New Developments in Generative Methods for Event Simulation

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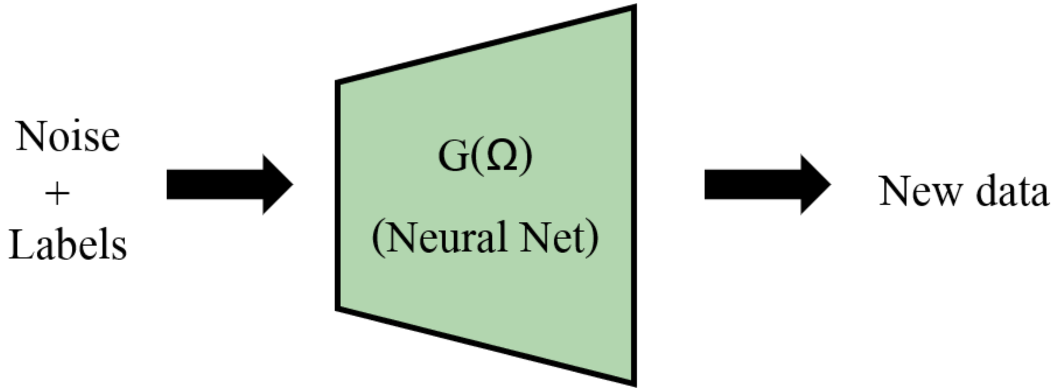
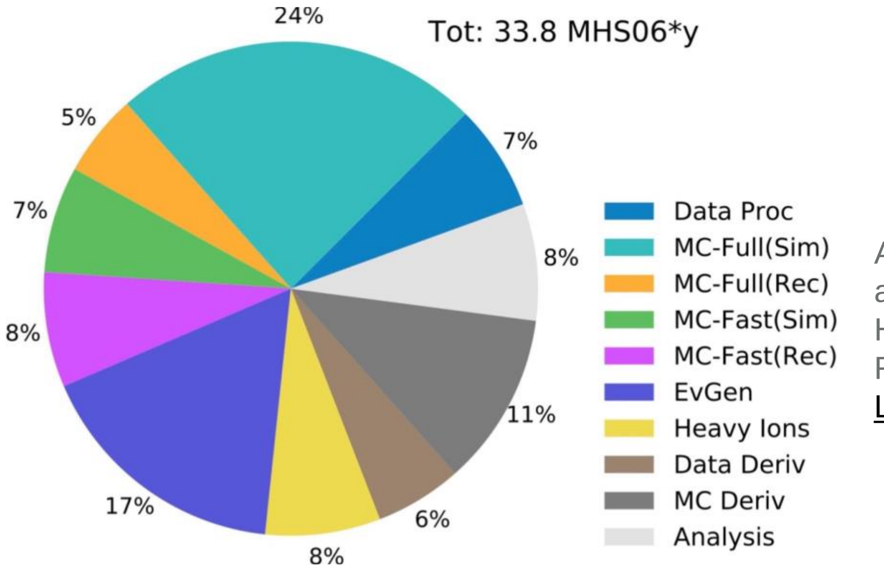
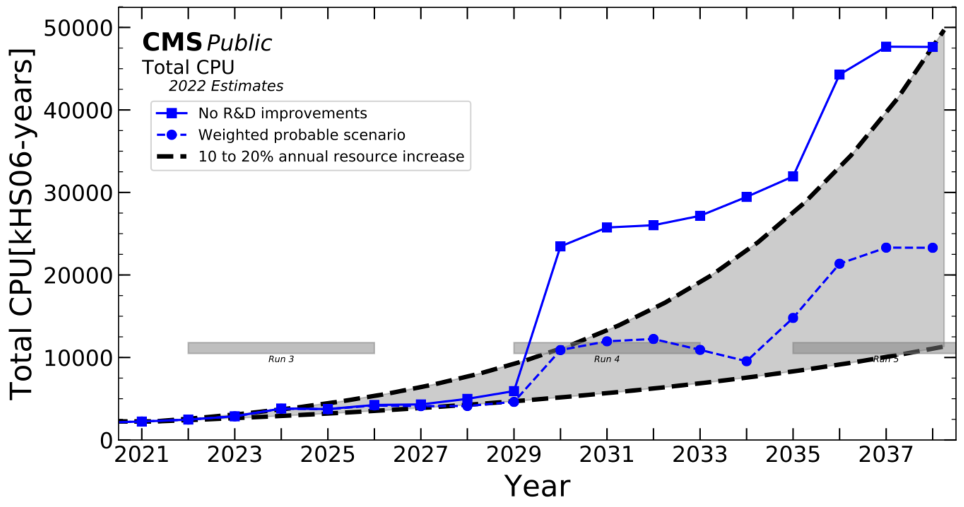
Introduction

- **Full MC simulation (Geant4)** is computationally **expensive**
  - Calorimeters most intensive part of detector simulation
- **Generative models** potentially offer **high fidelity** simulation with significant **speed up:**
  - More sustainable computing





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



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

Highly Granular Calorimeters for Future Experiments

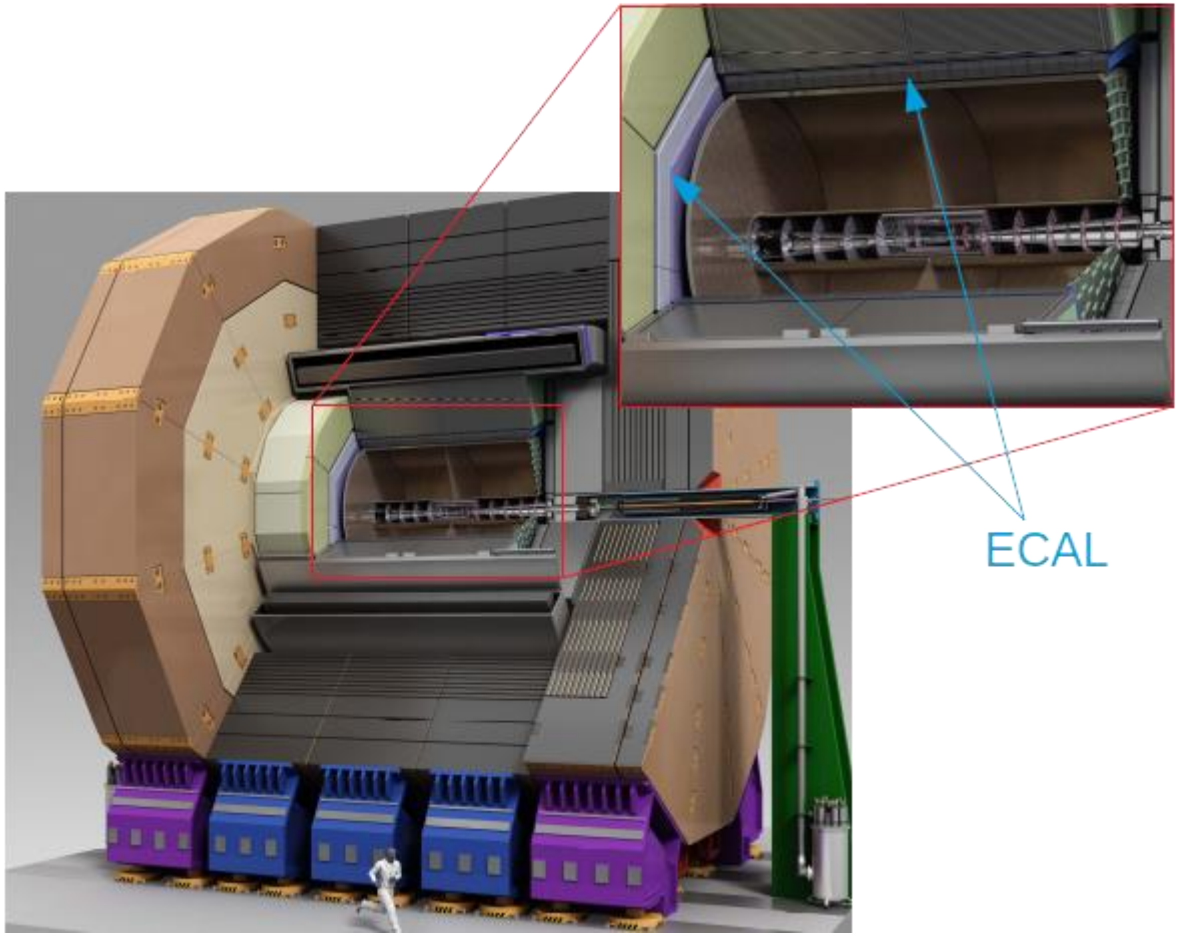
- Widely planned for future experiments: e.g. HL-LHC, e+e- Higgs Factories

- 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
  - **HCAL**: Sci-Fe - 30mm x 30 mm

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



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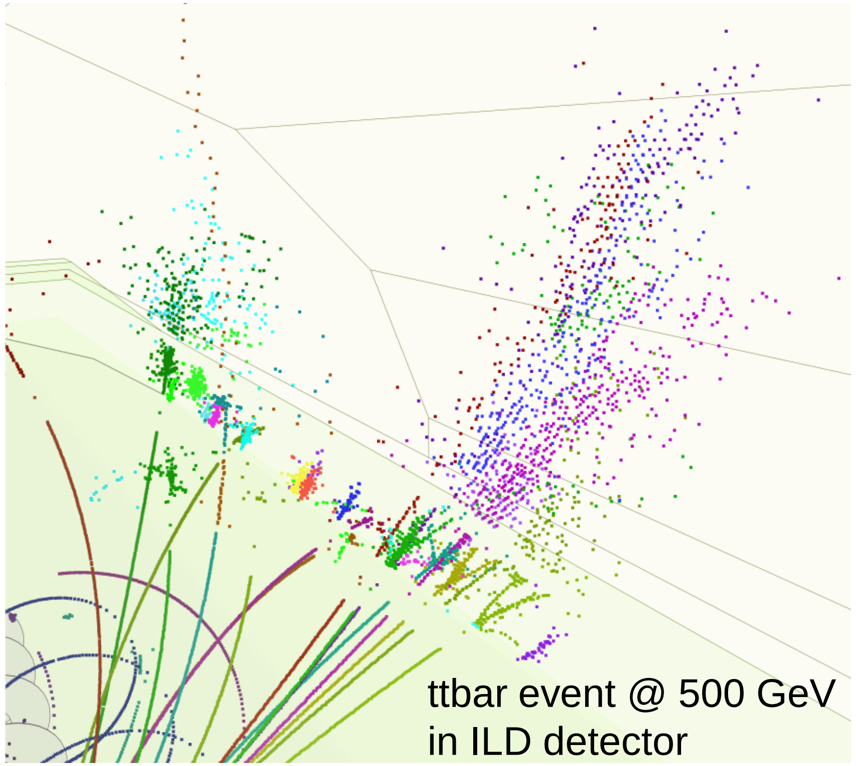
- High granularity calorimeters:
  - **ECAL**: Si-W - 5mm x 5mm - ~ 80 million channels
  - **HCAL**: Sci-Fe - 30mm x 30 mm - ~ 8 million channels

c.f. a few cm^2 for ATLAS/CMS ECAL (before High Lumi)

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

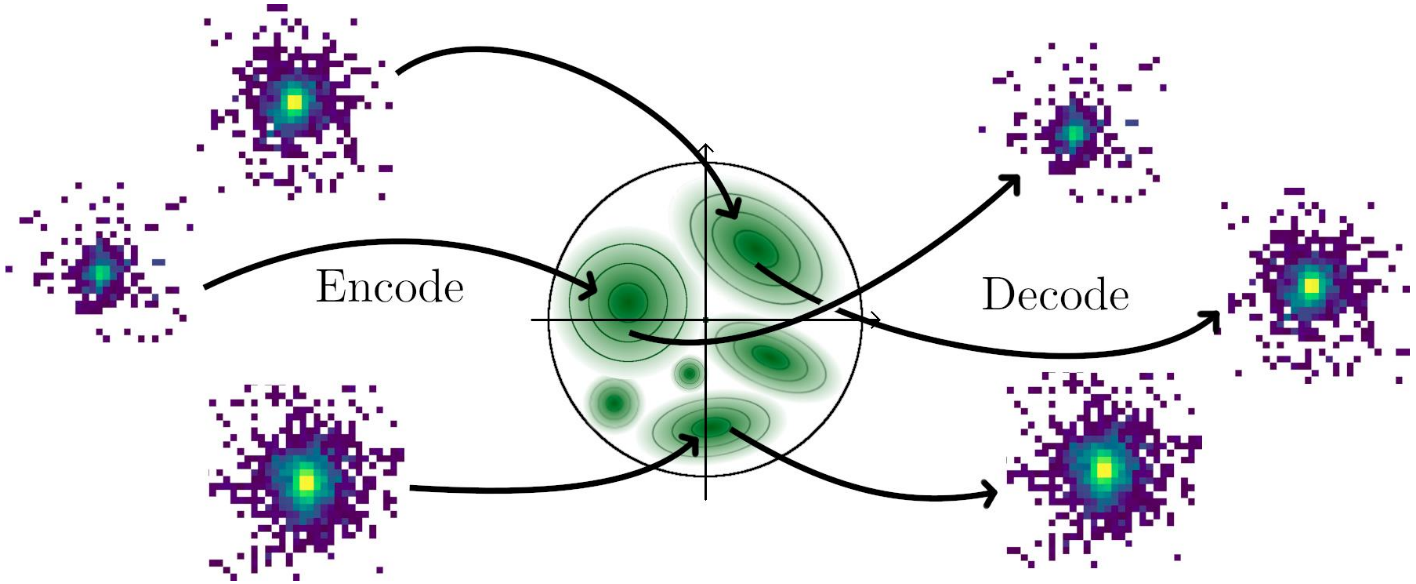


ttbar event @ 500 GeV in ILD detector

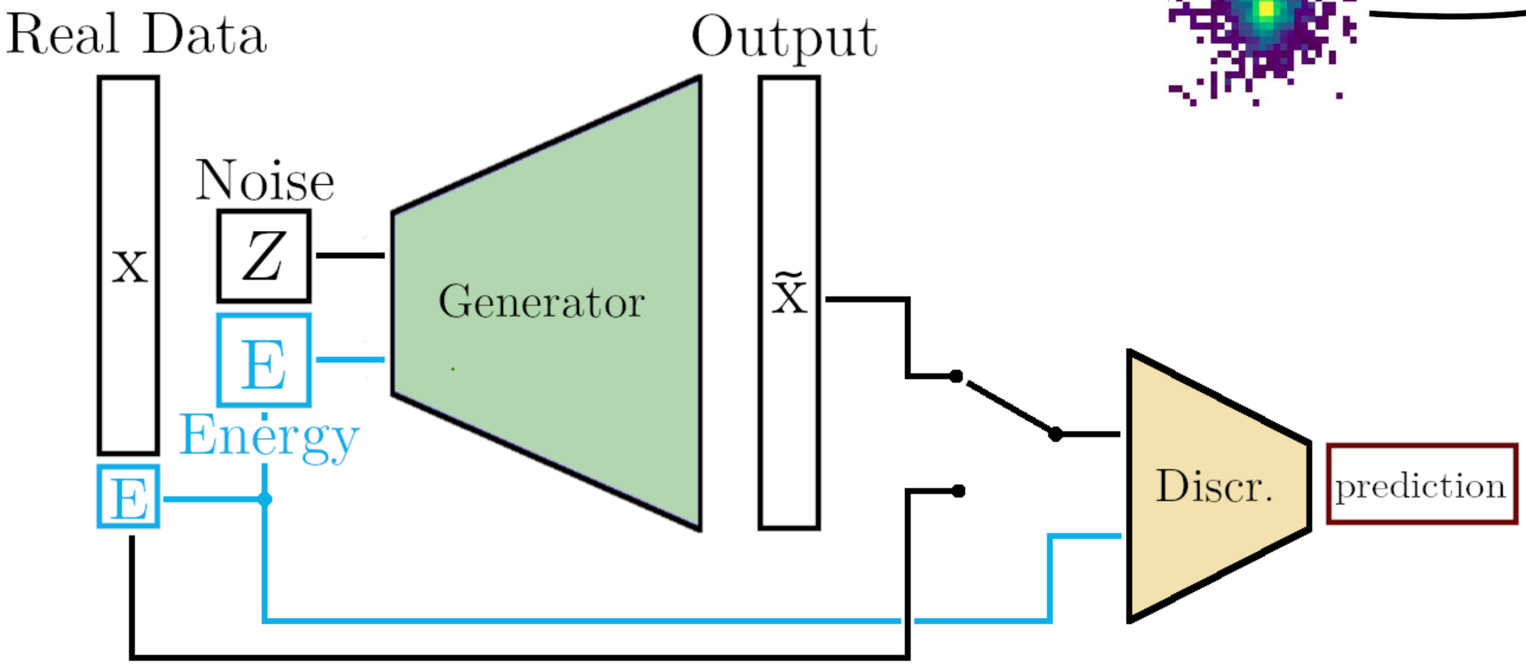
Common Generative Models

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

Variational Autoencoder (**VAE**)



Generative Adversarial Network (**GAN**)

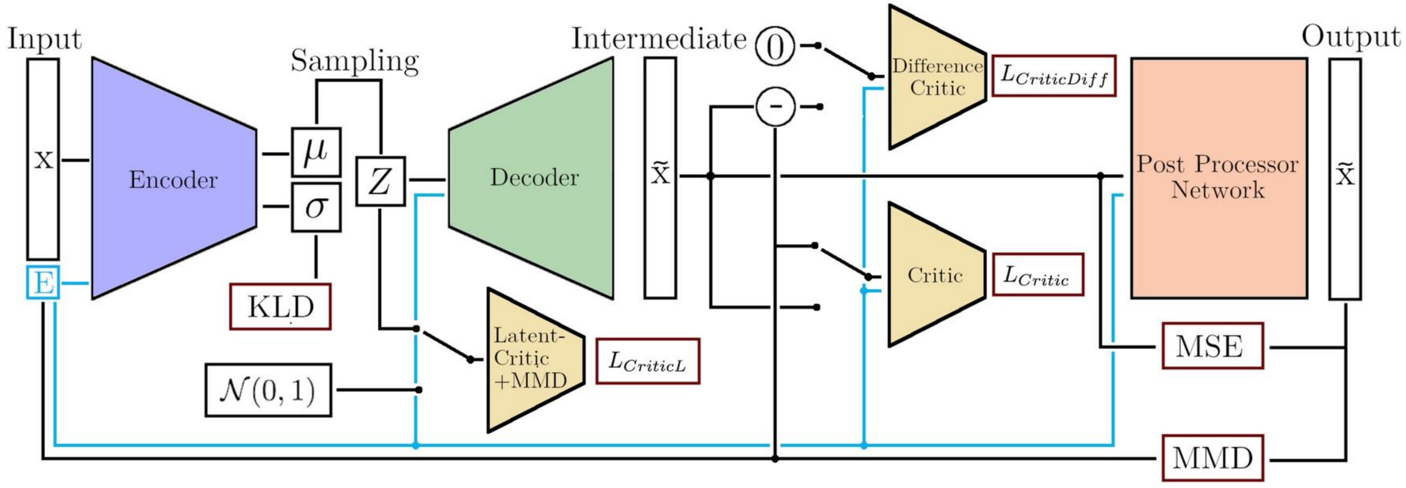


[1]D.P. Kingma, M. Welling. Auto-encoding Variational Bayes (2014), arXiv:1312.6114

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

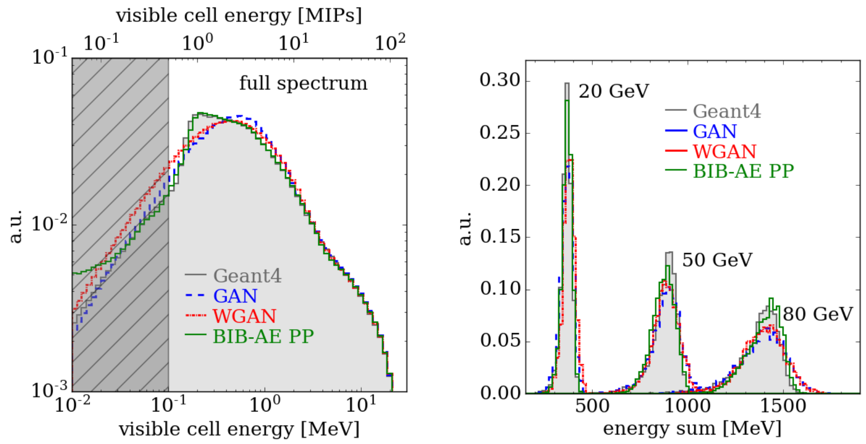
Initial Progress: Photons and Pions

- 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)



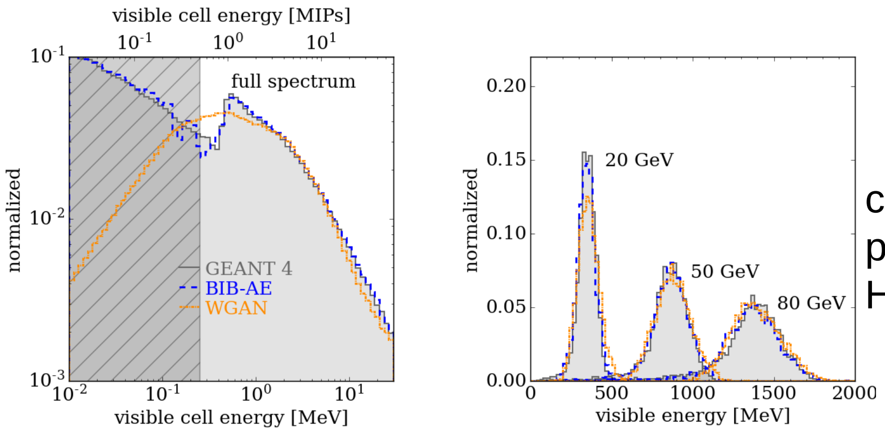
BIB-AE: Bounded Information Bottleneck Auto-Encoder

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)

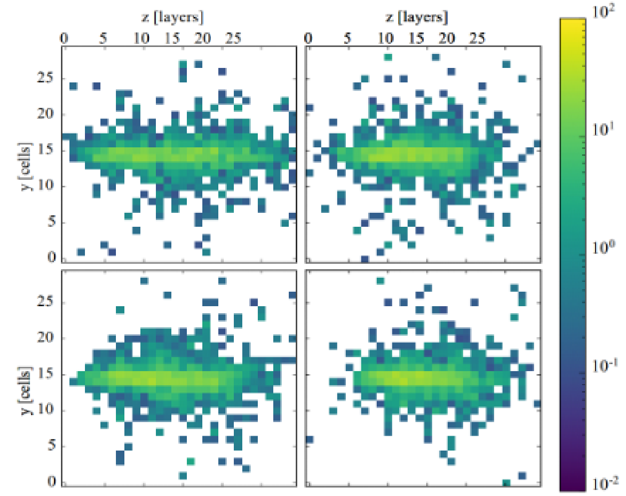


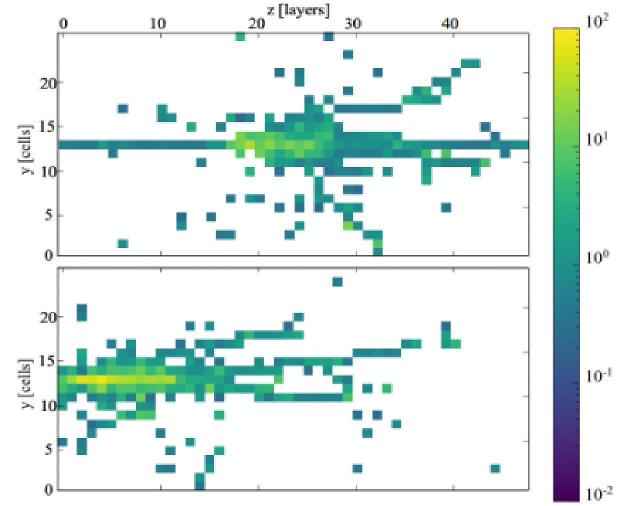
charged pions HCAL

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





		Energy	Angles	ECAL +HCAL	Reco
Photon showers	• Predominantly governed by EM interactions • Compact structure ↓ **Relatively easy to generalise**	✓	+	N/A	+
Pion showers	• Hadronic and EM interactions • Complex structure • Large event-to-event fluctuations ↓ **Hard to learn**	✓	X	X	–

✓ = Achieved
X = Yet to be done
– = Partially Addressed
\+ = Addressed here

For **realistic application** also need:

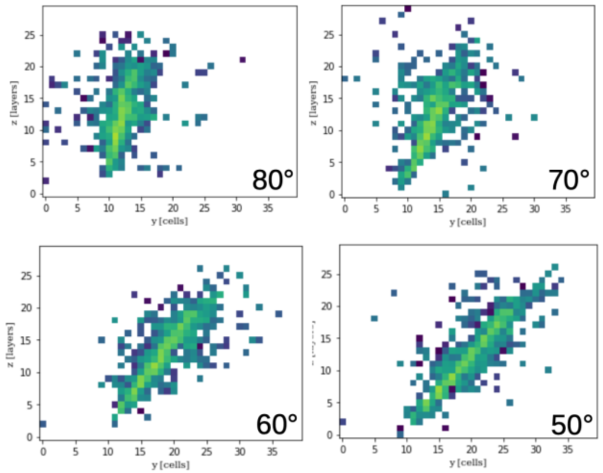
- **Angular conditioning**
- High performance after **reconstruction**
- …

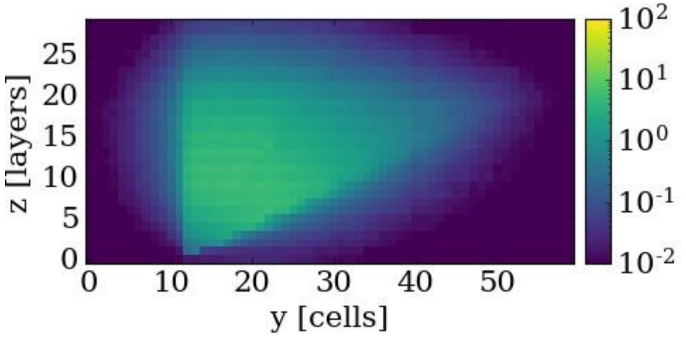
Also continue to investigate other promising **ML architectures**

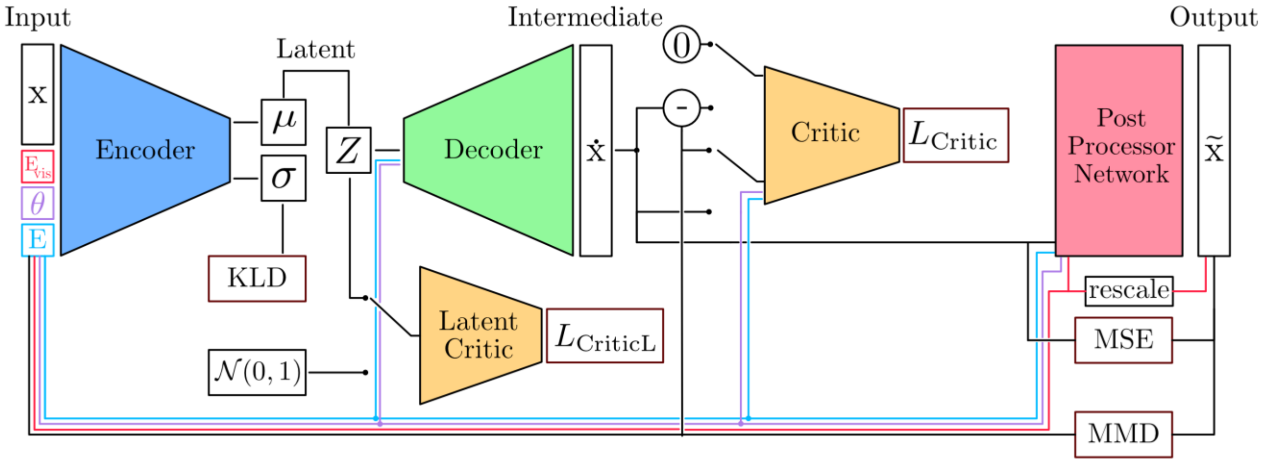
⟶ this talk

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

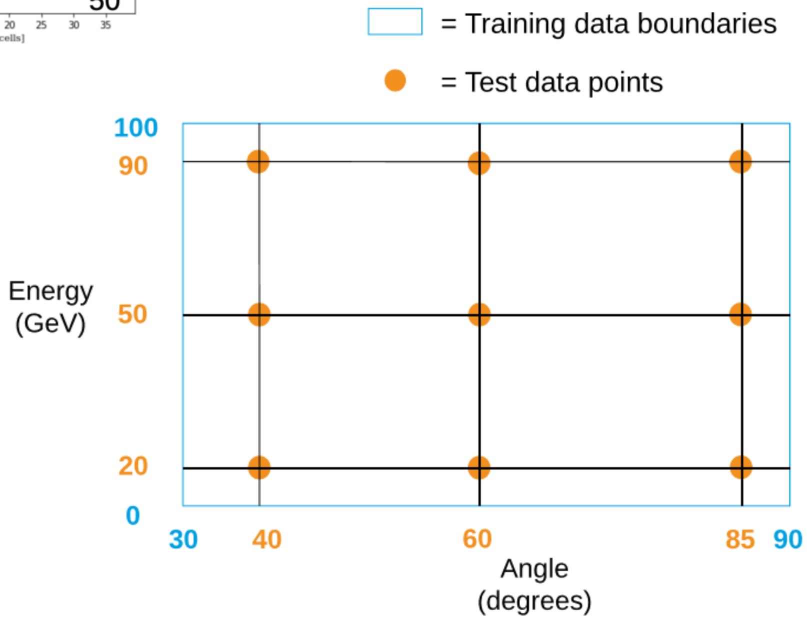






$$L_{\text{BIB-AE}} = \text{KLD} + L_{\text{CriticL}} + L_{\text{Critic}}$$

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

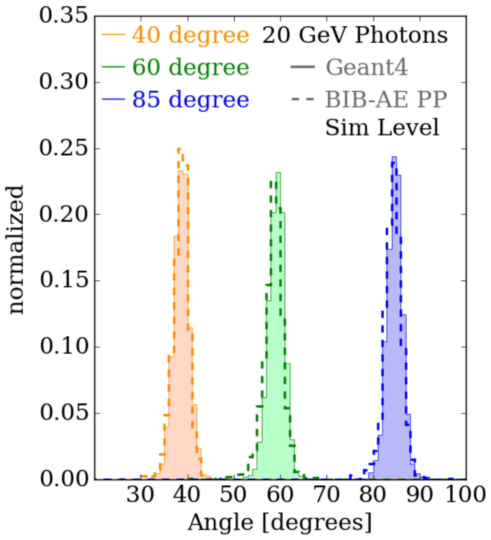


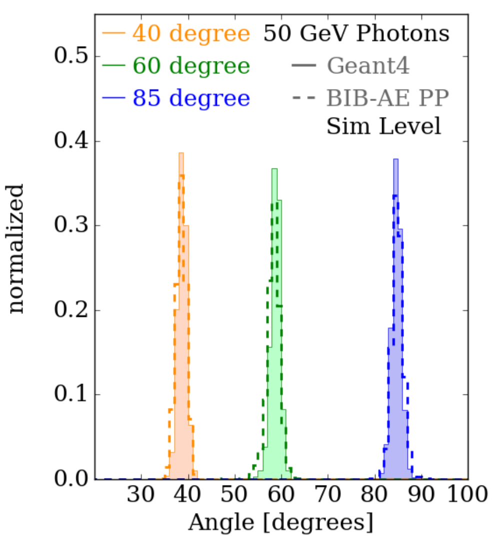
Training and validation samples - 30x60x30 grid

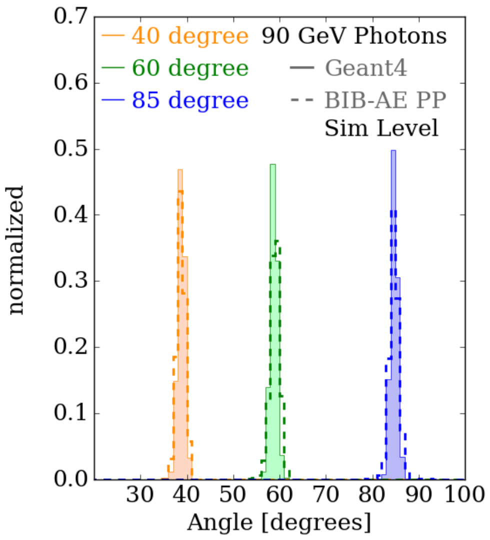
Angular Conditioning Performance

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

- **Sim** level angle reconstruction





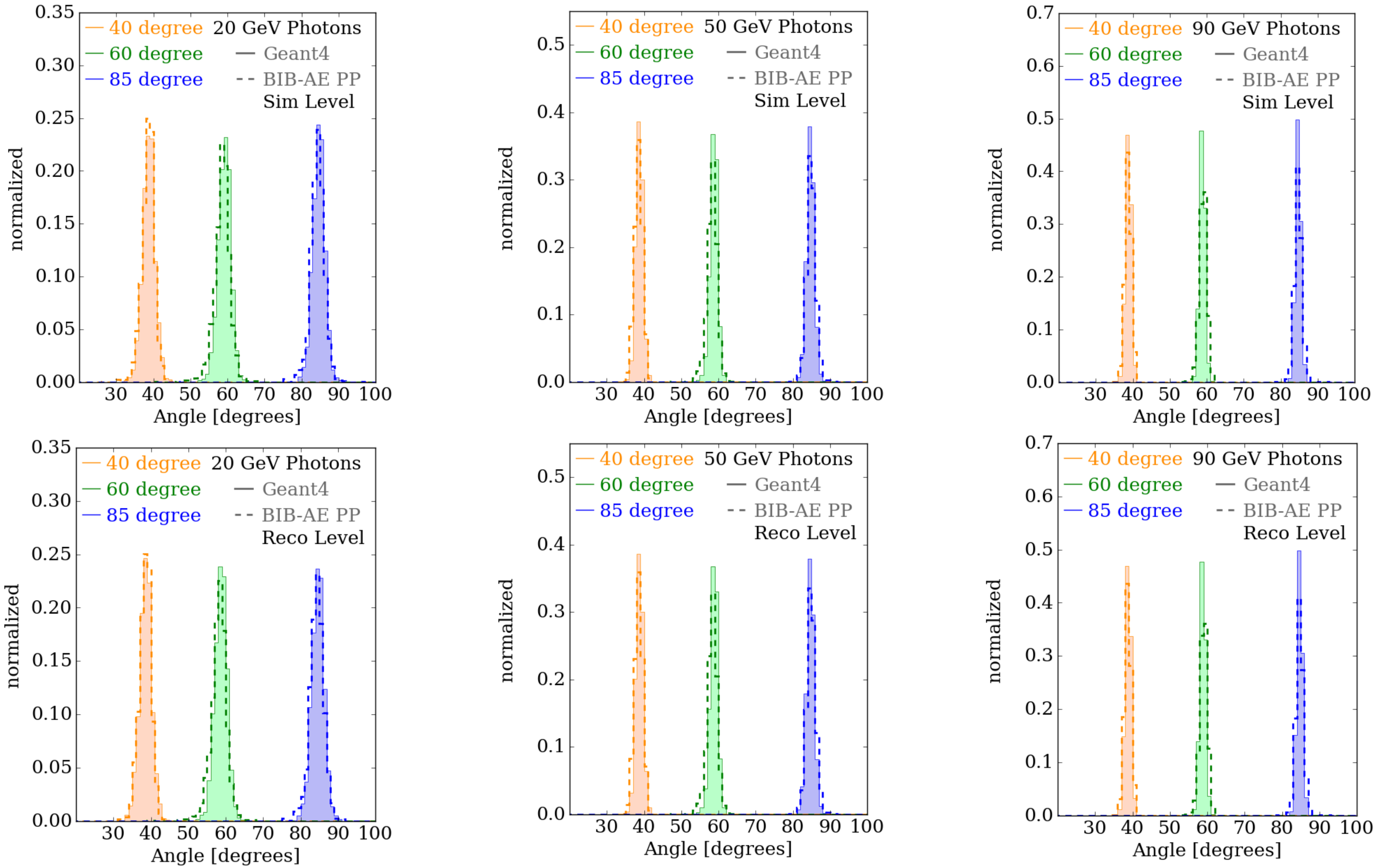


Angular Conditioning Performance

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

- **Sim** level angle reconstruction

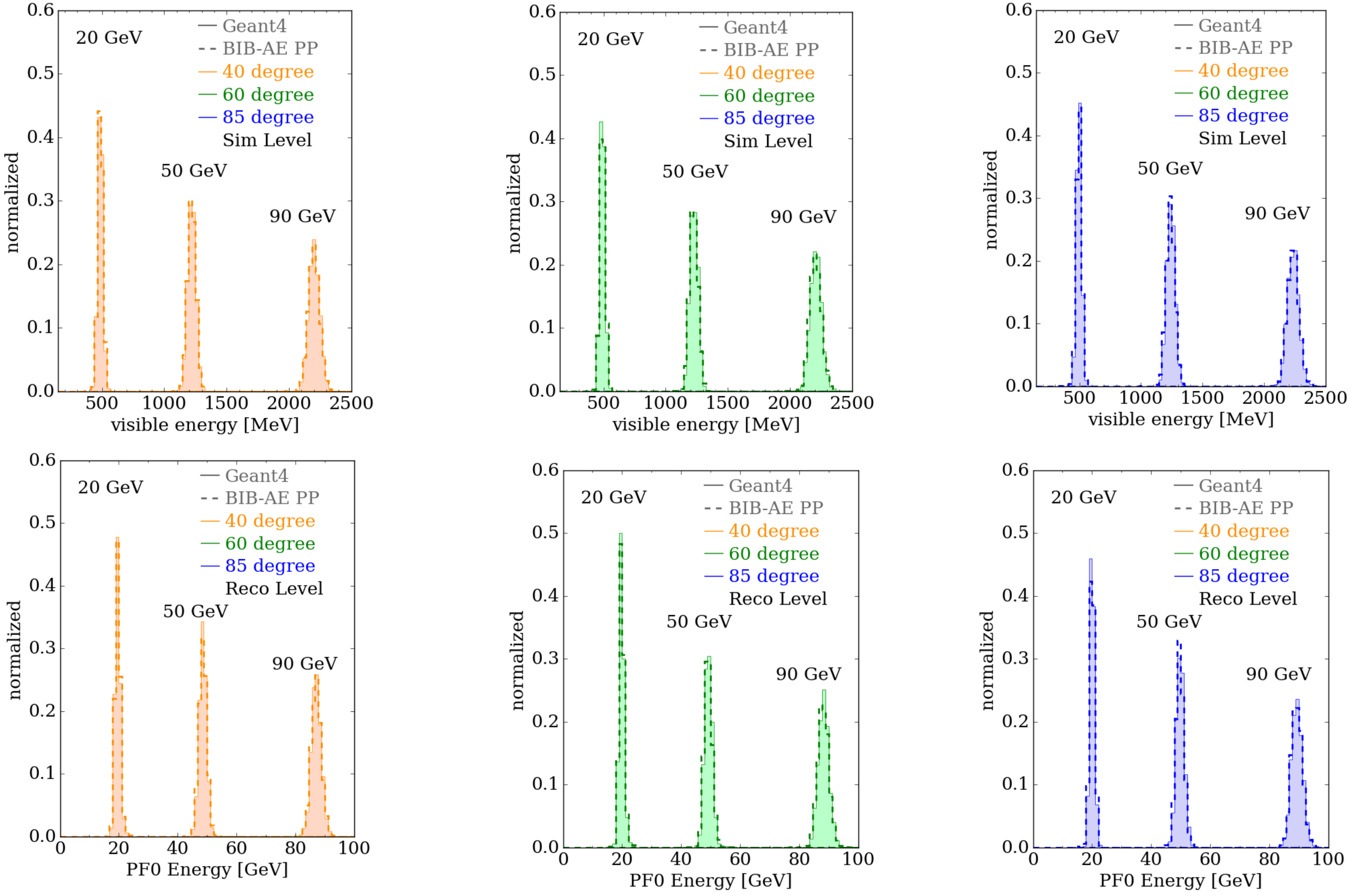
- **Rec** level angle reconstruction
  - After full reconstruction with PandoraPFA



Energy Conditioning Performance

New Angles on Fast Calorimeter Shower Simulation,
Diefenbacher, P.M. 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



Performance After Reconstruction

New Angles on Fast Calorimeter Shower Simulation, Diefenbacher, P.M. et al. 2023 MLST in press
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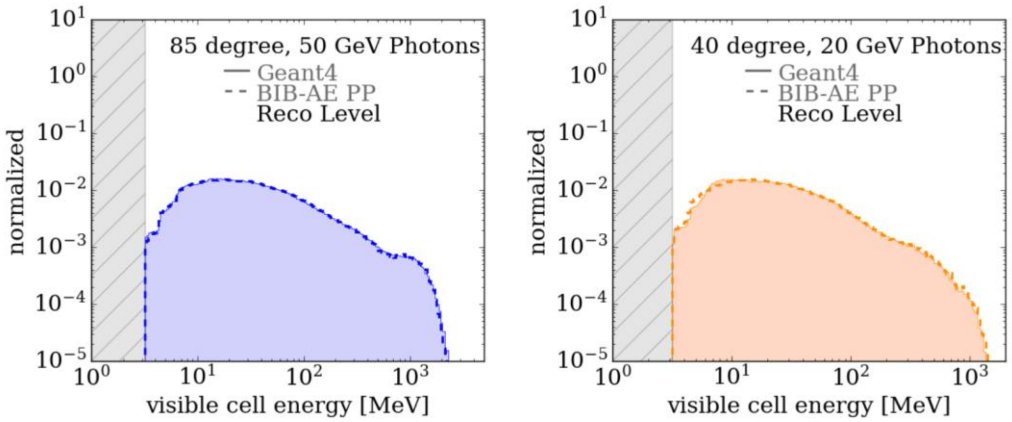
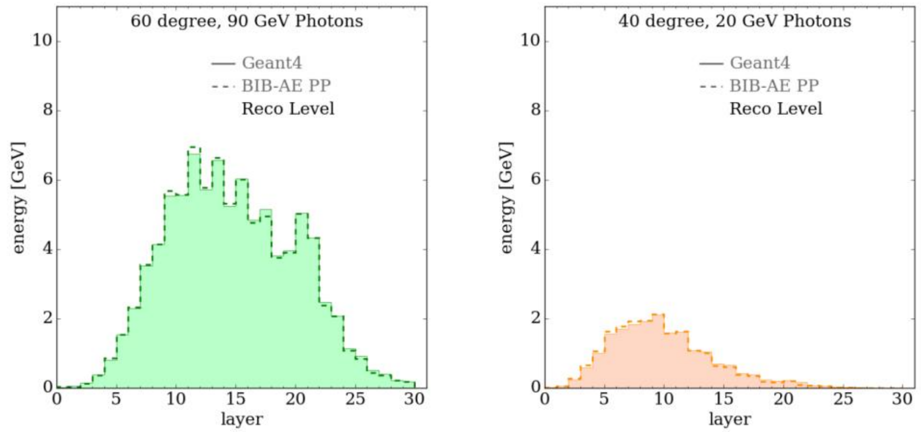
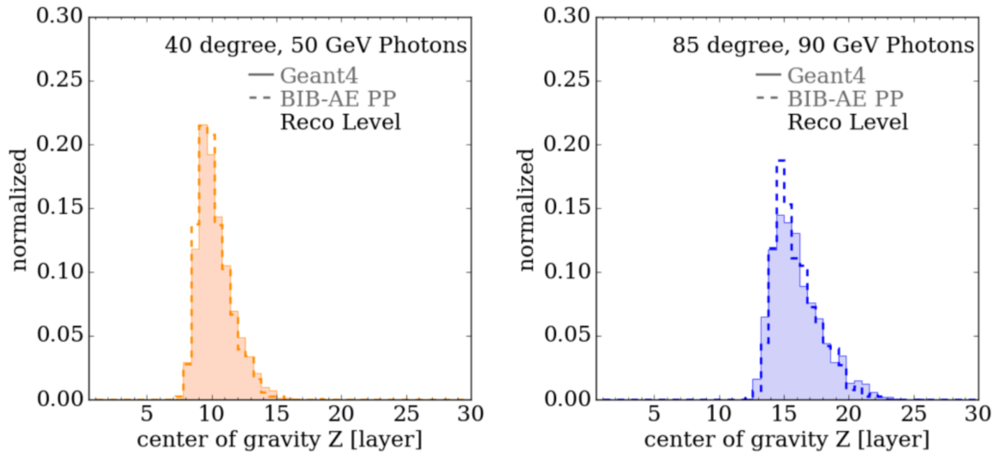


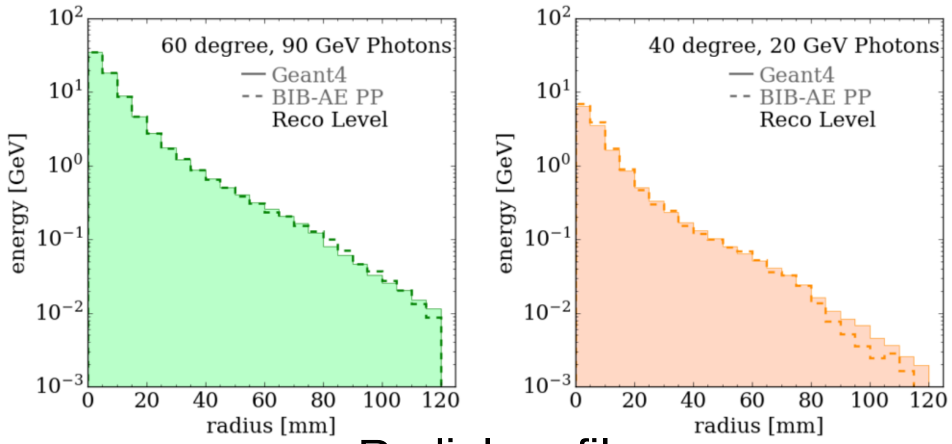
Hit energy spectrum



Longitudinal profile



Centre of gravity in z

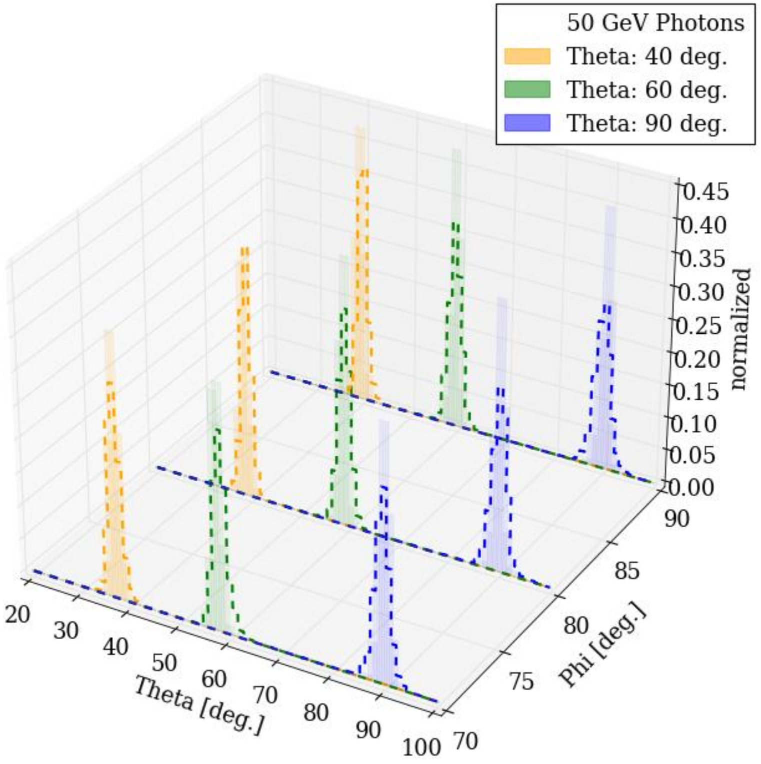


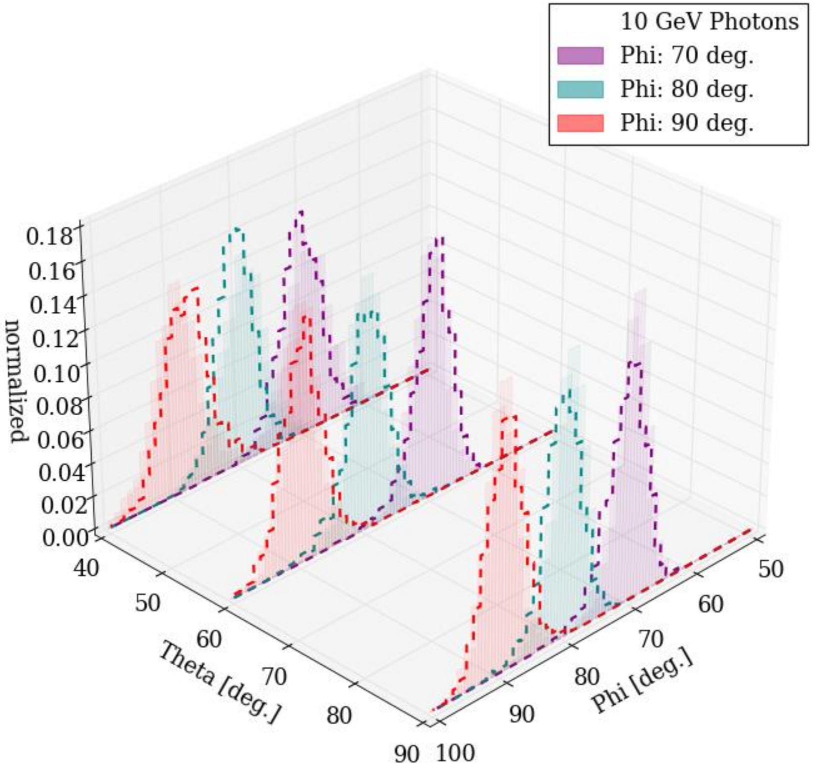
Radial profile

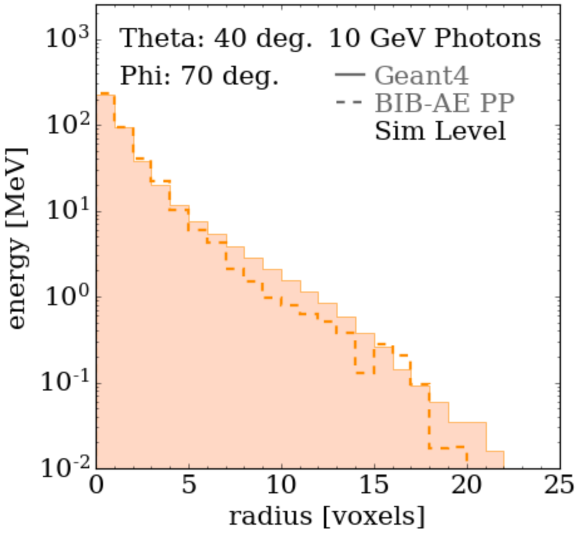
Best (left) and worst (right) test point ⟶ **Excellent** physics fidelity

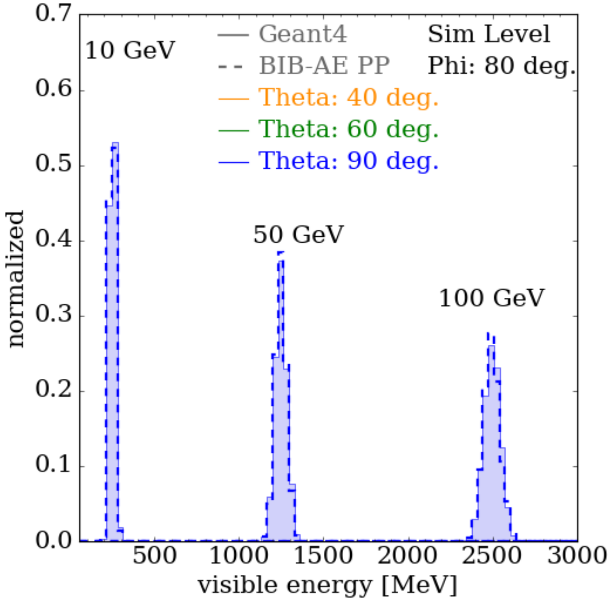
Adding Another Angle

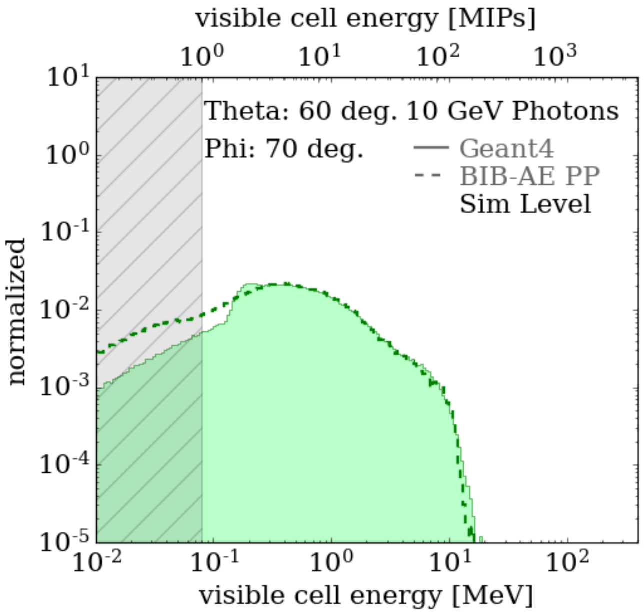
- Need to condition on **energy, theta and phi** for full application
- **Extending phase space** can be challenging
- **Work in progress**



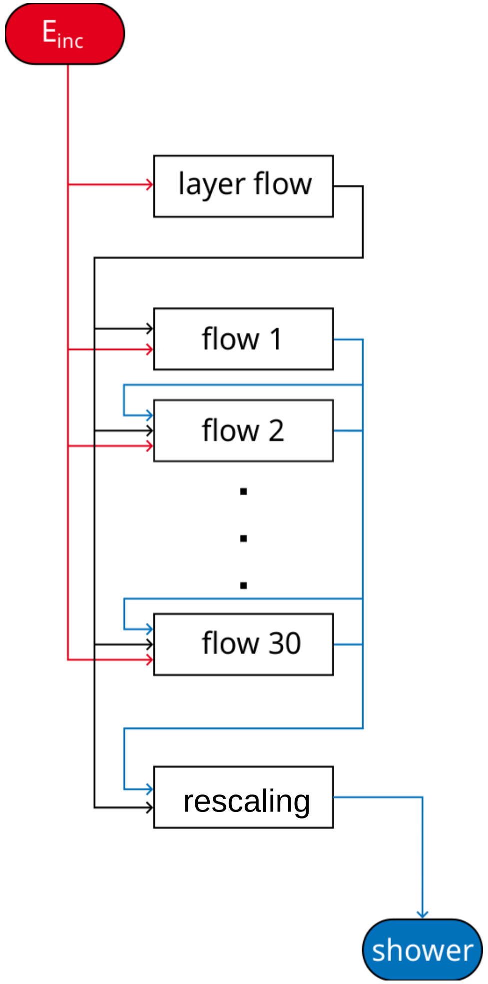


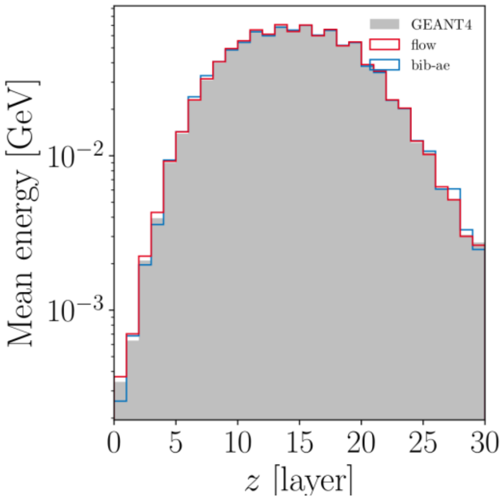


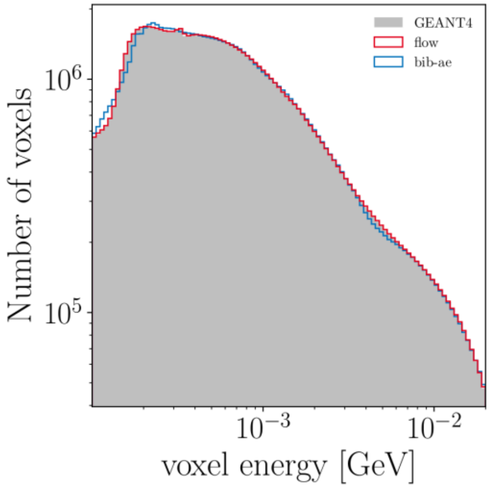


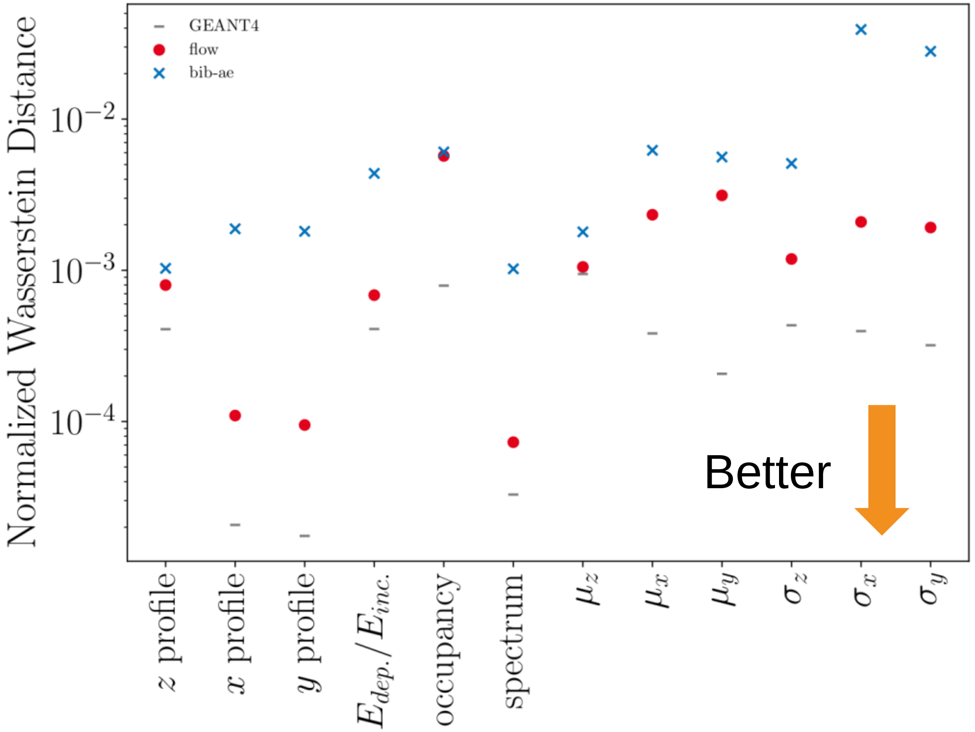


Layer-to-Layer Normalising Flow Model









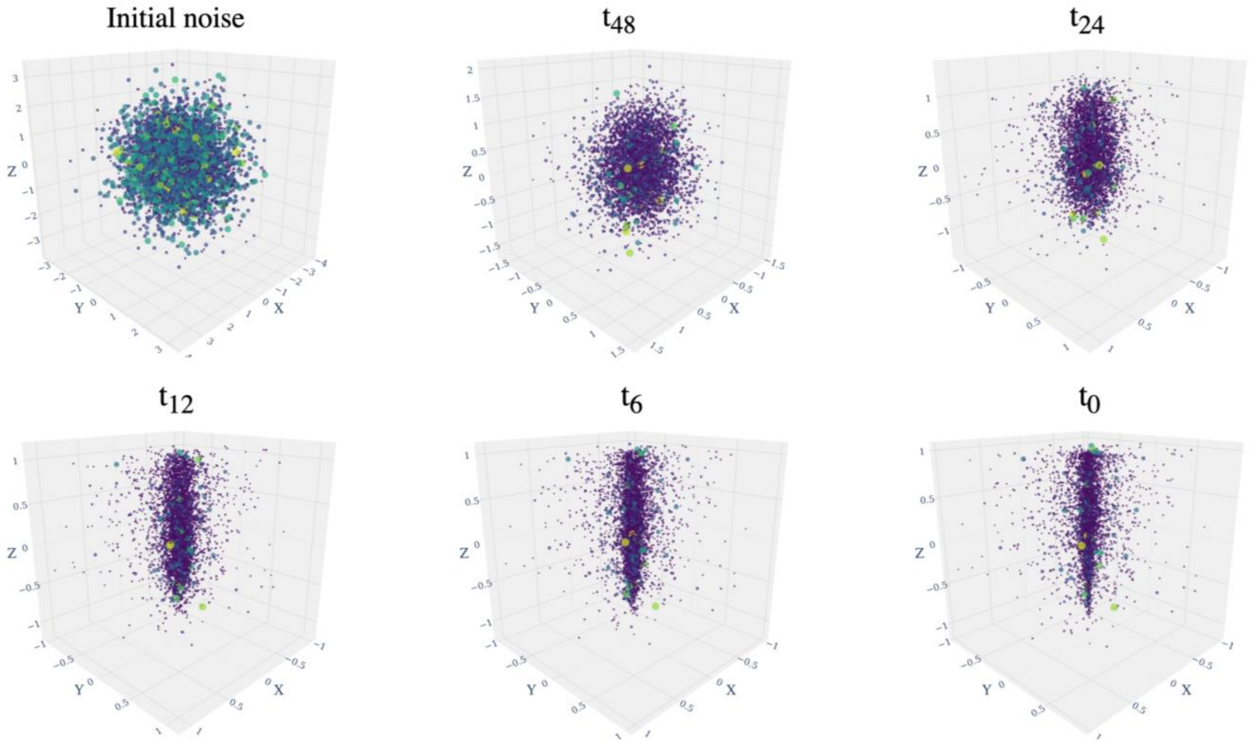
[1] **Fast and accurate simulations of calorimeter showers with normalizing flows**, Krause & Shih., Phys. Rev. D 107, 113003

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

- Fully **invertible model**
- Learns to **sequentially** produce shower shape in each layer
- Extends previous work[1] 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

Point Cloud Diffusion

- **Regular grid models** show very high physics fidelity - yet they have **two drawbacks**:
  - **Low occupancy** ⟶ lots of superfluous compute
  - **Irregular** detector **geometries** ⟶ back projection creates **artifacts**



- Solution: **point cloud** based models
- Use **additional information** in the Geant4 simulation:
  - Much **higher granularity** than **physical geometry**
  - Gain **geometry independence**

- Apply **diffusion model** to clustered Geant4 steps for **photon** showers

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, P.M. et al., arXiv:2305.04847, Submitted to JINST

Point Cloud Diffusion

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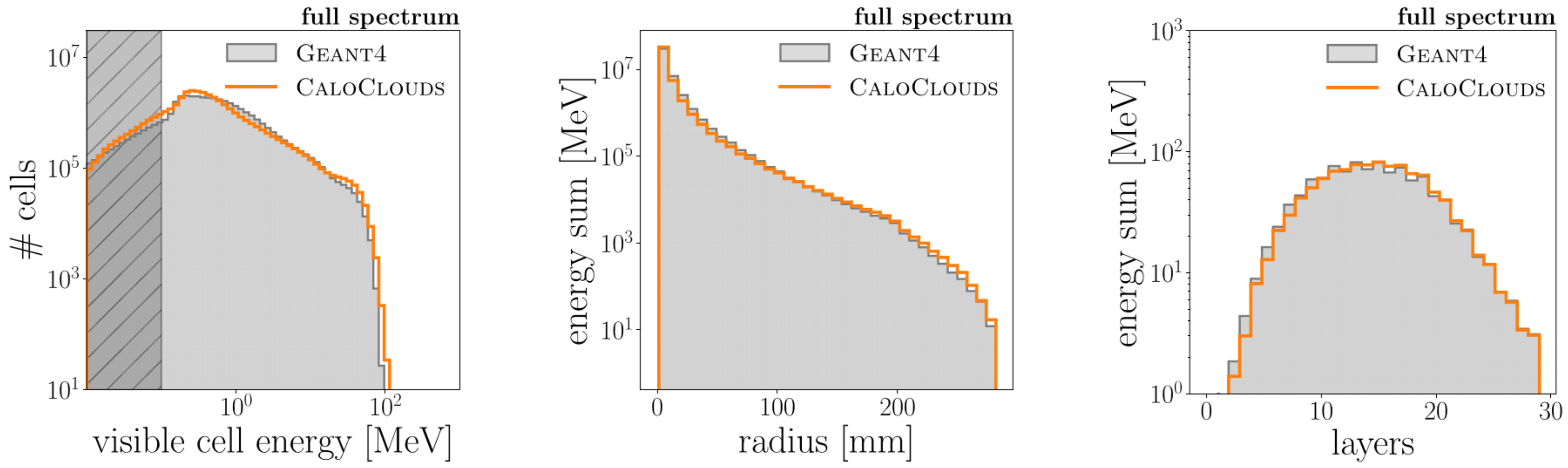

- Overall observe very good physics fidelity
- **First successful application of diffusion models to (high granularity) calorimeter simulation using point clouds**

Point Cloud Diffusion

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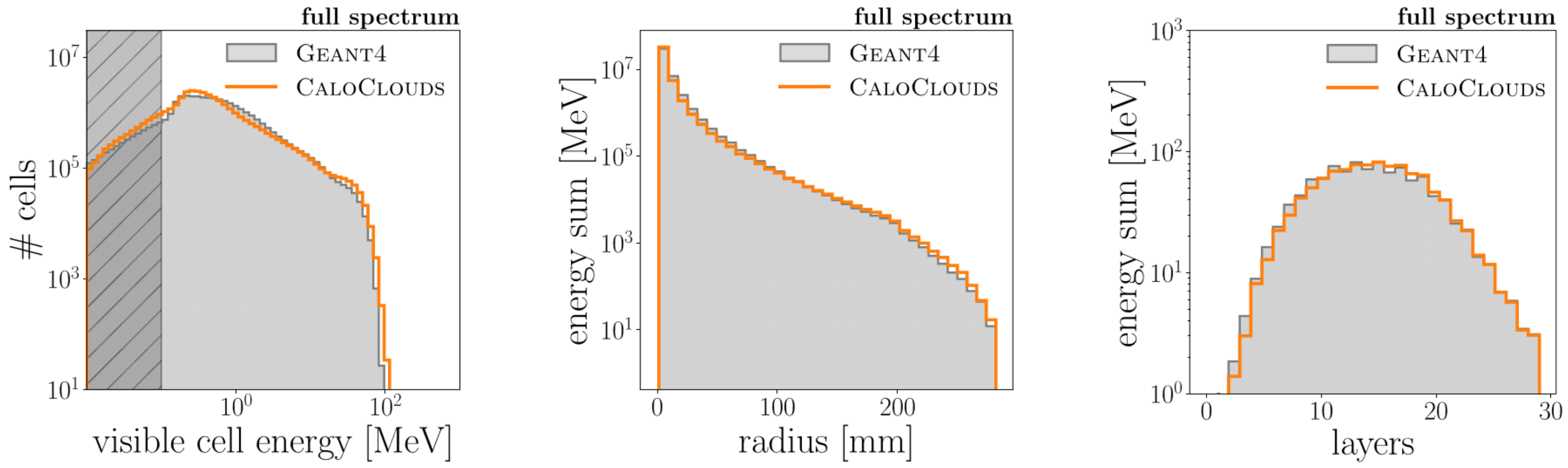

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- **First successful application of diffusion models to (high granularity) calorimeter simulation using point clouds**

- Problem: speed-up provided by original diffusion model is small

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

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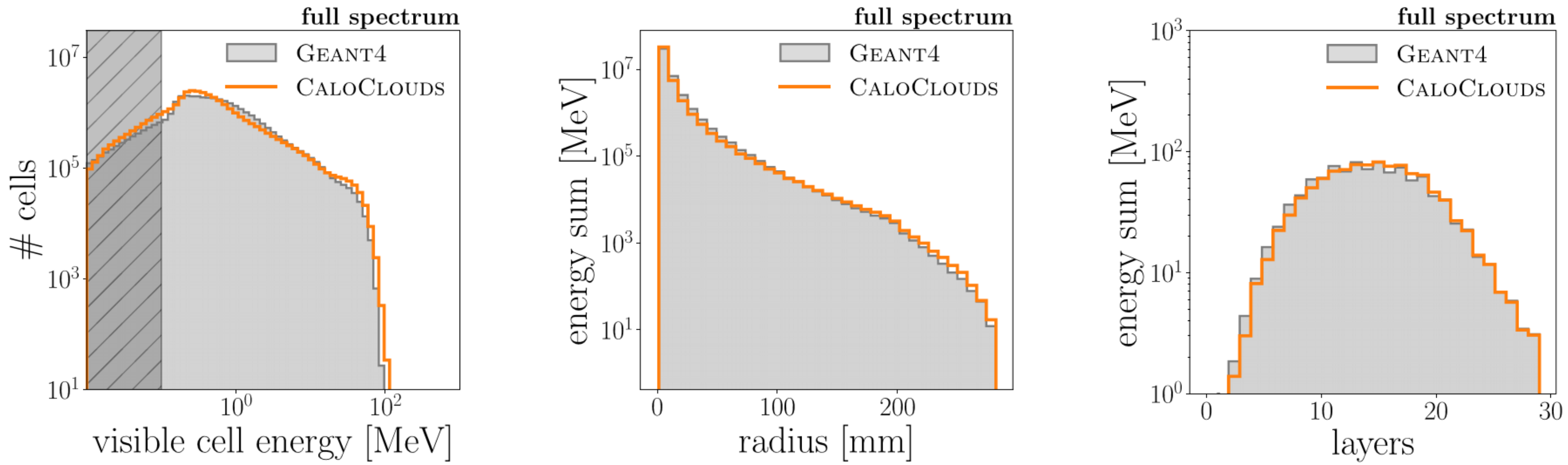

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Work in progress

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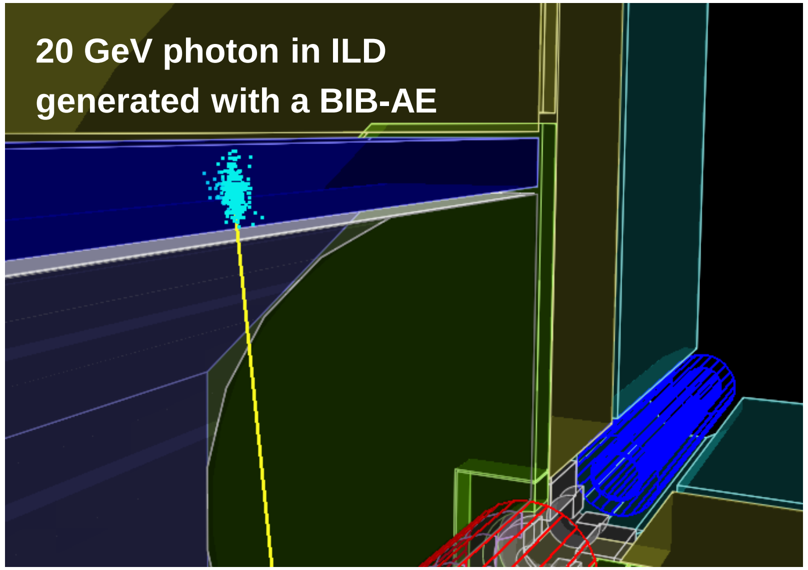
- Problem: speed-up provided by original diffusion model is small
- Solution: apply **consistency distillation**
  - Achieve **x46** faster simulation than Geant4 on **CPU**
  - Publication in preparation

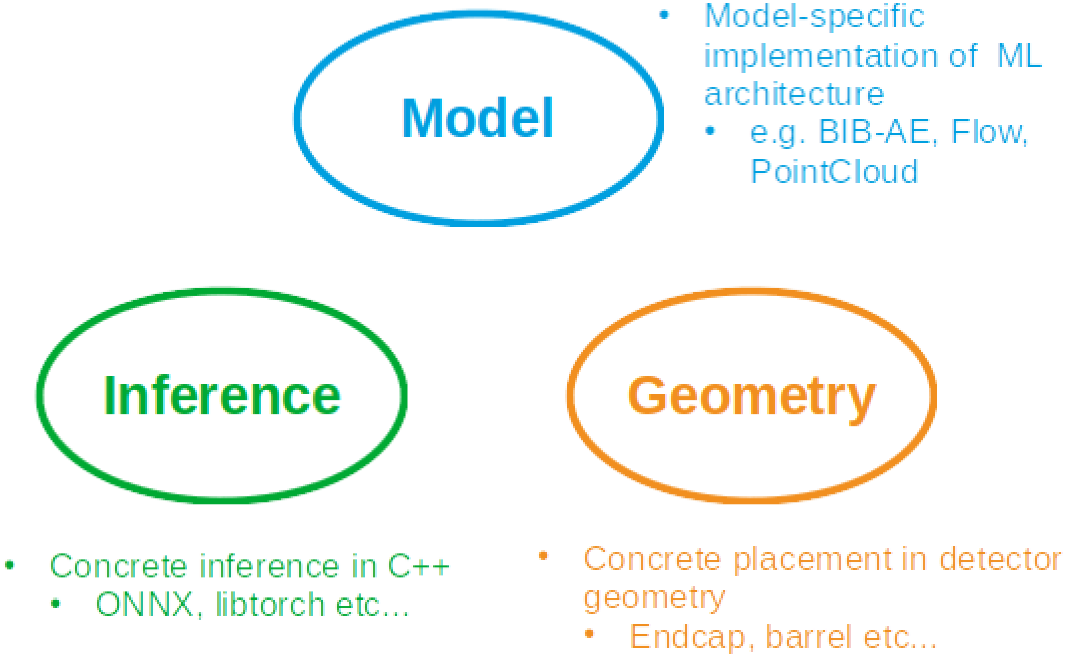
Integration into the Full Simulation Chain

- 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

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

- **Essential** step to be able to study performance of model with **full physics benchmarks**
  - Di-photon separations
  - Tau decays with photons





Conclusion

Achieved

- **Energy and angular** conditioning for EM showers with high physics fidelity
  - **Strong performance** after **reconstruction** with PandoraPFA
- **Normalising flow** model can reproduce shower observables with **increased fidelity**
- **First** successful generation of calorimeter showers as a **point cloud**
  - Achieve a high degree of **geometry independence**
- An initial implementation of a **prototype library** for interfacing with the full simulation chain

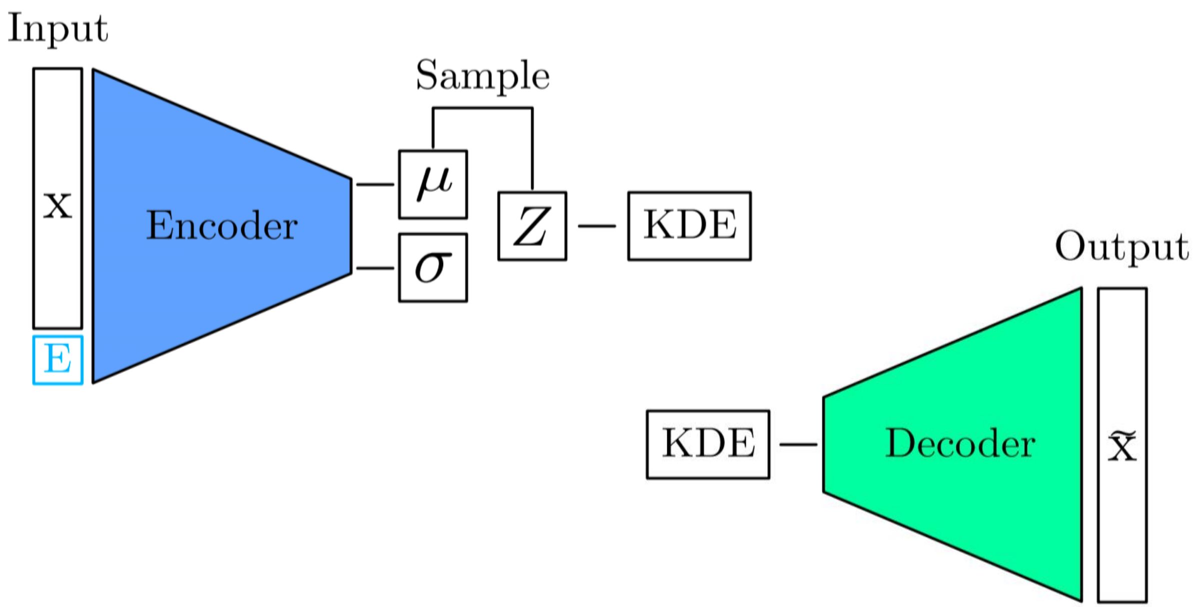
Next Steps

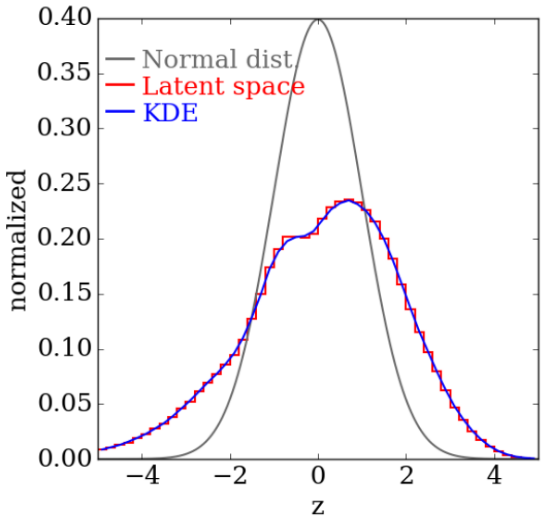
- Continue to improve simulation **speed** with models and **extend functionality** (e.g. additional angle)
- Study full **physics benchmarks**

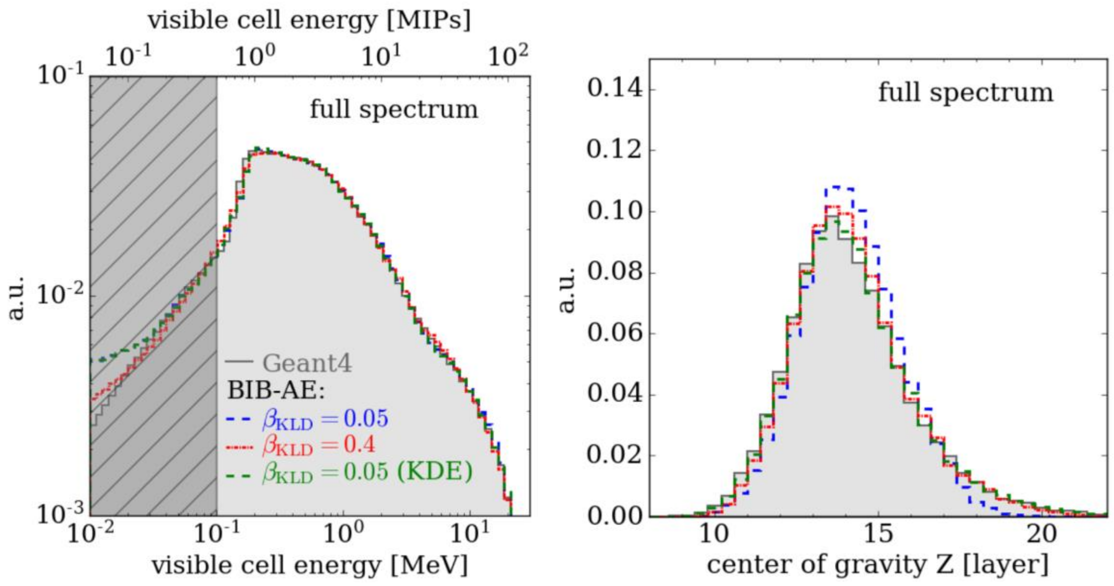
Backup

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)



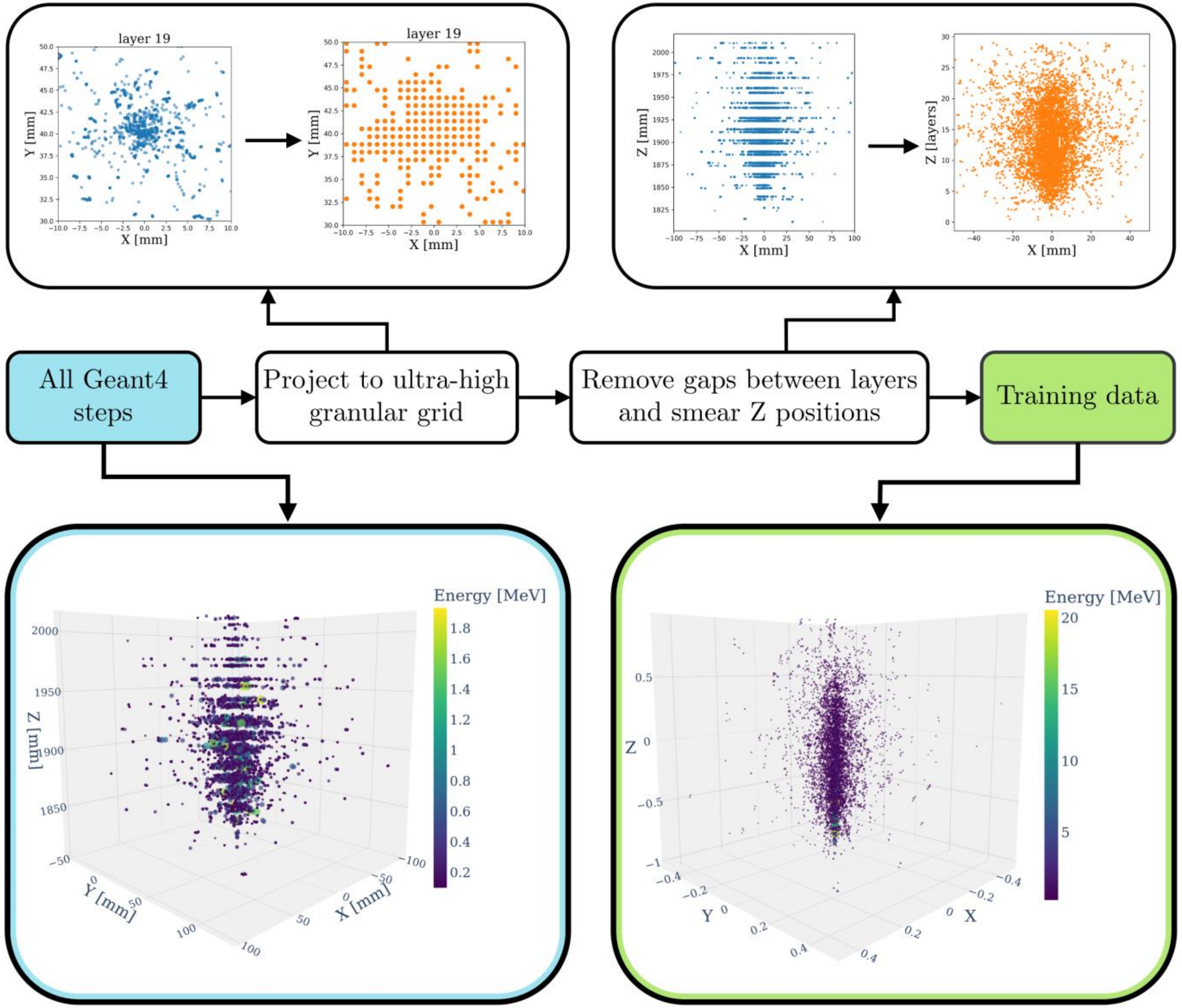




Buhmann et. al: **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network**, EPJ Web of Conferences 251, 03003 (2021)

CaloClouds: Data Preprocessing

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, P.M. et al., arXiv:2305.04847, Submitted to JINST



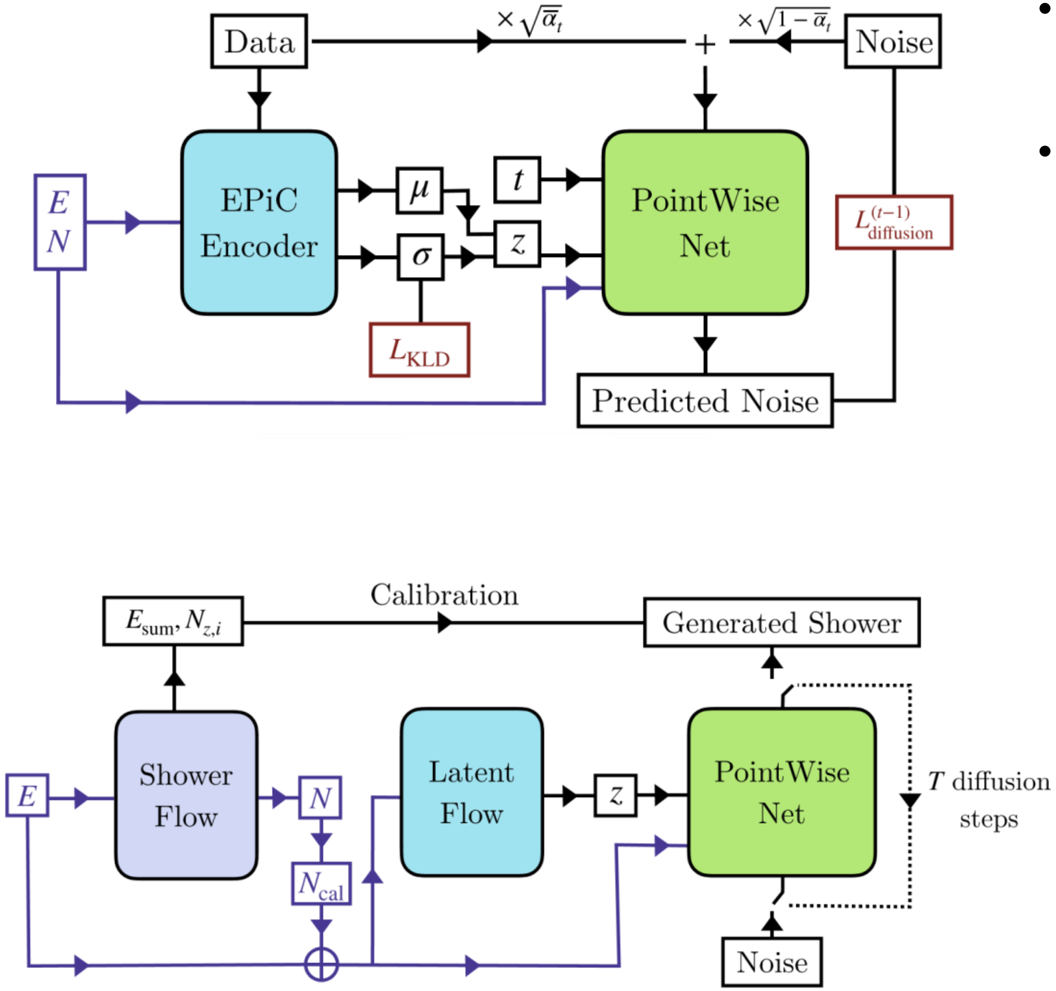
- Using all Geant4 steps directly is **computationally prohibitive**
  - 40k Geant4 steps at 90 GeV

- Apply preprocessing step:
  - Project Geant4 steps into **ultra-high granularity grid** (36 times more granular than ILD ECAL)
    - Reduce number of points by factor ~7:
    - Up to **6000 space points**

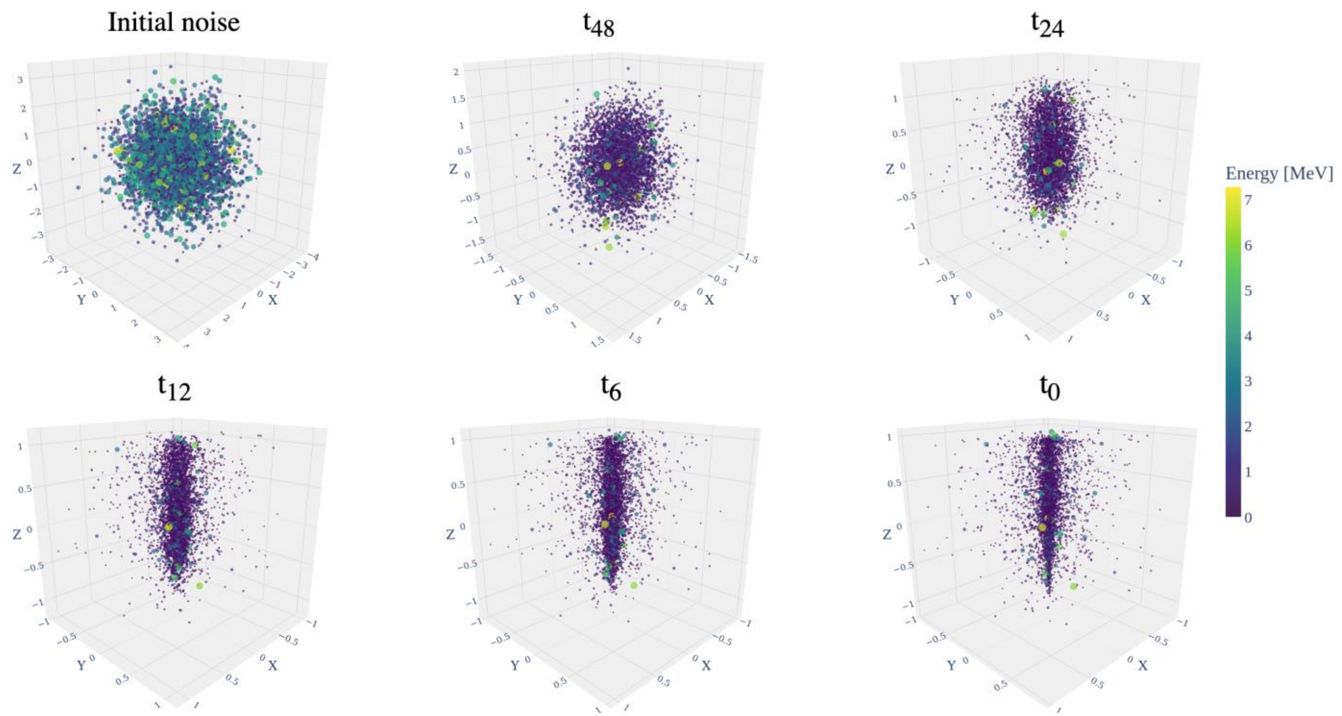
- Again study **photons** in ILD ECAL
  - 10-100 GeV, 90 deg impact
  - Additionally **check** the effects of **varying incident point** (hence geometry)

CaloClouds: Diffusion Model Architecture

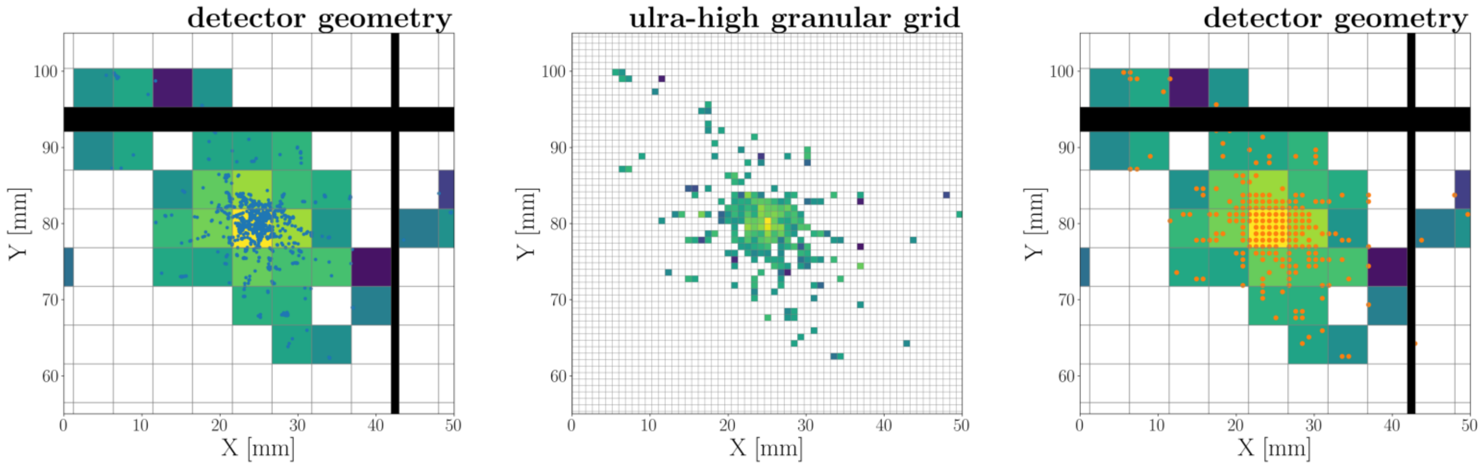
CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation, Buhmann, P.M. et al., arXiv:2305.04847, Submitted to JINST



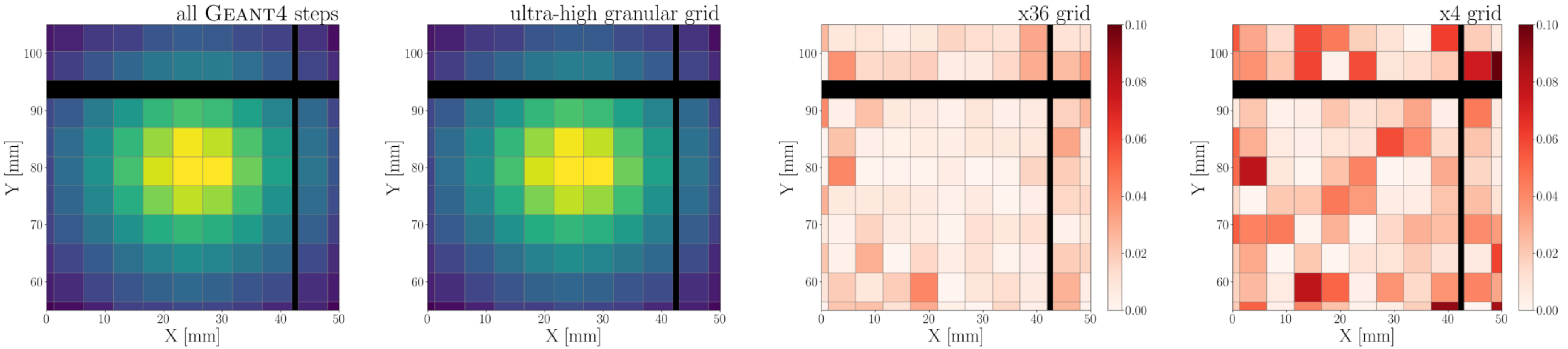
- Training of PointWise Net with EPiC Encoder (e-Print: 2301.08128)
- Inference uses two additional flows for number of space points, calibration and latent space



Effects Of Pre-clustering To Ultra-high Granularity



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

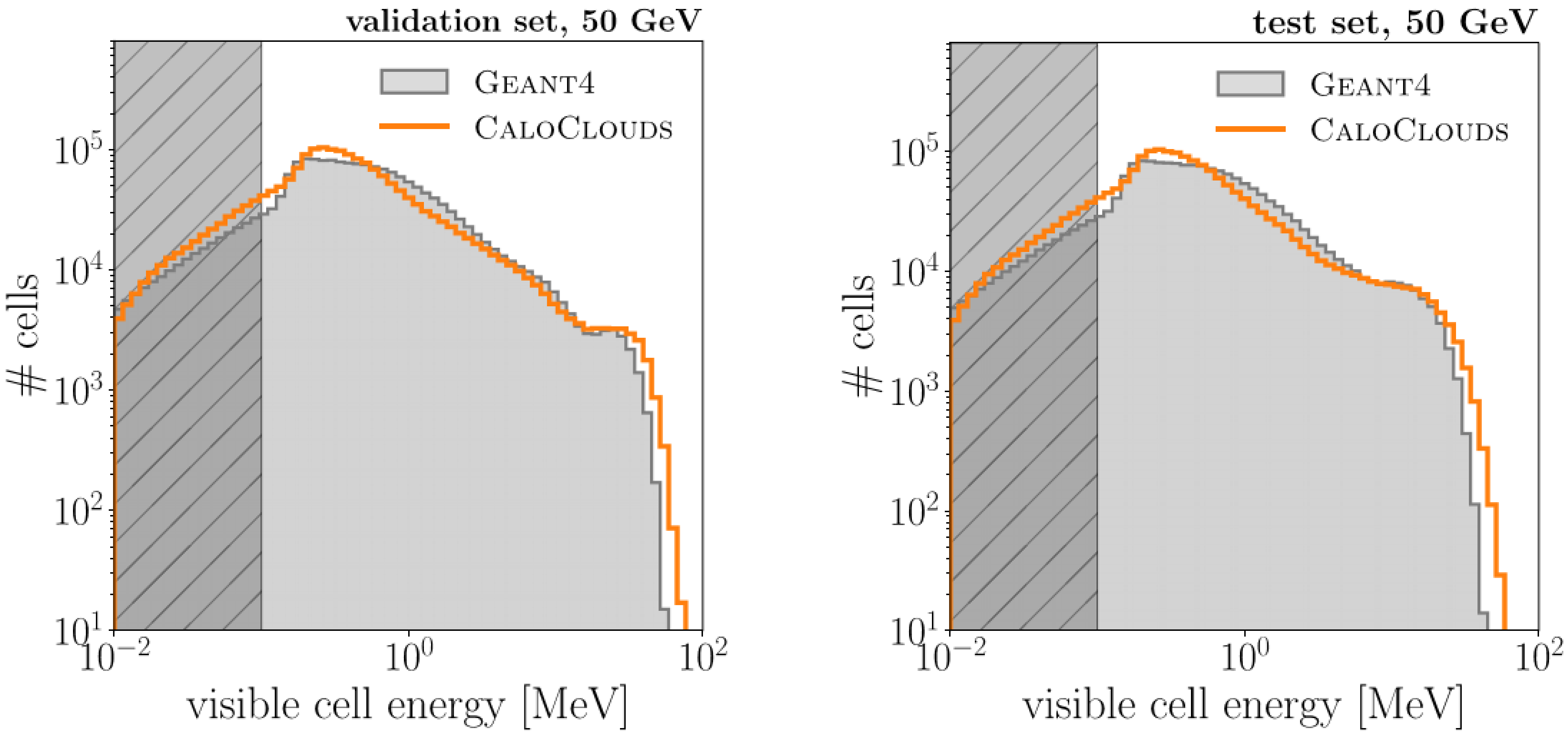


overlay of 2k Geant4 90 Gev showers in layer 21
with full round-trip pre-clustering and back-projection

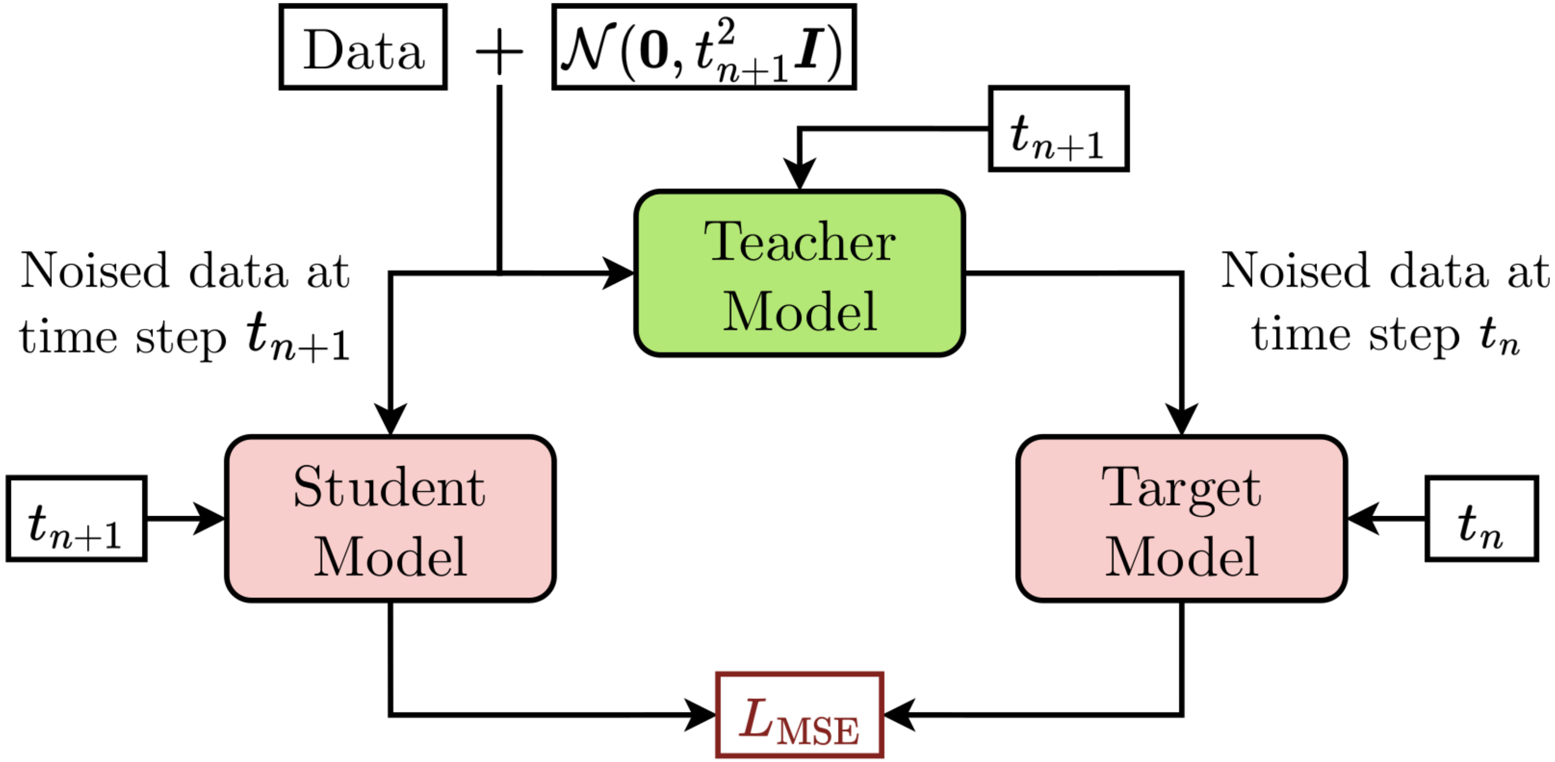
relative difference per cell
< 2% in core of shower

relative difference with
lower granularity

CaloClouds: Effects Of Varying Geometry



Consistency Model



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

Simulator	Hardware	Batch size	time [ms]	Speedup
GEANT4	CPU	1	4081.53 ± 169.92	×1.0
Flow	CPU	1	1746.61 ± 64.50	x2.3
		10	392.61 ± 0.34	x10.4
		100	228.86 ± 7.09	x17.8
		1000	275.55 ± 3.01	x14.8
Flow	GPU	1	2471.07 ± 70.20	x1.7
		1000	3.39 ± 0.09	×1202.3

Normalising Flow, photon showers 10-100 GeV, 90 deg