High Fidelity Simulation of High Granularity Calorimeters with High Speed

ML4Jets meeting
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E. Buhmann, S. Diefenbacher, E. Eren, F. Gaede, D. Hundhausen, G. Kasieczka,
W. Korcari, A. Korol, K. Krüger, P. McKeown and L. Rustige

DESY.

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

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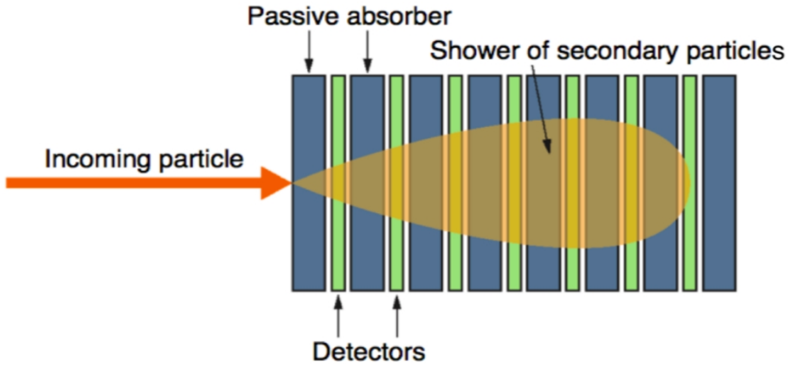
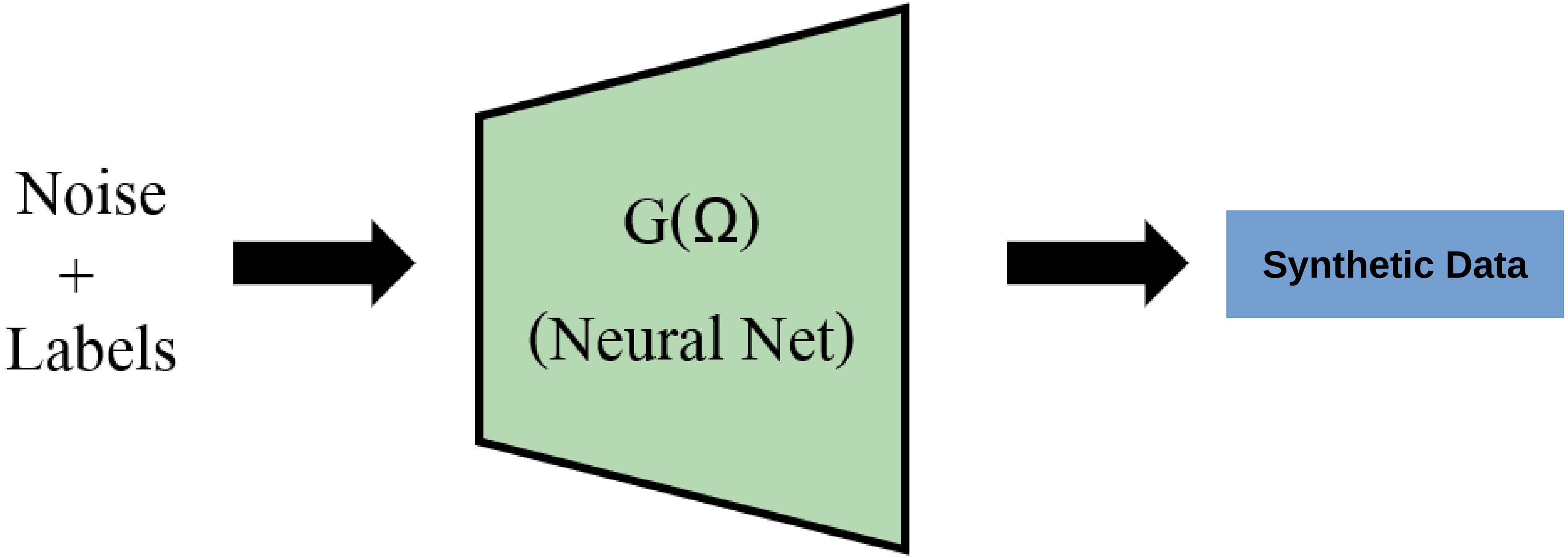
Deep Generative Models



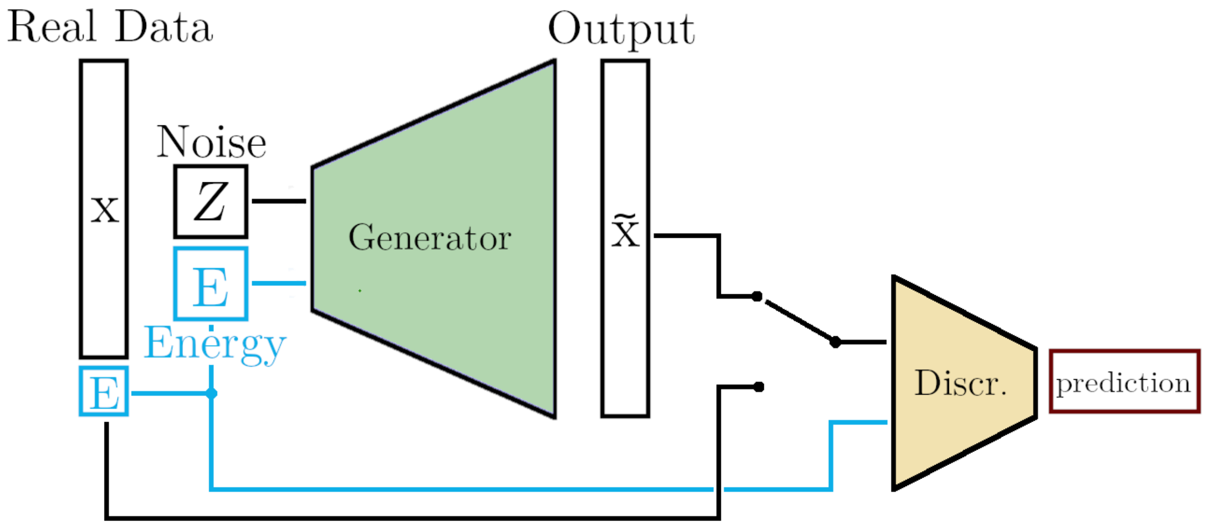
- Calorimeter simulation in HEP is CPU expensive!
- Promising solution for a **fast shower simulation**
  - Generate new samples by following the distribution of original data (i.e Geant4)
  - Map random noise to data
  - Conditioning



Recap: Generative Adversarial Neural Networks (GANs)

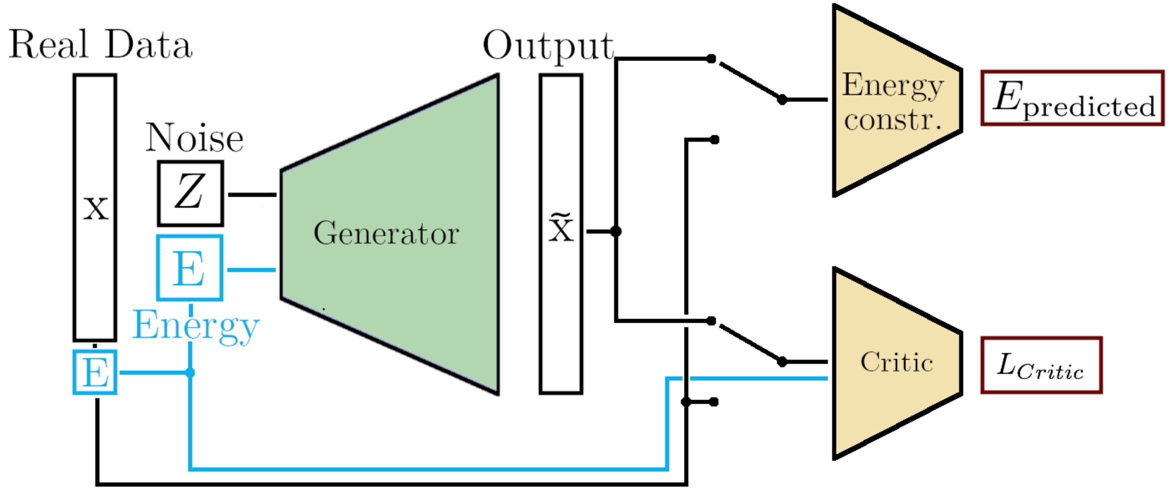
GAN

- First generative architecture used for simulating showers
- Discriminator tries to differentiate: Fake or Real ?
- Generator tries to fool the distriminator
- **New:** Apply mini-batch discrimination (pion)



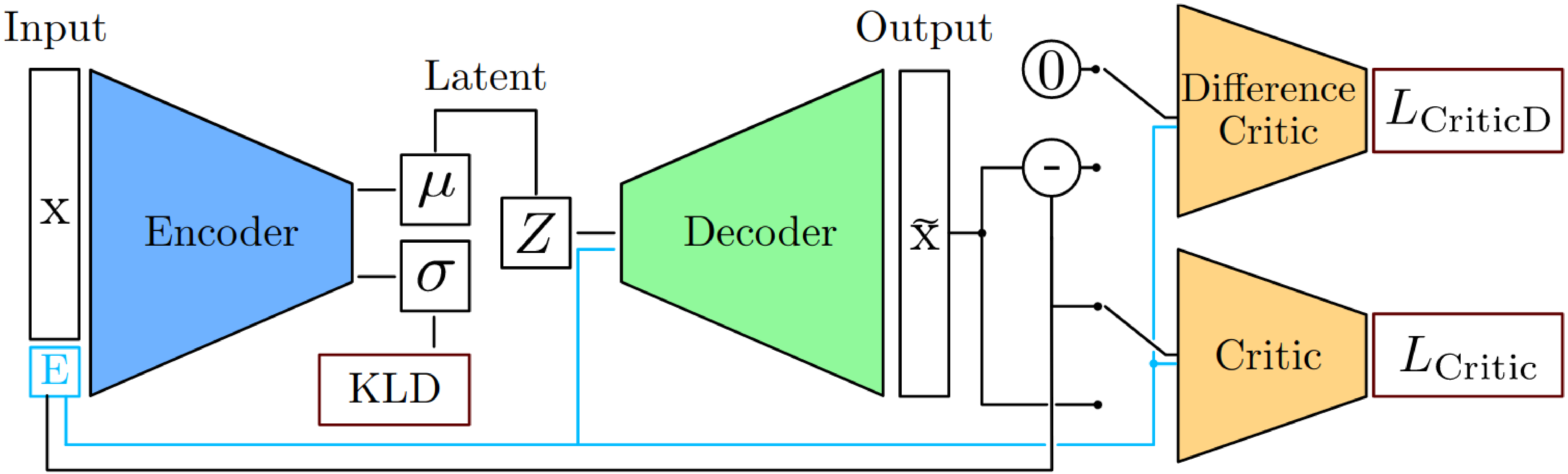
WGAN

- Alternative to classical GAN training:
  Helps improve the stability of the training
  Use Wasserstein-1 distance as a loss with gradient penalty
- Second network to constrain energy
- **New:** Latent optimization method (LO) is employed (pion)



Bounded-Information Bottleneck Autoencoder (BIB-AE)

- Unifies features of GANs and Autoencoders
- WGAN-like critics evaluate the quality of reconstructed images

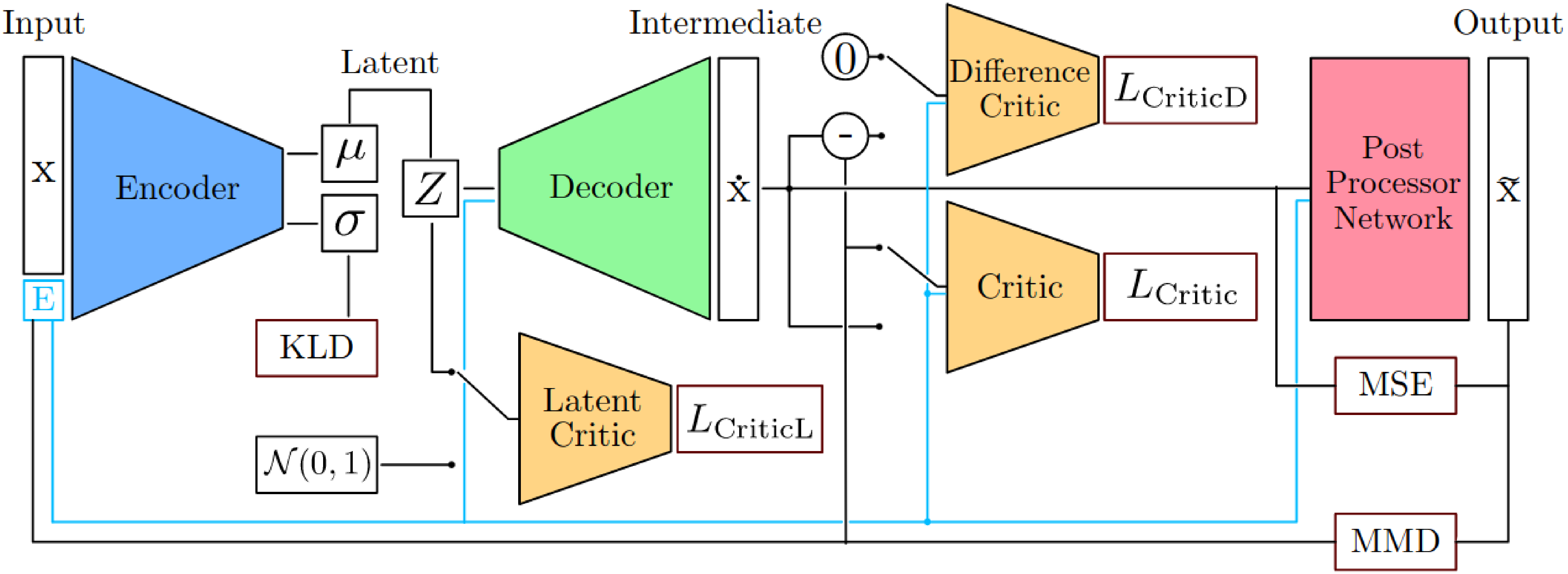


Buhmann, et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed.** Comput Softw Big Sci 5, 13 (2021)

Voloshynovskiy et al.: **Information bottleneck through variational glasses:** 1912.00830

Bounded-Information Bottleneck Autoencoder (BIB-AE)

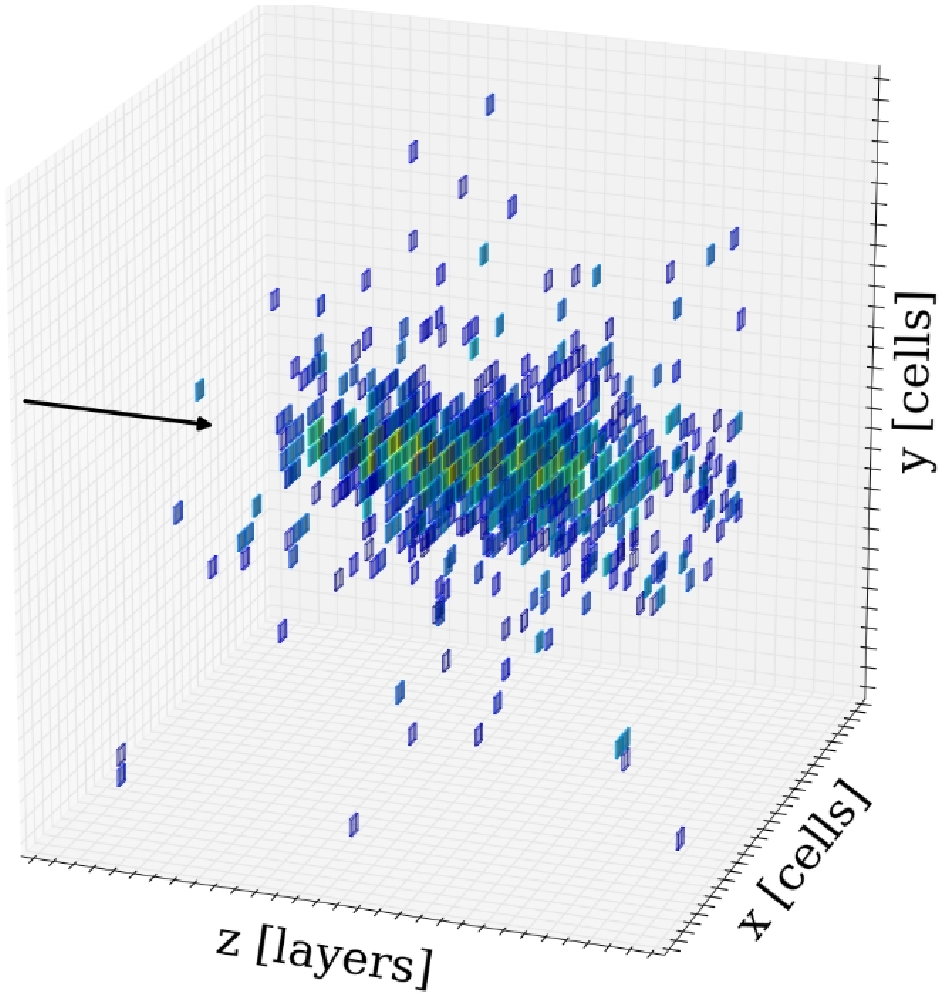
- Latent regularization is improved by an additional critic and a Maximum Mean Discrepancy (MMD) term
- Additional Post-Processor network, trained in a second step, is used to improved per-pixel energies
- **New**: Sampling from encoded latent space via multi-dimensional Kernel Density Estimation (KDE)
- **New**: Batch statistics involved in backward propagation



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

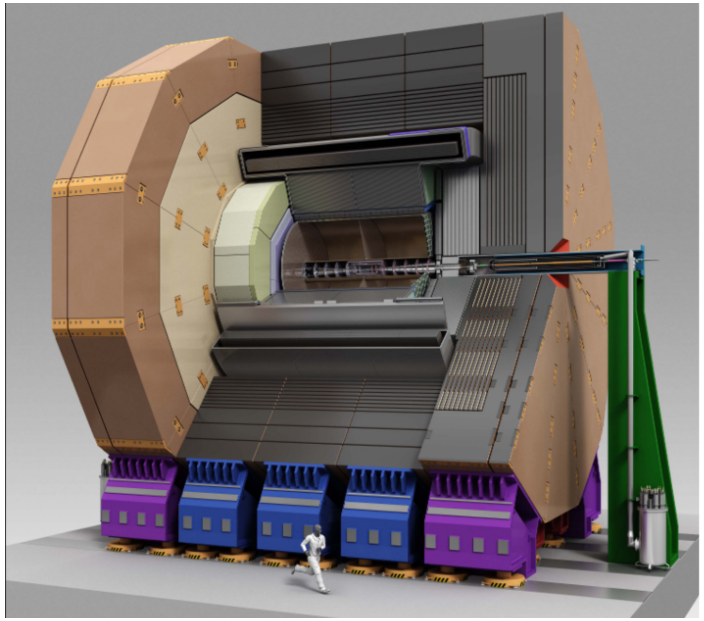
$$L_{\mathrm{Post}} = \mathrm{MMD} + \mathrm{MSE}$$

Photon Dataset



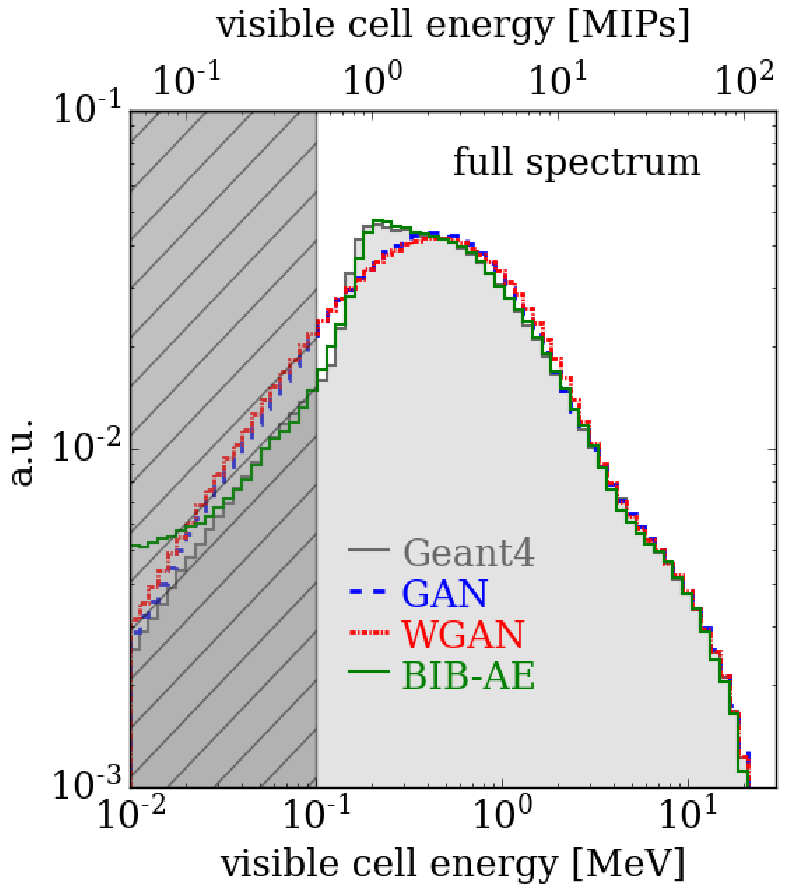
- 950k showers
- Fixed incident point and angle
- Uniform 10 GeV to 100 GeV
- 30x30x30 image

Highly Granular ECAL of ILD

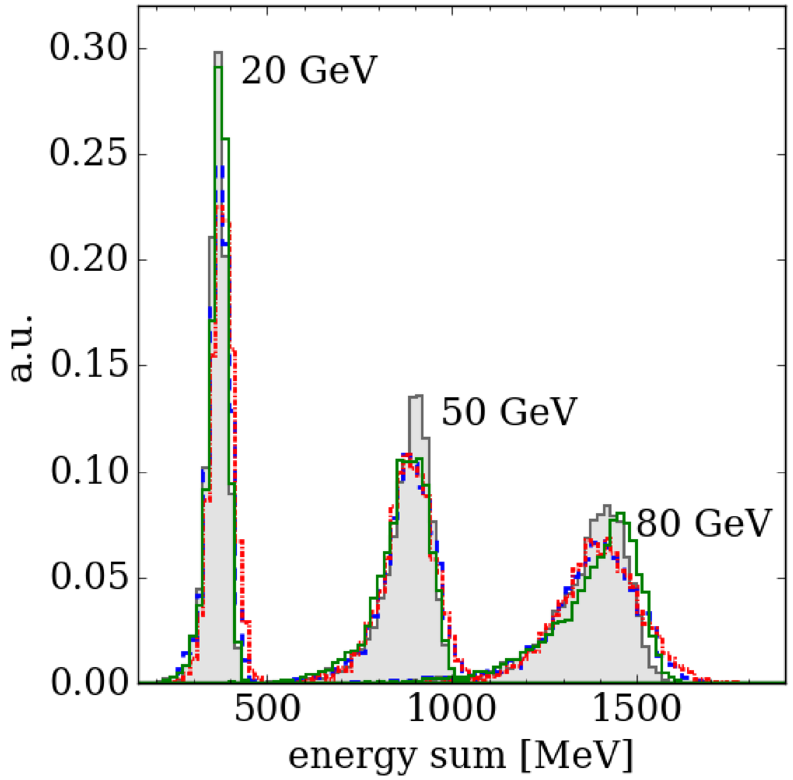


Zenodo Data Repository

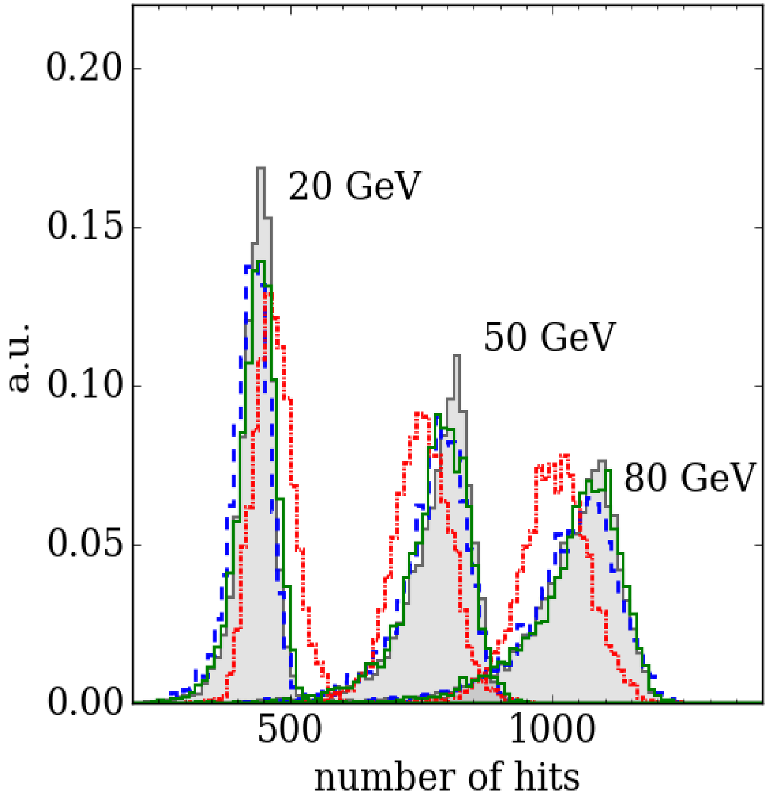
Photon Results



Very good agreement of MIP peak for BIB-AE with Post-Processing!

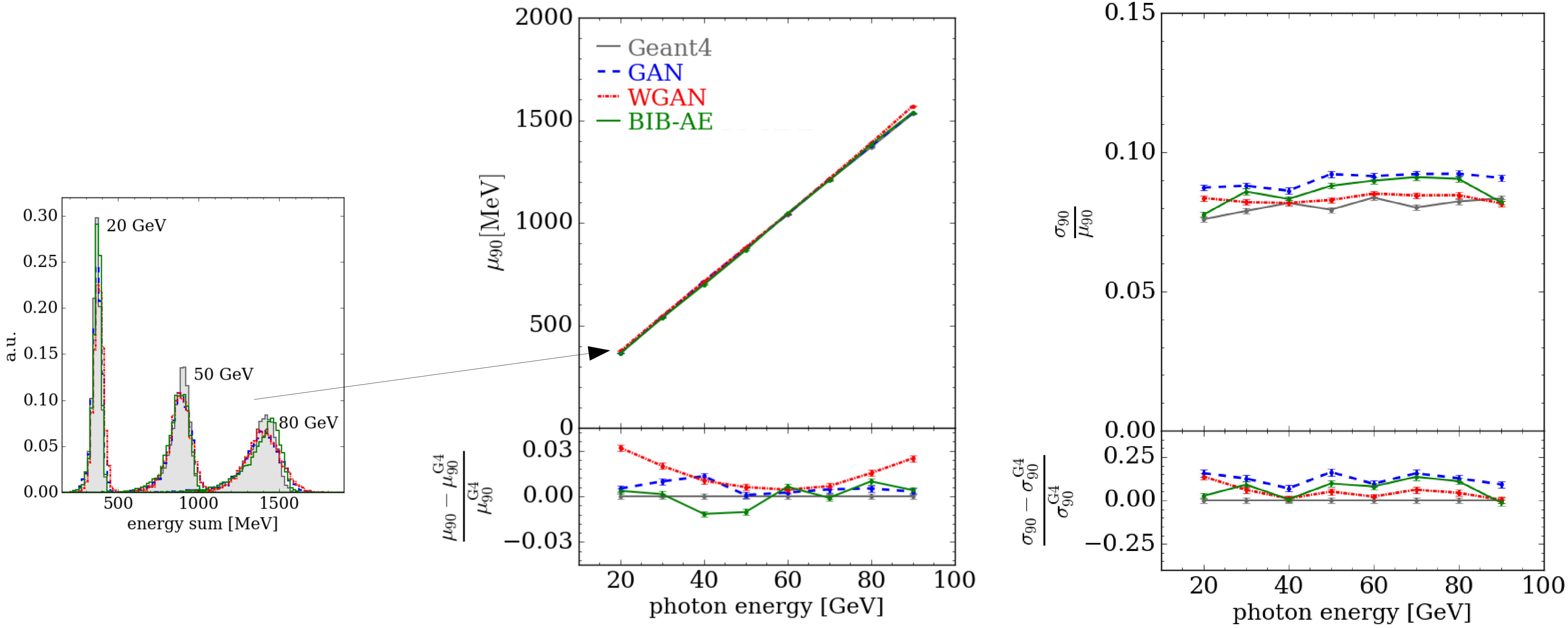


Peak and shape of the energy-sum is nicely reproduced by all models



BIB-AE and GAN correctly model number of hits

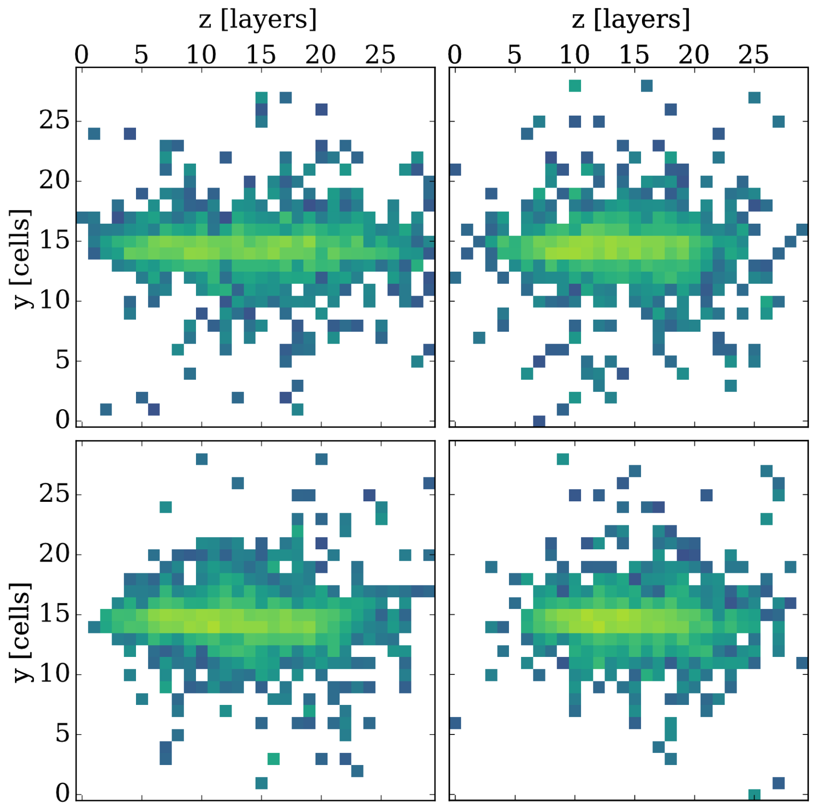
Linearity and Resolution*

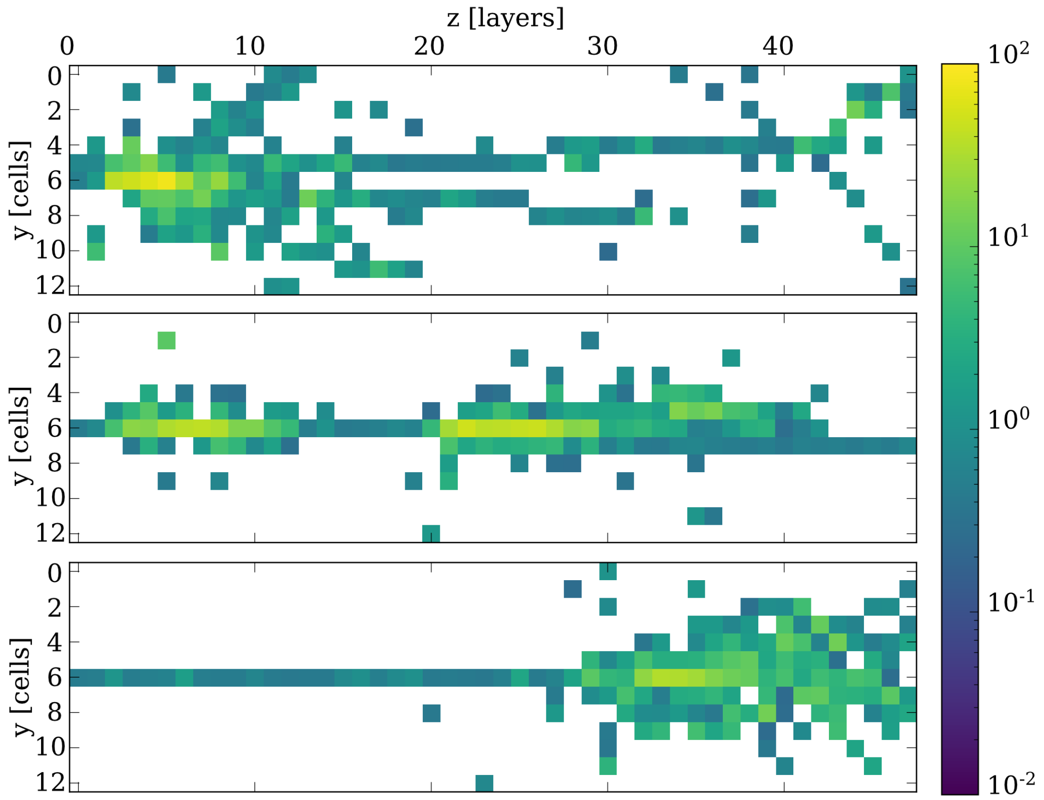


*not the actual ECAL resolution, no correction for sampling fraction variation performed

Hadron Showers

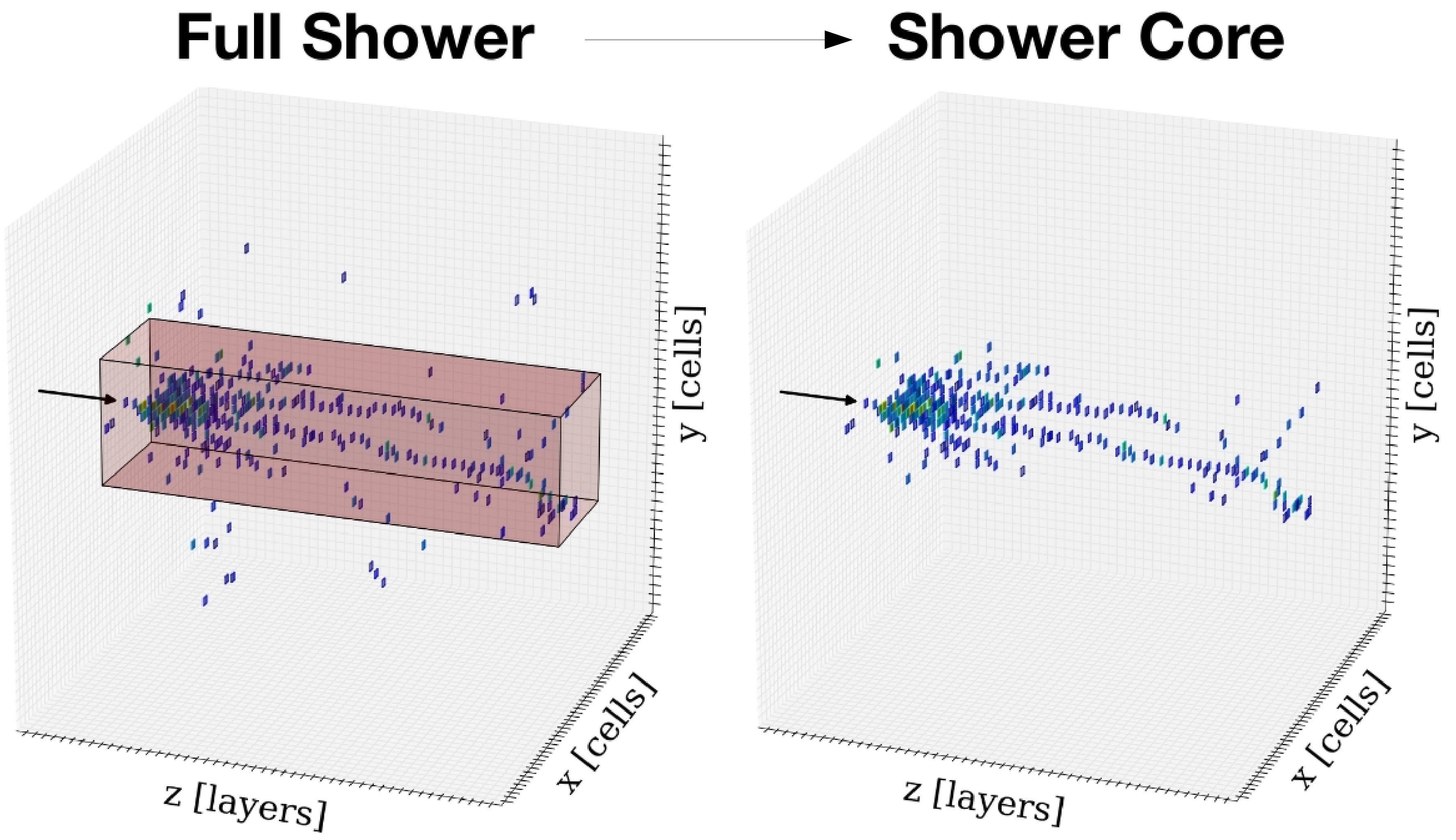
- Success for electromagnetic showers, now started to address hadronic (pion) showers:
  - Much more complex shower structure
  - Currently training with a smaller 3D image containing the active area (i.e shower core)
  - Started with GAN, WGAN, BIB-AE and alternatives





photon showers **vs.** **pion showers**

Pion Dataset



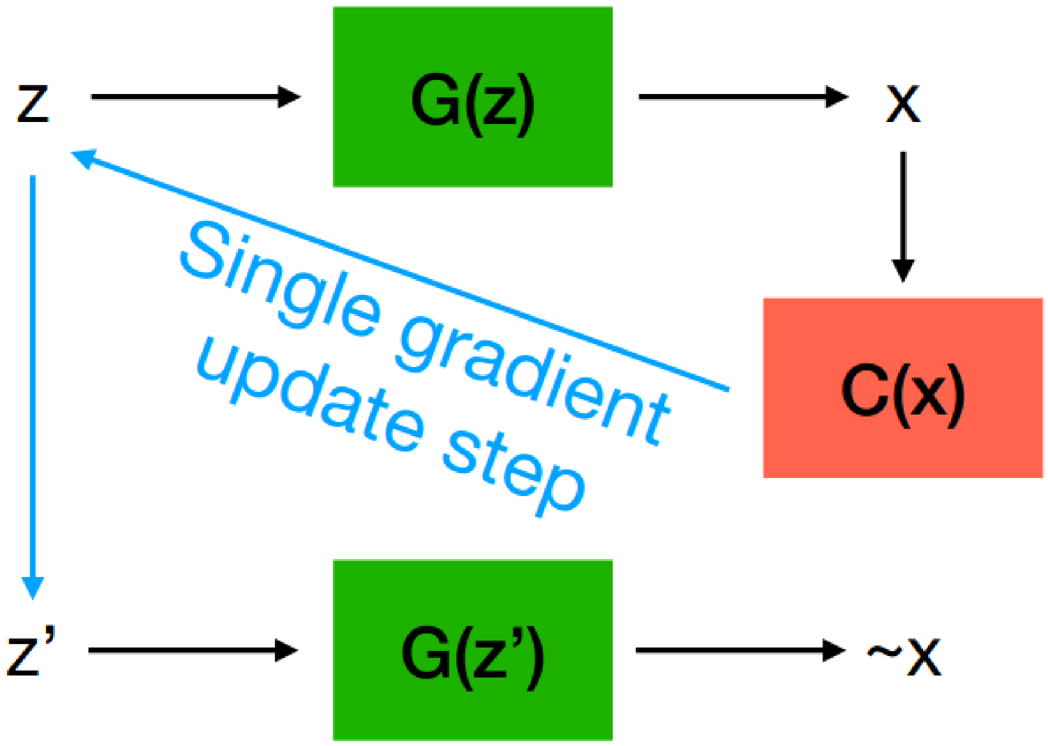
48x48x48 **48x13x13**

- 500k showers
- Fixed incident point and angle
- Uniform 10 GeV to 100 GeV

Latent Optimized WGAN

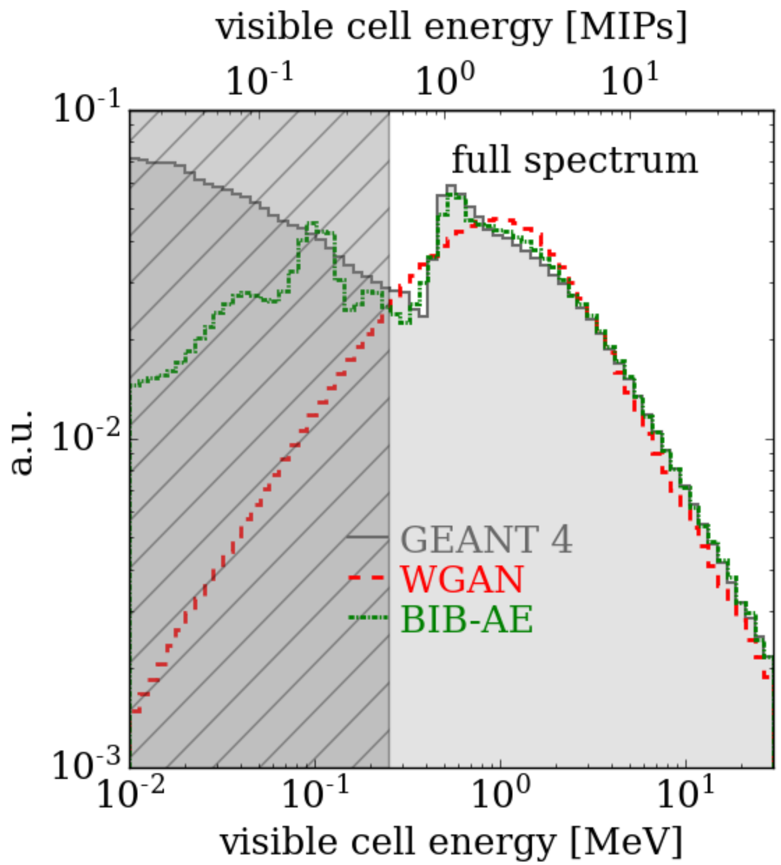
Standard WGAN

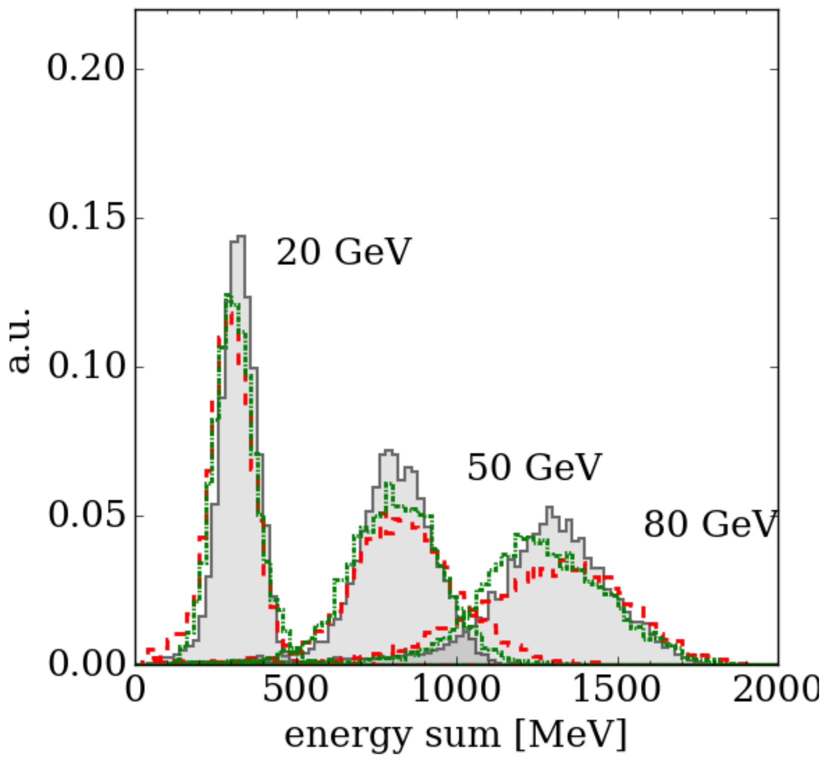
Latent Optimisation

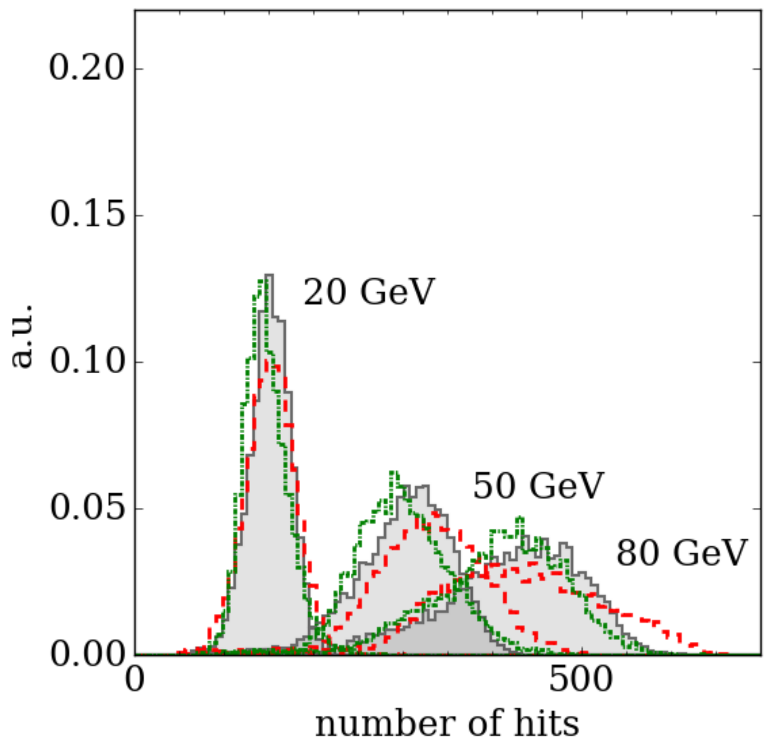


Wu et al.: **LOGAN: Latent Optimisation for Generative Adversarial Networks** 1912.00953

Pion Shower Results I



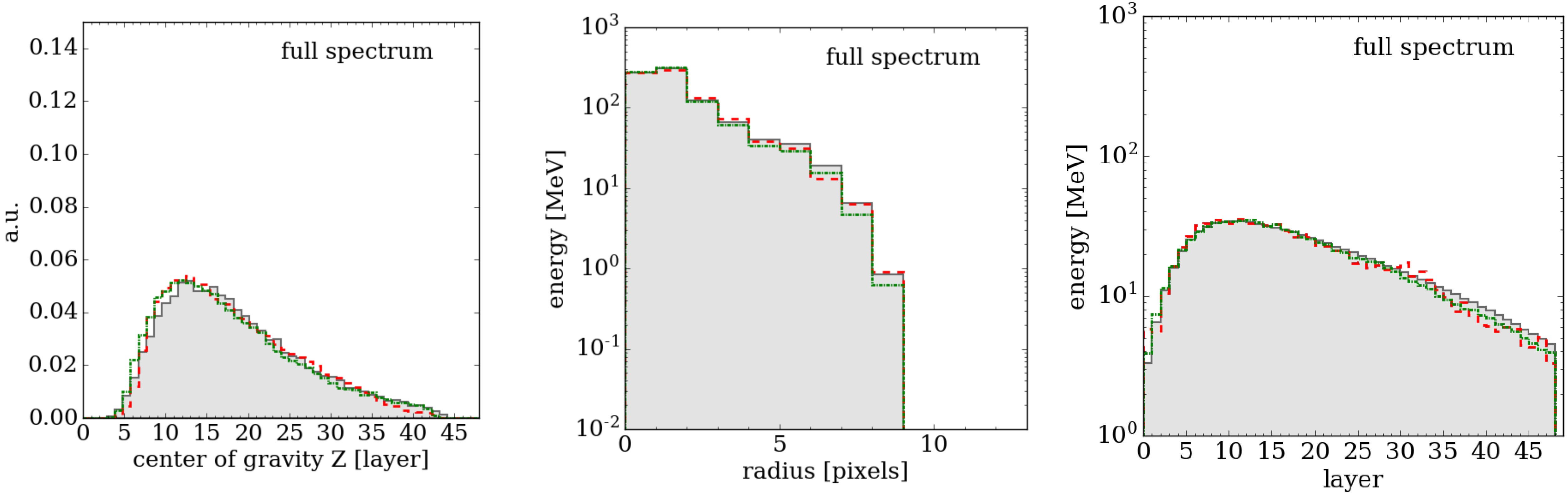




Very good agreement of MIP peak for BIB-AE with Post-Processing!

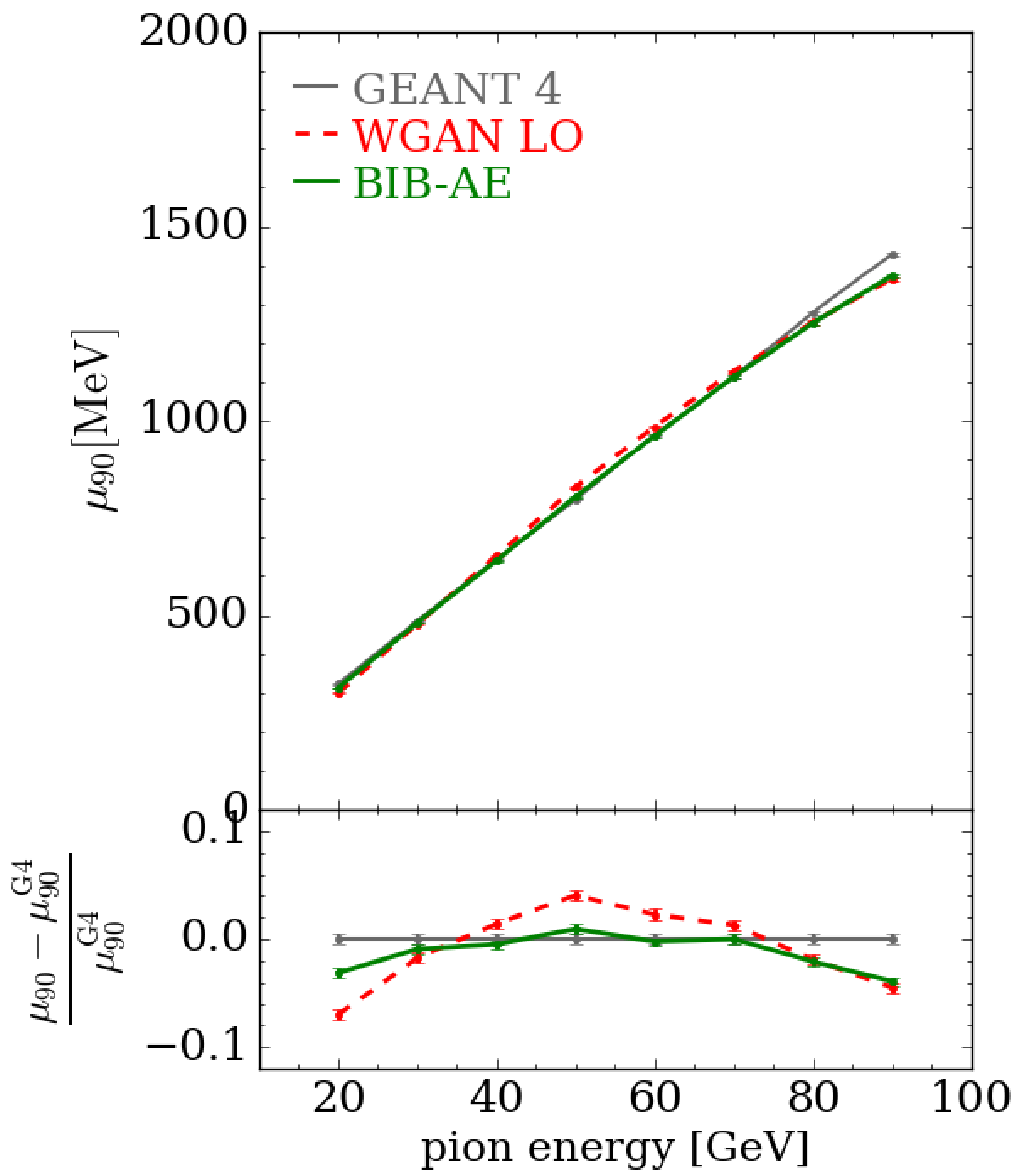
Overall good agreement with Geant4, still room for improvement

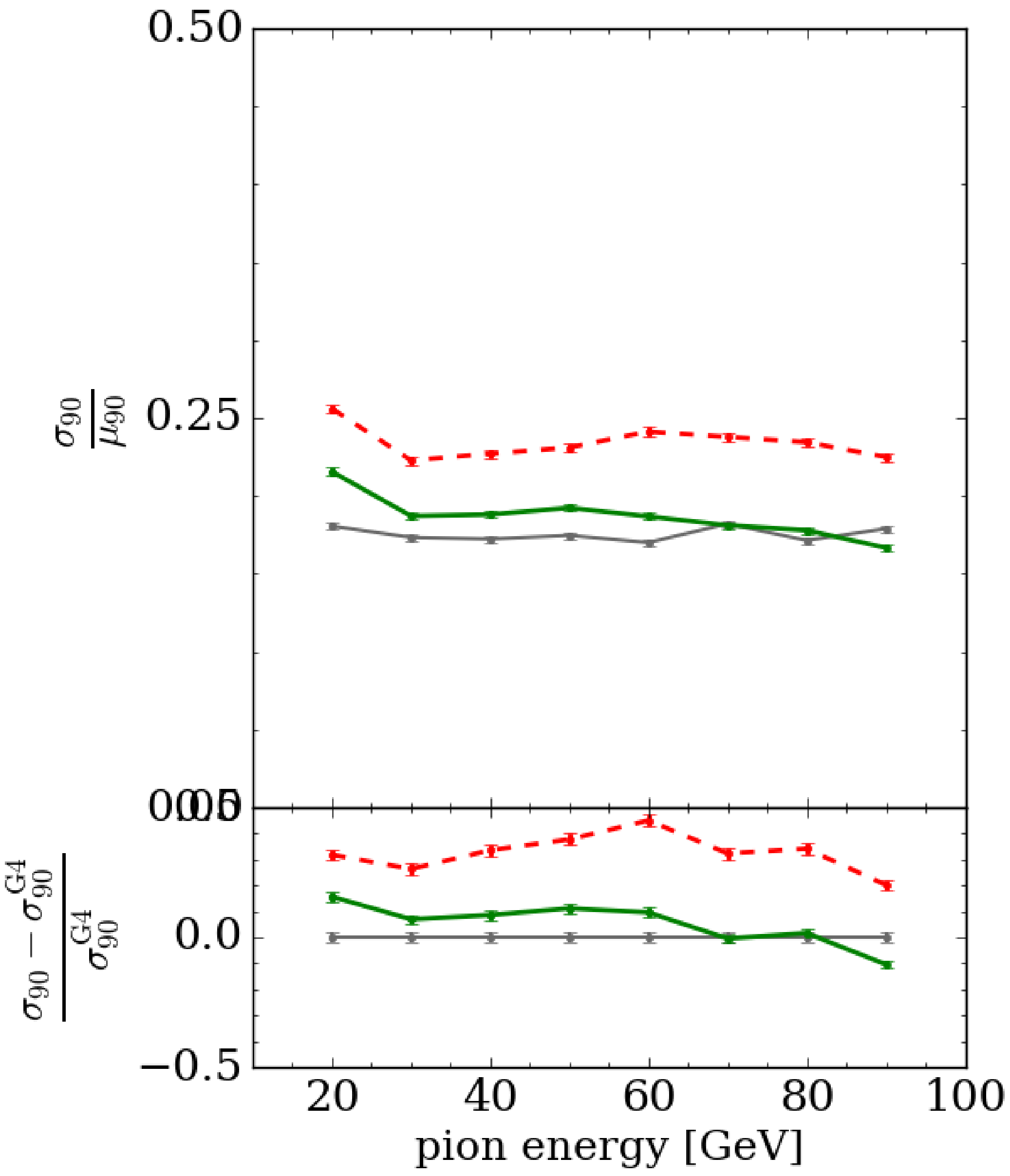
Pion Shower Results II



Both WGAN and BIB-AE fairly reproduces bulk of Geant4 distributions

Linearity and Resolution





Computation Time

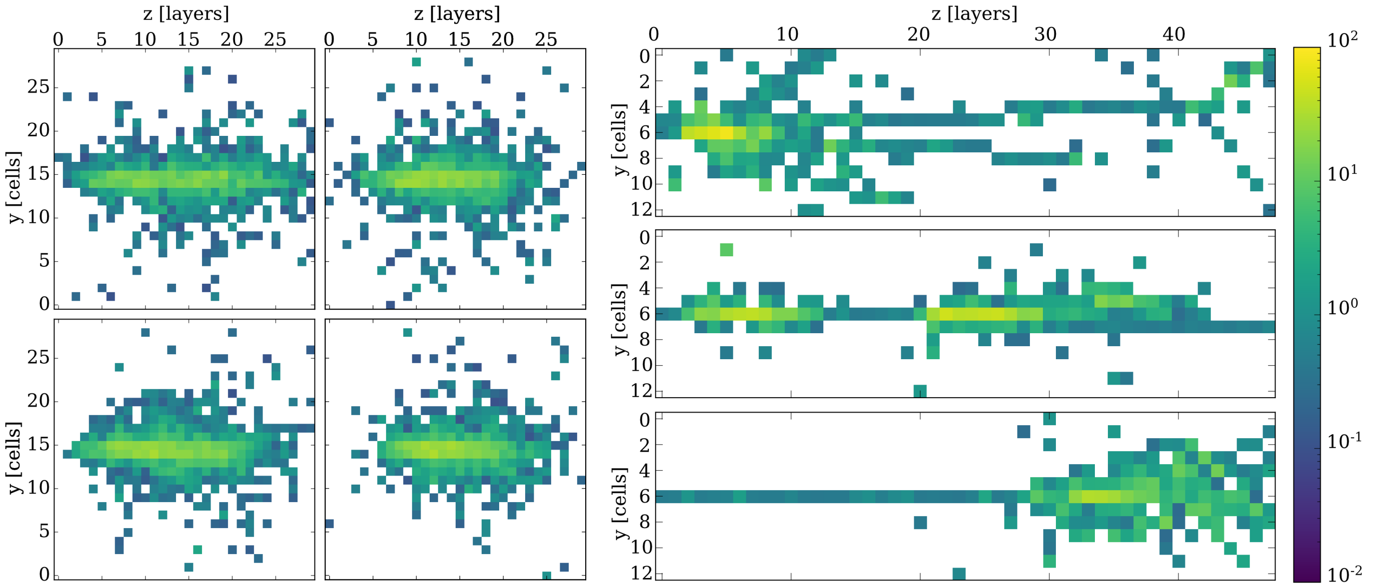
Hardware	Simulator	Photons		Pions	
		Time/shower[ms]	Speed-up	Time/shower[ms]	Speed-up
CPU	Geant4	4082±170	×1	2684±125	×1
	WGAN	61.44±0.03	×66	195.67±0.56	×14
	BIB-AE	95.98±0.08	×43	36.05±0.82	×74
GPU	WGAN	3.93±0.03	×1039	2.695±0.004	×996
	BIB-AE	1.60±0.03	×2551	1.101±0.004	×2438

We observe speed-ups of three orders of magnitude

Conclusions and Outlook

Application of generative models to high resolution EM and hadronic showers simulation

- ✔ Modelling of MIP peak and achieving high fidelity
- ✔ Speed-up: 3 orders of magnitude



Architectures and extensions:

- GAN (+ Mini-Batch discr.)
- WGAN (+ Latent Opt.)
- BIB-AE (+ KDE sampl. + Mini-Batch discr.)

Future plans:

- Condition on incident position / angle
- More focus on hadron showers and full size-showers
- Integrate into existing tools / frameworks

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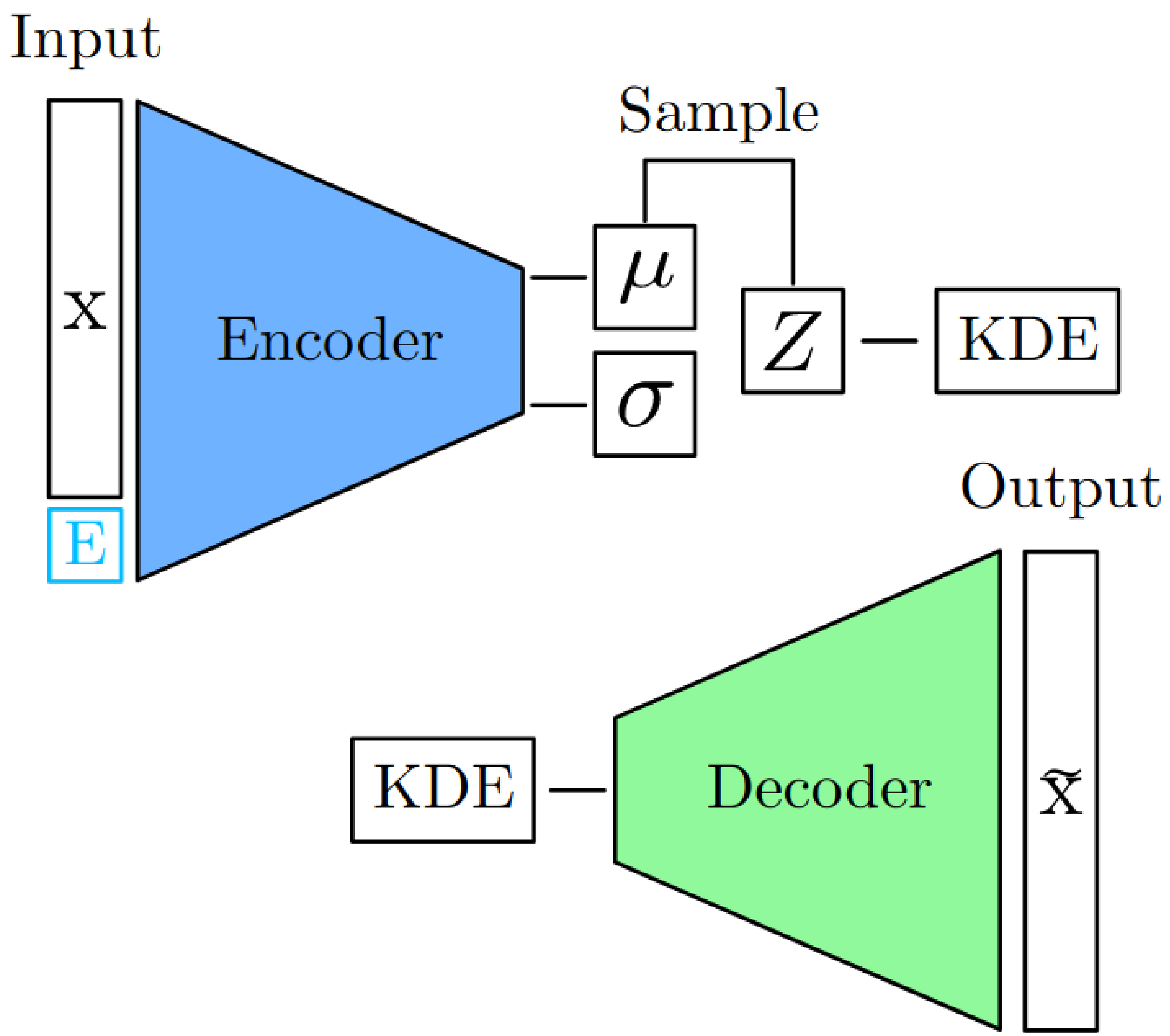
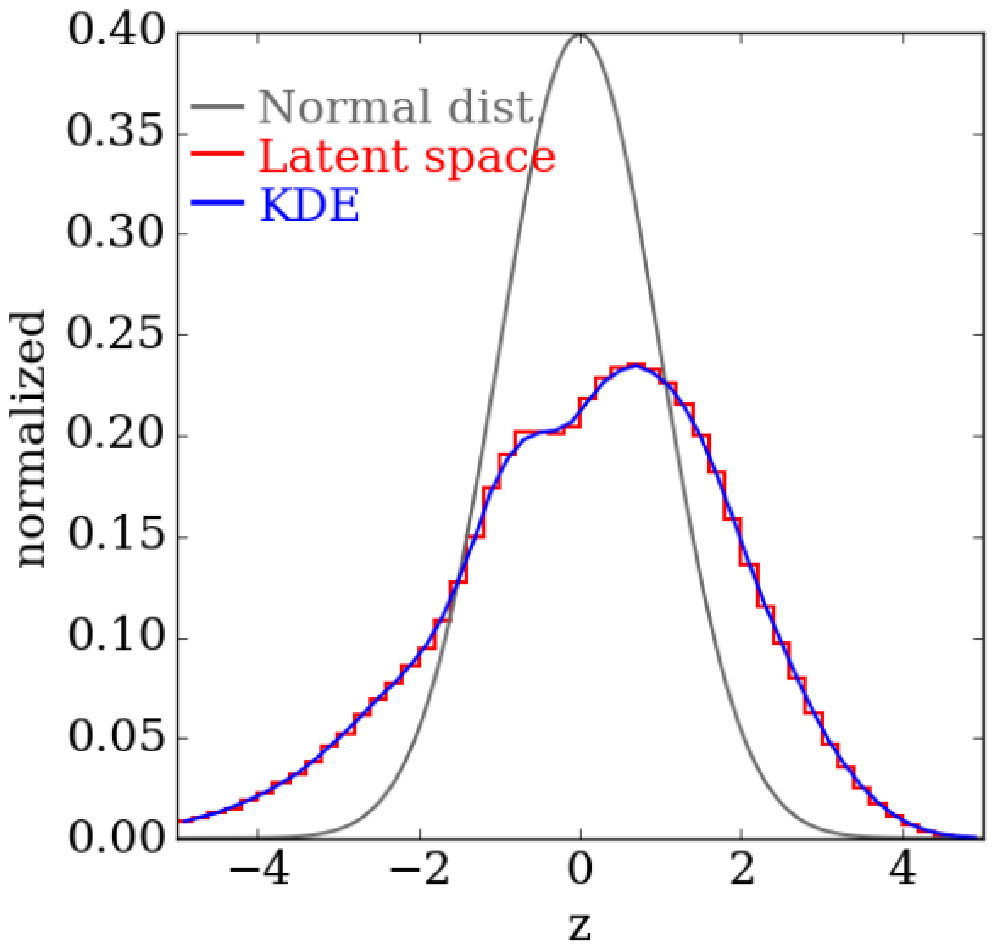
Thank you

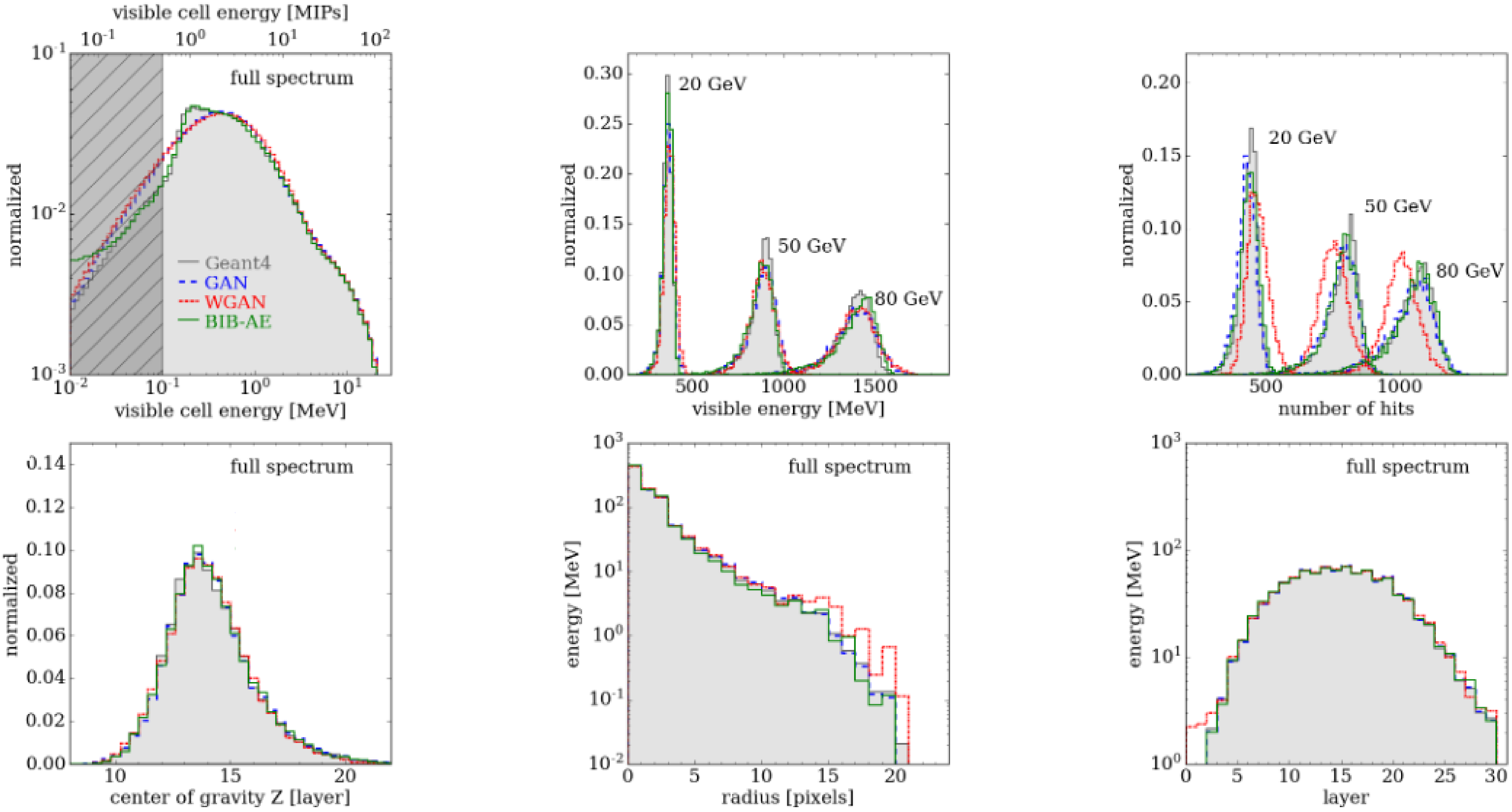
Kernel Density Estimation BIB-AE





Buhmann et. al. **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network:** 2102.12491

Photon all



visible cell energy [MIPs]
full spectrum
Geant4
GAN
WGAN
BIB-AE
normalized
visible cell energy [MeV]
20 GeV
50 GeV
80 GeV
visible energy [MeV]
number of hits
center of gravity Z [layer]
energy [MeV]
radius [pixels]
layer

Correlations (Pion)

GEANT4 - BIB-AE PP KDE

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.06	0.00										
$m_{1,z}$	0.00	-0.02	0.00									
$m_{2,x}$	-0.06	-0.00	-0.04	0.00								
$m_{2,y}$	-0.01	0.11	-0.03	-0.04	0.00							
$m_{2,z}$	0.00	0.04	-0.11	-0.04	-0.05	0.00						
E_{vis}	0.02	-0.02	-0.02	0.02	-0.00	-0.01	0.00					
E_{inc}	0.01	0.01	-0.02	0.08	0.04	-0.03	0.01	0.00				
n_{hit}	0.04	0.03	-0.02	0.08	0.02	-0.02	0.00	0.01	0.00			
E_1/E_{vis}	-0.00	0.04	0.00	0.02	0.01	0.09	0.02	0.01	0.02	0.00		
E_2/E_{vis}	-0.00	-0.05	-0.03	0.03	0.03	-0.03	-0.01	-0.01	-0.01	0.02	0.00	
E_3/E_{vis}	0.00	0.00	0.01	-0.06	-0.05	-0.11	-0.01	-0.01	-0.01	-0.01	-0.02	0.00

GEANT4 - WGAN LO

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.17	0.00										
$m_{1,z}$	0.01	-0.12	0.00									
$m_{2,x}$	0.07	0.07	-0.14	0.00								
$m_{2,y}$	-0.07	0.05	-0.23	-0.02	0.00							
$m_{2,z}$	-0.07	0.04	-0.08	0.02	-0.06	0.00						
E_{vis}	-0.01	0.11	0.05	0.11	0.12	0.06	0.00					
E_{inc}	-0.00	0.19	0.04	0.03	0.01	0.03	0.06	0.00				
n_{hit}	-0.02	0.08	-0.01	0.23	0.23	0.14	-0.02	0.05	0.00			
E_1/E_{vis}	-0.01	0.12	0.01	0.12	0.17	0.06	-0.06	-0.06	0.00	0.00		
E_2/E_{vis}	-0.02	-0.08	-0.09	-0.02	-0.01	-0.03	0.06	0.05	0.00	0.05	0.00	
E_3/E_{vis}	0.02	-0.10	0.00	-0.14	-0.24	-0.09	0.02	0.01	-0.01	0.02	-0.10	0.00