

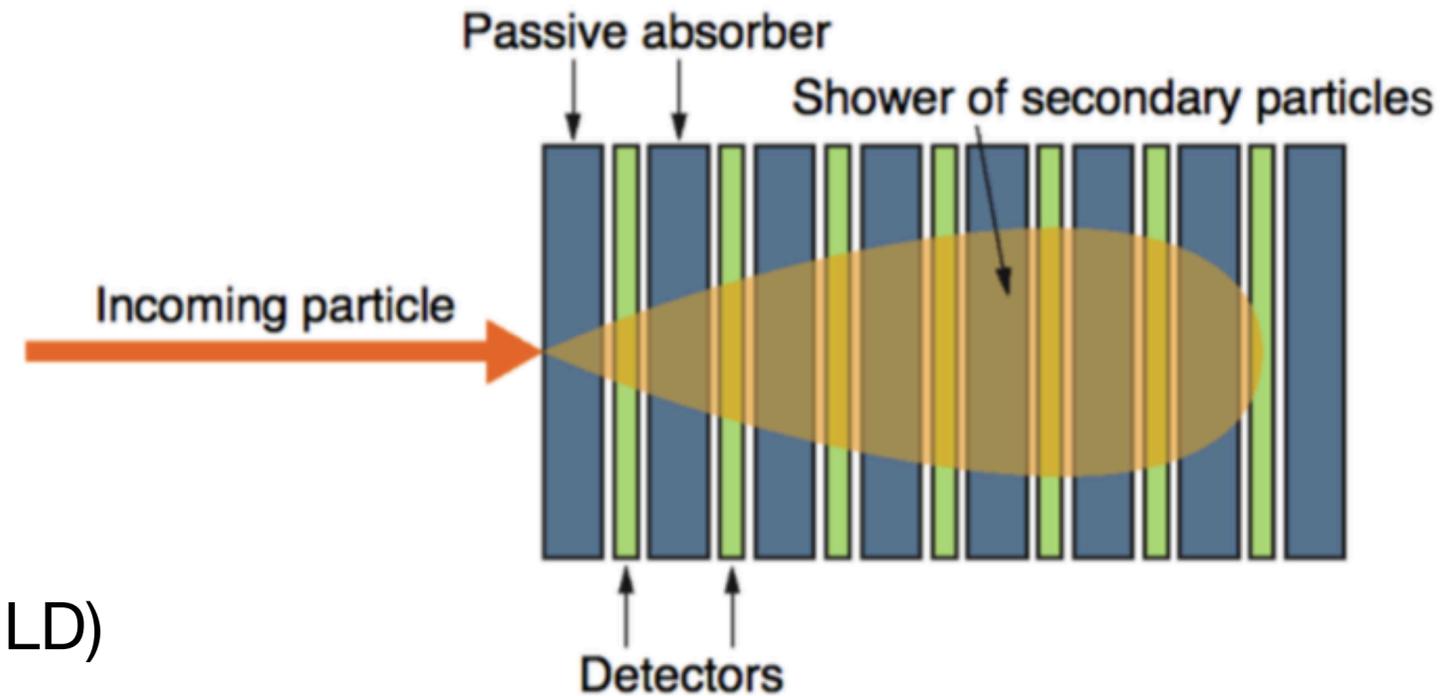
# Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network

Erik Buhmann\*

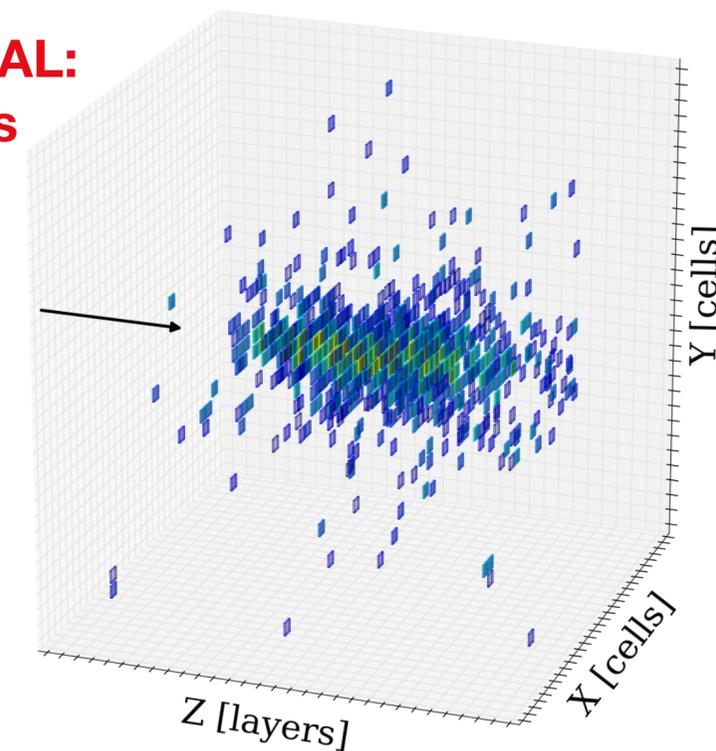
*with* Sascha Diefenbacher, Engin Eren, Frank Gaede,  
Gregor Kasieczka, Anatolii Korol, and Katja Krüger

arXiv: 2102.12491

# Fast Simulation of Particle Showers in Calorimeters



**highly granular ECAL:  
30 x 30 x 30 cells**

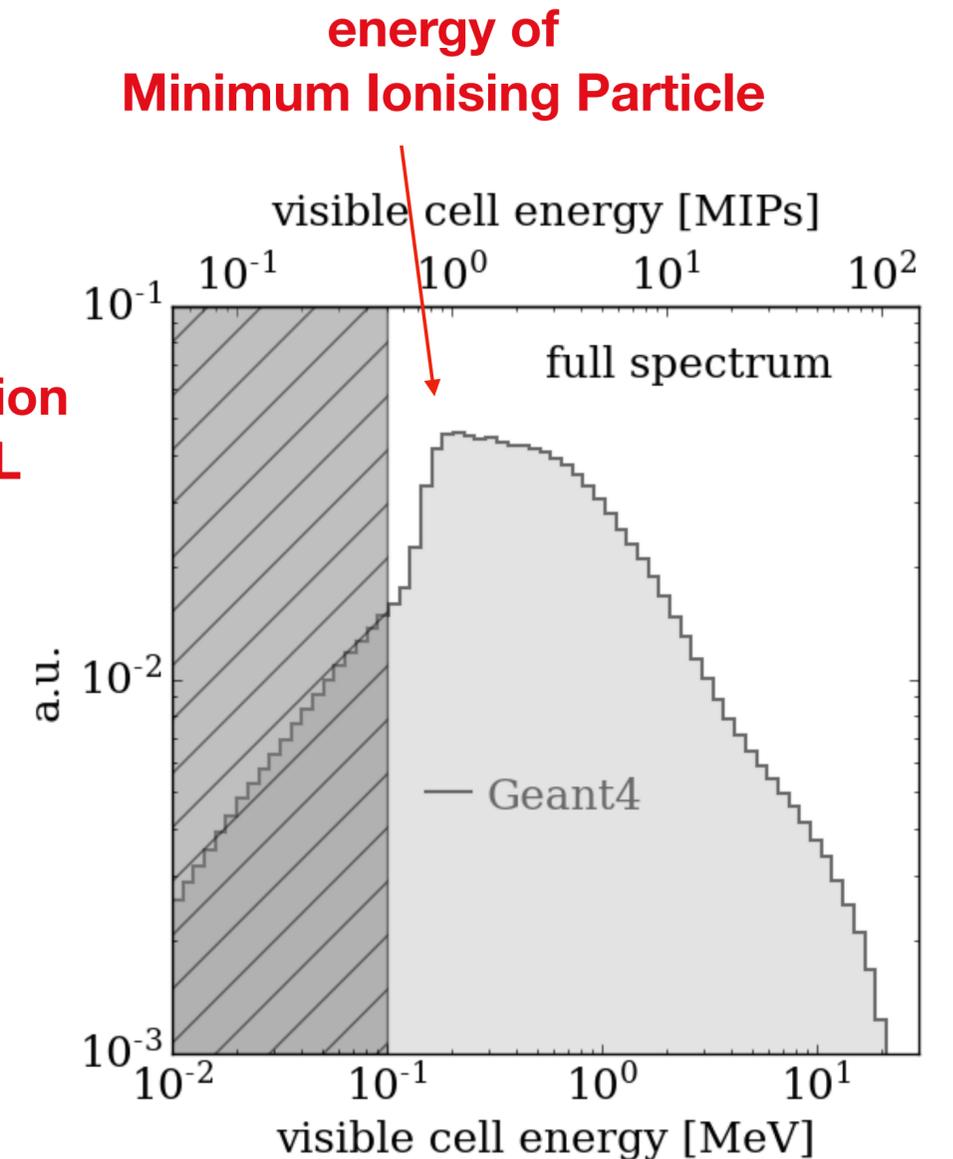
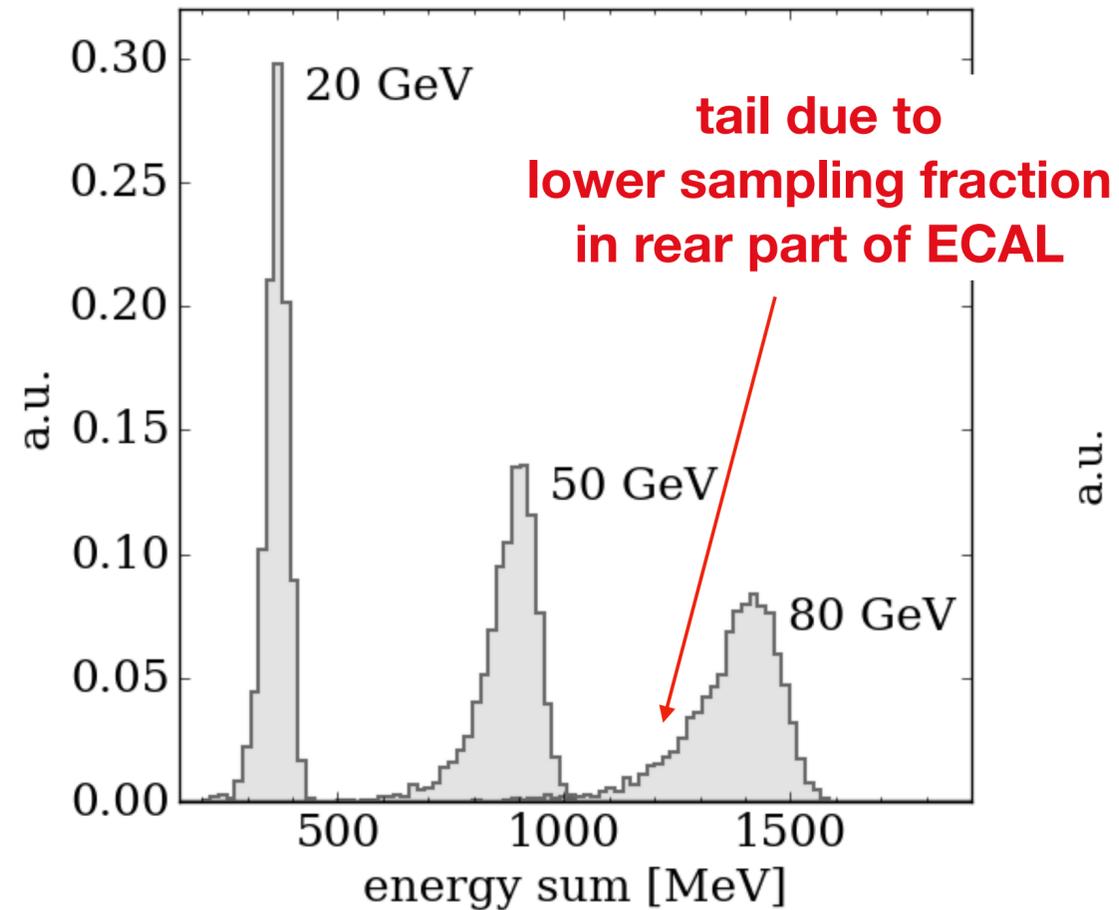
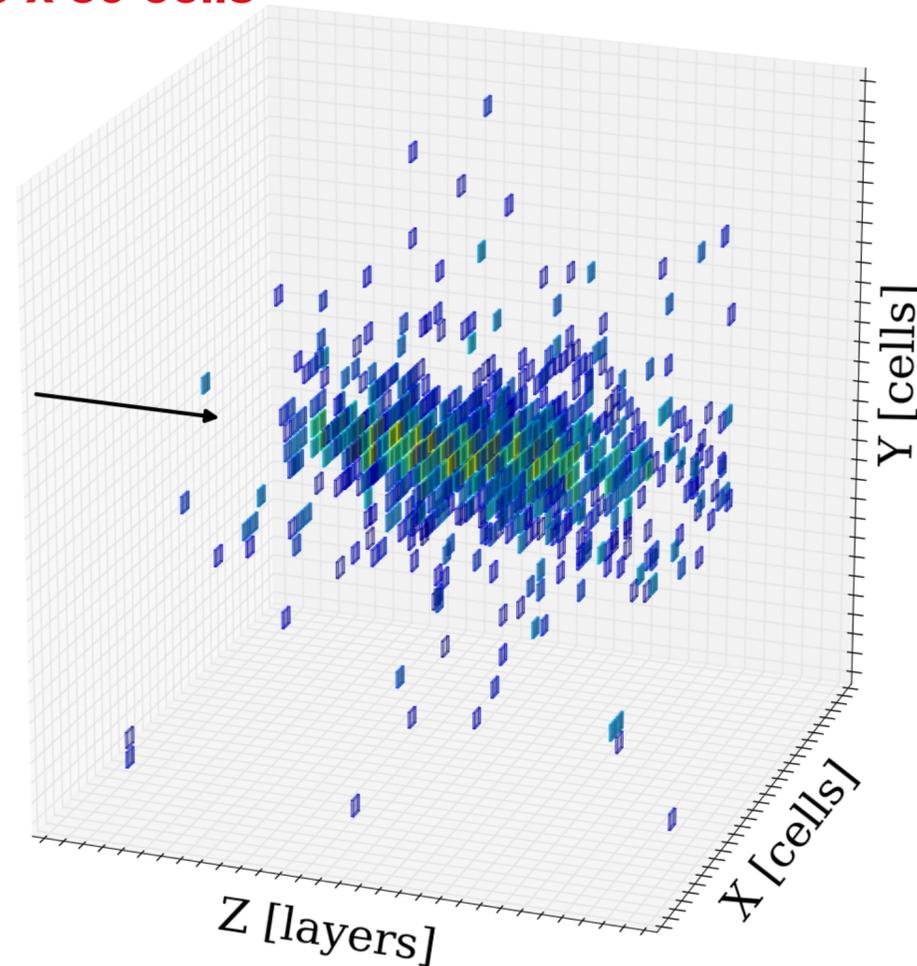


- Photons entering Electromagnetic Calorimeter (ECAL)
  - Electromagnetic particle cascade = particle shower
- Geant4 simulation of ECAL of International Large Detector (ILD)
  - For proposed International Linear Collider (ILC)
  - Highly granular SiW calorimeter optimised for Particle Flow
- Large-scale Geant4 simulations computationally expensive
  - Promising idea: Augment with Generative Neural Networks (VAEs, GANs)
  - Training statistics 950k samples → Generative model amplifies statistic\*

\* Butter et al.: *Amplifying Statistics using Generative Models*: NeurIPS ML4PS 2020

# Challenges of Generating Particle Showers: Individual Showers & Global Distributions

highly granular ECAL:  
30 x 30 x 30 cells



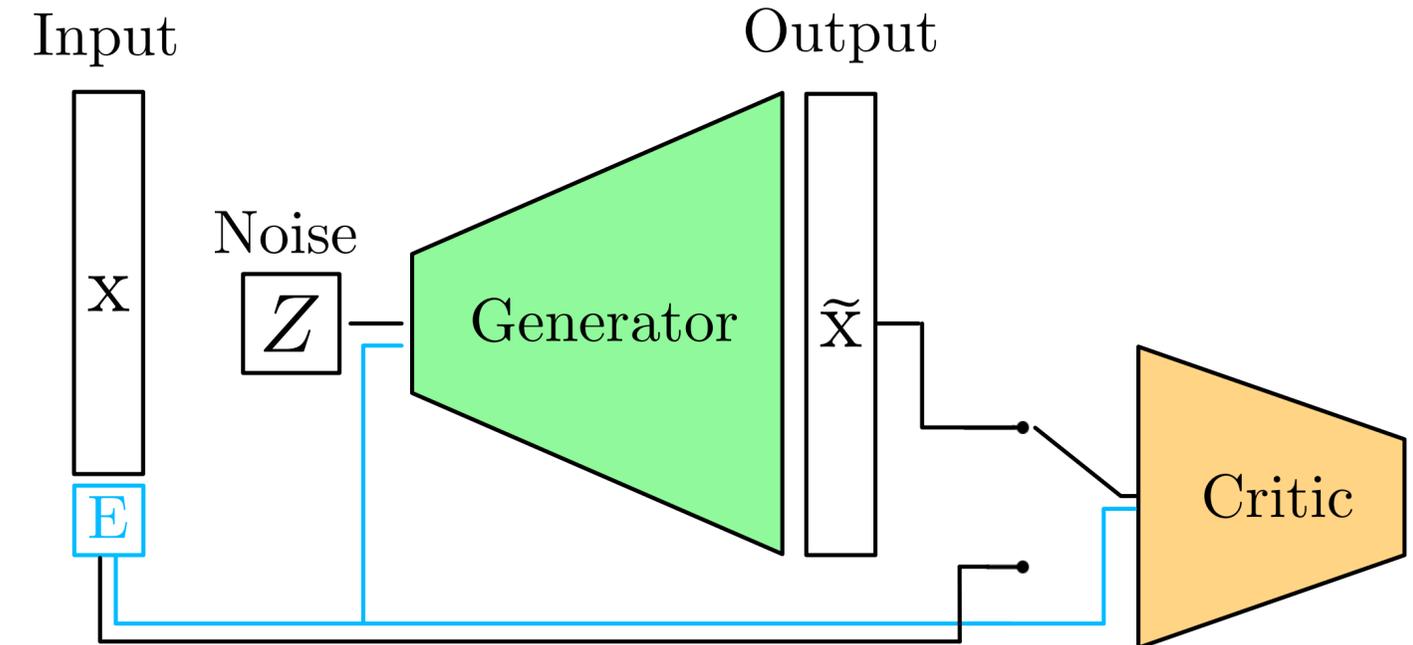
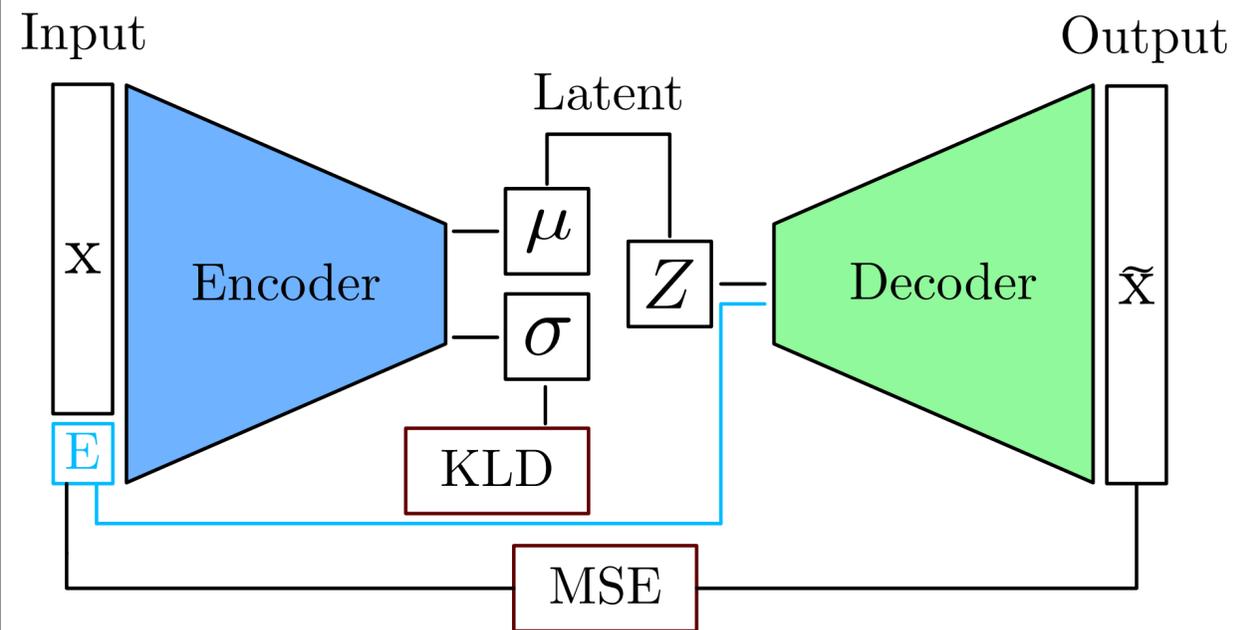
- Accurate shower feature representation in 3D necessary
- Many global distributions: total energy, cell energy, center of gravity, ...

# Generative Models: VAEs and GANs

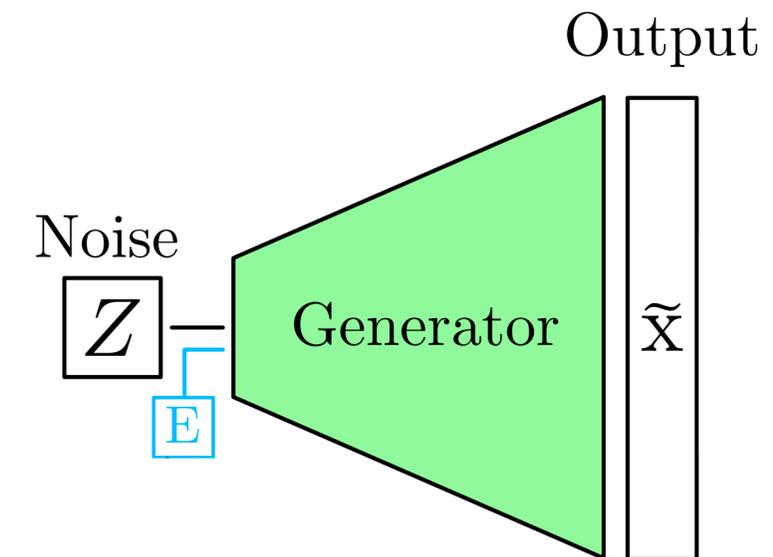
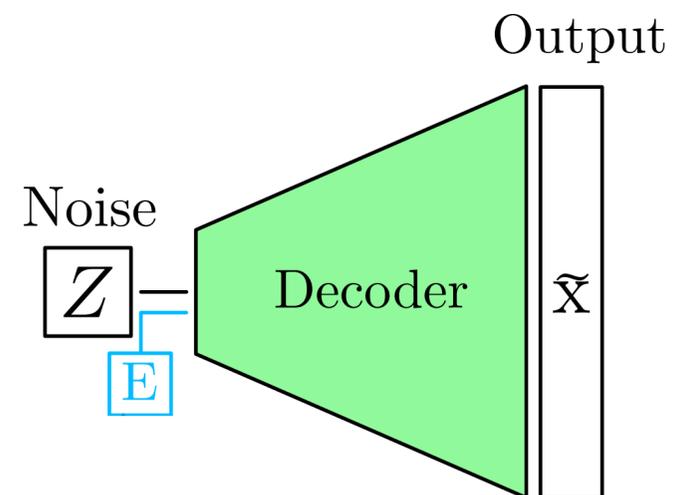
## Variational Autoencoder (VAE)

## Generative Adversarial Network (GAN)

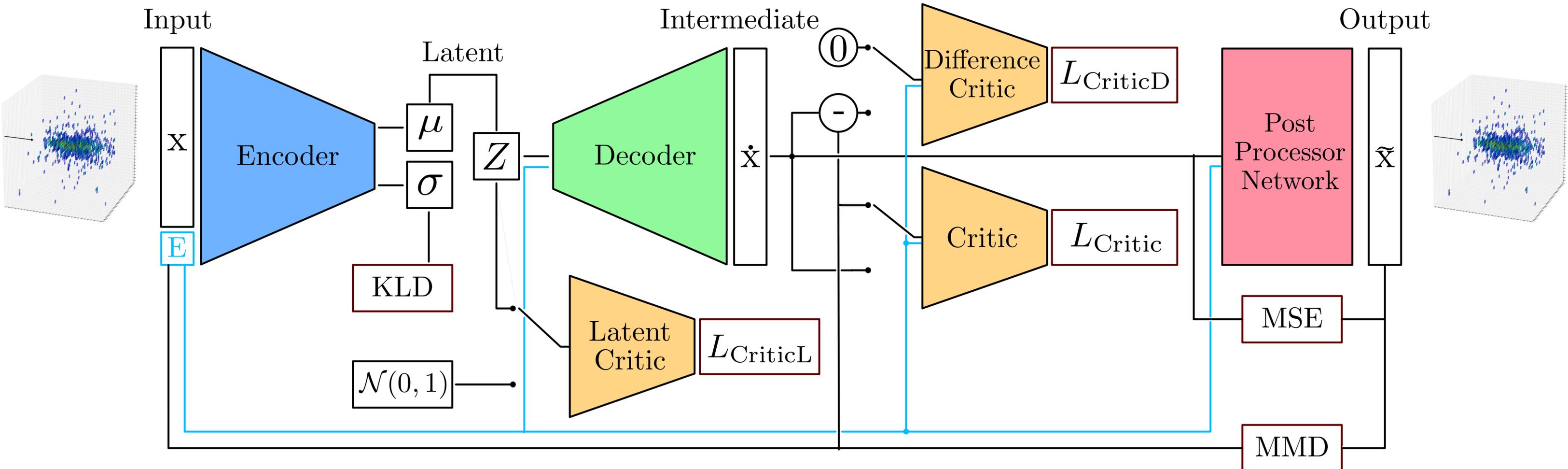
**Training:**



**Generation:**



# Bounded Information Bottleneck Autoencoder (BIB-AE)

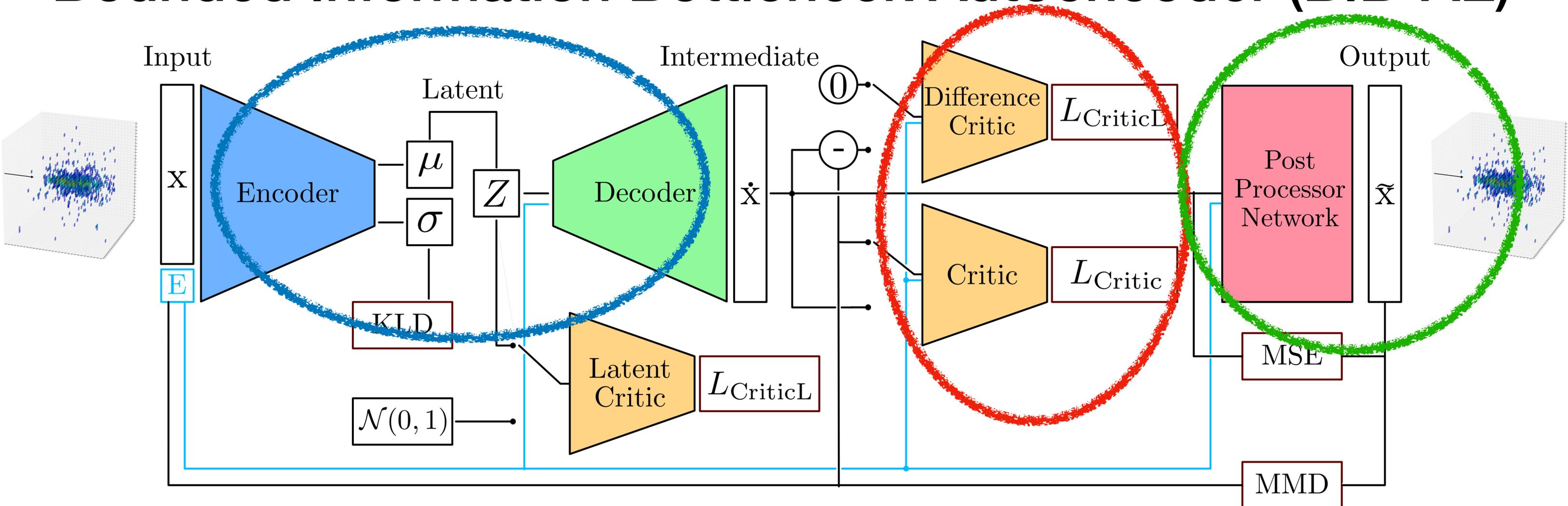


$$L_{\text{BIB-AE}} = \text{KLD} + L_{\text{CriticL}} + L_{\text{Critic}} + L_{\text{CriticD}}$$

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

- Advanced generative architecture inspired by [arXiv:1912.00830](https://arxiv.org/abs/1912.00830) [CS]
- Combination of **VAE**, **GAN**, and a **Post Processor network** (among others)
- ~ 70 million trainable parameters (Decoder about 35M)

# Bounded Information Bottleneck Autoencoder (BIB-AE)

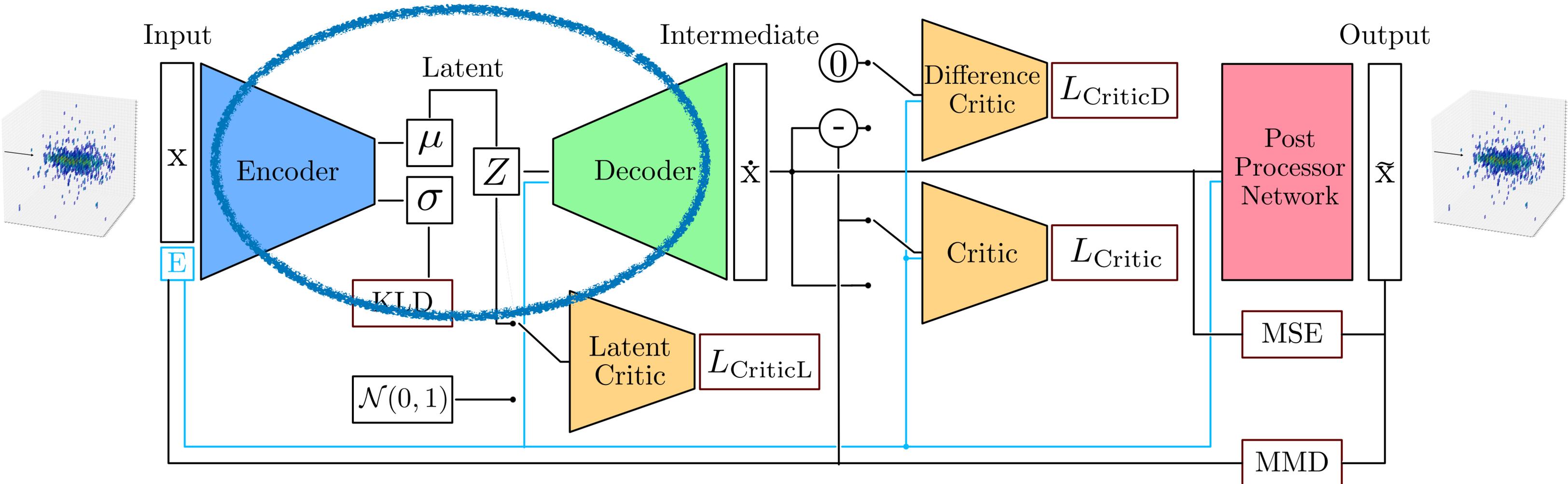


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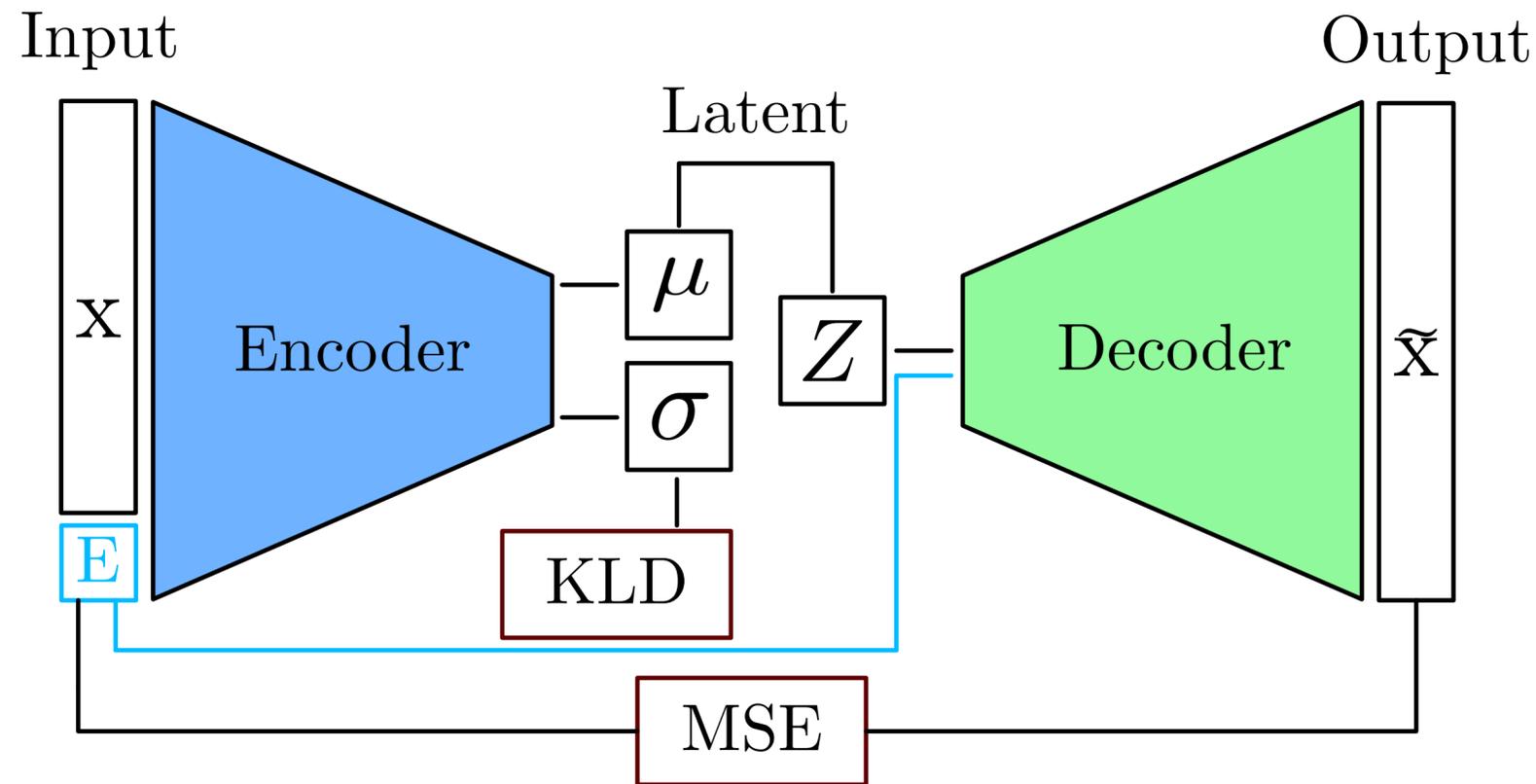


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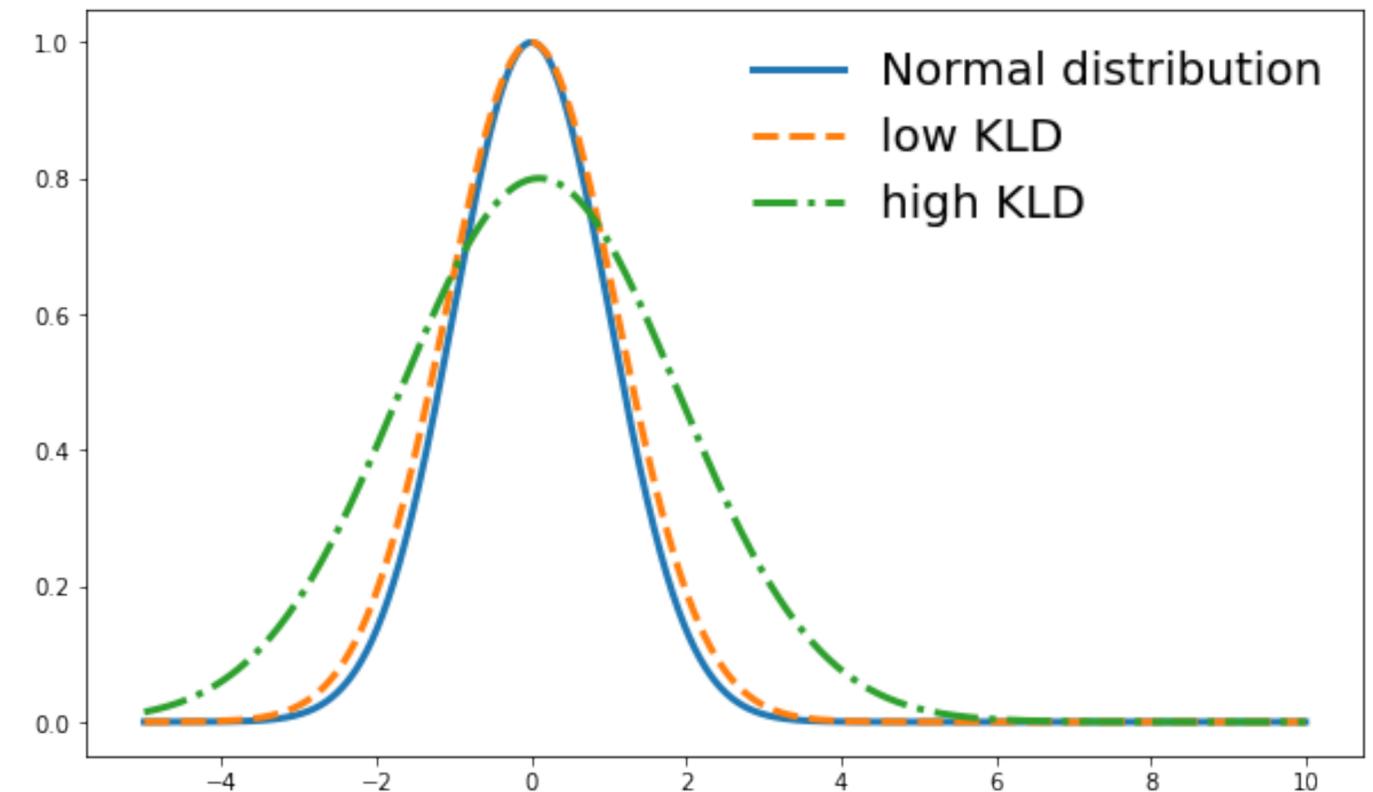
# Variational Autoencoder & Kullback-Leibler Divergence



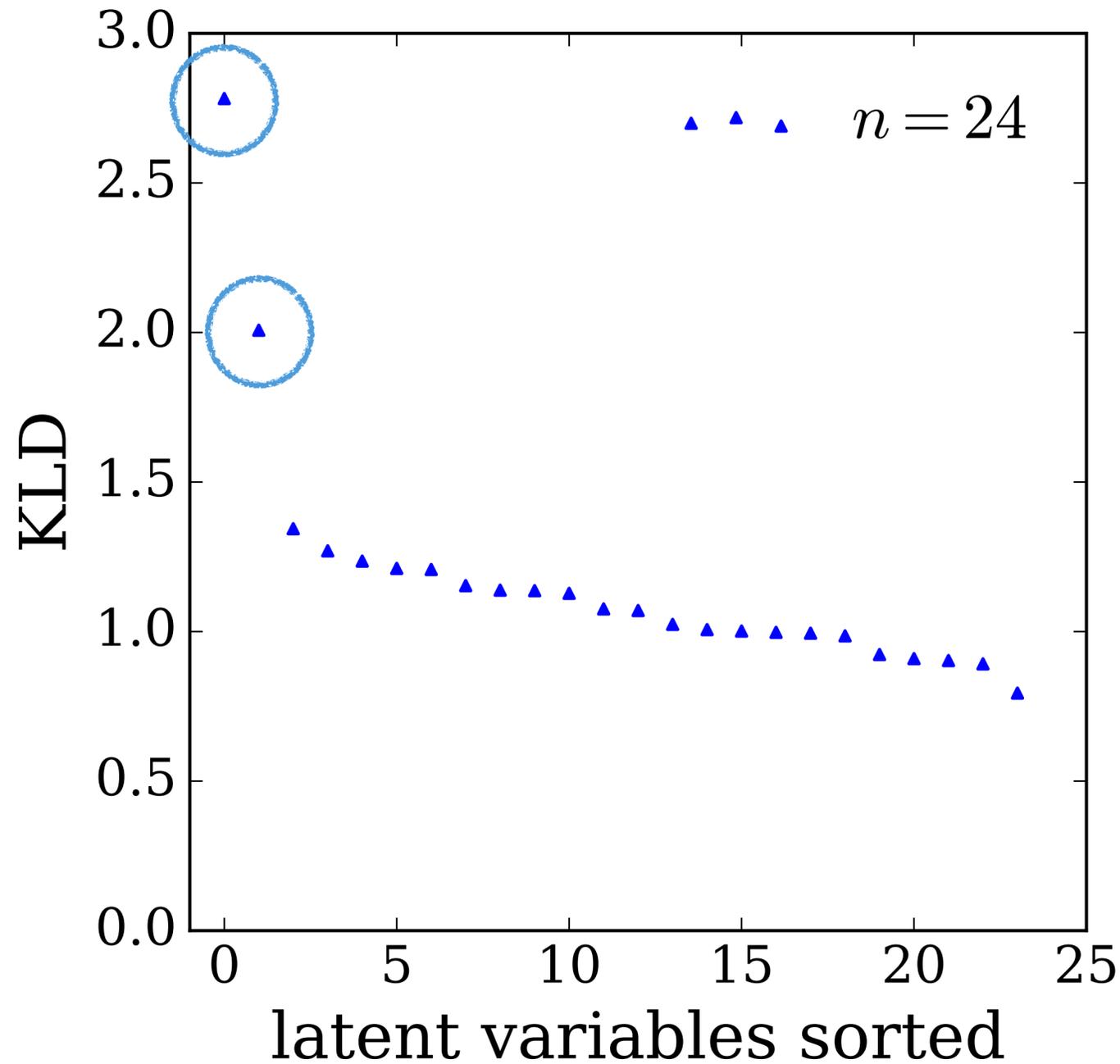
$$\text{Total Loss: } L_{\text{VAE}} = L_{\text{reco}} + \beta_{\text{KLD}} \cdot L_{\text{KLD}}$$

- **Hyperparameter  $\beta_{\text{KLD}}$  optimisation:**  
Balance between well regularised latent space & good reconstruction loss
- KLD measure for **information** encoded in latent space
  - What physics information is encoded?

- **Reconstruction loss:**  
Often Mean Squared Error, in our case: Critic network
- **KLD loss (Kullback-Leibler divergence):**  
Regularises latent space ( $\mu_i$  and  $\sigma_i$ ) towards Standard Normal distributions



# High KLD variables vs. Physics observables



Few latent variables encode most information

High KLD variables correlated to shower physics observables (i.e. centre of gravity in z)

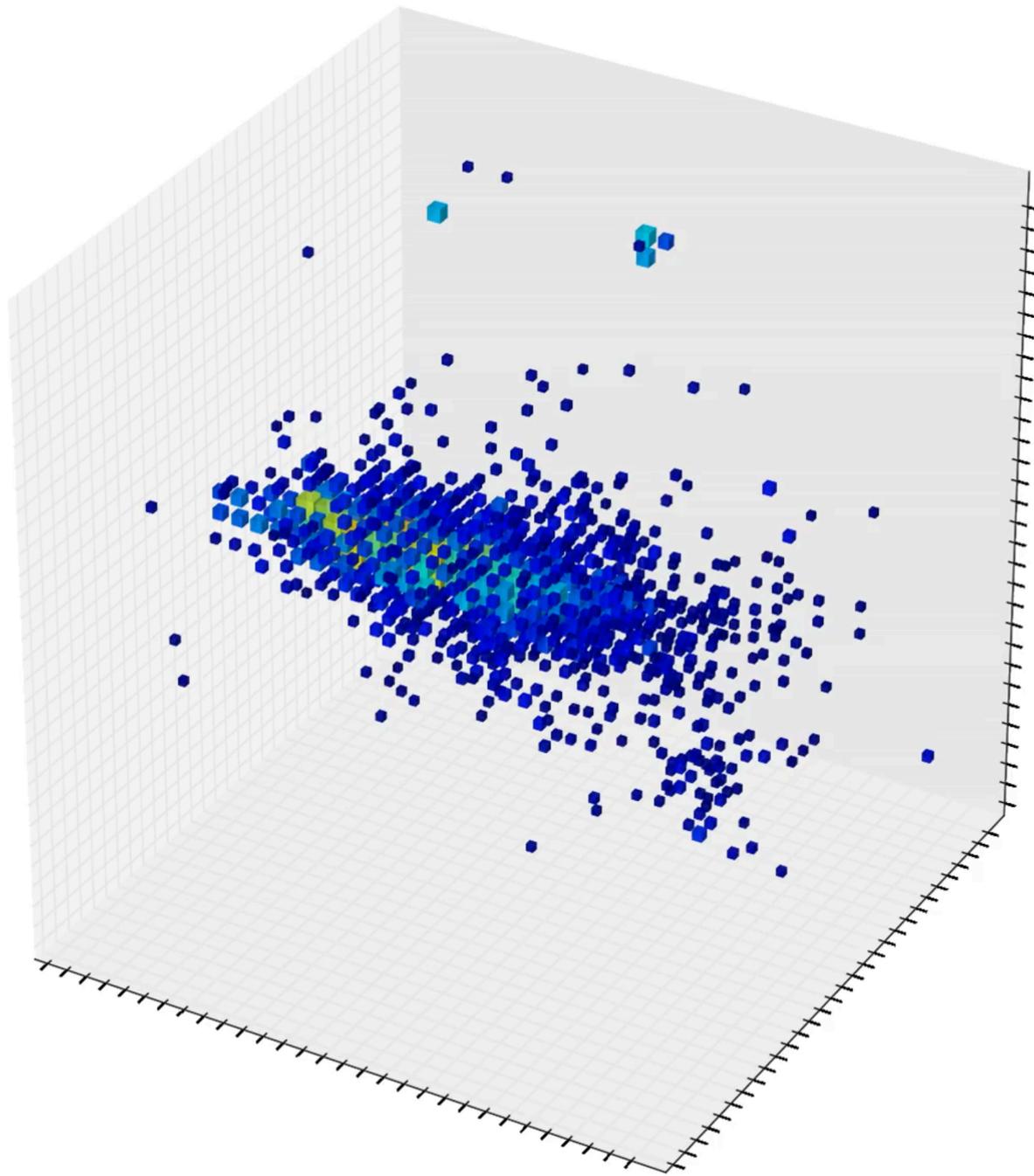
1st moment = center of gravity

Encoding behaviour consistent over multiple BIB-AE trainings & hyperparameter changes!

$m_{1,x}$	0.1	0.1	0.1
$m_{1,y}$			
$m_{1,z}$	0.9	0.1	0.4
$m_{2,x}$	0.3		0.1
$m_{2,y}$	0.3		0.1
$m_{2,z}$	0.3	0.4	
$E_{vis}$	0.1	0.1	1.0
$E_{inc}$	0.1	0.1	1.0
$n_{hit}$	0.1	0.1	1.0
$E_1/E_{vis}$	0.9	0.2	0.4
$E_2/E_{vis}$	0.2	0.8	0.2
$E_3/E_{vis}$	0.8	0.4	0.3
	$z_0$	$z_1$	$E$

# High KLD variables vs. Physics observables

$$z_0 = -3.0$$



1st moment  
= center of gravity

Few latent variables  
encode most information

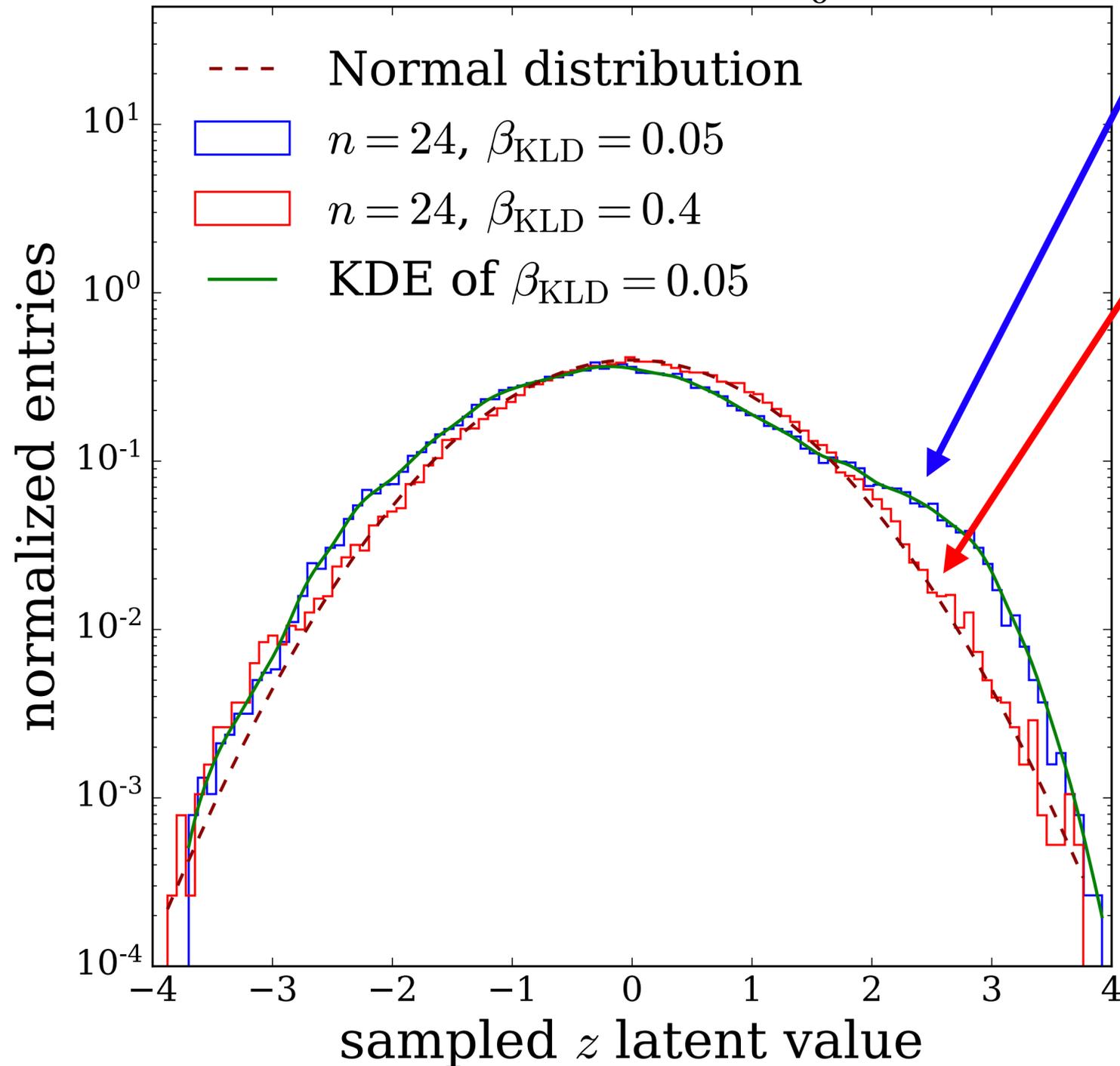
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# The highest KLD variable & Optimal Sampling

latent var.  $\mathcal{Z}_0$



Lower  $\beta_{\text{KLD}} \rightarrow$  Higher  $L_{\text{KLD}}$

▸ *Latent space  $\neq$  Normal distribution*

Higher  $\beta_{\text{KLD}} \rightarrow$  Lower  $L_{\text{KLD}}$

▸ *Latent space  $\approx$  Normal distribution*

• Goal for optimal generation:

▸ *Latent space = Sampling space*

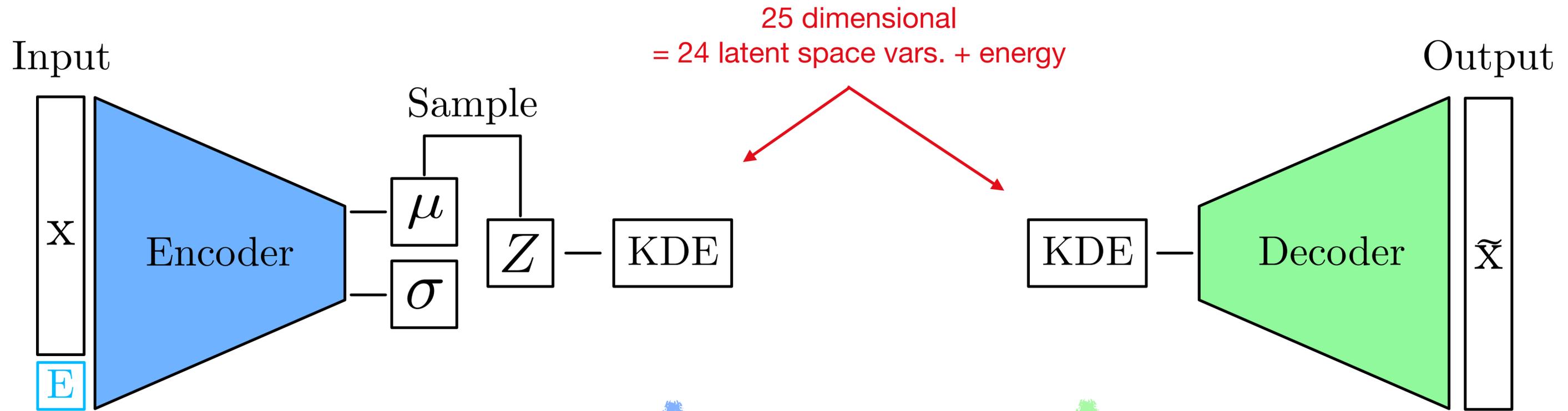
• Implementation by either:

1. **Tight regularisation with higher  $\beta_{\text{KLD}} = 0.4$**   
or

2. **Sampling from the encoded latent space**  
(i.e. via Kernel Density Estimation (KDE))

1. is motivated by [beta-VAE, ICLR 2017](#) | 2. mirrors method in [1901.00875](#)

# BIB-AE + Density Estimation Sampling



Estimate encoded latent space density with Kernel Density Estimator (KDE)

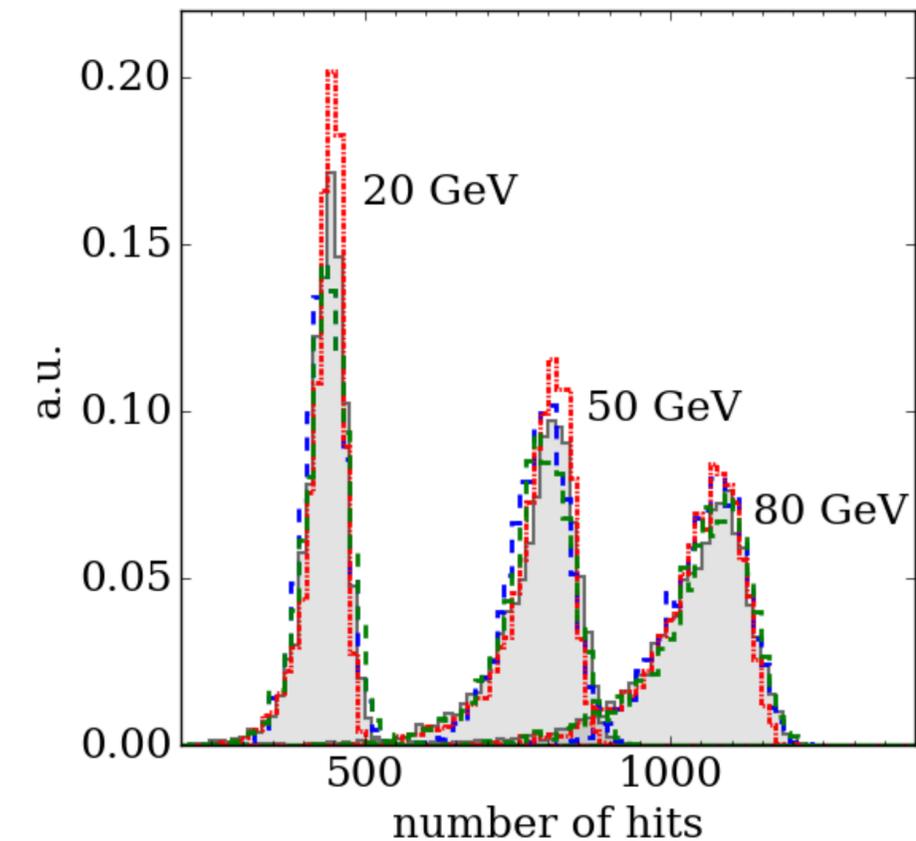
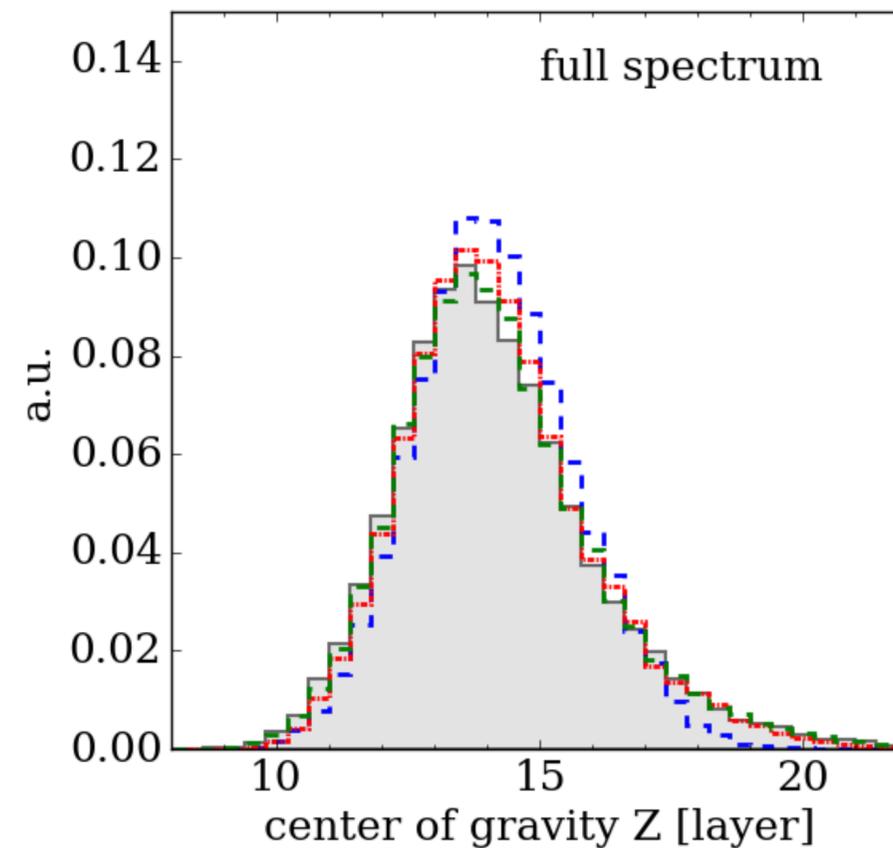
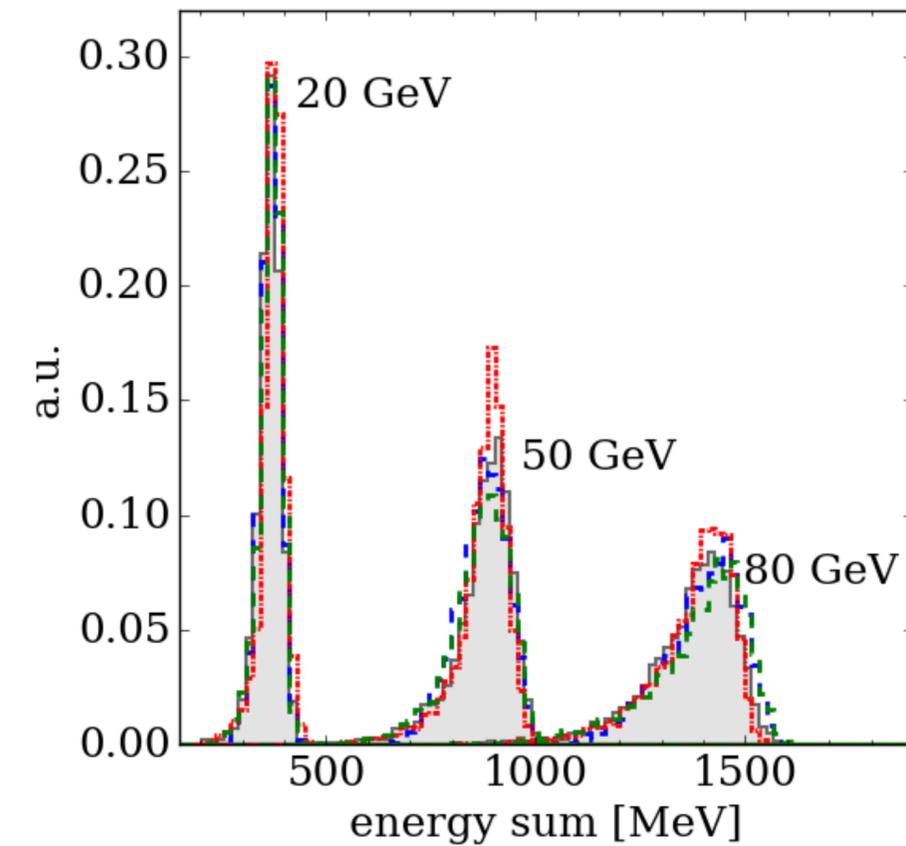
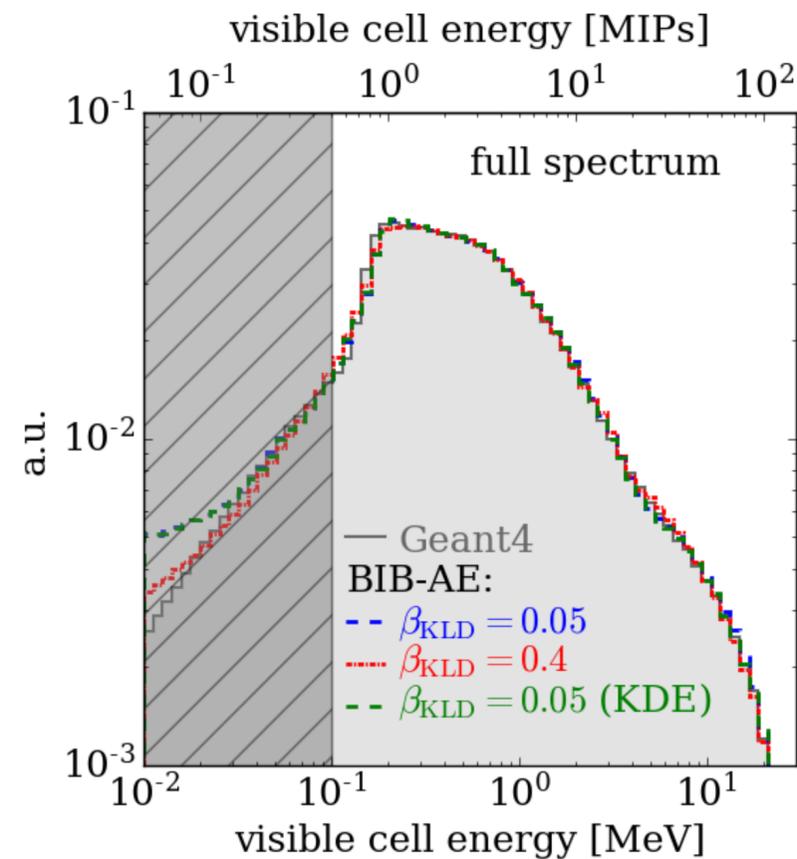
Generation:

Sample latent space from this KDE

- > Preserves all latent space correlations
- > Applicable to already trained models

# Generative Fidelity

- Comparing three models:
  - Previous baseline  $\beta_{\text{KLD}} = 0.05$
  - Tight regularisation  $\beta_{\text{KLD}} = 0.4$
  - KDE sampling  $\beta_{\text{KLD}} = 0.05$  (KDE)
- All models get MIP peak right (thanks to Post Processor network)
- Center of gravity improved for both optimised models
- Too narrow single energy distributions with tight regularisations



# Summary

- BIB-AE generates highly granular photon showers with high fidelity at high speed
- Accurate MIP peak with Post Processor network
- Correlations between physics observables and latent variables yield interpretable latent space
- Improvement of shower shape (i.e. center of gravity) from optimised latent space sampling
- KDE sampling promising method for all VAE-based architectures & applicable to models without retraining

arXiv: [2005.05334](https://arxiv.org/abs/2005.05334) & [2102.12491](https://arxiv.org/abs/2102.12491)

