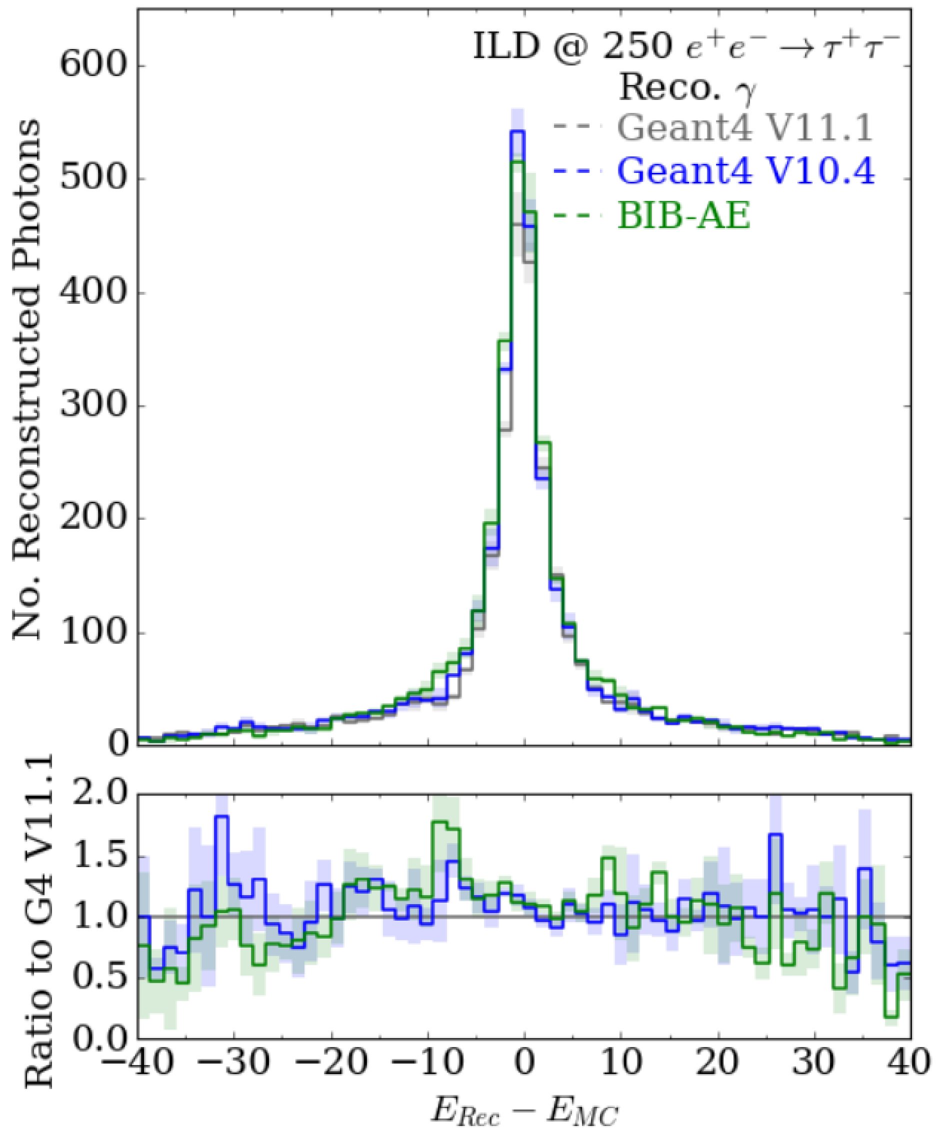
Benchmark: Reconstruction performance (π^0s)

π^0s	No. True	No. Reco	No. Good (π^0 correctly recoed)	No. Missed (π^0 missed)	No. Confused (π^0 incorrectly recoed)	No. Fake (No. Reco – No. Good – No. Confused)
Geant4 V11.1	16693	8942 ± 69	2452 ± 33	12843 ± 27	1398 ± 33	5092 ± 80
Geant4 V10.4	16693	9021 ± 119	2545 ± 35	12789 ± 35	1359 ± 10	5117 ± 96
BIB-AE	16693	9192 ± 130	2576 ± 16	12720 ± 2	1397 ± 16	5219 ± 128

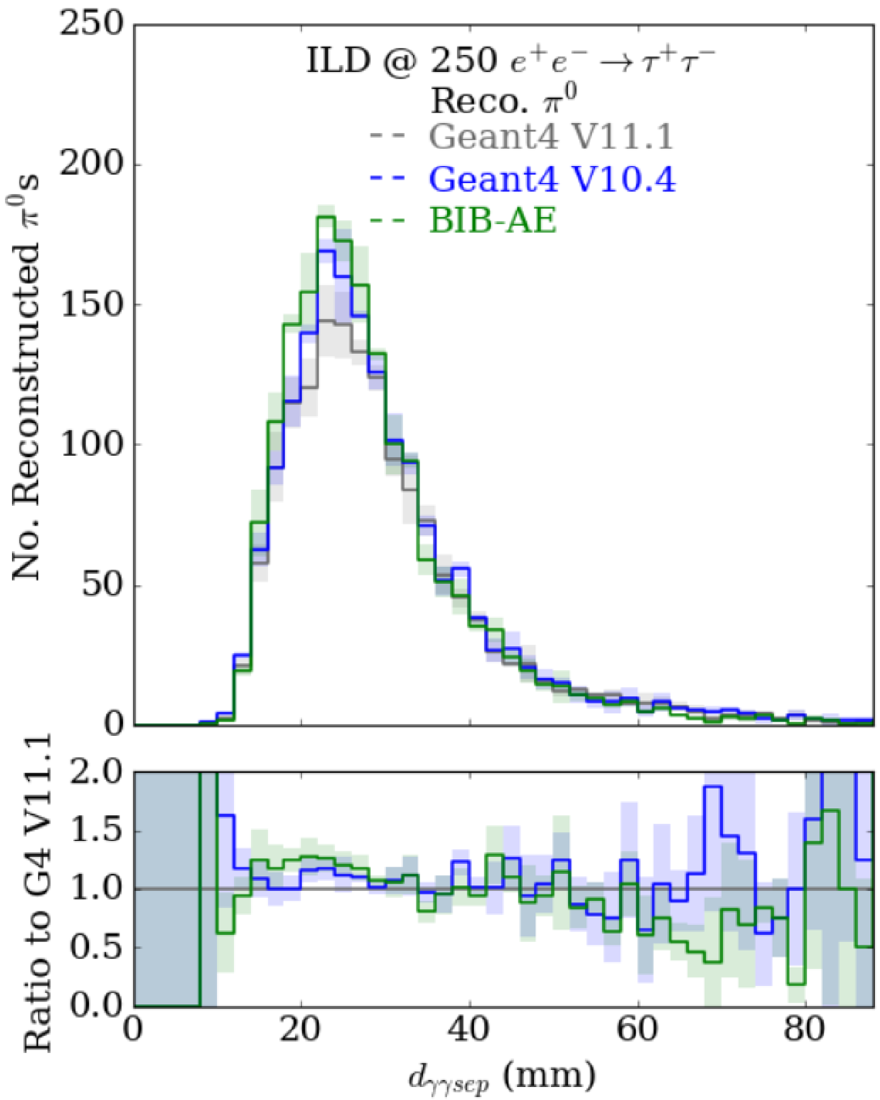
- Now look at $\boldsymbol{\pi^0}$ **reco-candidates** with criteria on MC-Truth link:
  - Only take **pi0s linked to a tau**
  - Both γs have **E>10 GeV** and **passed geometry** fast sim **triggers**

Photons from Tau pi0s

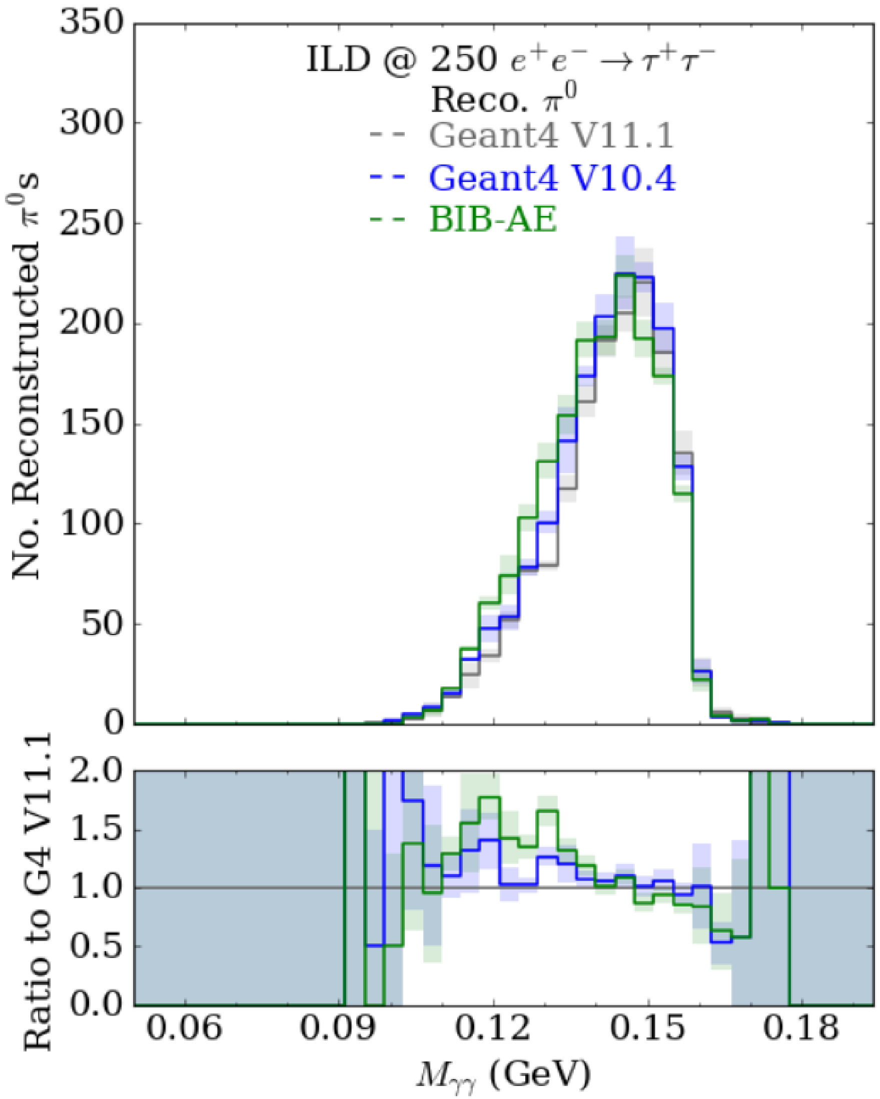




Tau pi0s



ILD @ 250 $e^+e^- \rightarrow \tau^+\tau^-$
Reco. π^0
Geant4 V11.1
Geant4 V10.4
BIB-AE
No. Reconstructed π^0s
Ratio to G4 V11.1
$d_{\gamma\gamma sep}$ (mm)



ILD @ 250 $e^+e^- \rightarrow \tau^+\tau^-$
Reco. π^0
Geant4 V11.1
Geant4 V10.4
BIB-AE
No. Reconstructed π^0s
Ratio to G4 V11.1
$M_{\gamma\gamma}$ (GeV)

Conclusion

Achieved

- **Energy and angular** conditioning for EM showers with high physics fidelity
- **Additional angle** added in conditioning- **reduce grid size** (compute) and remove artefacts from **regular-irregular** projection
- An initial implementation of a **prototype library** for interfacing with the full simulation chain
- **First physics benchmark** for generative fast sim in high granularity calorimeter
  - π^0 from taus- **similar level of performance** to differences between Geant4 versions
  - Some deviations in reconstruction performance still visible

Next Steps

- **Extend** functionality of library (batching, GPU support etc.)
- Other generative models based on **point clouds**- naturally handle irregular geometries
- **Hadronic** showers in **ECAL+HCAL**
- …

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, P.M. et al., arXiv:2305.04847, JINST 18 (2023) 11, P11025

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

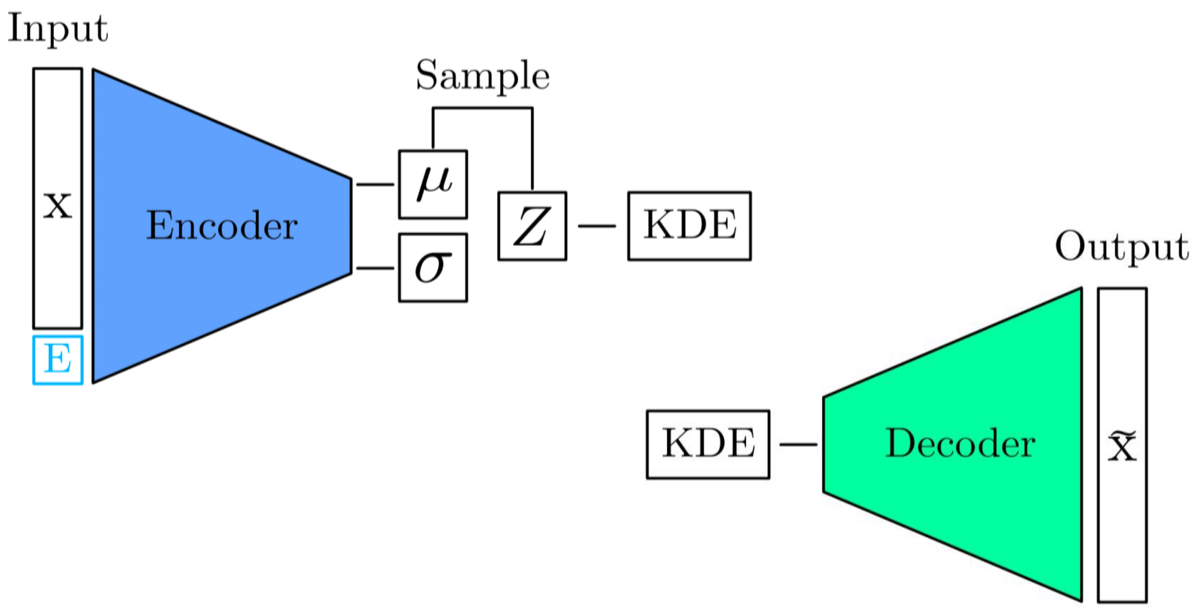
Backup

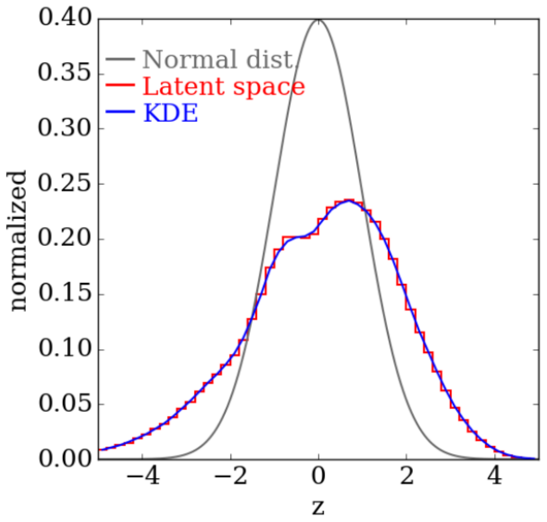
Latent Space sampling

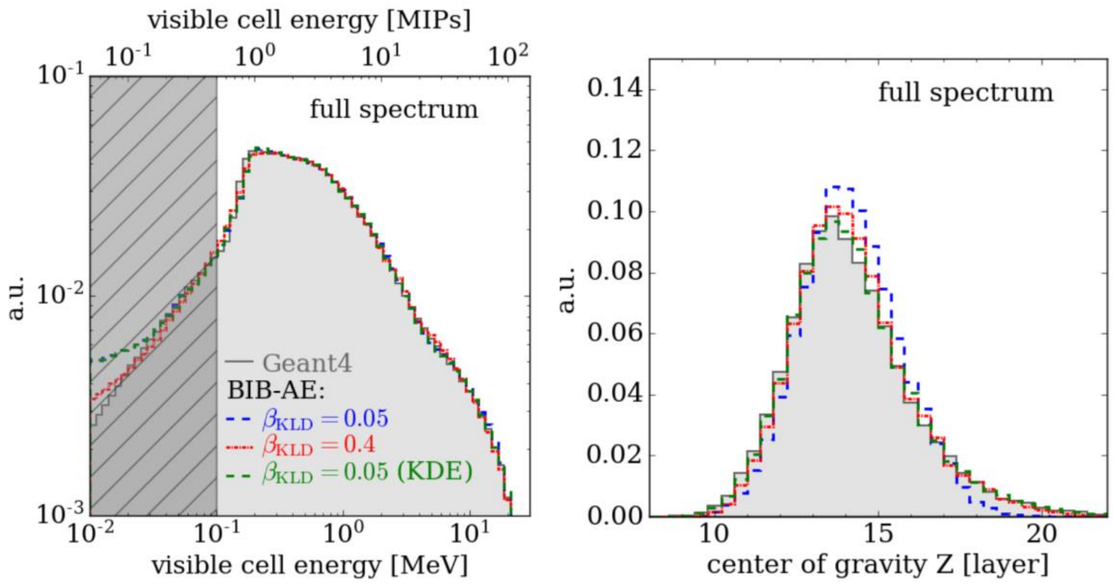
- **Relaxing regularisation** of latent space allows more information to be stored
  - Latent space deviates from a Normal distribution

- Employ **density estimation** to produce latent sample (**normalising flow**)

- **Improve** modeling of **shower shape** (center of gravity)

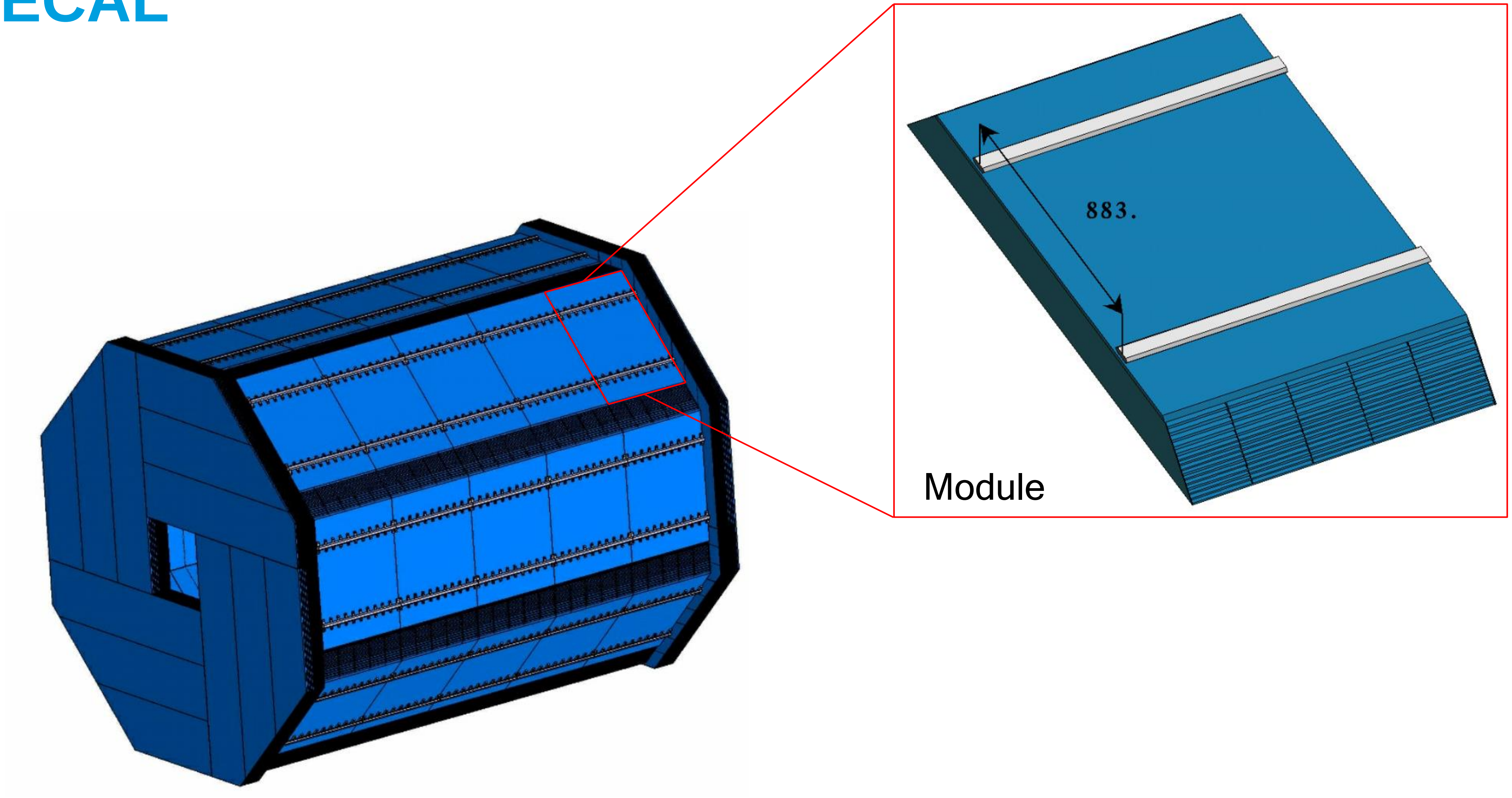




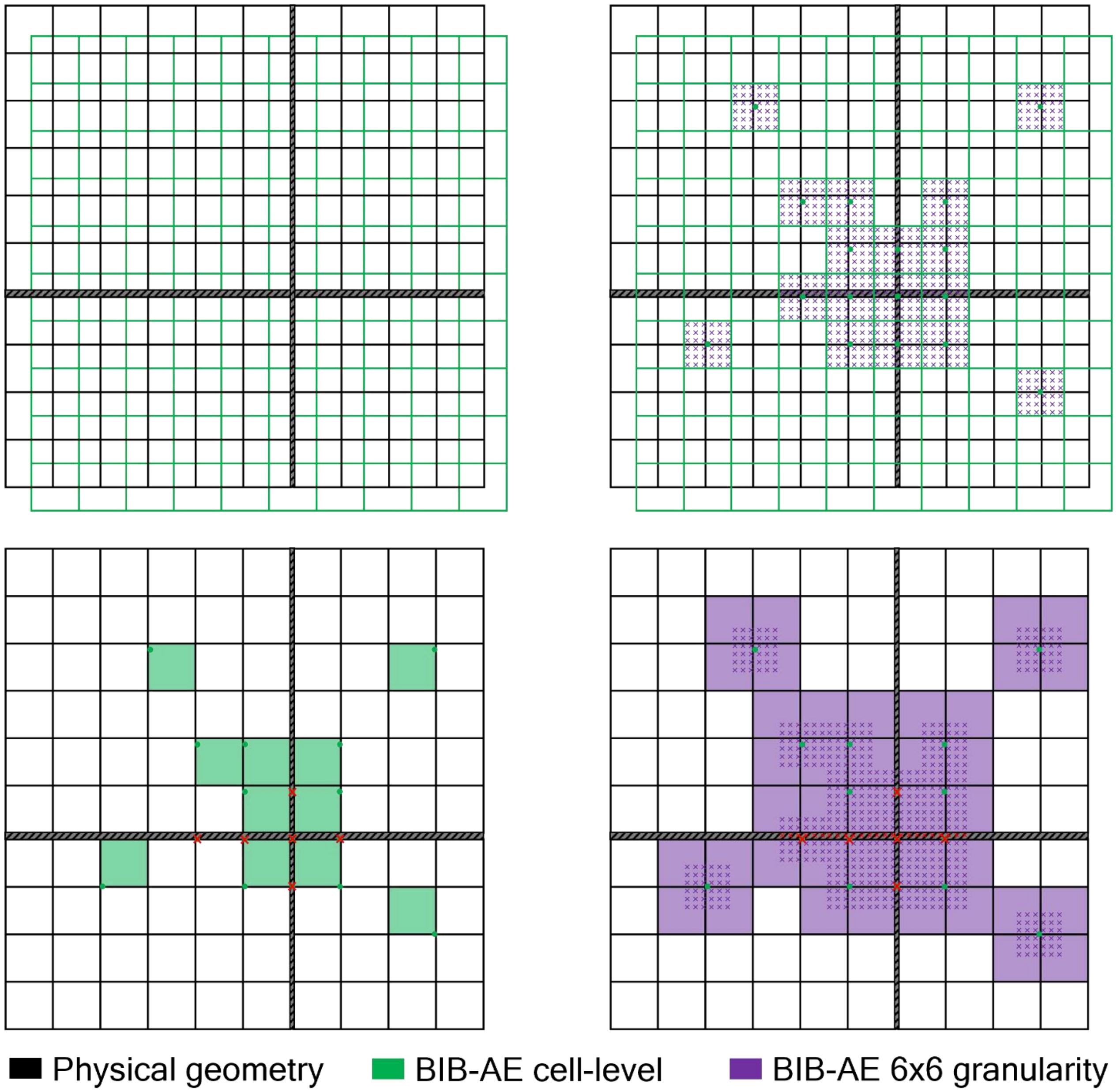


Buhmann et. al: **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network**, EPJ Web of Conferences 251, 03003 (2021)

ILD ECAL



Tackling Irregular Geometries



Timing Of Generative ML Methods

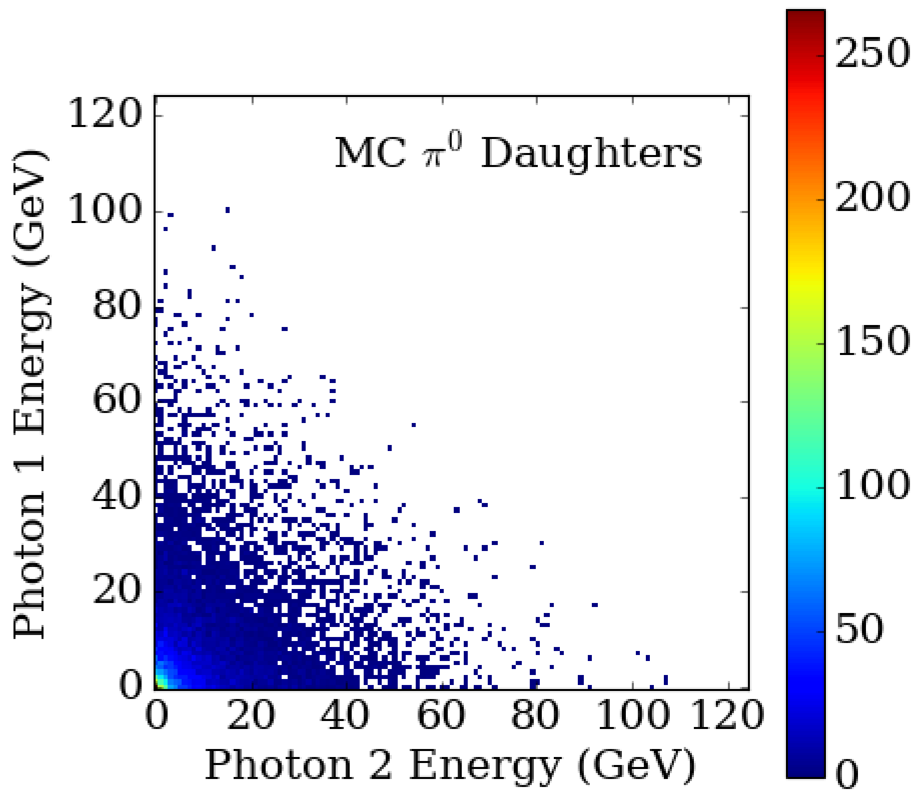
Hardware	Simulator	Time / Shower [ms]	Speed-up
CPU	GEANT4	2684 ± 125	×1
	WGAN	47.923 ± 0.089	×56
	BIB-AE	350.824 ± 0.574	×8
GPU	WGAN	0.264 ± 0.002	×10167
	BIB-AE	2.051 ± 0.005	×1309

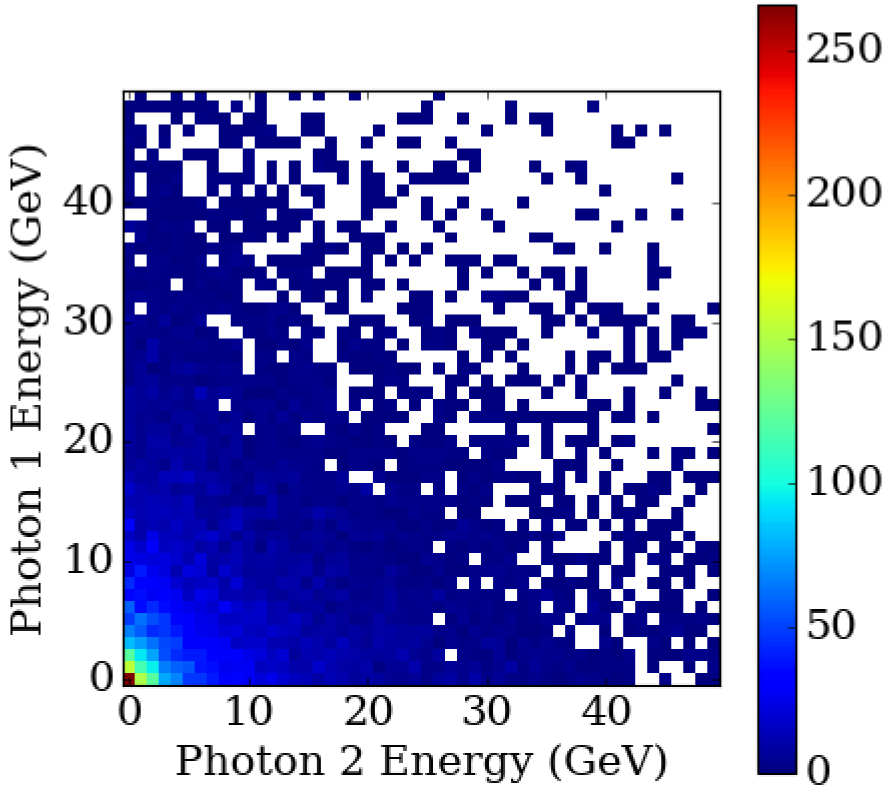
BIB-AE/WGAN, pion showers 10-100 GeV uniform

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

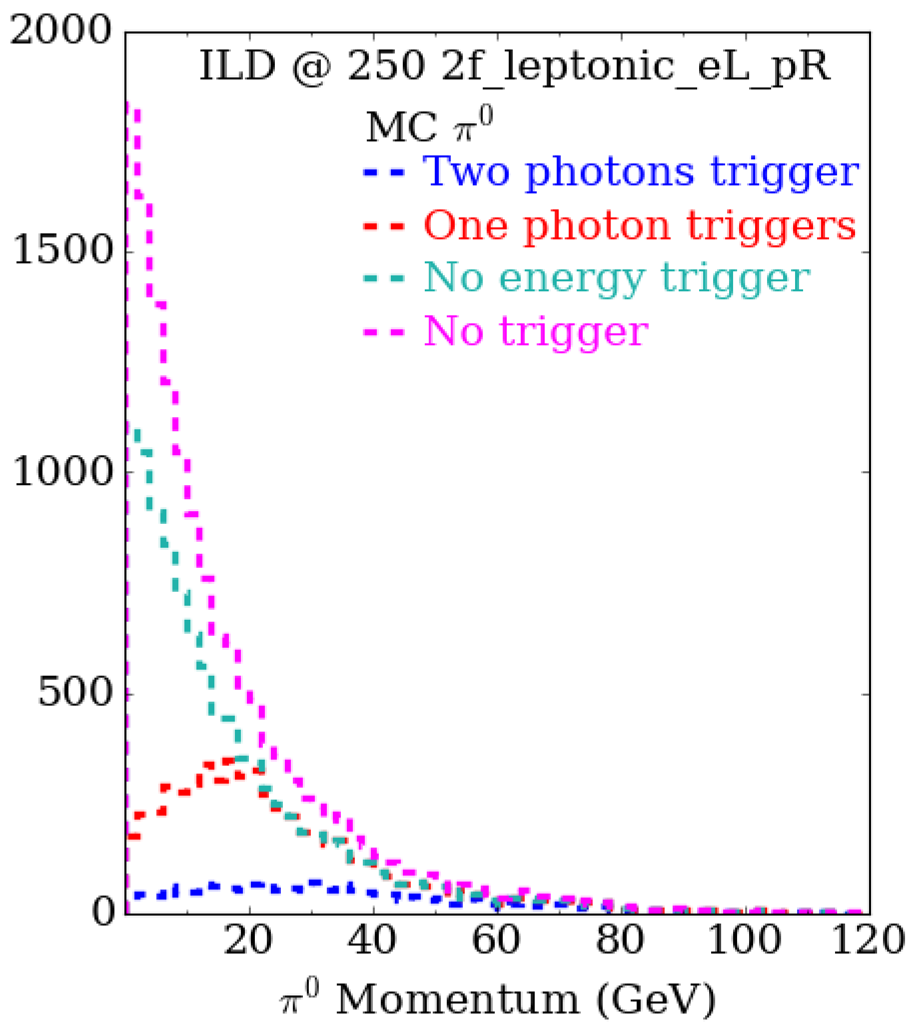
BIB-AE, photon showers 10-100 GeV - 30-90 deg uniform

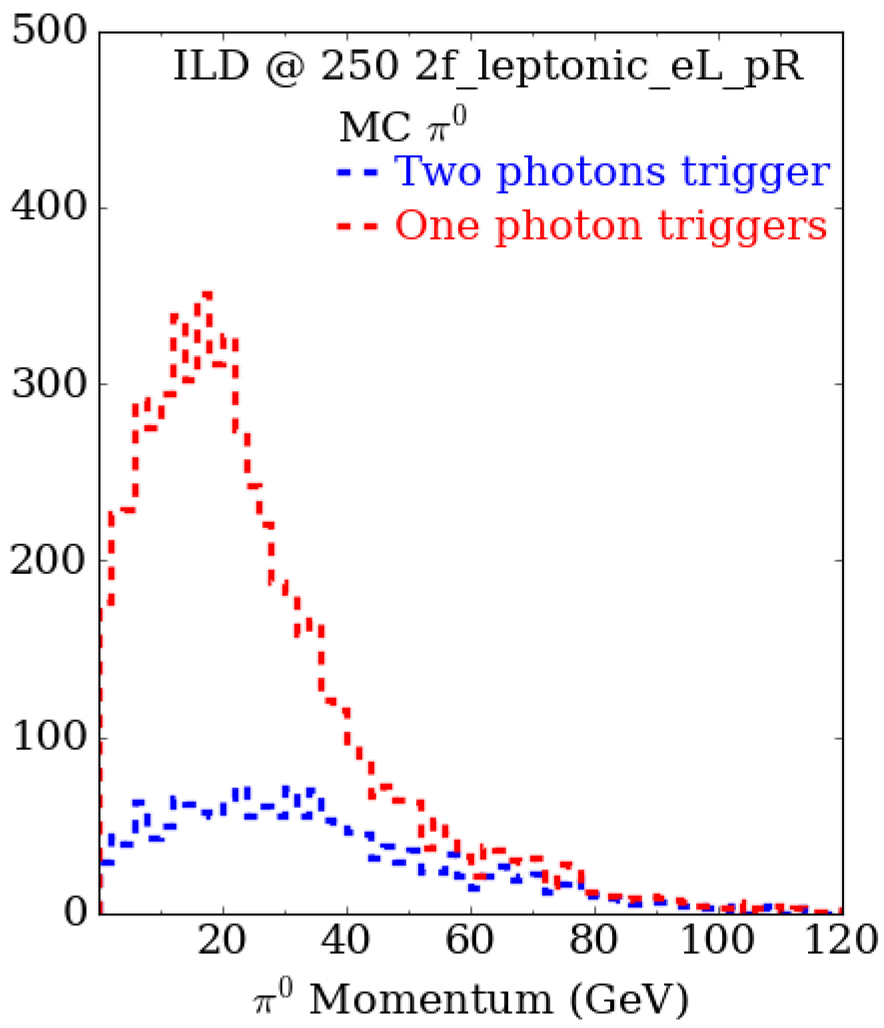
MC Pi0– daughter correlations



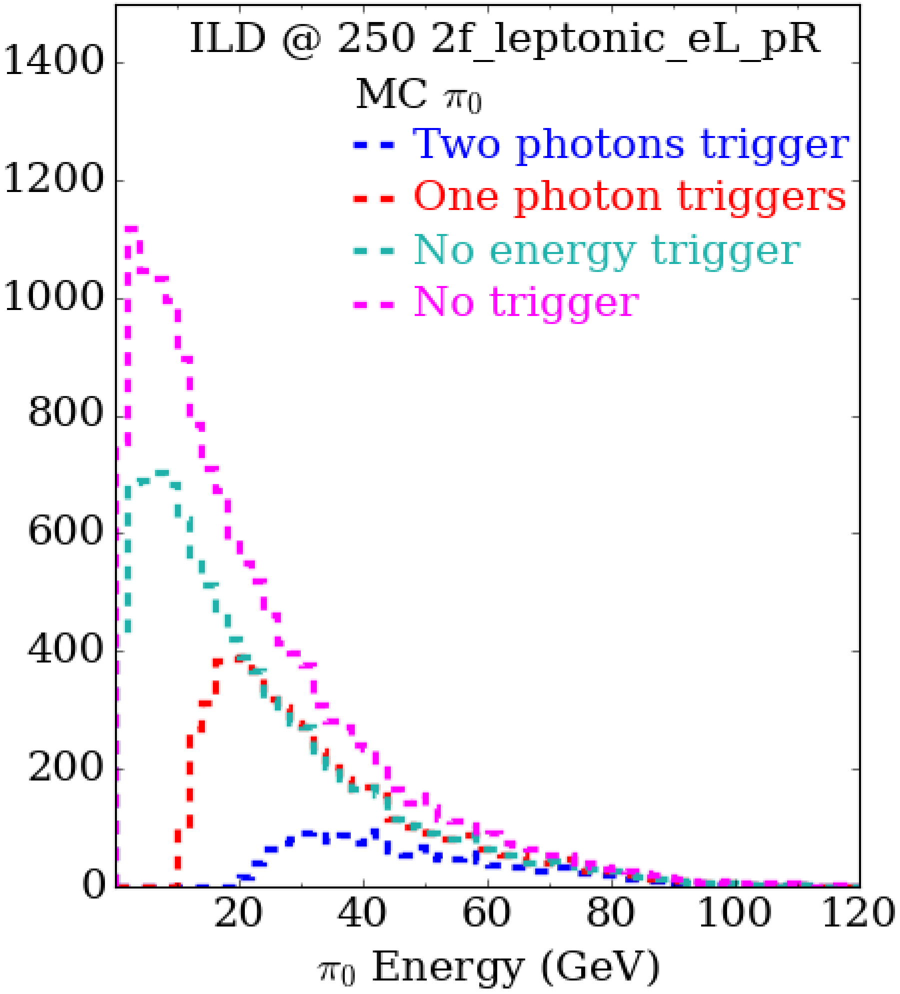


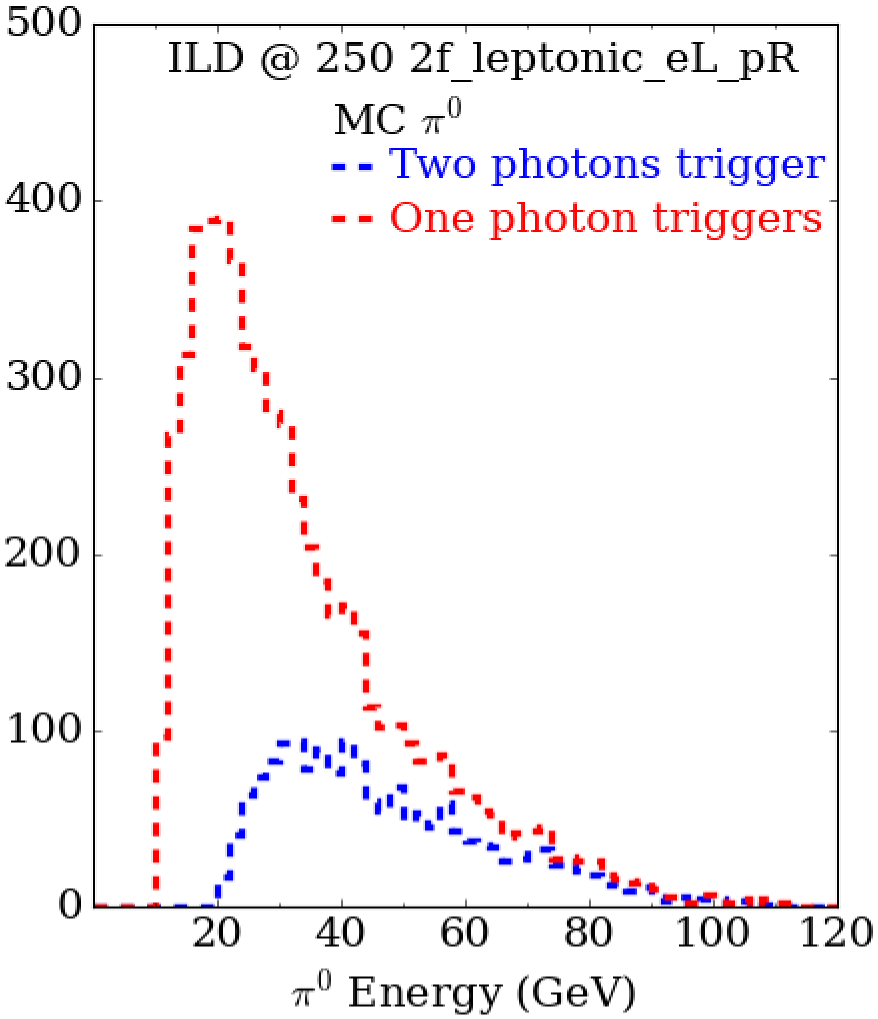
MC Pi0 – Momentum



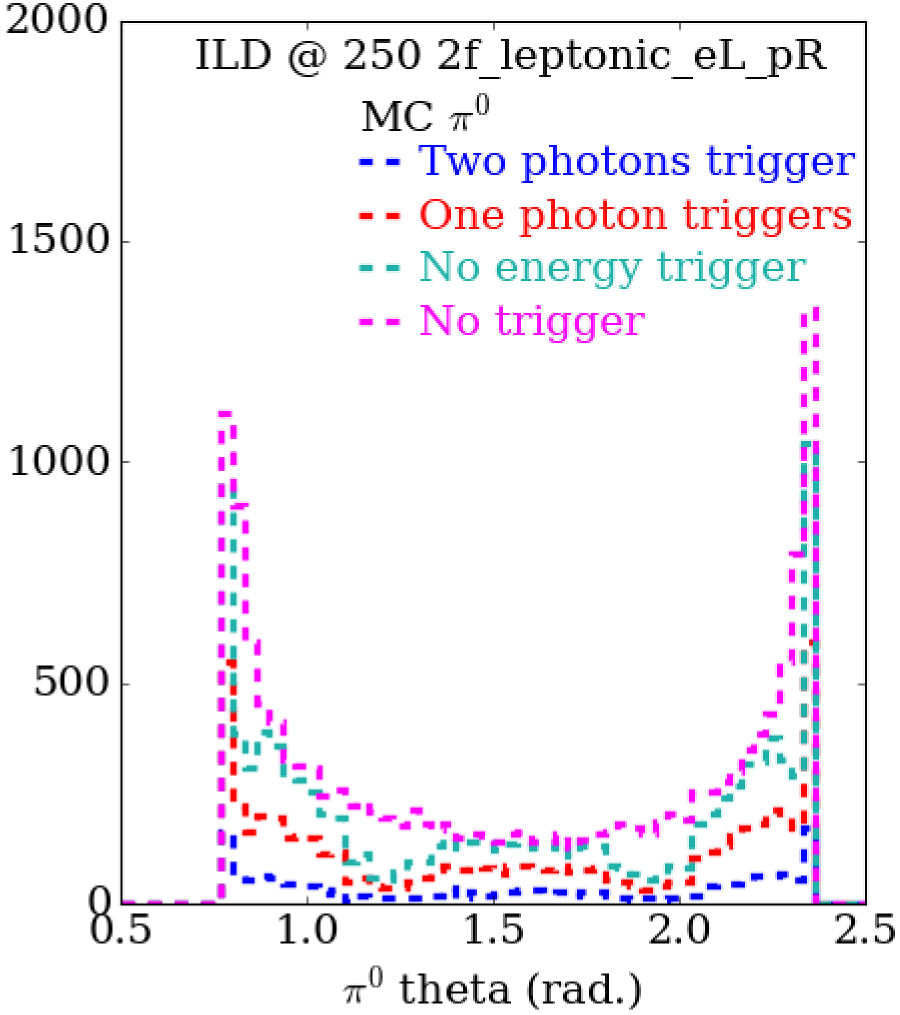


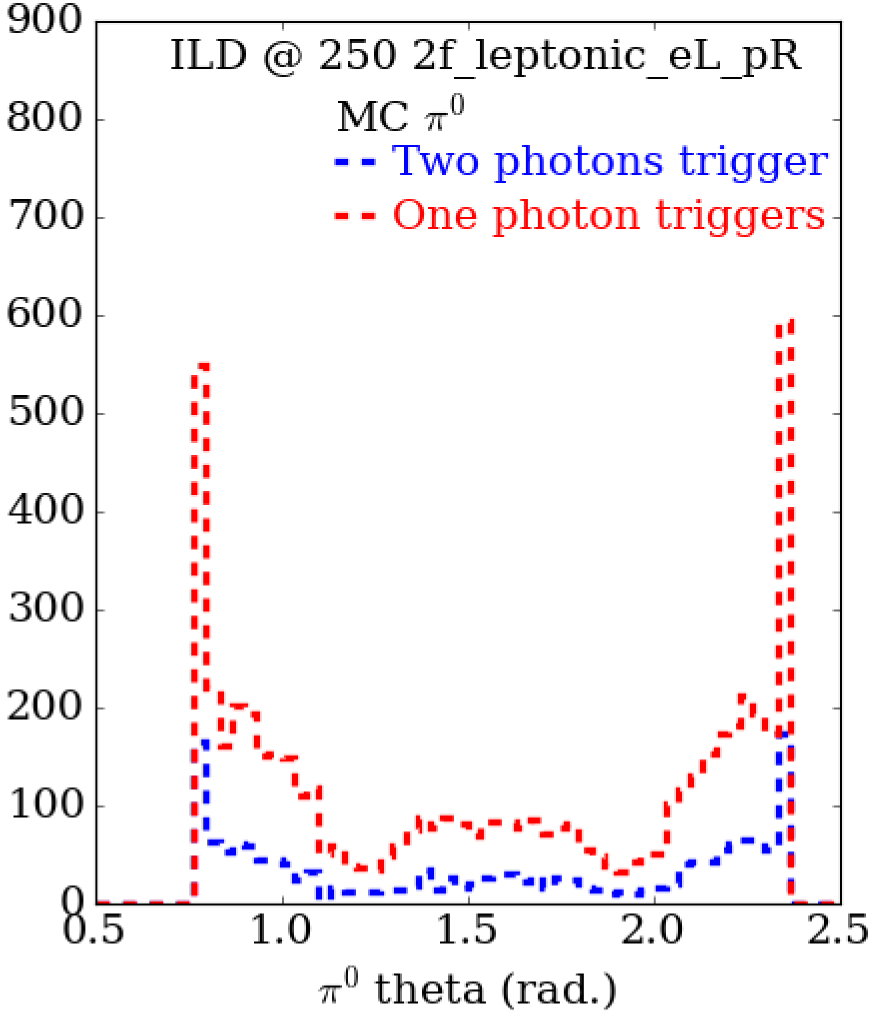
MC Pi0 – Energy



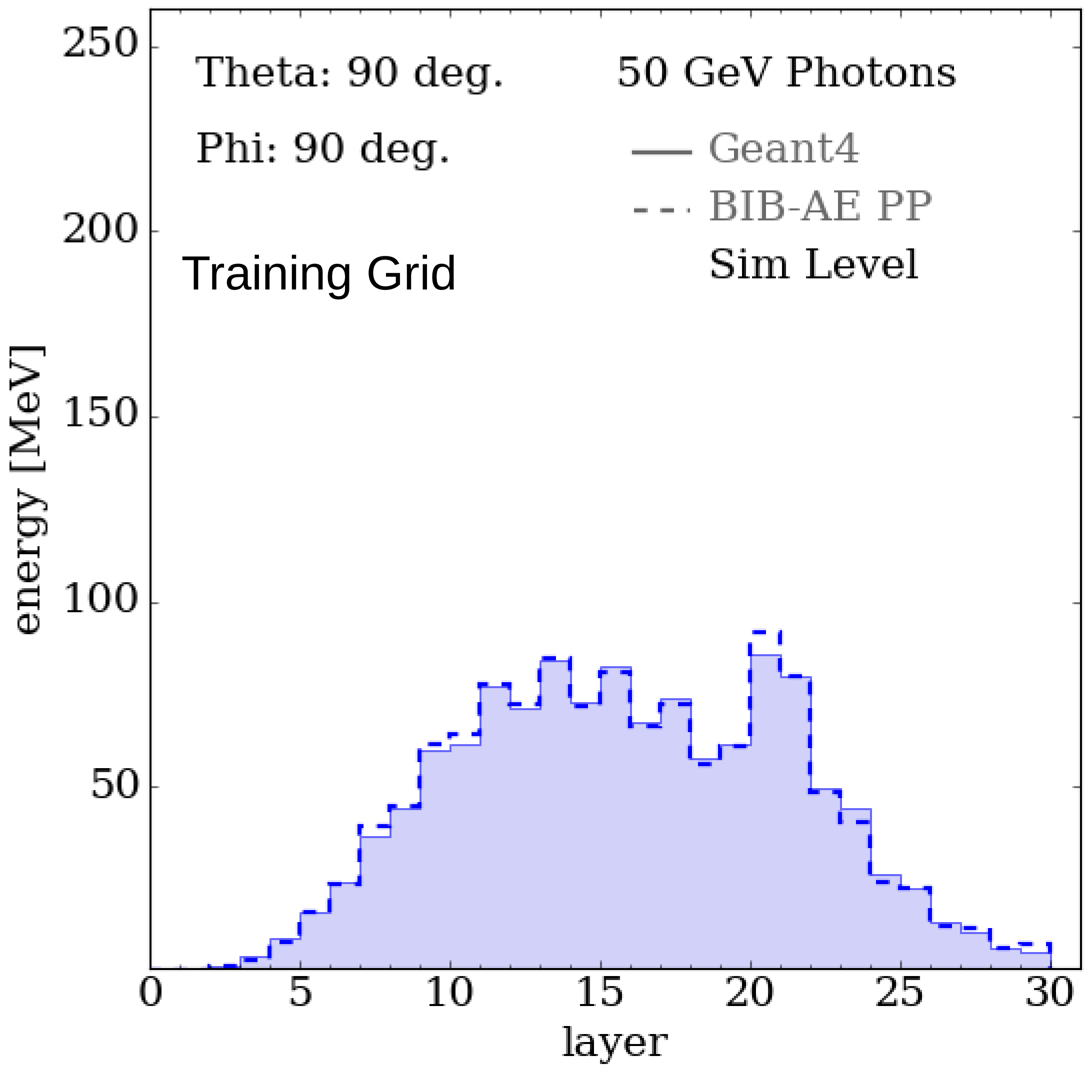


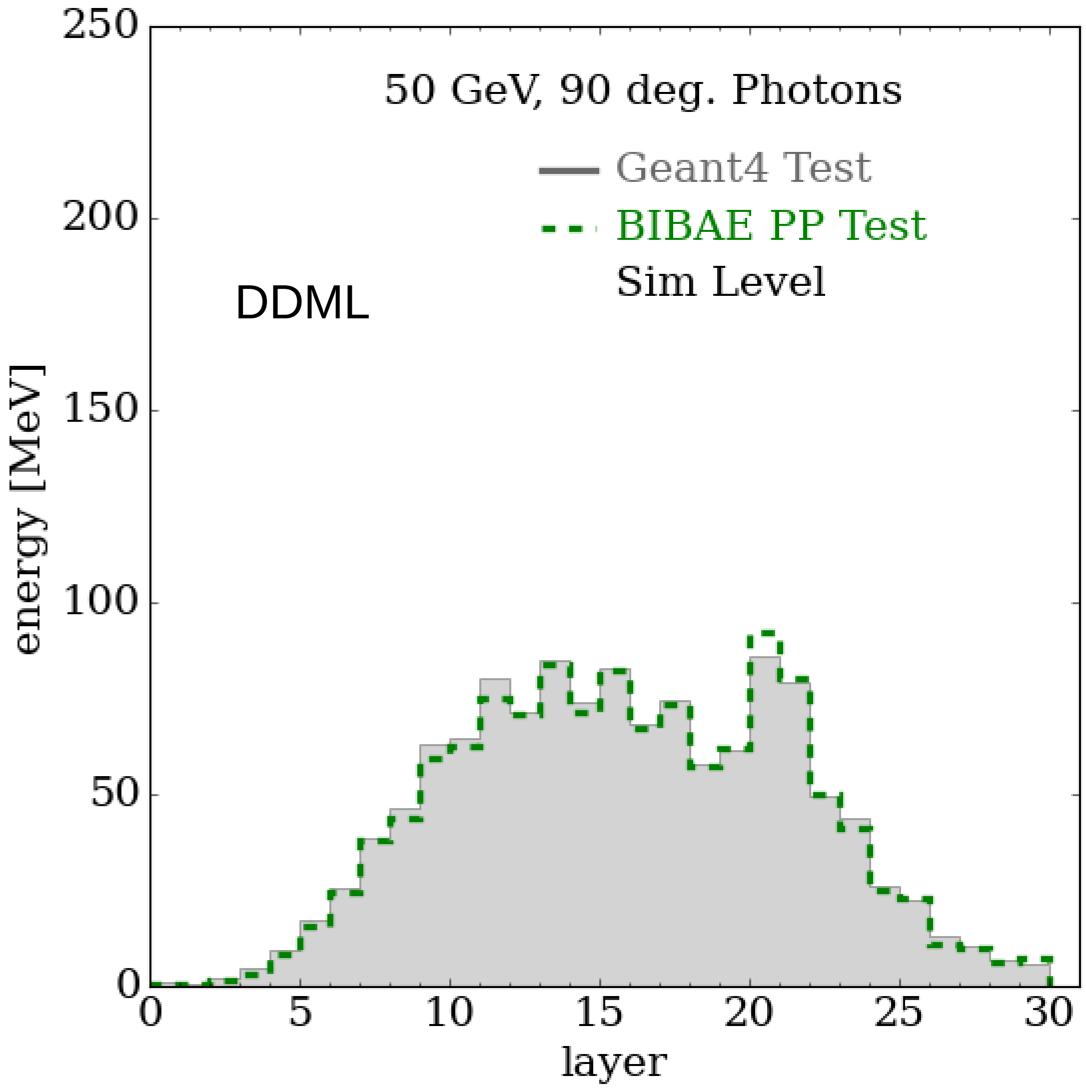
MC Pi0 – Theta


ILD @ 250 2f_leptonic_eL_pR
MC π^0
Two photons trigger
One photon triggers
No energy trigger
No trigger
2000
1500
1000
500
0
0.5
1.0
1.5
2.0
2.5
π^0 theta (rad.)

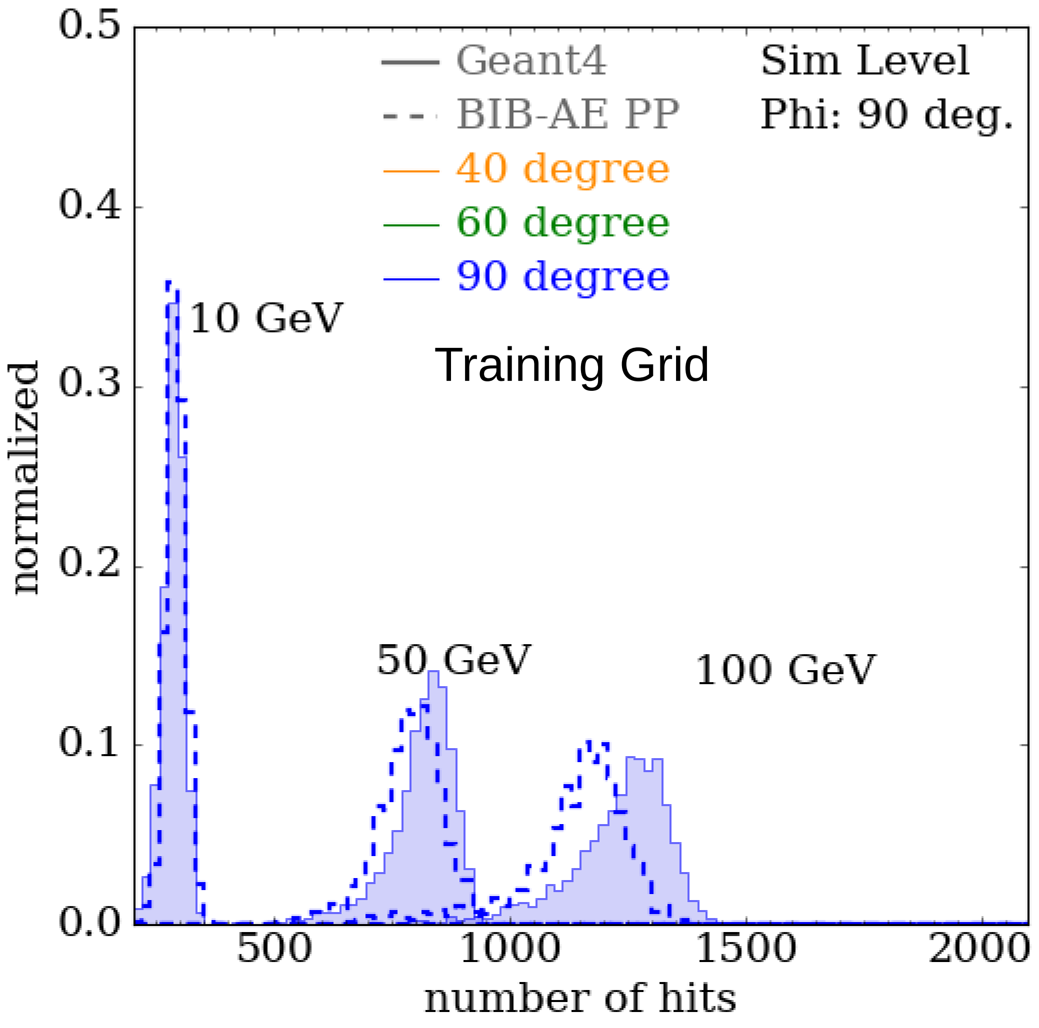

ILD @ 250 2f_leptonic_eL_pR
MC π^0
Two photons trigger
One photon triggers
900
800
700
600
500
400
300
200
100
0
0.5
1.0
1.5
2.0
2.5
π^0 theta (rad.)

Longitudinal

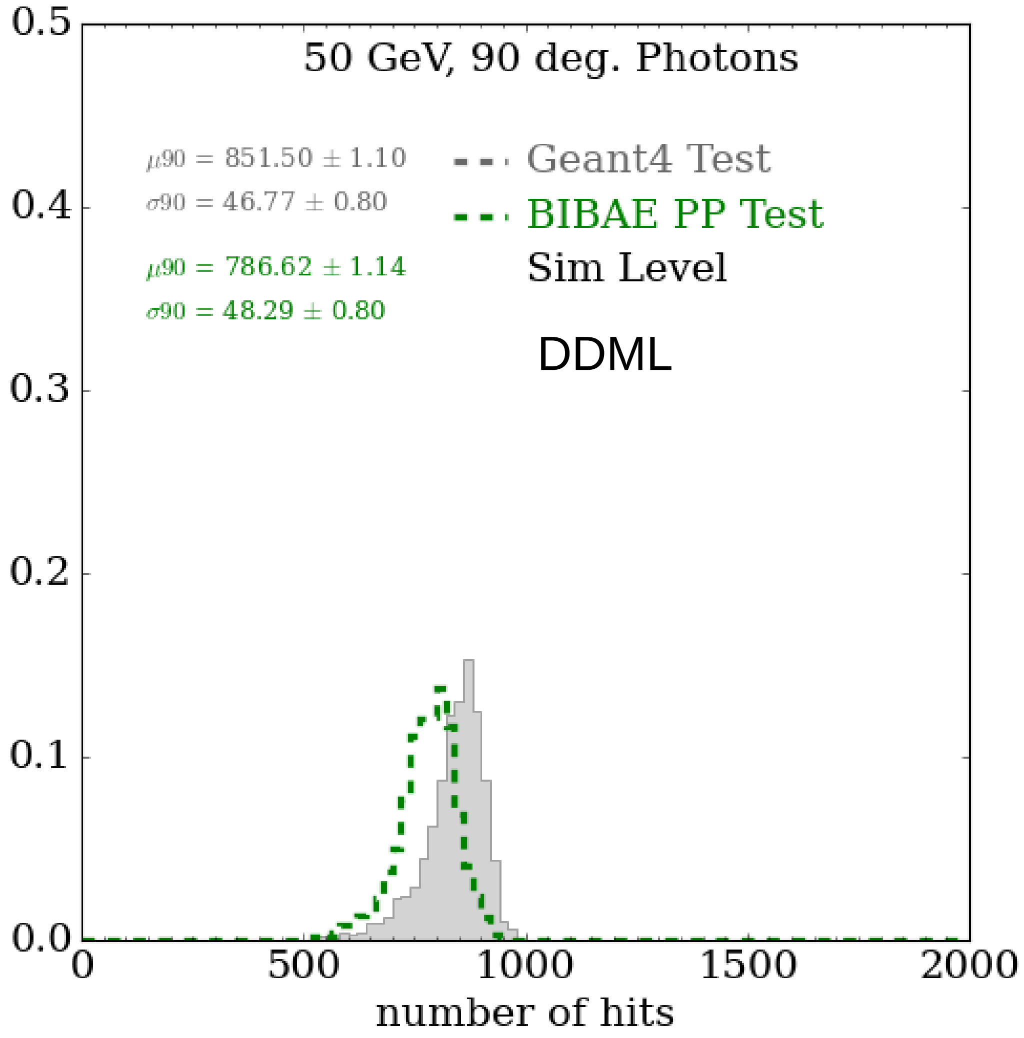




Nhits

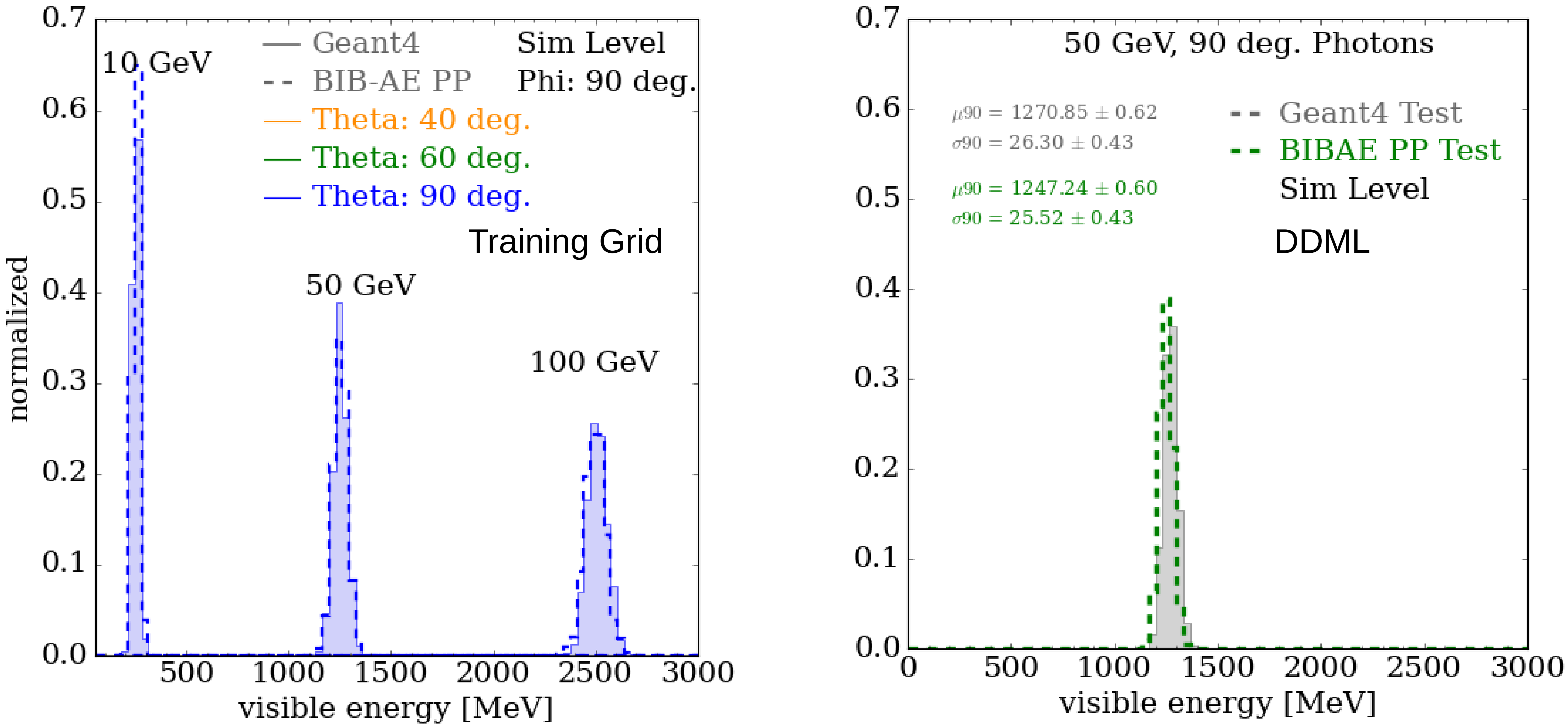


Geant4
BIB-AE PP
40 degree
60 degree
90 degree
Sim Level
Phi: 90 deg.
10 GeV
Training Grid
50 GeV
100 GeV
normalized
number of hits
0.5
0.4
0.3
0.2
0.1
0.0
500
1000
1500
2000

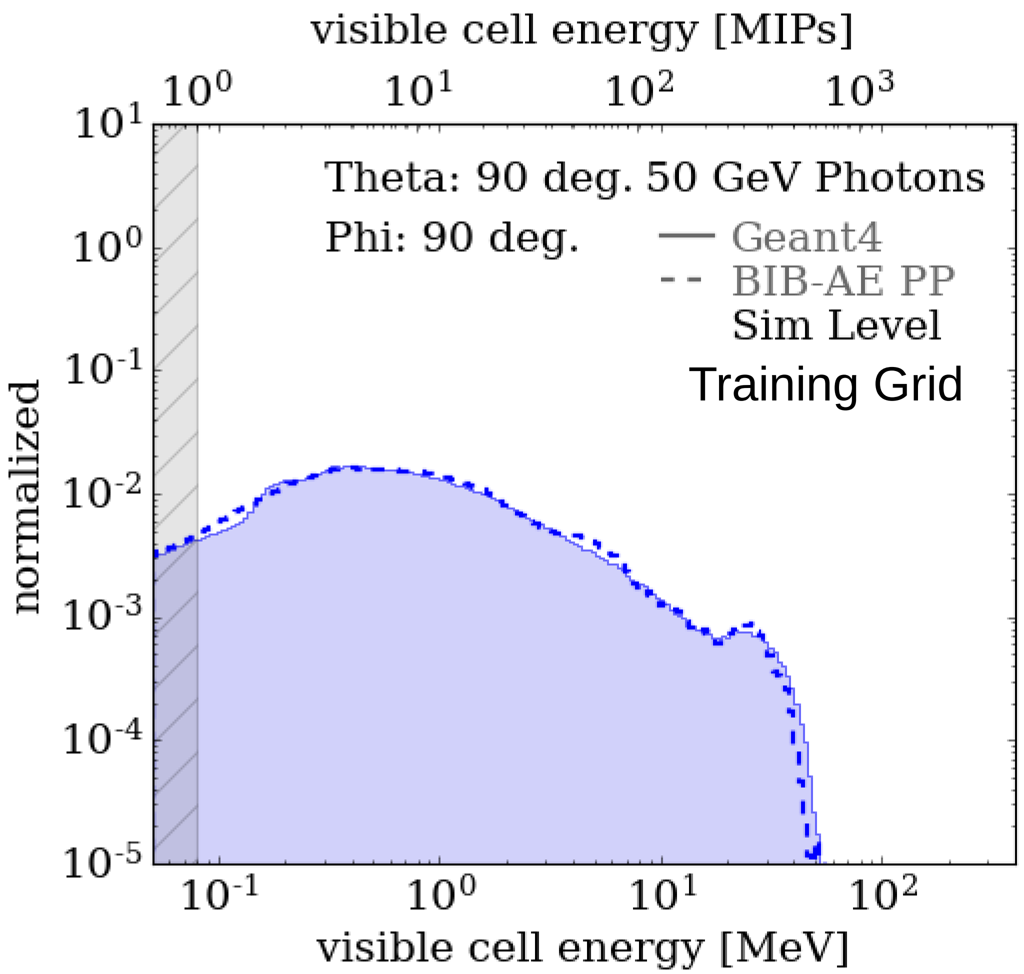


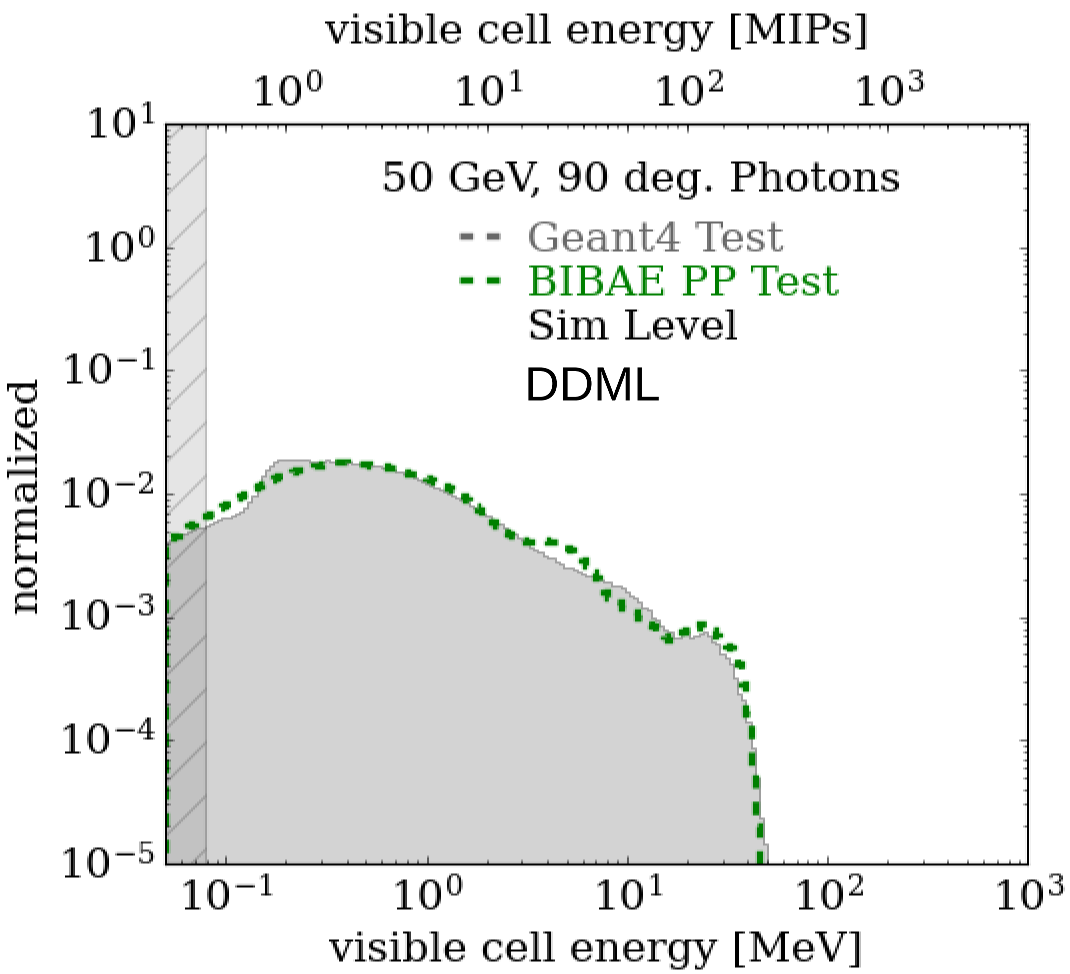
50 GeV, 90 deg. Photons
μ90 = 851.50 ± 1.10
σ90 = 46.77 ± 0.80
μ90 = 786.62 ± 1.14
σ90 = 48.29 ± 0.80
Geant4 Test
BIBAE PP Test
Sim Level
DDML
number of hits
0.5
0.4
0.3
0.2
0.1
0.0
0
500
1000
1500
2000

Visible energy



Cell Energy


visible cell energy [MIPs]
10^0 10^1 10^2 10^3
10^1 10^0 10^{-1} 10^{-2} 10^{-3} 10^{-4} 10^{-5}
normalized
Theta: 90 deg. 50 GeV Photons
Phi: 90 deg.
Geant4
BIB-AE PP
Sim Level
Training Grid
10^{-1} 10^0 10^1 10^2
visible cell energy [MeV]


visible cell energy [MIPs]
10^0 10^1 10^2 10^3
10^1 10^0 10^{-1} 10^{-2} 10^{-3} 10^{-4} 10^{-5}
normalized
50 GeV, 90 deg. Photons
Geant4 Test
BIBAE PP Test
Sim Level
DDML
10^{-1} 10^0 10^1 10^2 10^3
visible cell energy [MeV]

Radial Energy