The Bounded Information Bottleneck Autoencoder (BIB-AE)

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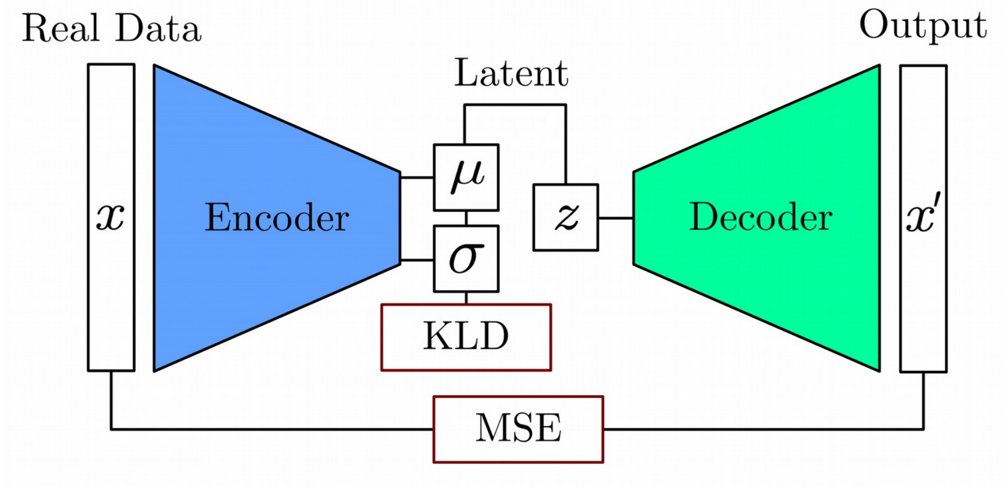
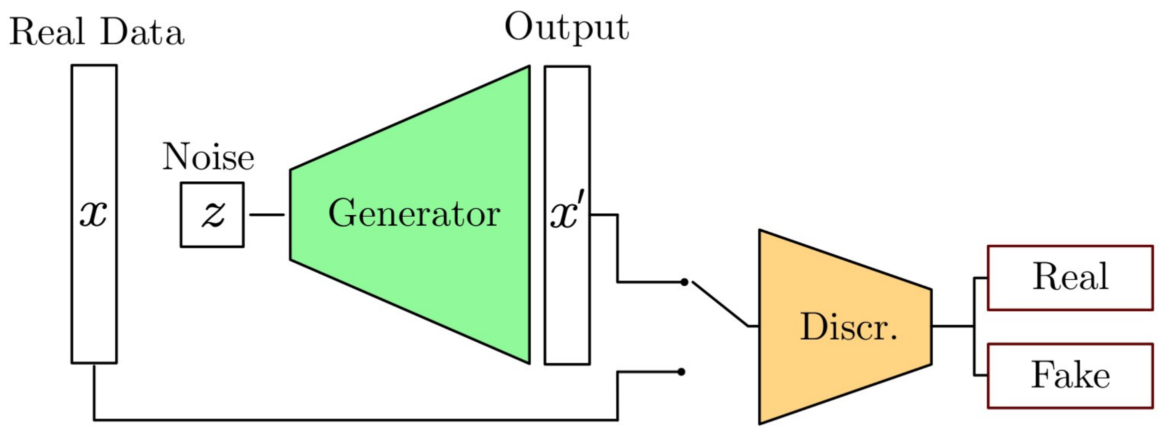
VAE vs GAN Architectures





- **Encoder/decoder** pair
- Data mapped to regular Gaussians
- Decoder generates samples from **latent space**

✓ Easier to train

X Less expressive

- **Generator/discriminator** pair
- **Adversarial feedback** from discriminator trains generator
- Generator produces samples

X Hard to train

✓ Can be rather expressive

Scalable to high dimensions!

Bounded Information Bottleneck Autoencoder: Motivation

- Motivated by information theory: the **Information Bottleneck Principle**[1],[2]
  - Optimise **trade-off** between **compression** and **retention** of useful information
  - For the BIB-AE: $\mathscr{L}(\phi,\theta)=I_{\phi}(\boldsymbol{X};\boldsymbol{Z})-\beta I_{\phi,\theta}(\boldsymbol{Z};\boldsymbol{X})$
  - $I_{\phi}(\boldsymbol{X};\boldsymbol{Z})$ = mutual information between training data vector $\boldsymbol{X}$ and latent vector $\boldsymbol{Z}$; ϕ = encoder params., θ = decoder params.
  - β controls the compression/information retention balance

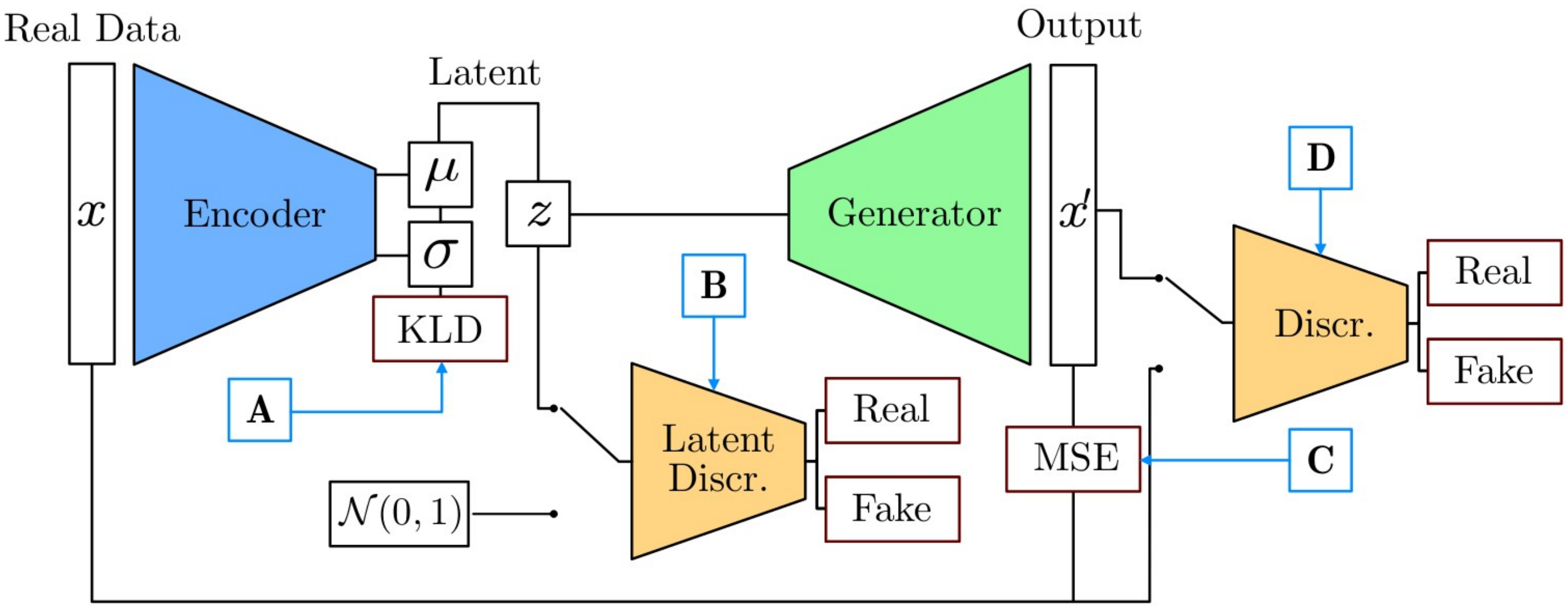
- BIB-AE: **Unifies** features of common **GANs** and **VAEs**[3]

[1] Tishby et al.: **The information bottleneck method**, arXiv:physics/0004057 (2000)

[2] Tishby and Zaslavsky: **Deep Learning and the Information Bottleneck Principle**, arXiv:1503.02406 (2015)

[3] Voloshynovskiy et. al: **Information bottleneck through variational glasses**, arXiv:1912.00830 (2019)

Components of the Core BIB-AE Architecture



- **A**: latent space KL-divergence term
- **B** : latent space discriminator/MMD term
- **C**: data space MSE term
- **D**: data space discriminator

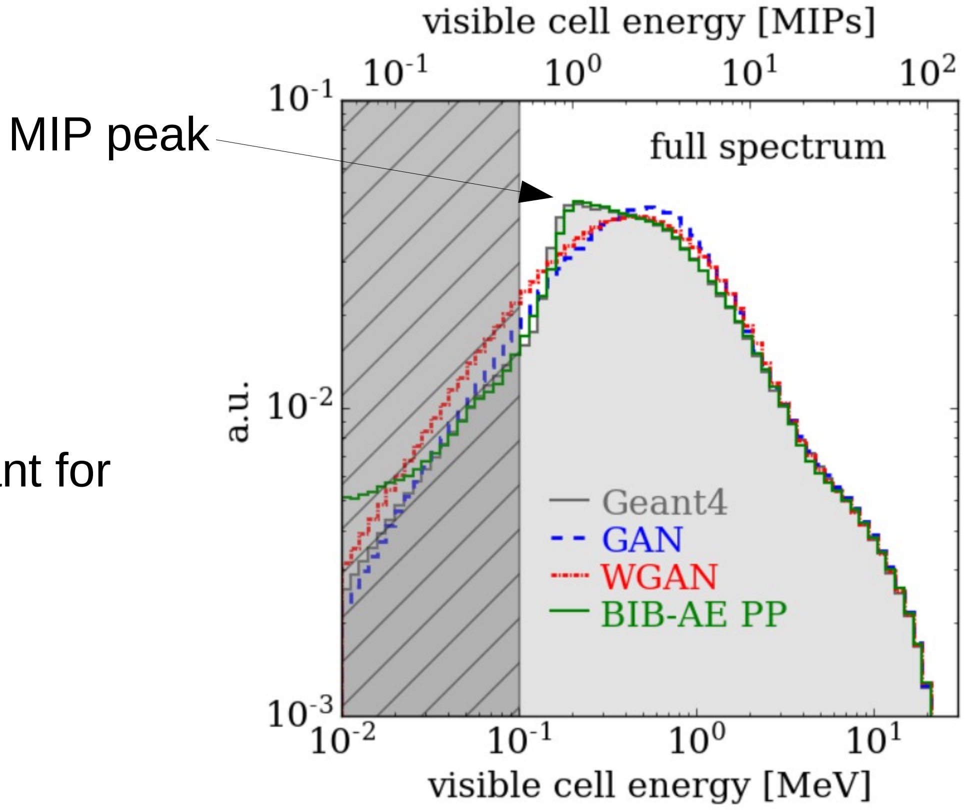
Voloshynovskiy et. al: **Information bottleneck through variational glasses**, arXiv:1912.00830 (2019)

Adaption to Highly Granular Calorimeter Shower Data

- **Highly granular** calorimeter data is very **sparse**
  - Causes problems for an MSE based loss
  - Switch to a discriminator based approach

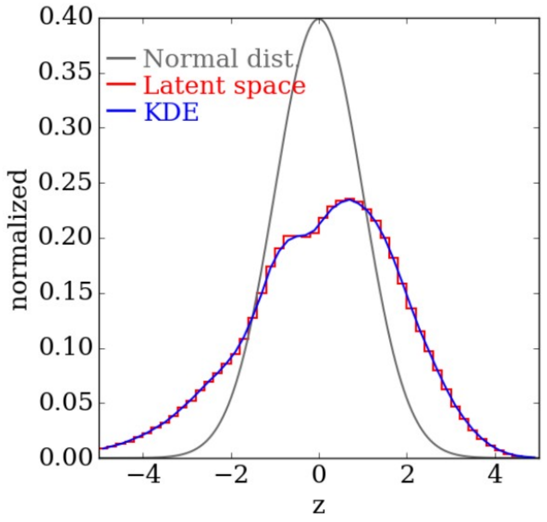
- **Cell energy spectrum** has a very steep rise (MIP peak- important for calibration)
  - Difficult to model with an adversarial approach...

- Offload to separate **Post Processor** network:
  - 3D convolutions, kernel size 1
  - MSE loss and Sorted Kernel MMD loss
  - Encourage network to modify individual pixels

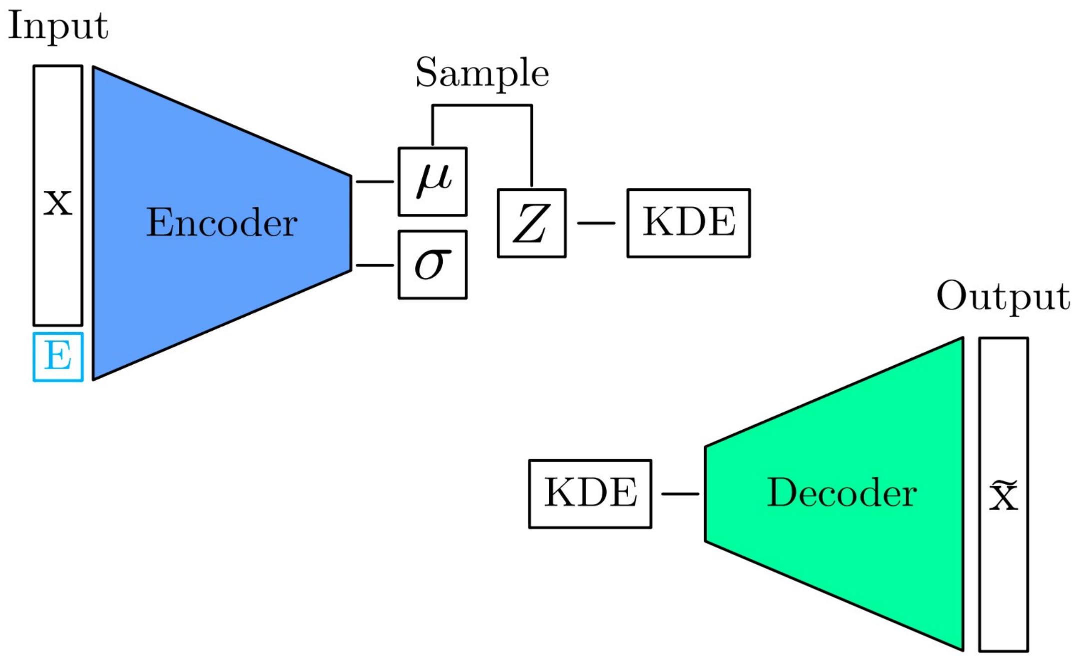


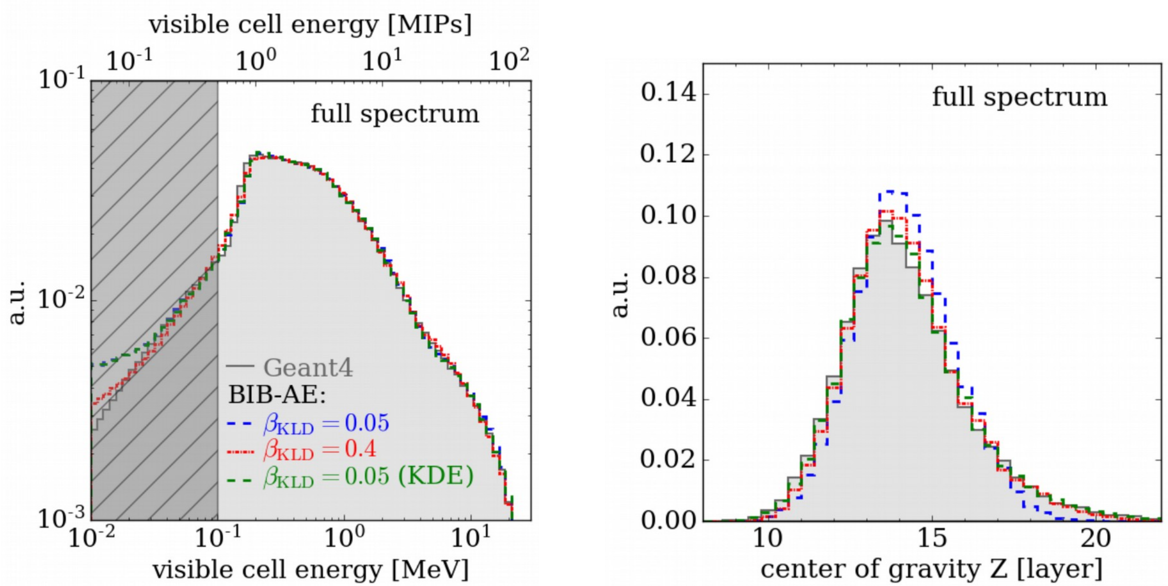
Buhmann et. al: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed**, CSBS 5, 13 (2021)

Latent Space sampling



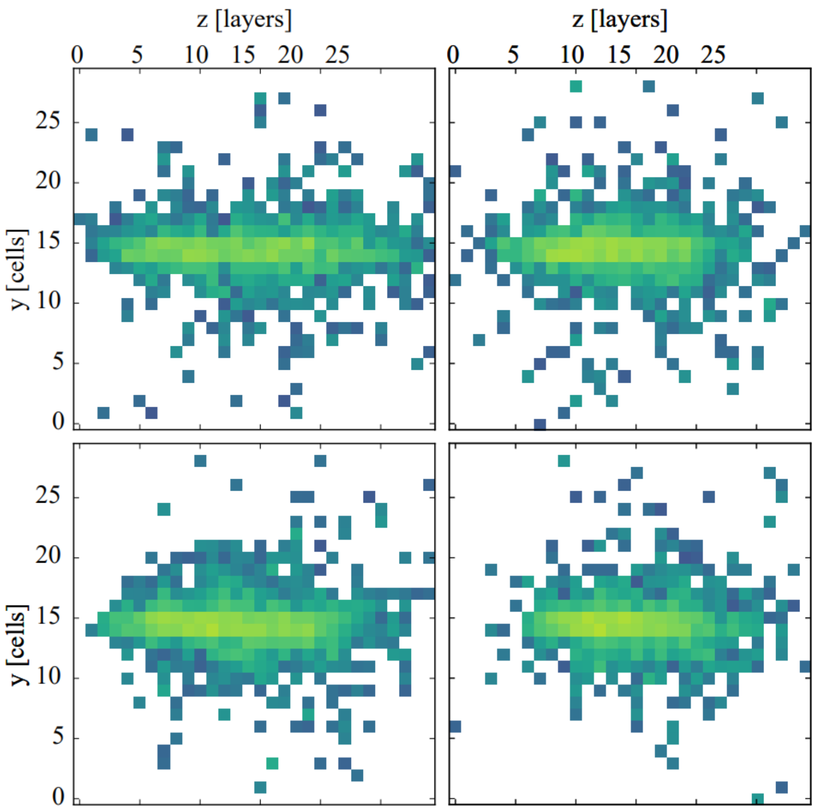
- **Relaxing regularisation** of latent space allows more information to be stored
  - Latent space deviates from a Normal distribution
- Employ **density estimation** to produce latent sample (e.g. KDE)
- **Improve** modeling of **shower shape** (center of gravity)

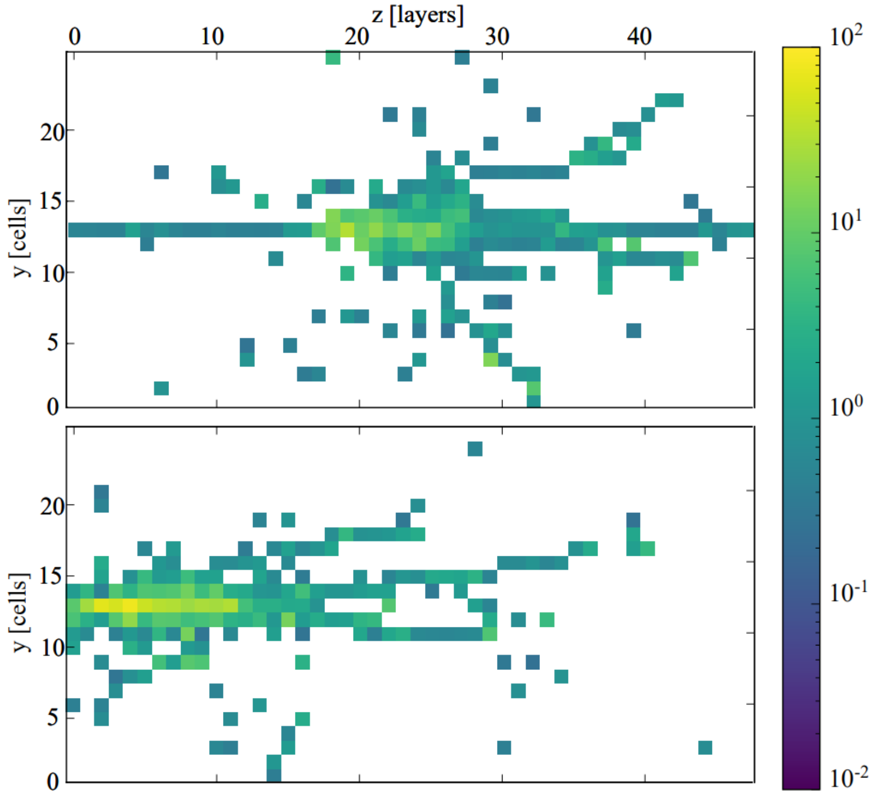




Buhmann et. al: **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network**, EPJ Web of Conferences 251, 03003 (2021)

From Photons to Pions





Photon showers

- Predominantly governed by **EM** interactions
- **Compact** structure → **Easy to generalise**

Pion showers

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

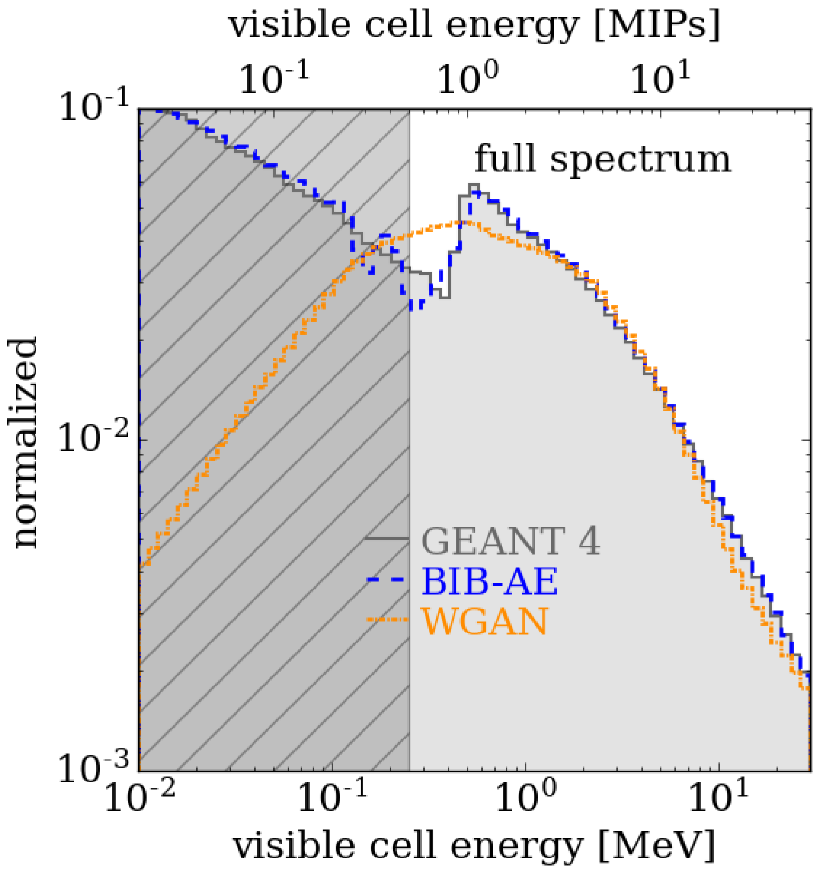
→ **Hard to learn**

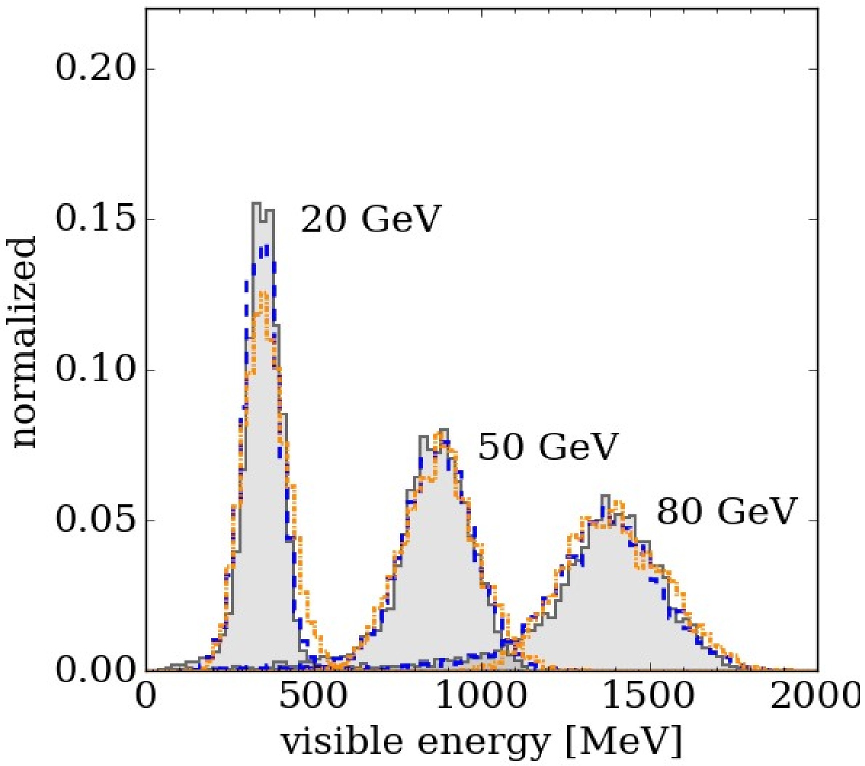
Pion Showers: Sim Level Results

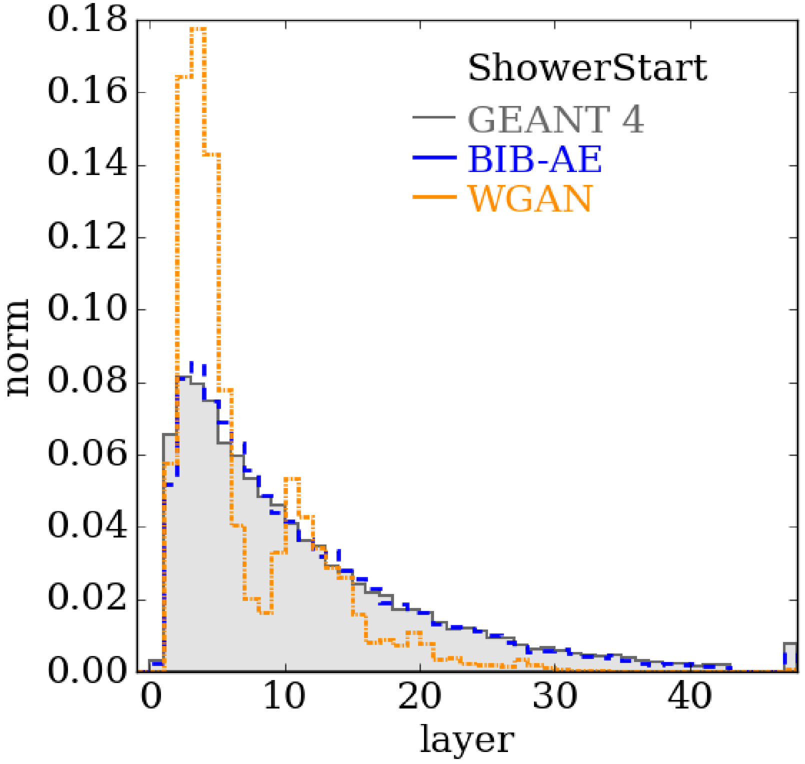
Buhmann et. al.,
Hadrons, Better, Faster, Stronger,
MLST 3 025014, (2022)

- **BIB-AE** shows consistently **high performance**; WGAN performance is mixed

MIP = Minimum Ionizing Particle

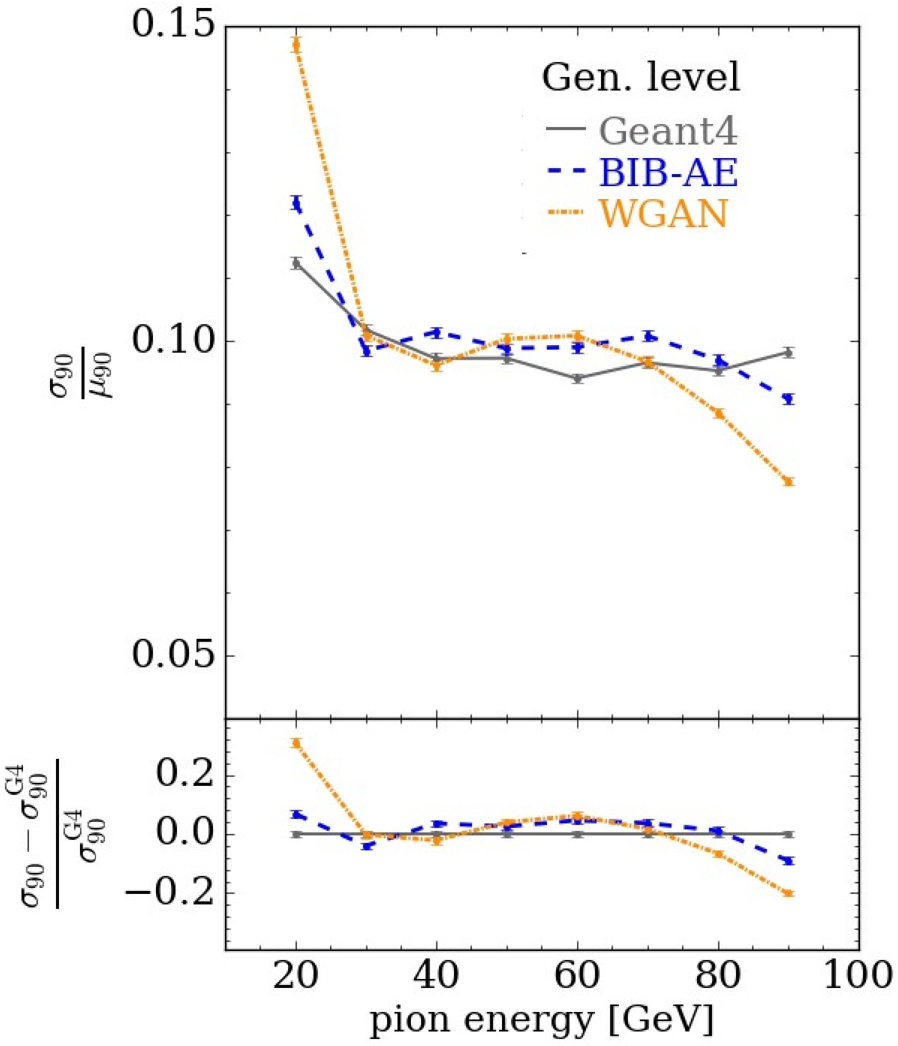


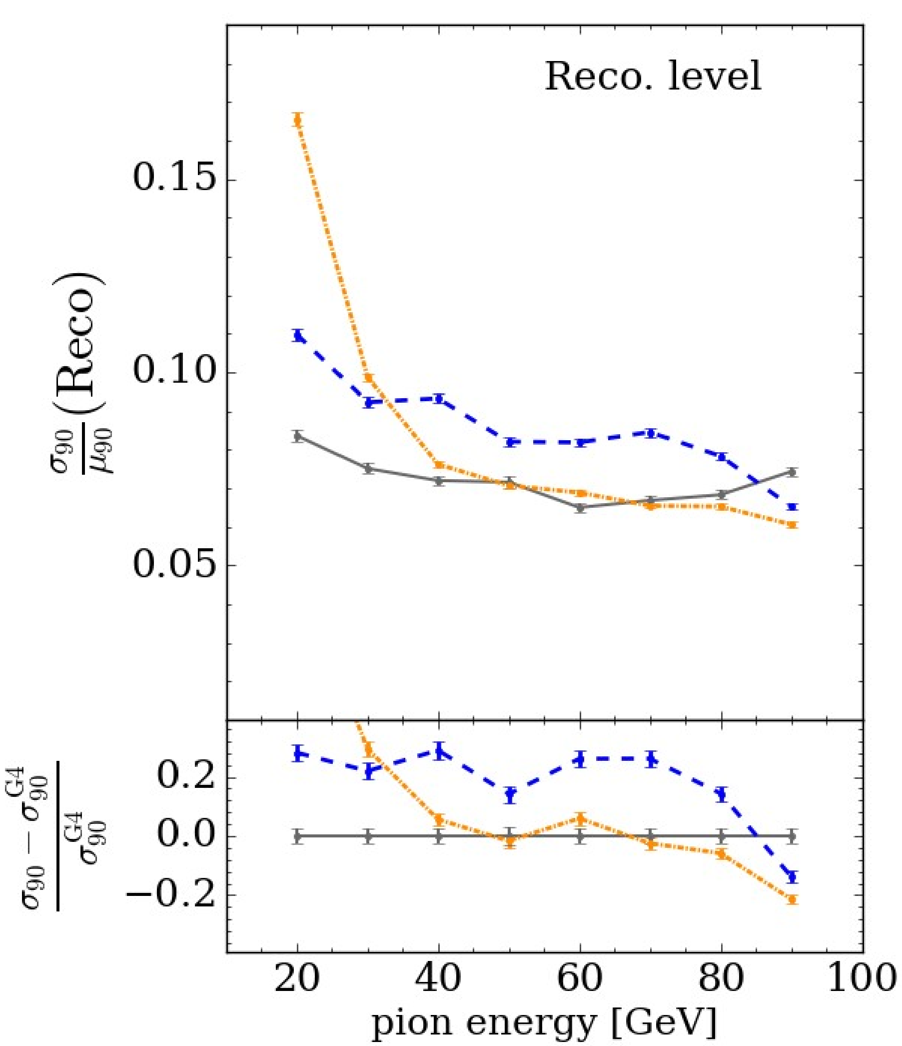




Pion Showers: Resolution Before and After Reconstruction

- Interface with **Pandora PFA**; after reconstruction BIB-AE performance reduces- requires further study!





Buhmann et. al., **Hadrons, Better, Faster, Stronger**, [MLST 3 025014](), (2022)

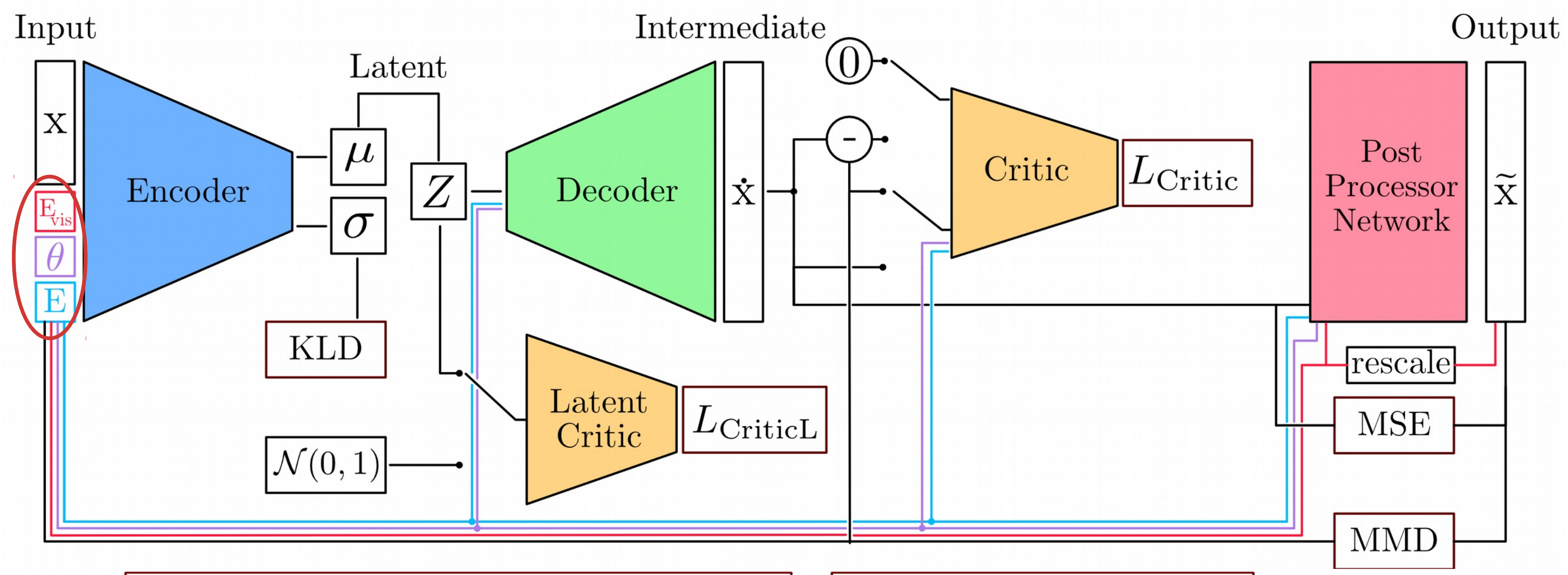
Pion Showers: Computing Time for Inference

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	$\times 1309$

Speed-up of as much as four orders of magnitude on single core of Intel® Xeon® CPU E5-2640 v4 and NVIDIA® A100 for the best performing batch size

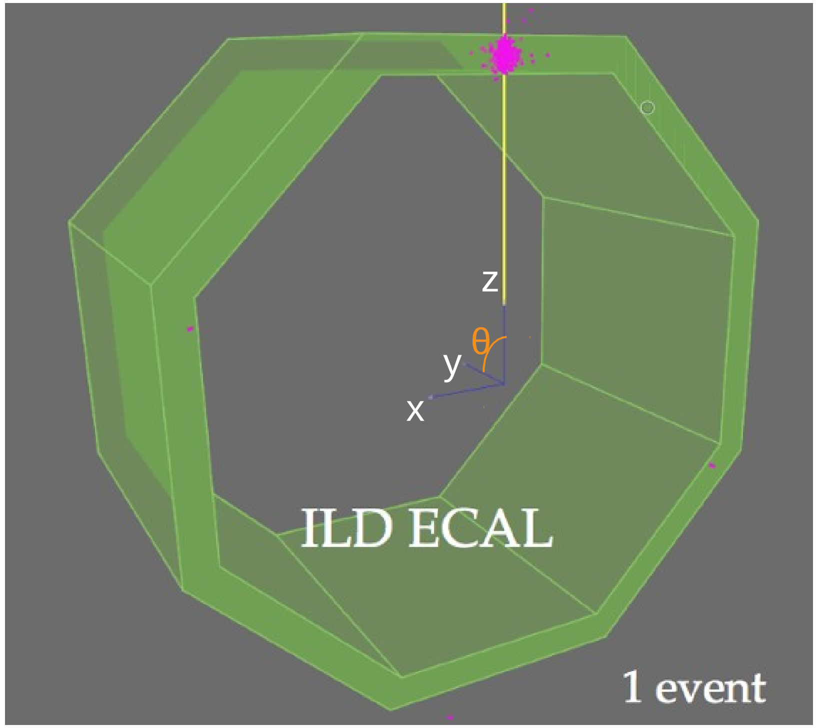
Angle and Energy Conditioning

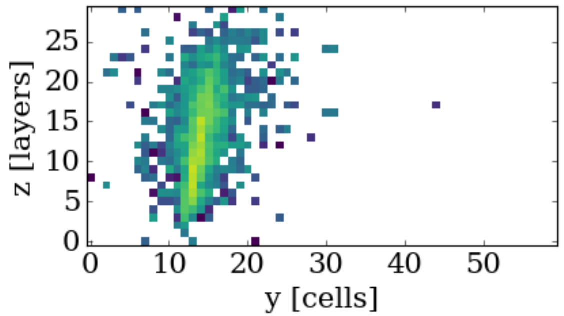
- **Multi-parameter conditioning** essential to **generalise** simulation tool
- **Normalising Flow** for latent sampling- **fast** sampling with multiple conditioning parameters
- Flow generates latent variables + Esum given angle and energy
- Additional **energy sum** conditioning in Post Processor- rescale per shower energy to pin down energy sum

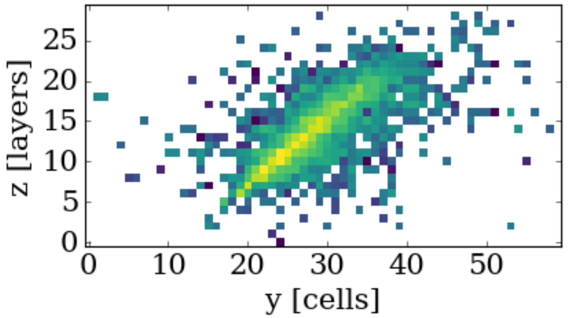


$L_{BIB-AE} = KLD + L_{CriticL} + L_{Critic}$

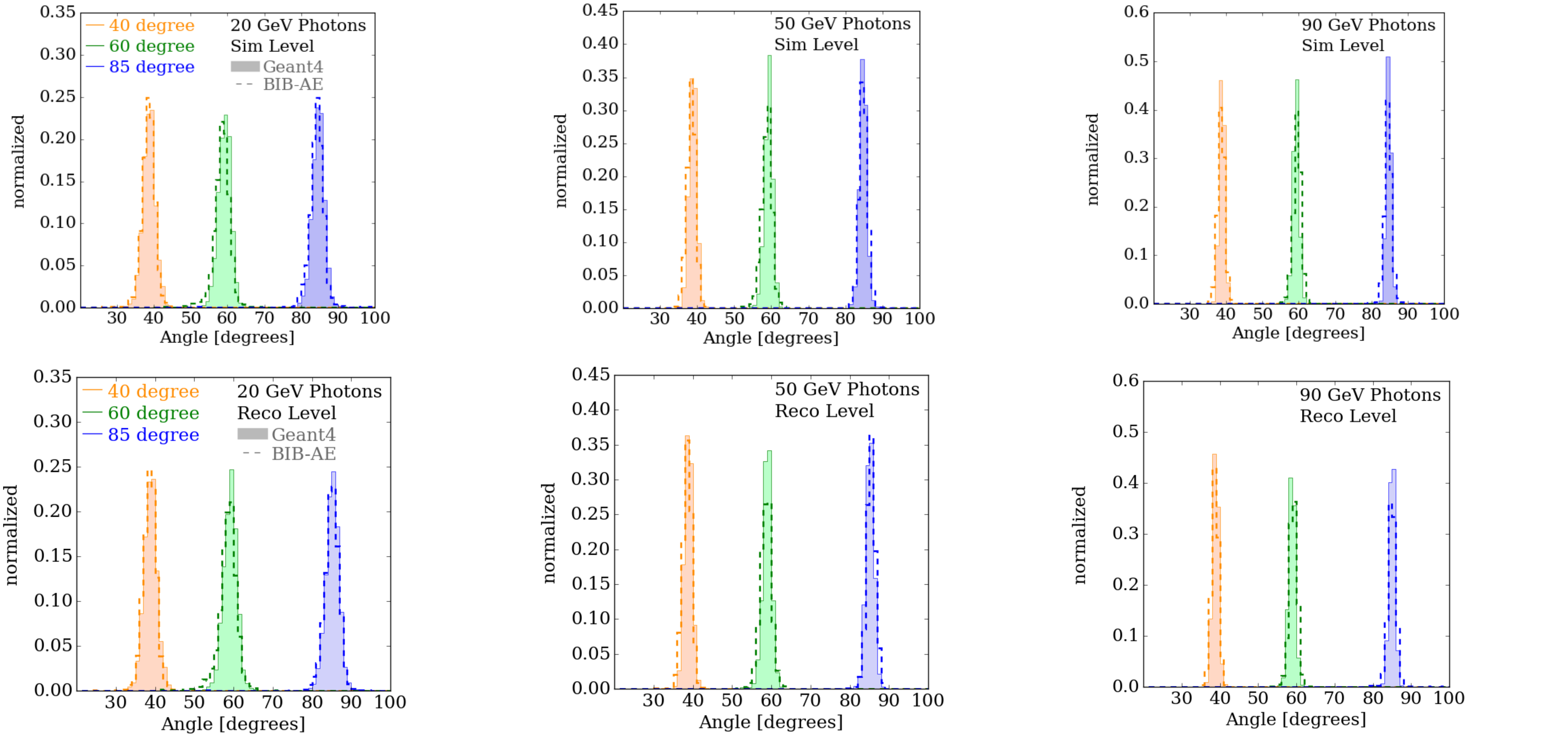
$L_{Post} = MMD + MSE$



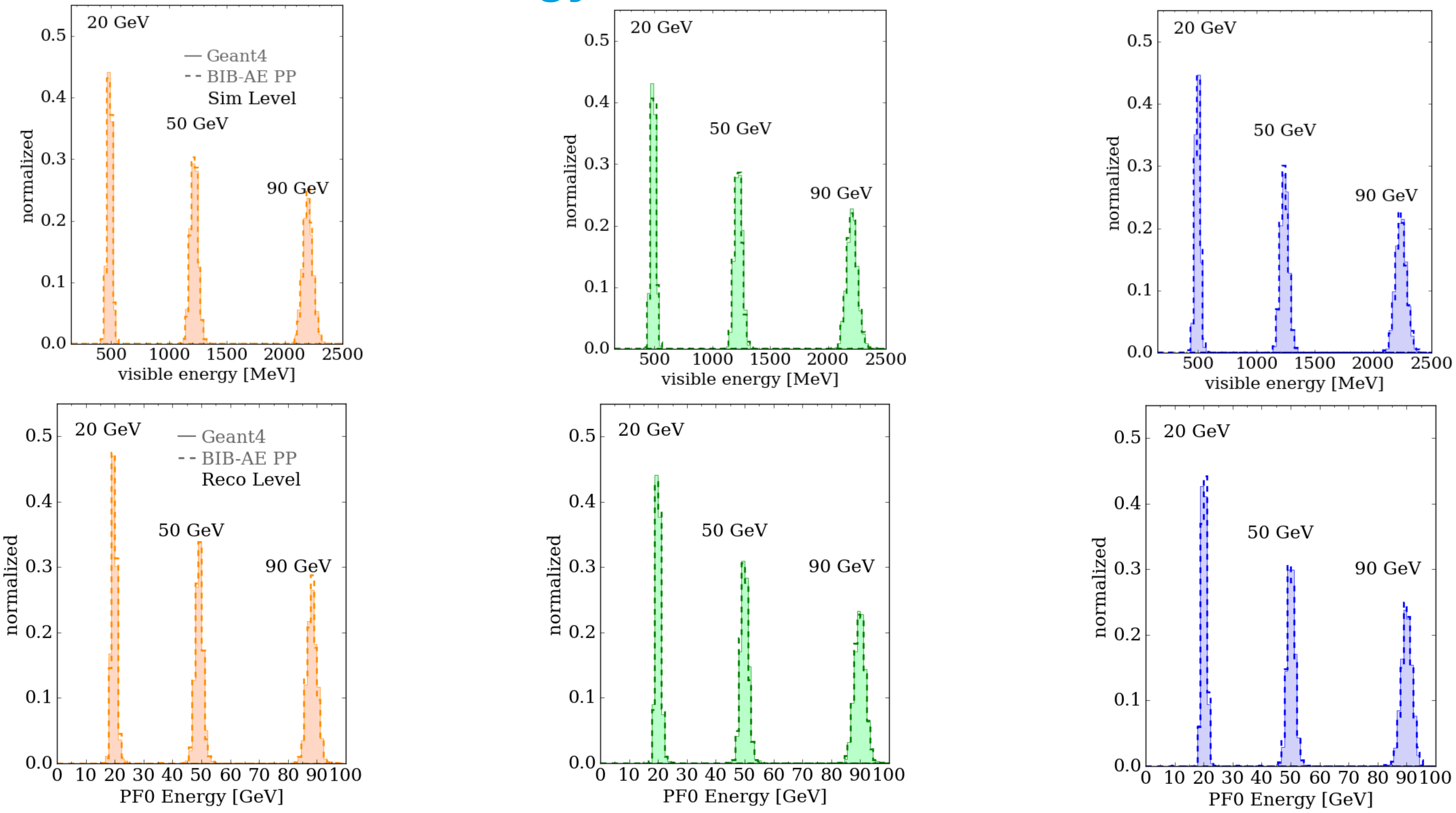




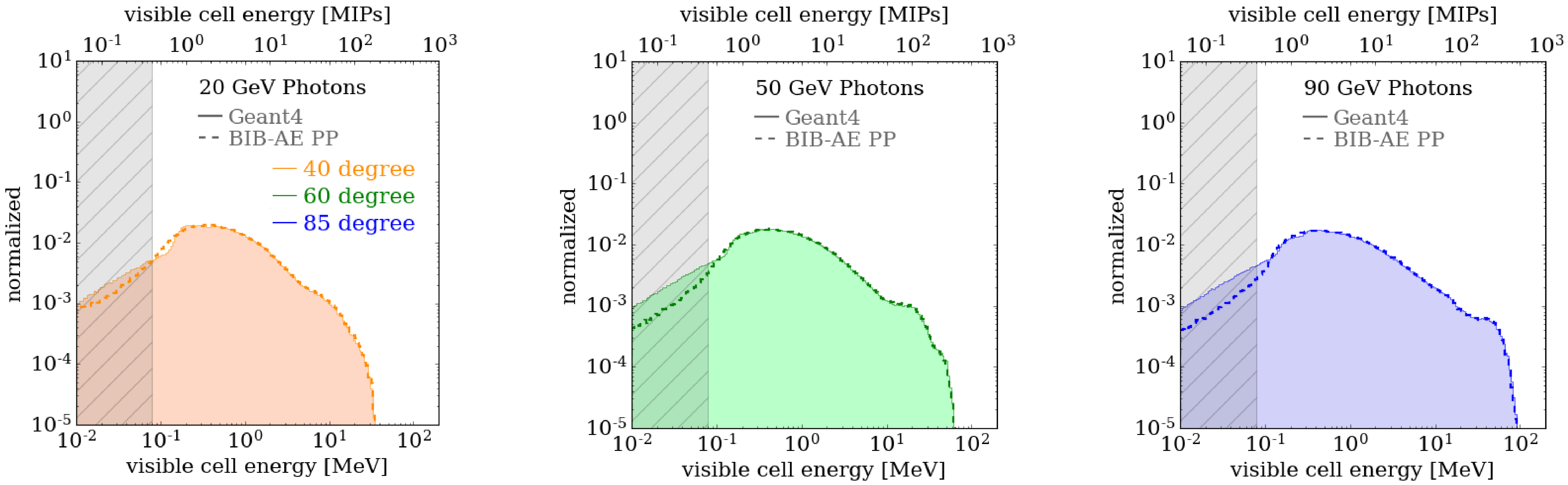
Results: Angular resolution- Sim vs Reco



Results: Visible Energy Sum- Sim vs Reco



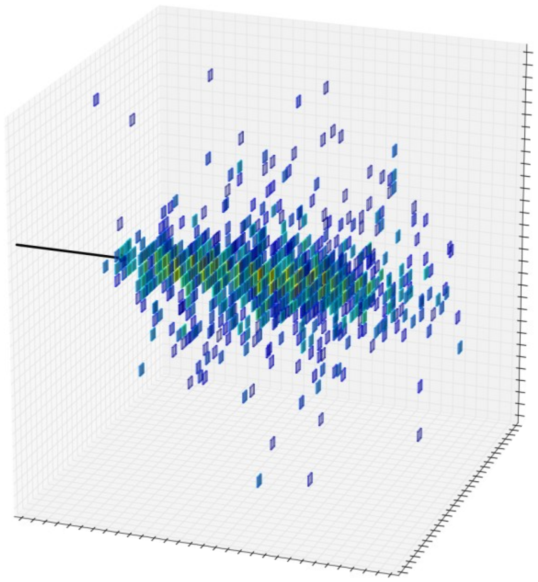
Results: Cell Energy Examples at Sim Level



Conclusion: Pros and cons

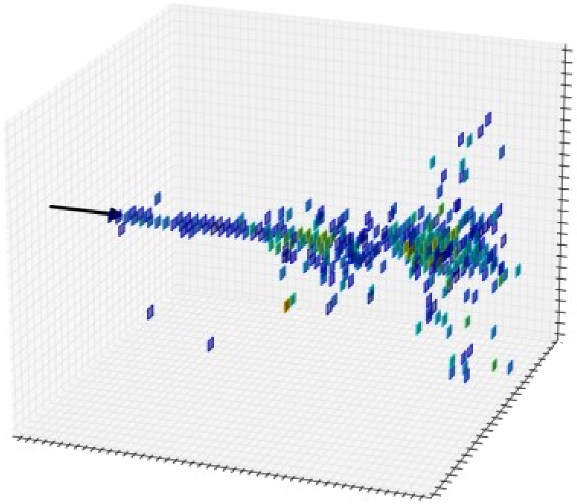
Pros

- Highly **expressive** architecture
- Permits **application-specific** modifications for increased performance
- Strong **theoretical motivation** enables targeted hyper-parameter tuning
- Capable of tackling multiple **different physics** cases (electromagnetic + hadronic showers)
- Possible to extend the framework to **multi-parameter conditioning**



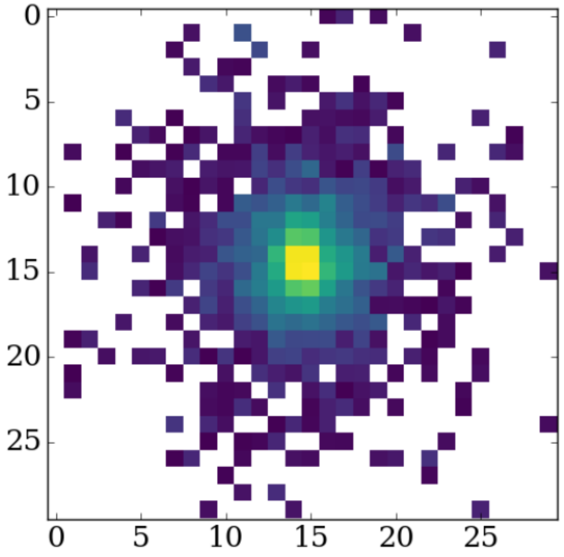
Cons

- Very **complex** architecture- lots of moving parts
- Quite a lot of **parameters**: ~10 million in current setups- **reduced** sampling **speed** (compared to e.g. a WGAN)
- Despite significantly increased stability, **adversarial training** still requires some care

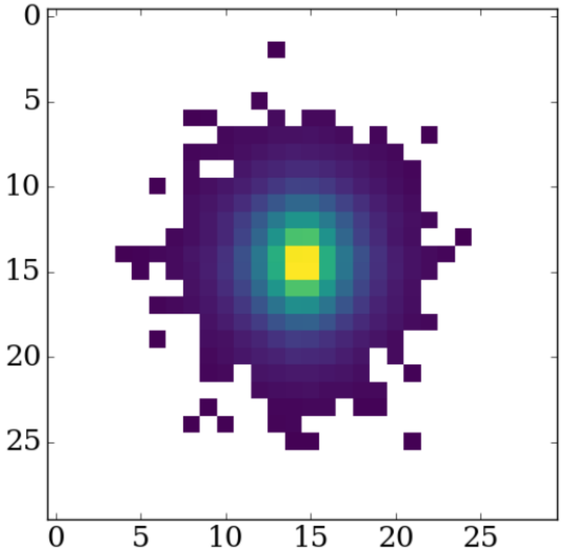


Backup

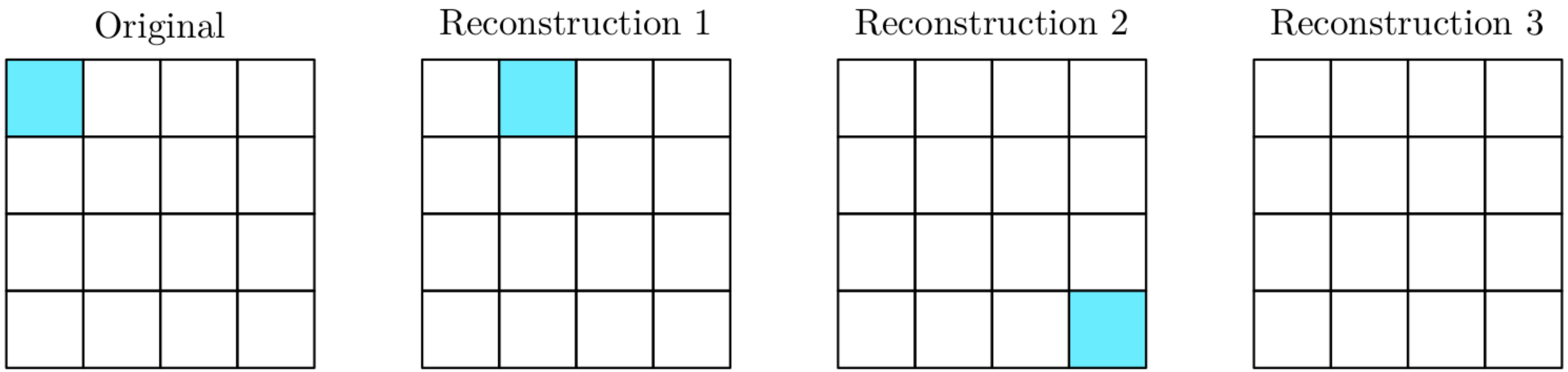
Problem with MSE



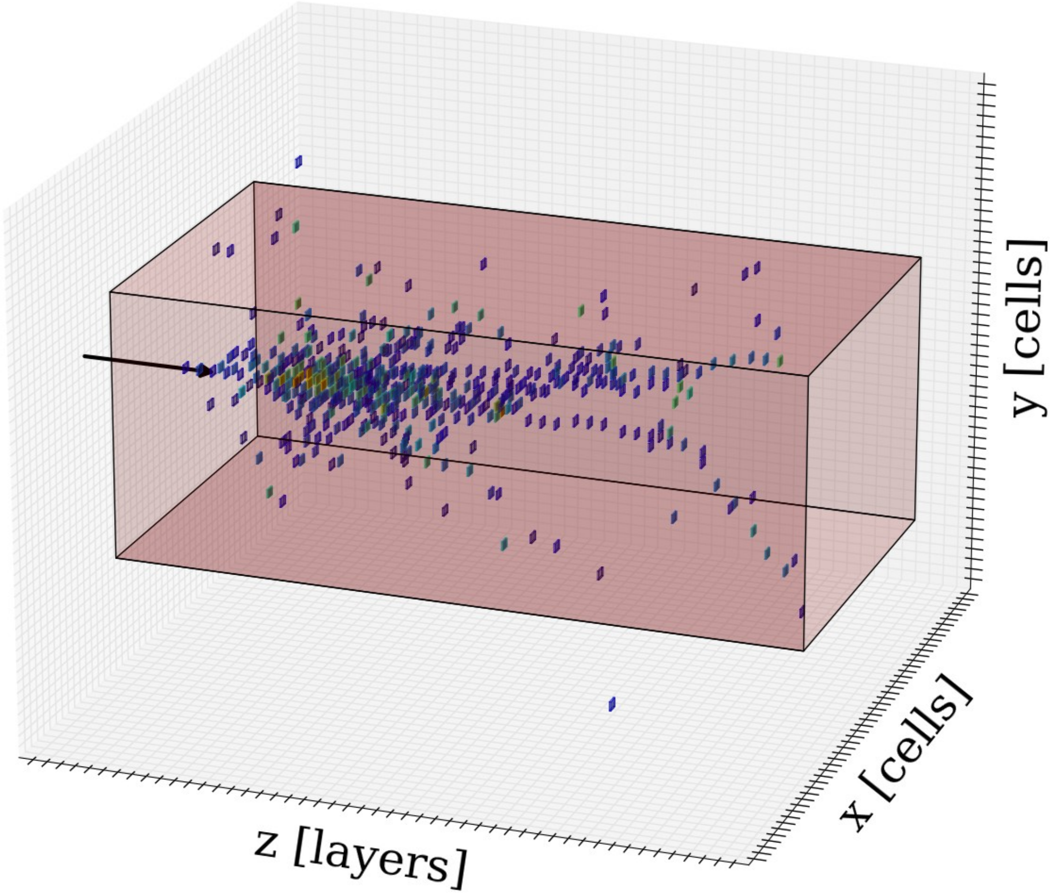
Geant 4 shower



MSE trained Autoencoder



Pion Dataset

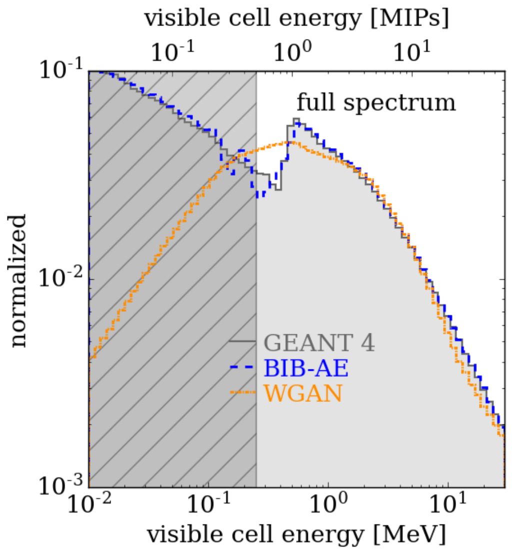


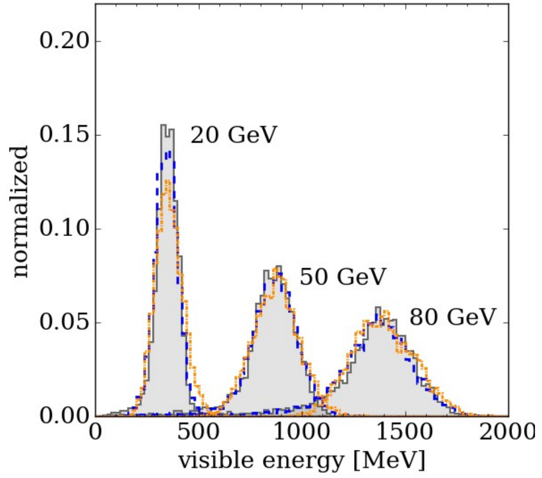
- Remove ECal from geometry
- Training data generation with Geant4

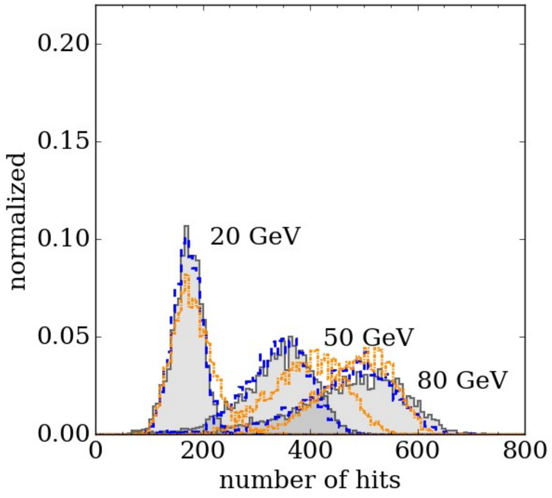
- Irregular HCAL geometry projected into 25x25x48 regular grid
  - Significantly reduce sparsity
  - Barely lose any hits

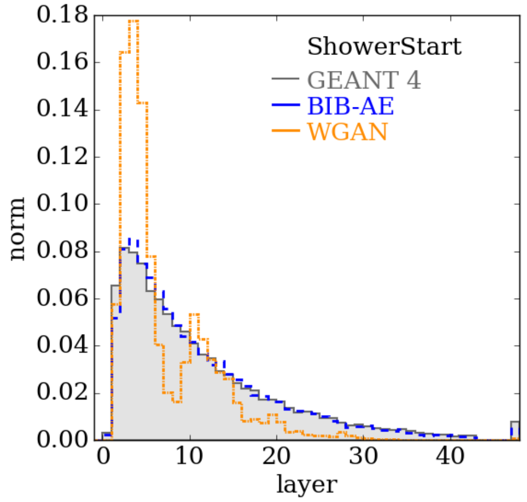
- 500k **pion** showers
- Fixed incident point and angle
- Uniform **energy**: **10-100 GeV**

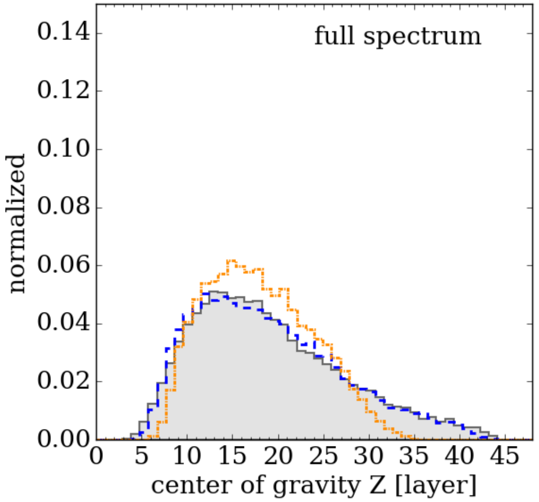
Pion Showers: Sim Level Results

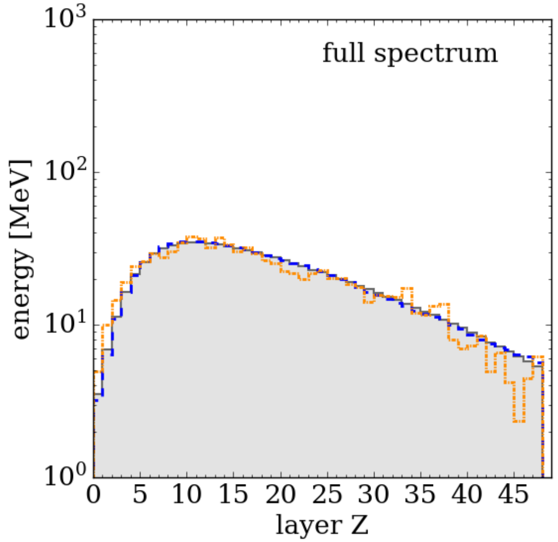




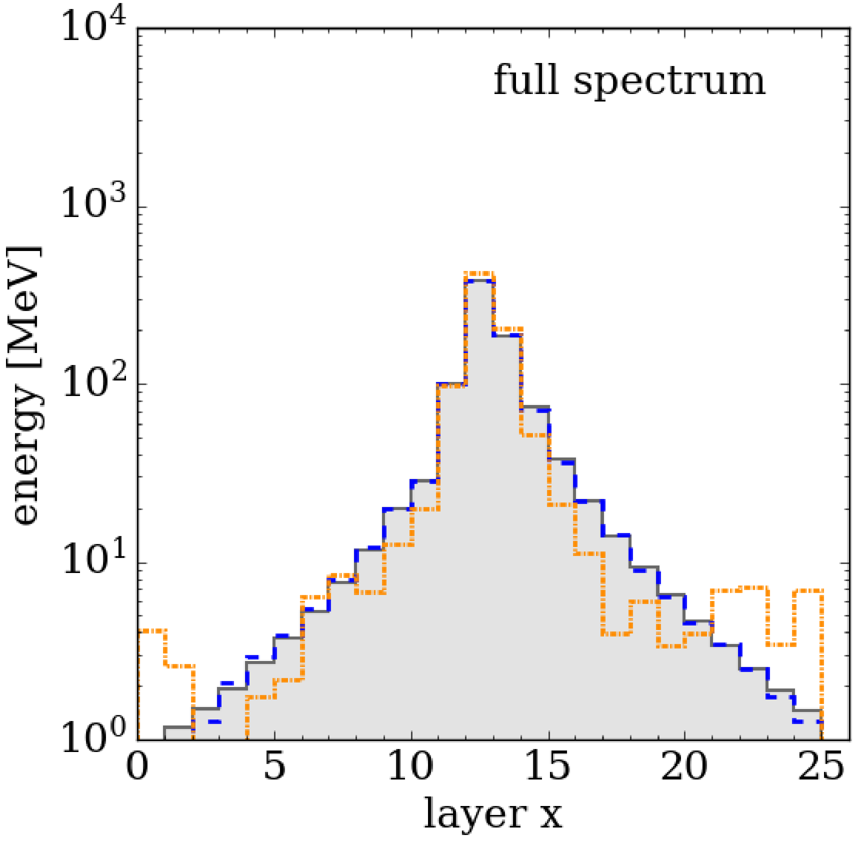


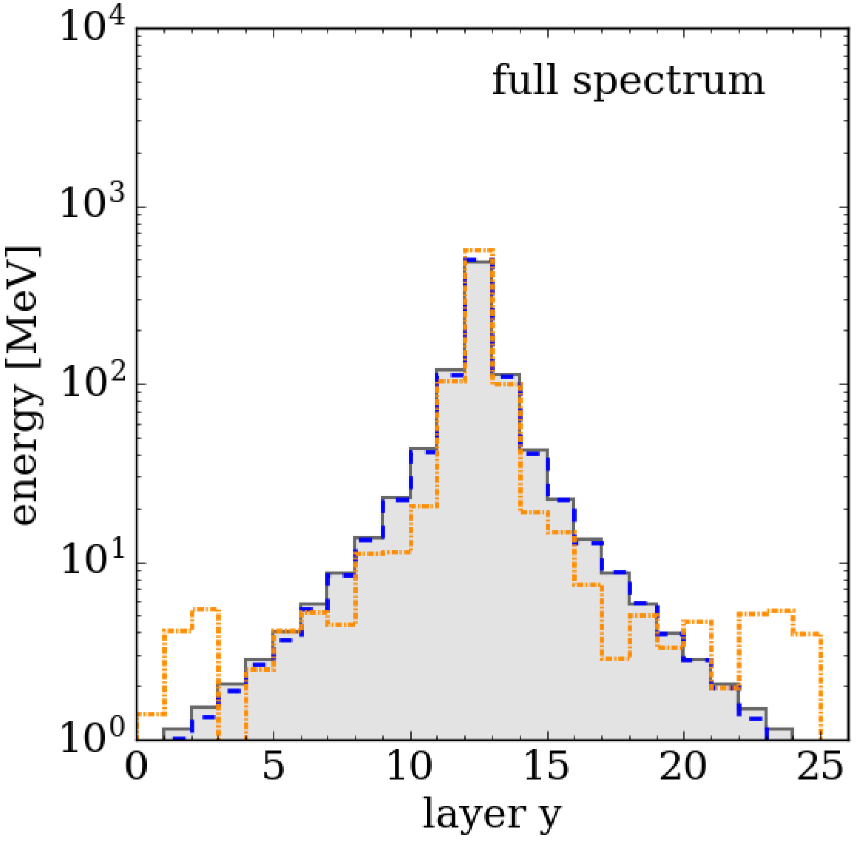






Pion Showers: Sim Level Results (continued)





Pion correlations

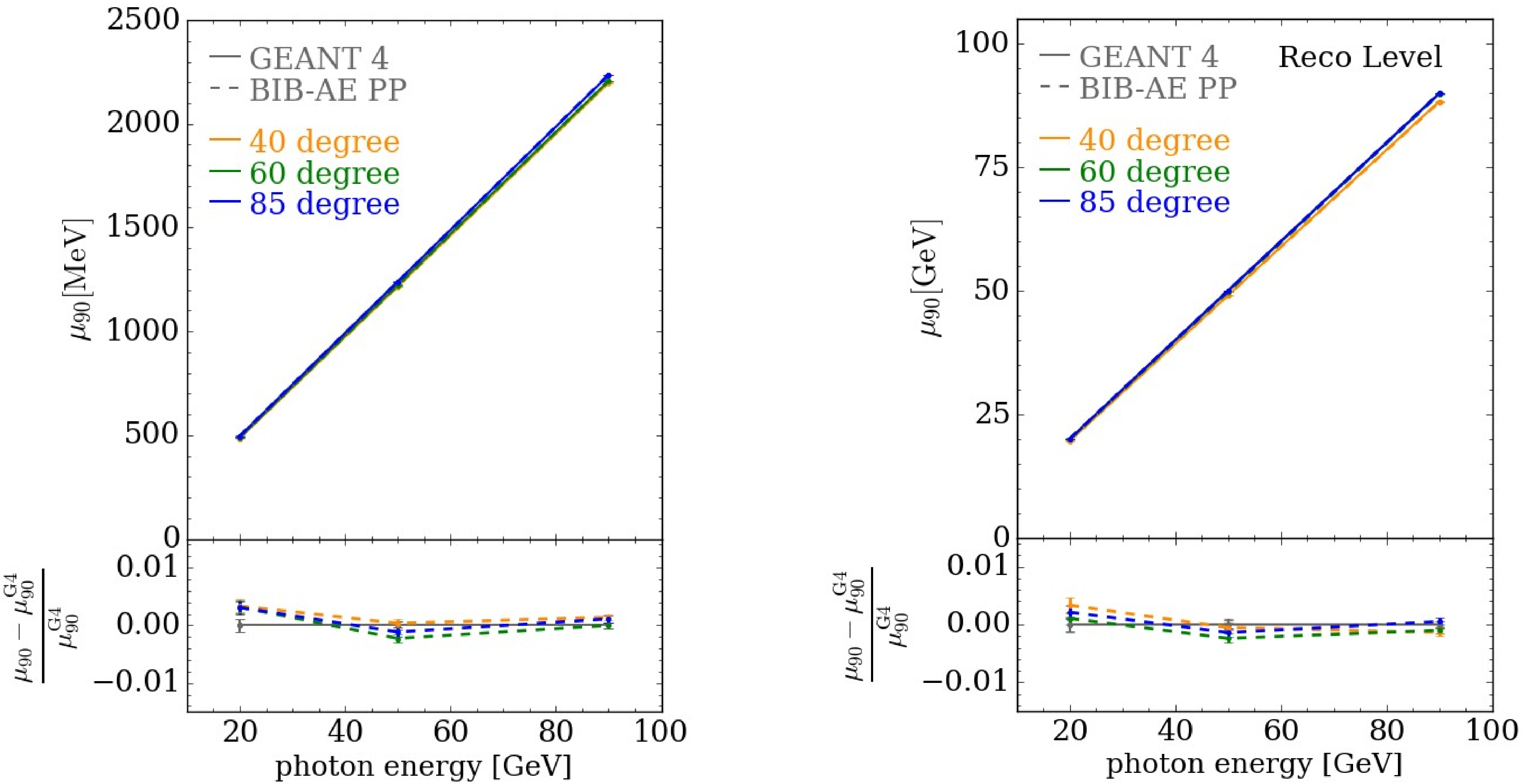
GEANT4 - BIB-AE

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.00	0.00										
$m_{1,z}$	-0.01	-0.04	0.00									
$m_{2,x}$	-0.08	-0.00	-0.06	0.00								
$m_{2,y}$	-0.10	-0.03	-0.05	0.01	0.00							
$m_{2,z}$	-0.06	0.01	-0.06	-0.08	-0.05	0.00						
E_{vis}	0.03	-0.02	-0.01	0.09	0.09	0.06	0.00					
E_{inc}	0.01	-0.03	-0.00	0.08	0.09	0.06	-0.01	0.00				
n_{hit}	0.03	-0.02	-0.02	0.13	0.14	0.06	0.00	-0.01	0.00			
E_1/E_{vis}	0.00	0.03	0.00	0.04	0.04	0.04	0.01	0.00	0.02	0.00		
E_2/E_{vis}	-0.01	-0.00	-0.03	0.02	-0.02	0.01	-0.02	-0.02	-0.01	0.02	0.00	
E_3/E_{vis}	-0.01	-0.04	0.00	-0.07	-0.04	-0.07	0.00	0.01	-0.01	-0.00	-0.03	0.00

GEANT4 - WGAN

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.21	0.00										
$m_{1,z}$	0.20	-0.10	0.00									
$m_{2,x}$	-0.14	-0.17	-0.20	0.00								
$m_{2,y}$	-0.20	-0.28	-0.21	-0.18	0.00							
$m_{2,z}$	-0.14	-0.24	-0.17	-0.20	-0.23	0.00						
E_{vis}	0.14	0.19	-0.21	0.11	0.18	0.06	0.00					
E_{inc}	0.11	0.17	-0.13	0.01	0.09	0.03	-0.03	0.00				
n_{hit}	0.10	0.07	-0.26	-0.02	0.05	-0.09	0.04	-0.00	0.00			
E_1/E_{vis}	-0.17	0.05	0.02	0.16	0.15	0.14	0.14	0.10	0.15	0.00		
E_2/E_{vis}	0.11	0.09	-0.28	-0.00	0.03	-0.01	-0.06	-0.12	-0.01	0.15	0.00	
E_3/E_{vis}	0.09	-0.22	0.03	-0.26	-0.29	-0.31	-0.15	-0.06	-0.27	0.03	-0.28	0.00

Results: Energy linearity Sim vs Rec



Results: Energy resolution Sim vs Rec