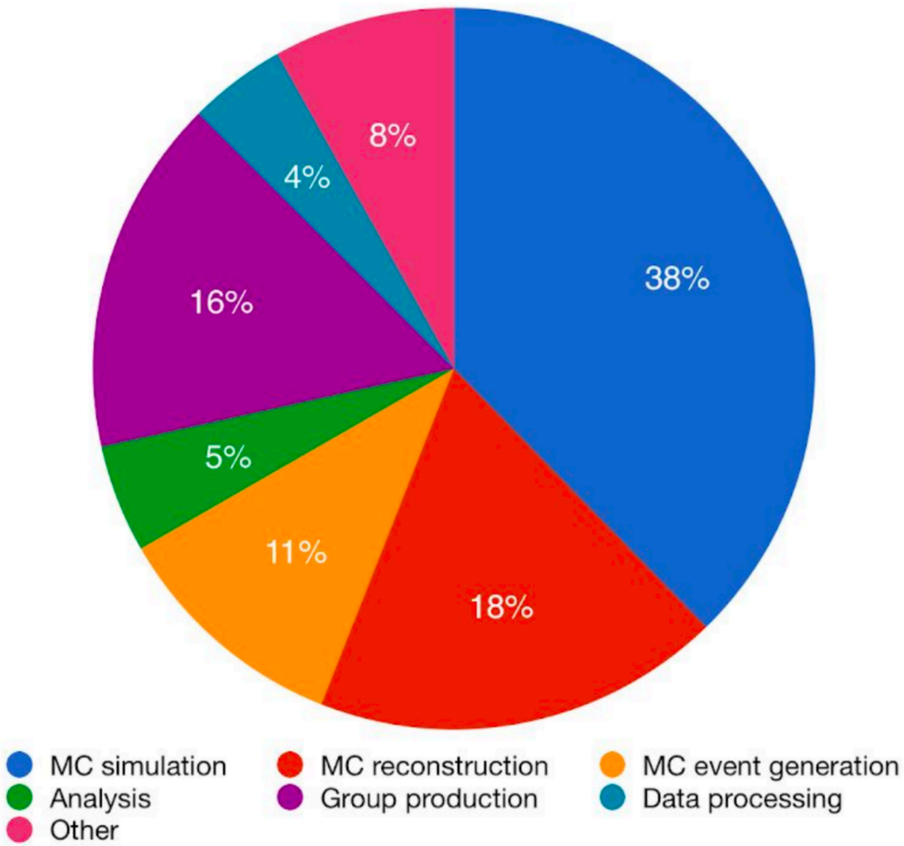
Generative Models for Shower Simulation on Testbeam Data

Erik Buhmann, **Sascha Diefenbacher**, Engin Eren, Frank Gaede, Gregor Kasieczka, William Korcari, Katja Krüger, Peter McKeown, Lennart Rustige

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG
CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE
HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES
DESY.

Shower Simulation



- MC simulation large part of computing
- Speed up:
  - Train ML model on small dataset
  - Draw majority of samples form ML model

➡ Amplify original data set

➡ Significantly faster

Catmore et. al. **ATLAS HL-LHC Computing Conceptual Design Report,** CERN-LHCC-2020-015 ; LHCC-G-178

Butter et al.: **Amplifying Statistics using Generative Models:** NeurIPS ML4PS 2020, 2008.06545

Classification

High Dim. Data

Classification

High Dim. Data

Low Dim. Label

Dog

Cat

Classification

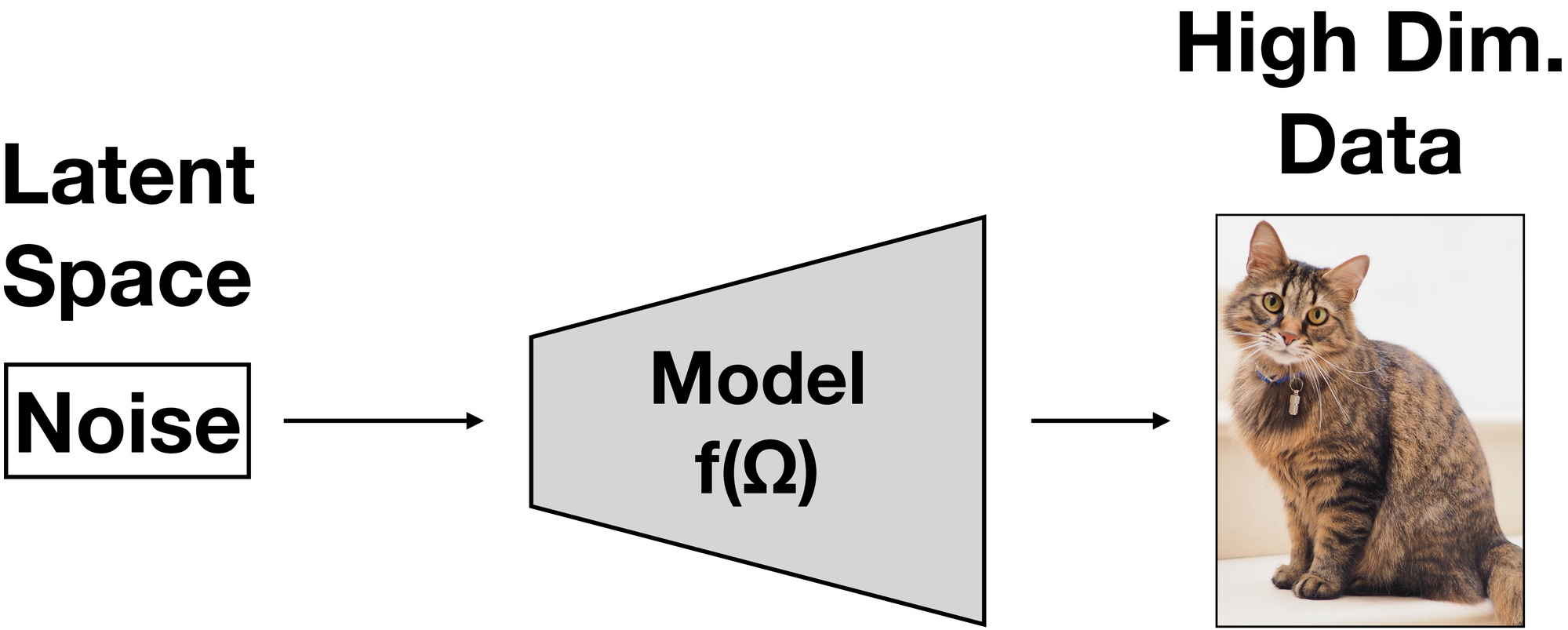
High Dim. Data

Model f(Ω)

Prediction

Cat/Dog?

Generation



Choice of Loss Function

- Generative:
  - How do you measure the model performance?
  - How is this expressed mathematically (and differentiable)

Choice of Loss Function

- Generative:
  - How do you measure the model performance?
  - How is this expressed mathematically (and differentiable)

http://thesecatsdonotexist.com

Generation Difficulties

- Image Set:
  - Does the new set have the same properties as the data?

Training Data:

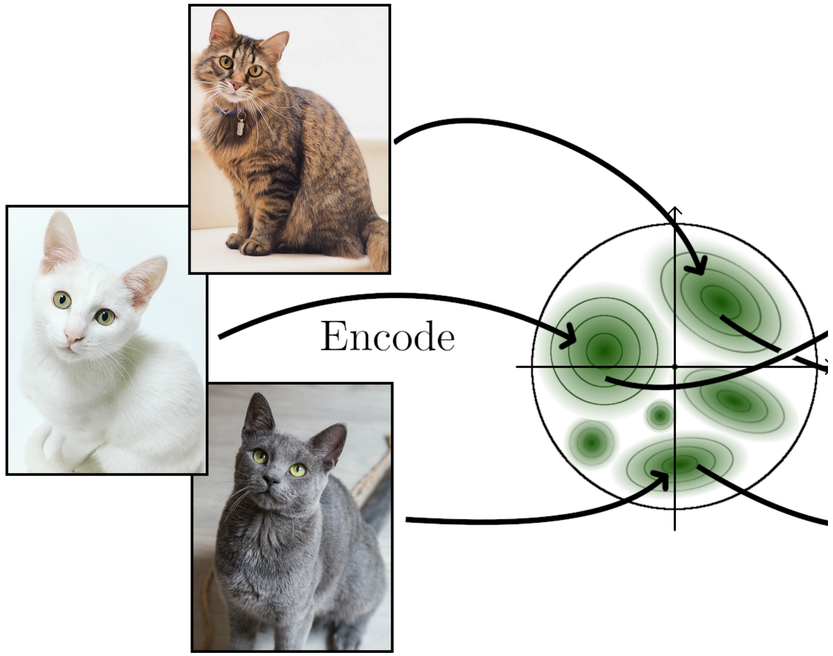
Generation Difficulties

- Image Set:
  - Does the new set have the same properties as the data?

Training Data:

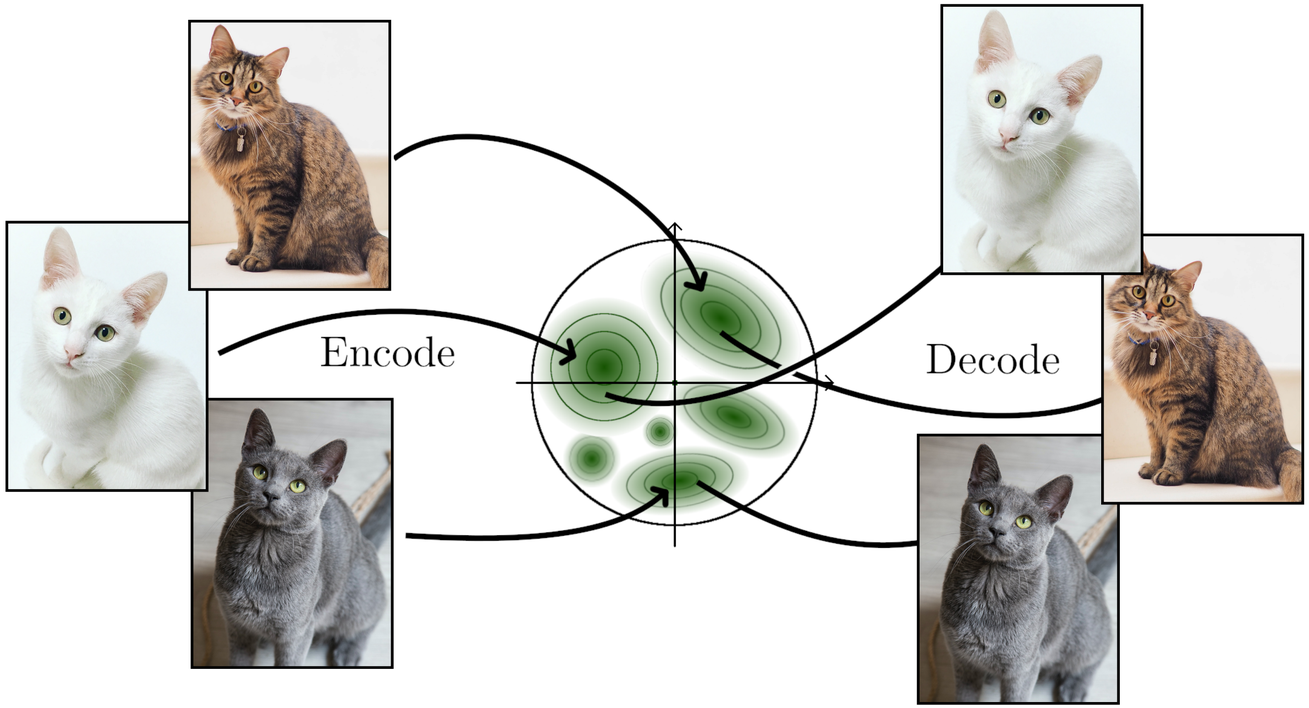
Generated Data:

AutoEncoder



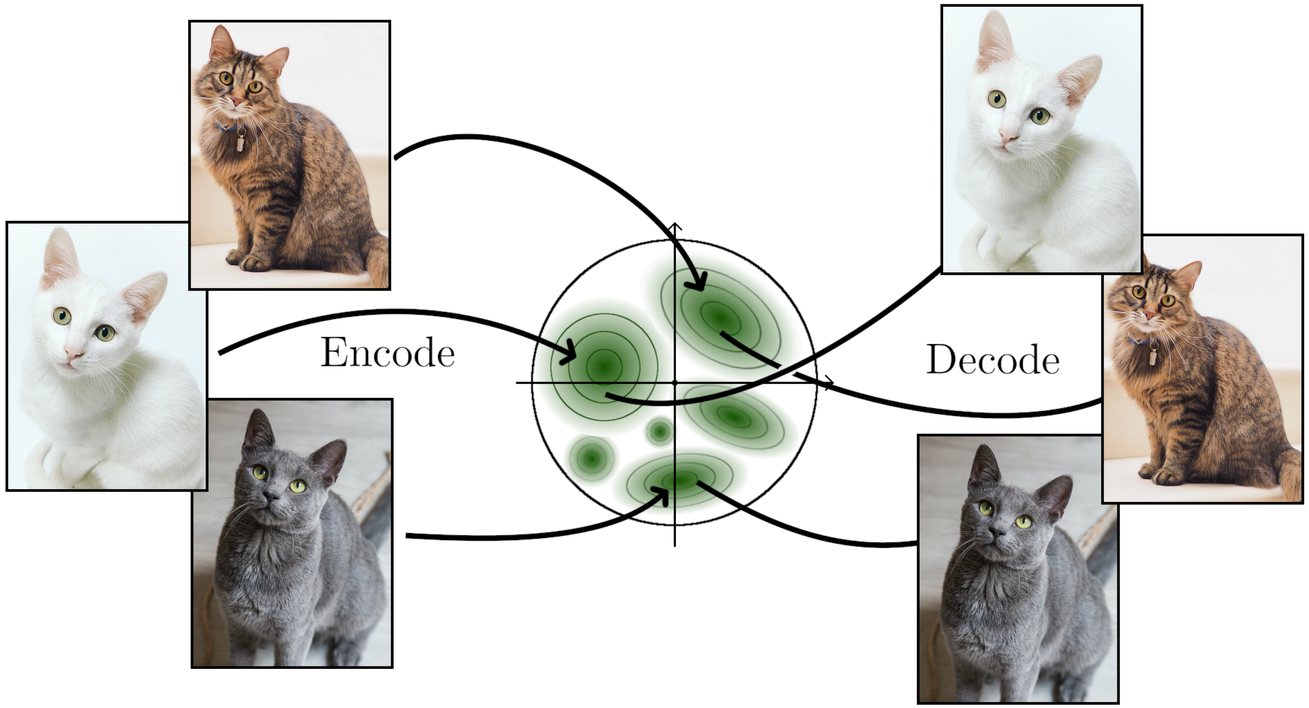
- Encoding function E(x)=z map high dimensional data X to low dimensional latent space Z

AutoEncoder



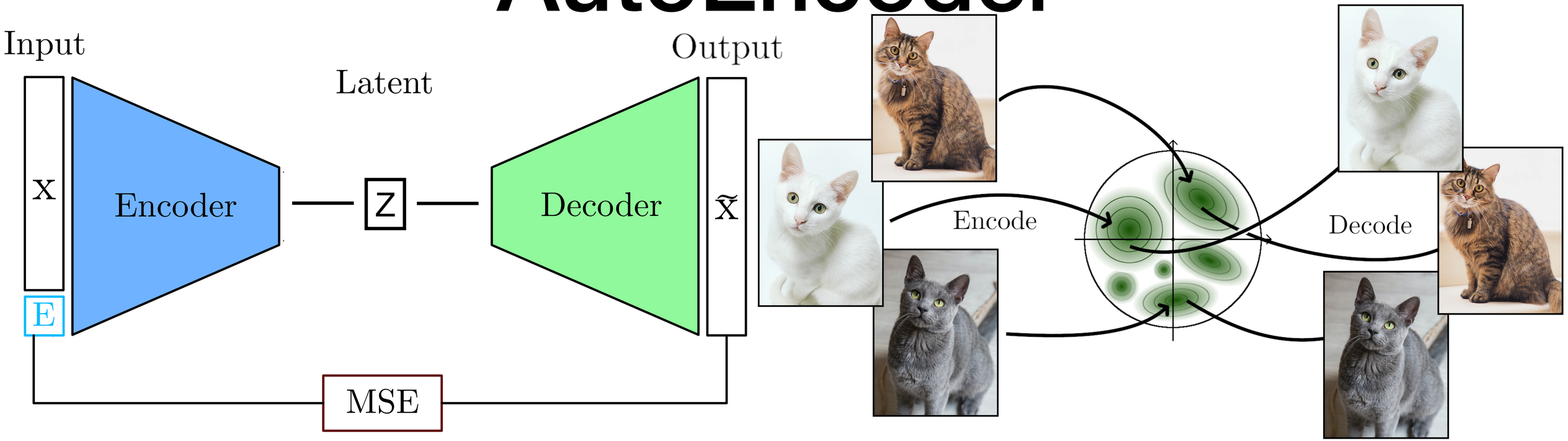
- Encoding function E(x)=z map high dimensional data X to low dimensional latent space Z
- Decoding function D(z)=x map latent space Z back to data X

AutoEncoder



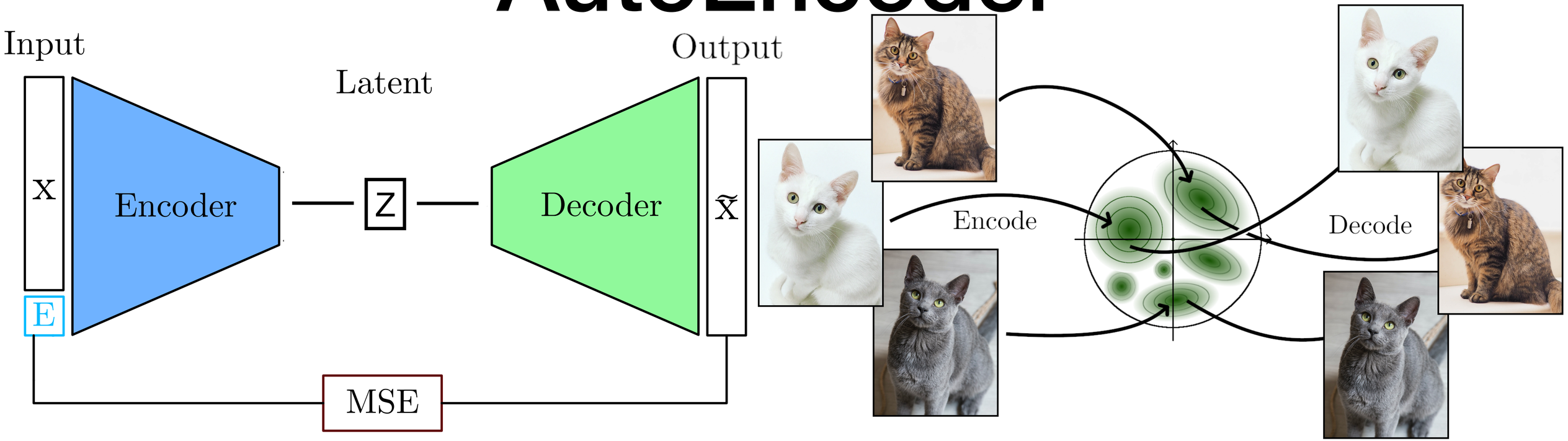
- Encoding function E(x)=z map high dimensional data X to low dimensional latent space Z
- Decoding function D(z)=x map latent space Z back to data X
- Compare Input and Output pixel by pixel with mean squared error

AutoEncoder



- Sample from Z and pass it to D(Z) ➡ Generate new samples

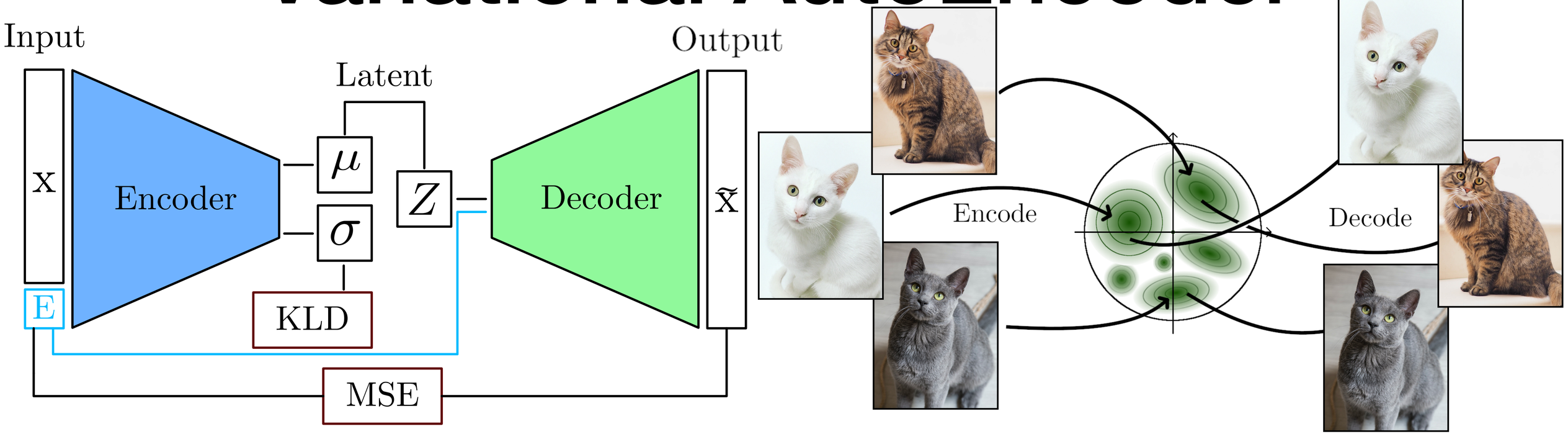
AutoEncoder



- Sample from Z and pass it to D(Z) ➡ Generate new samples
- Problem: Need regularised later space to sample form

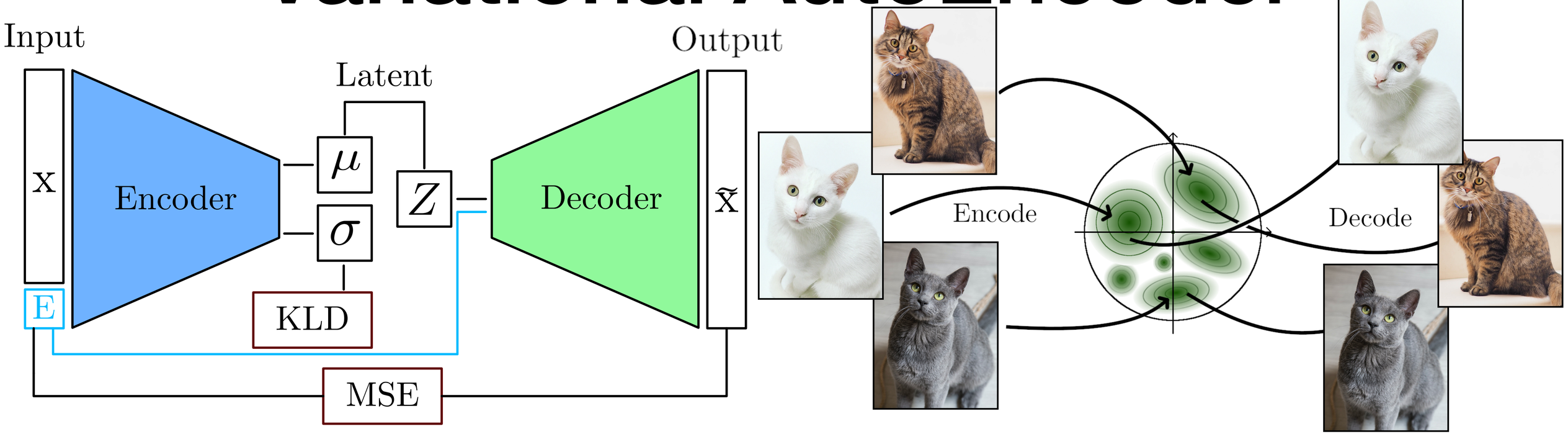
  Variational AutoEncoder

Variational AutoEncoder



- Latent space: Series of Gaussians, regularised match N(μ=0, σ=1)

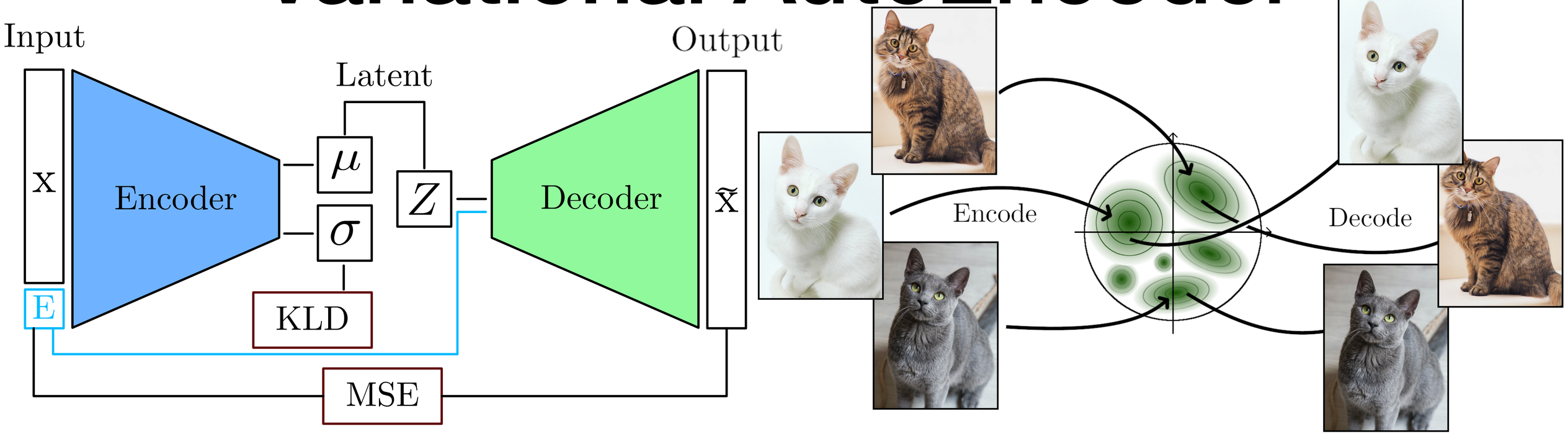
Variational AutoEncoder



- Latent space: Series of Gaussians, regularised match N(μ=0, σ=1)
  - Using Gaussians lets us use Kullback–Leibler divergence

$$\sum_{i=1}^{n} \sigma_i^2 + \mu_i^2 - \log(\sigma_i) - 1$$

Variational AutoEncoder

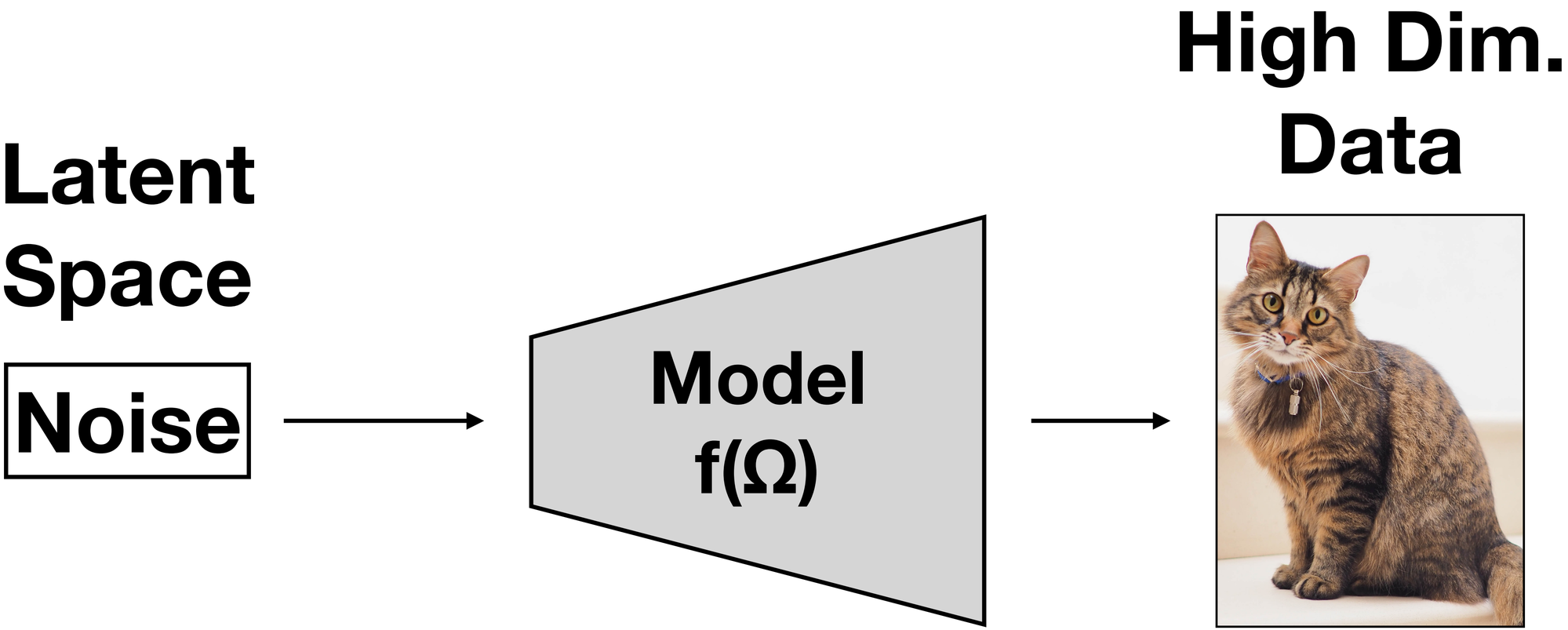


- Latent space: Series of Gaussians, regularised match N(μ=0, σ=1)
  - Using Gaussians lets us use Kullback–Leibler divergence

$$\sum_{i=1}^{n} \sigma_i^2 + \mu_i^2 - \log(\sigma_i) - 1$$

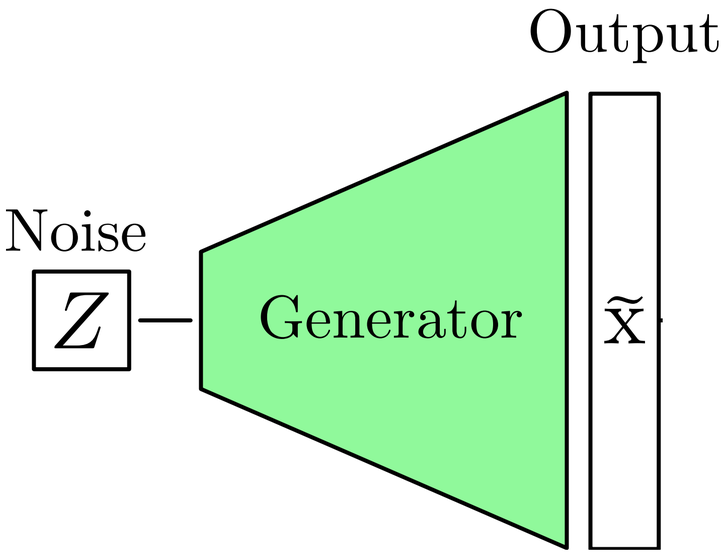
- Compare Input and Output again using MSE

Generative Adversarial Network



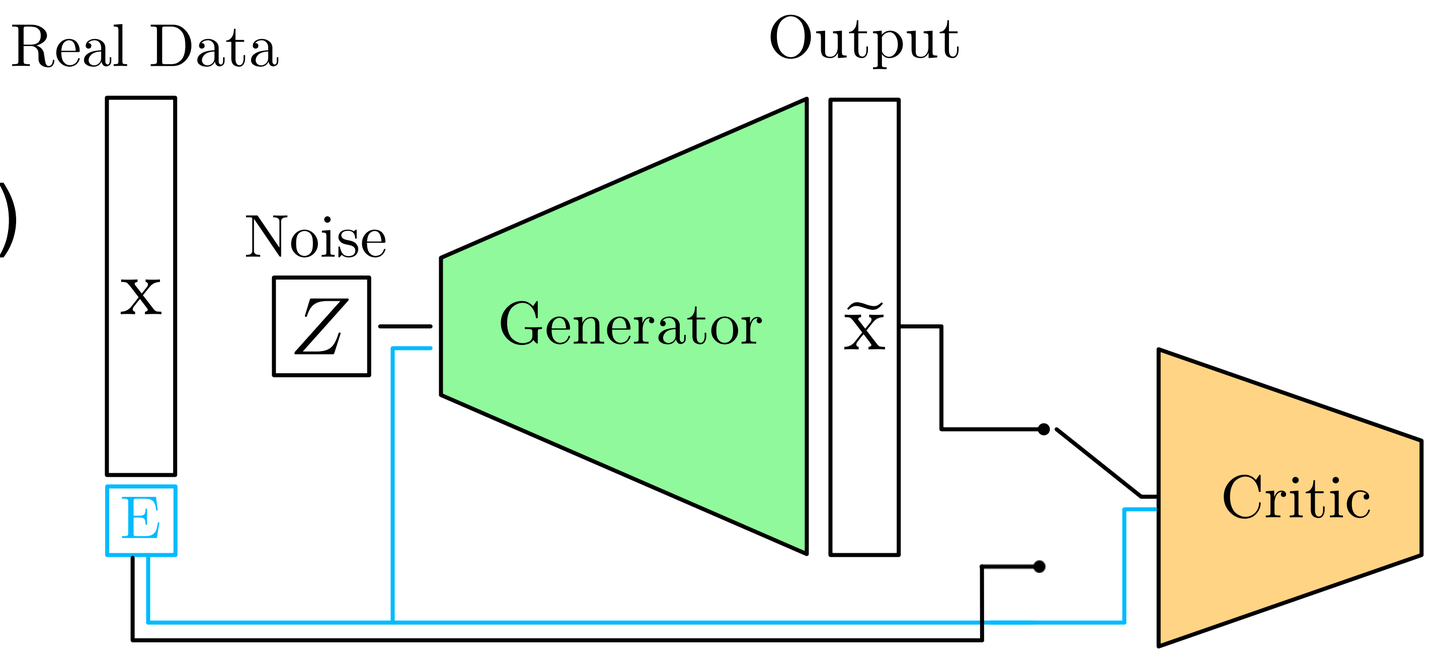
Generative Adversarial Network

- Generator Network G(z)=x
  - Maps noise Z to Data X



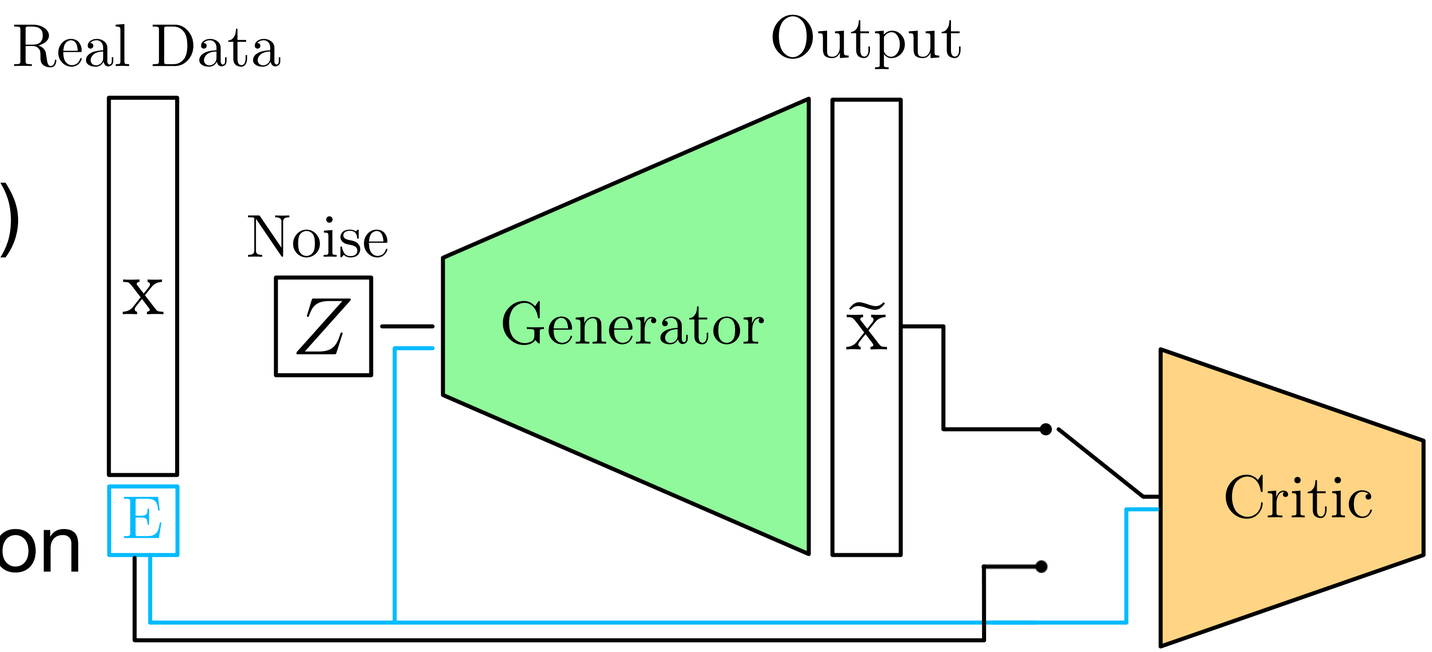
Generative Adversarial Network

- Generator Network G(z)=x
  - Maps noise Z to Data X
- Discriminator D(G(z)) and D(x)
  - Learns difference between real and fake



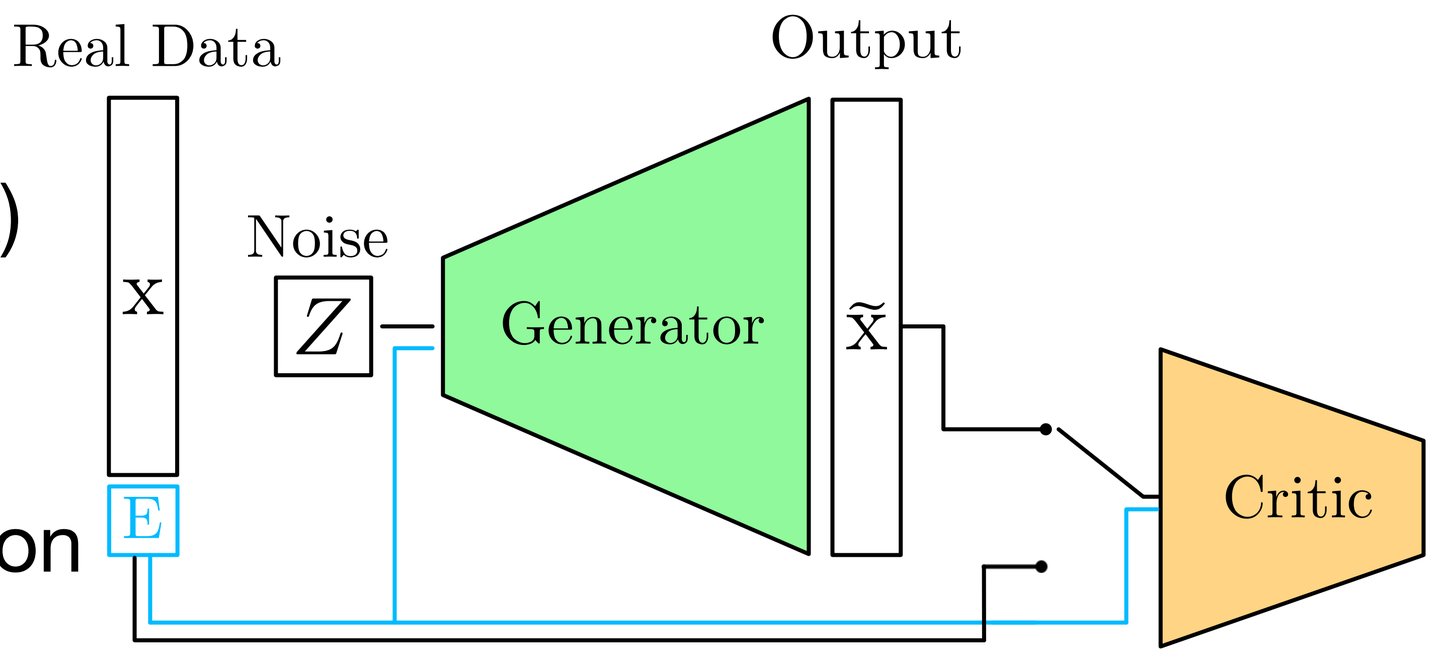
Generative Adversarial Network

- Generator Network G(z)=x
  - Maps noise Z to Data X
- Discriminator D(G(z)) and D(x)
  - Learns difference between real and fake
- D(G(z)) is differentiable function measuring performance

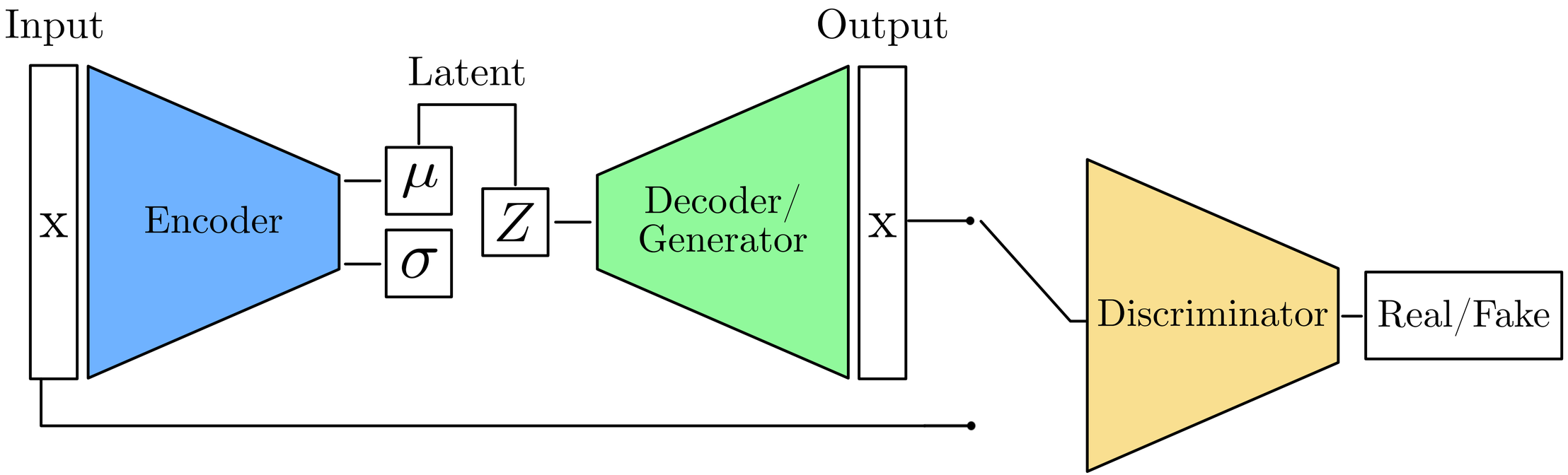


Generative Adversarial Network

- Generator Network G(z)=x
  - Maps noise Z to Data X
- Discriminator D(G(z)) and D(x)
  - Learns difference between real and fake
- D(G(z)) is differentiable function measuring performance
- Use D(G(z)) as loss to update G

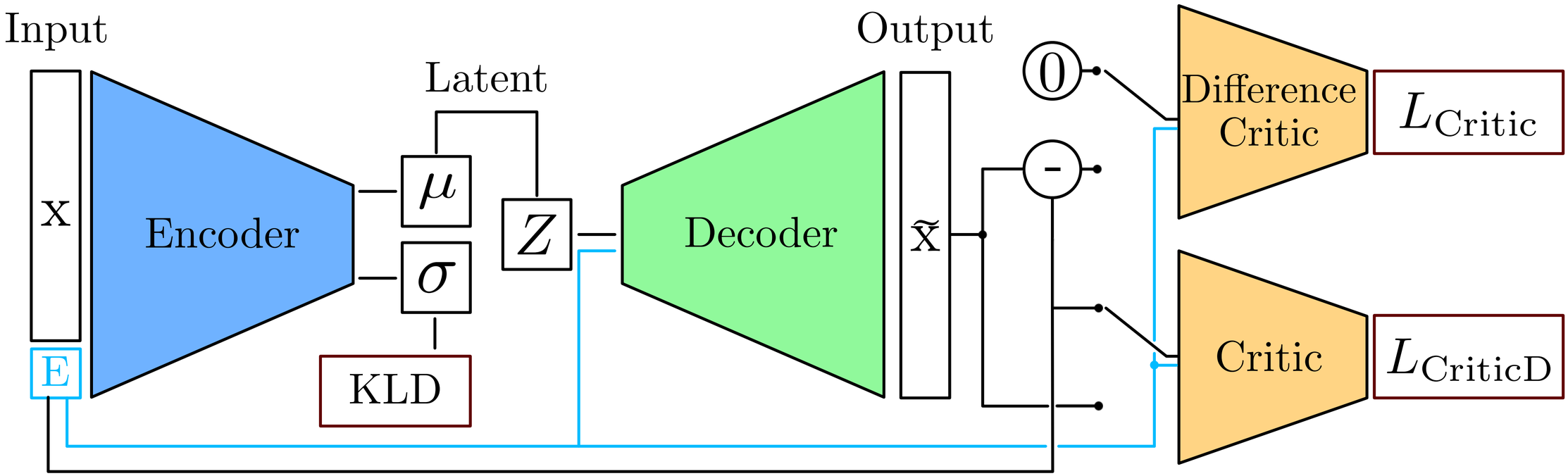


VAE-GAN



- Combines VAE and GAN ideas
  - Significant improvement in generated shower quality
  - No reconstruction loss, no meaningful latent space

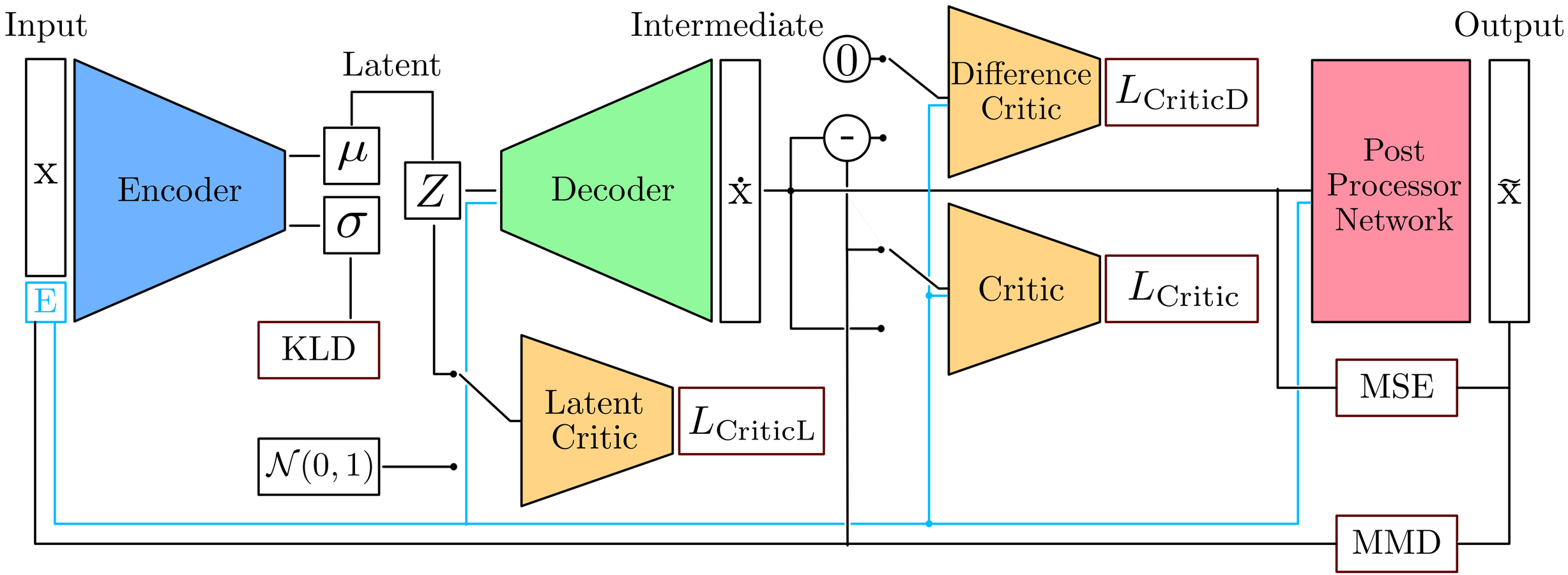
Bounded Information Bottleneck AutoEncoder



- Further expansion of the VAE-GAN structure
- Critic network that judges shower quality
- Second critic that judges reconstruction

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

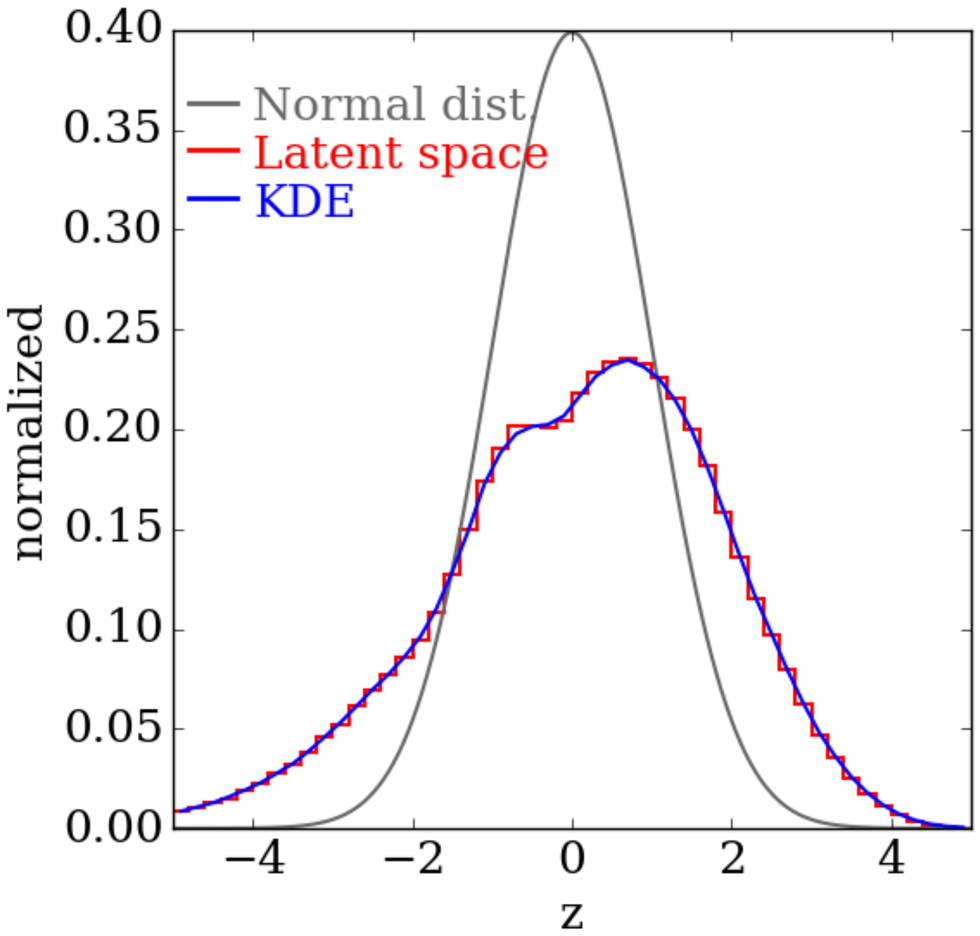
BIB-AE Post Processor



- Additional Critic for latent regularisation
- Final Post Processor Network for fine tuning

Latent Space Modelling

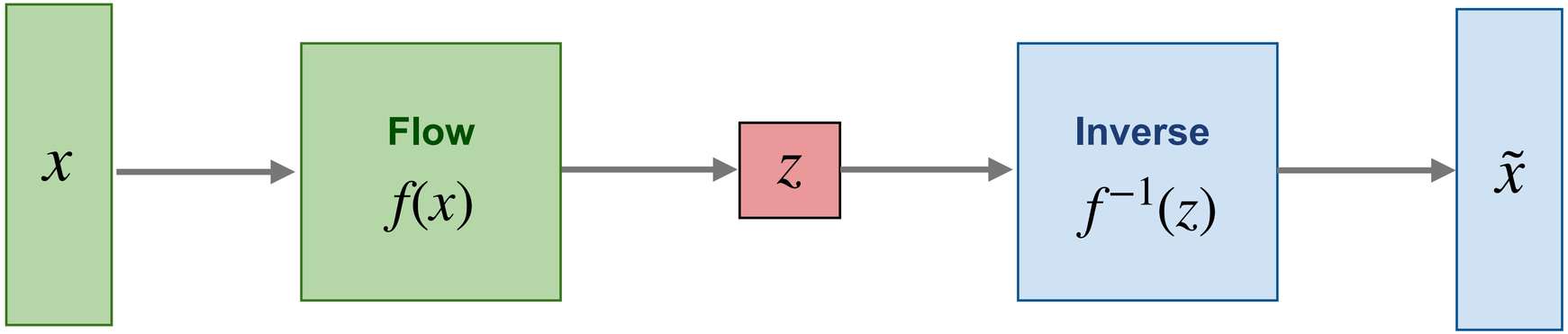
- Initial results underwhelming:
  - Check latent space encoding
  - Highly non Gaussian
- Two options:
  - Increase latent regularisation
    - Worsens shower quality
  - Fit latent space and sample
    - ~~Kernel Density Estimator (KDE)~~
    - Normalising Flow



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

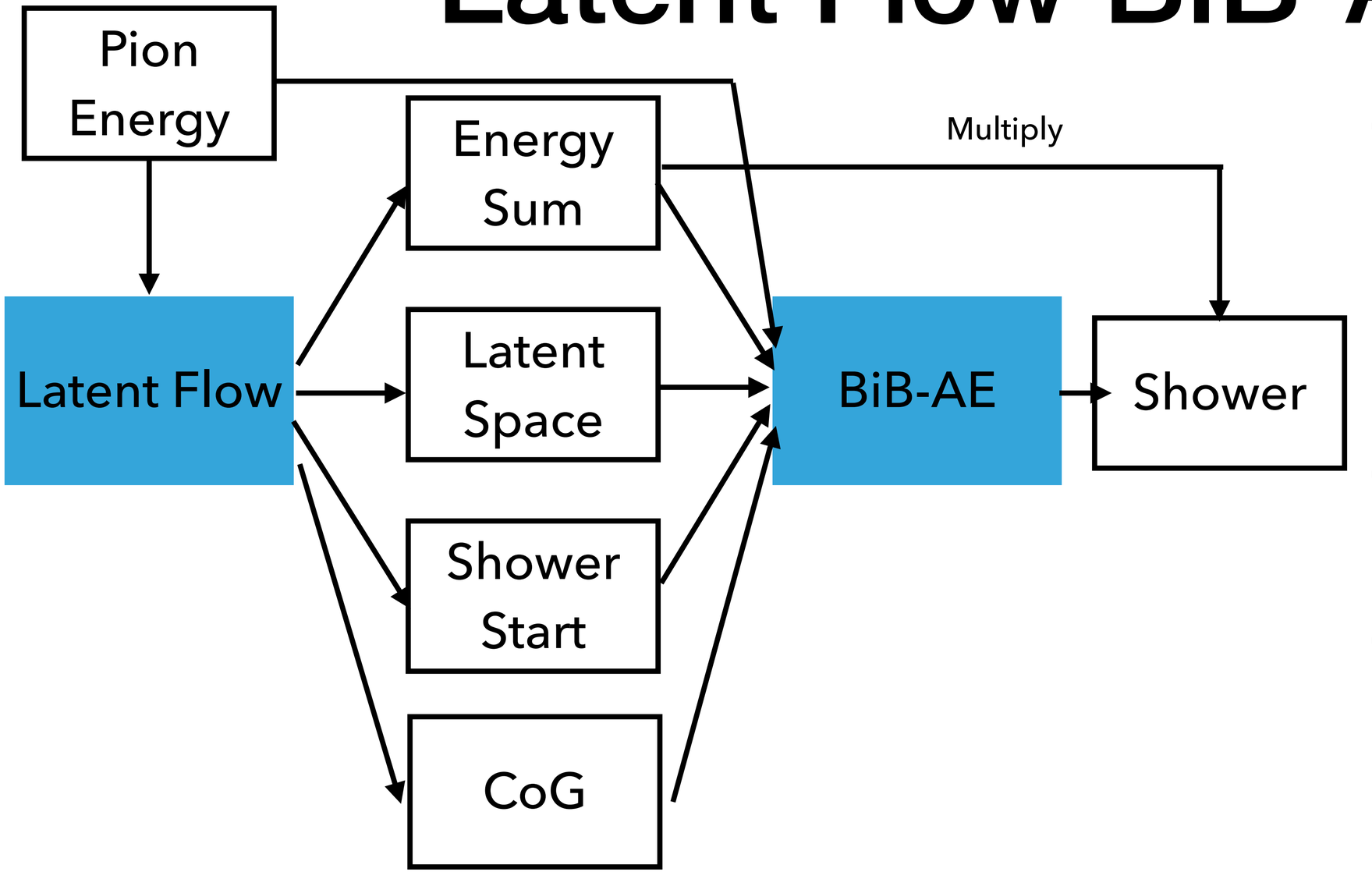
Latent Space Modelling

Normalising Flow



- Train invertible transformation to map data to latent space
- Use inverse to generate new data from new latent samples
- Very accurate for modelling low dimensionality problems

Latent Flow BIB-AE



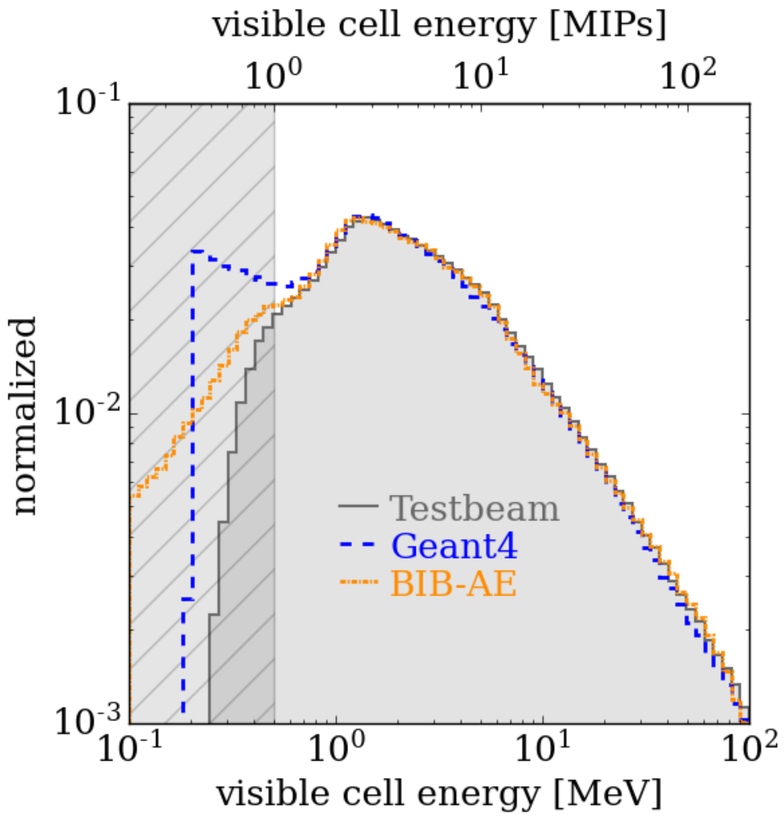
- Flow Generates:
  - Latent space
  - High-level observables
- Use Flow output as BIB-AE input
- Multiply with energy sum in the end

Hadronic Calorimeter

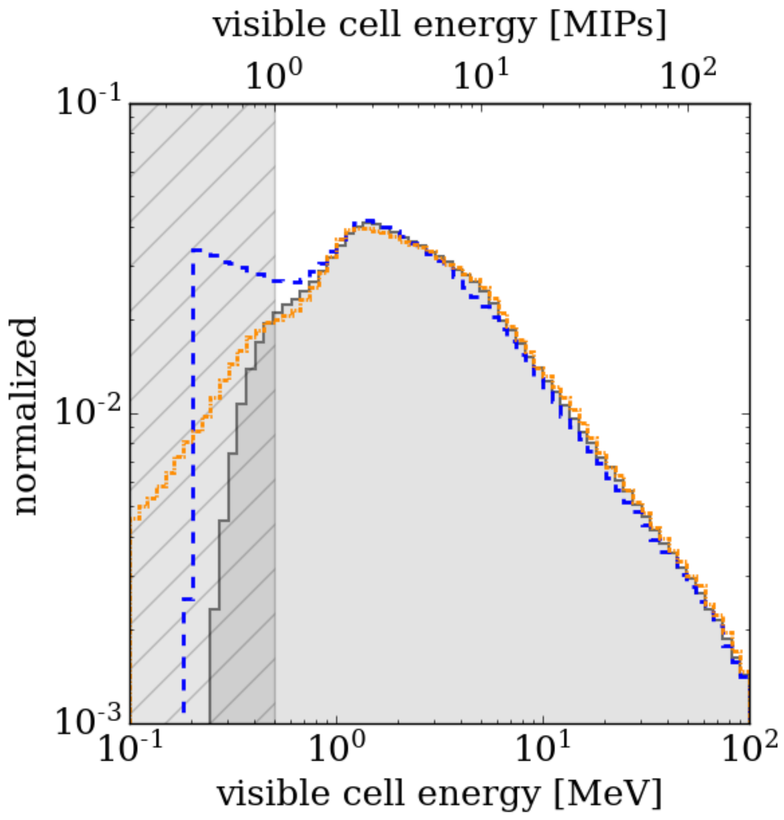
- CALICE H-cal prototype:
  - 24x24 cells
  - 39 layers, 2nd to last layer only 12x12 cell
  - ➡ Only use 37 layers
  - Data taken from June 2018 SPS testbeam
  - Comparison: Geant4 simulation, QGSP_BERT_HP physics list
  - For now 3 energies: 80GeV, 120GeV, 160GeV
  - 57k Showers per energy, 171k in total

Visible Cell Energy Spectrum

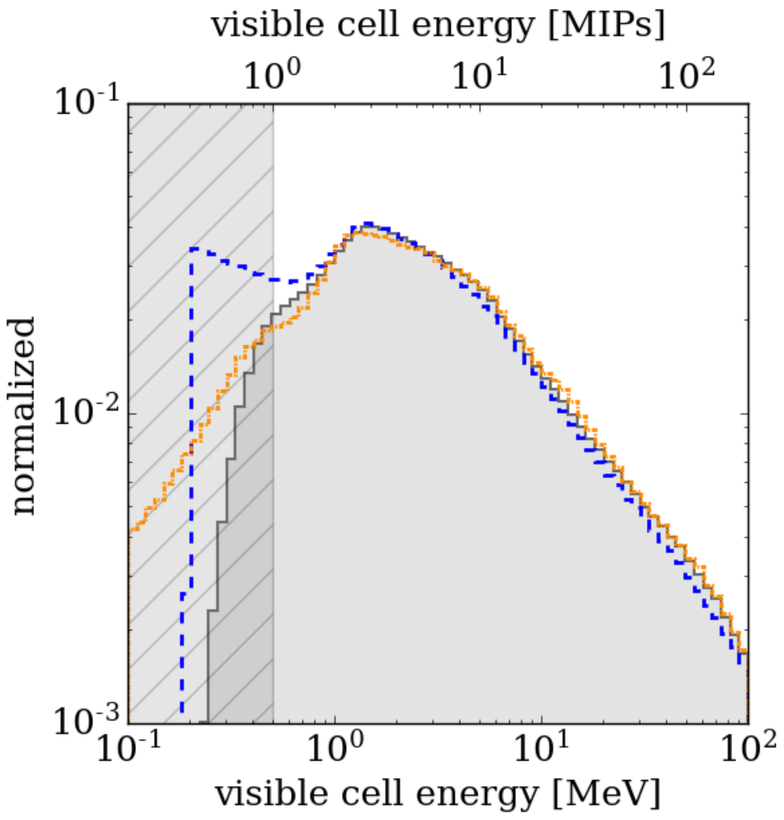
80GeV



120GeV

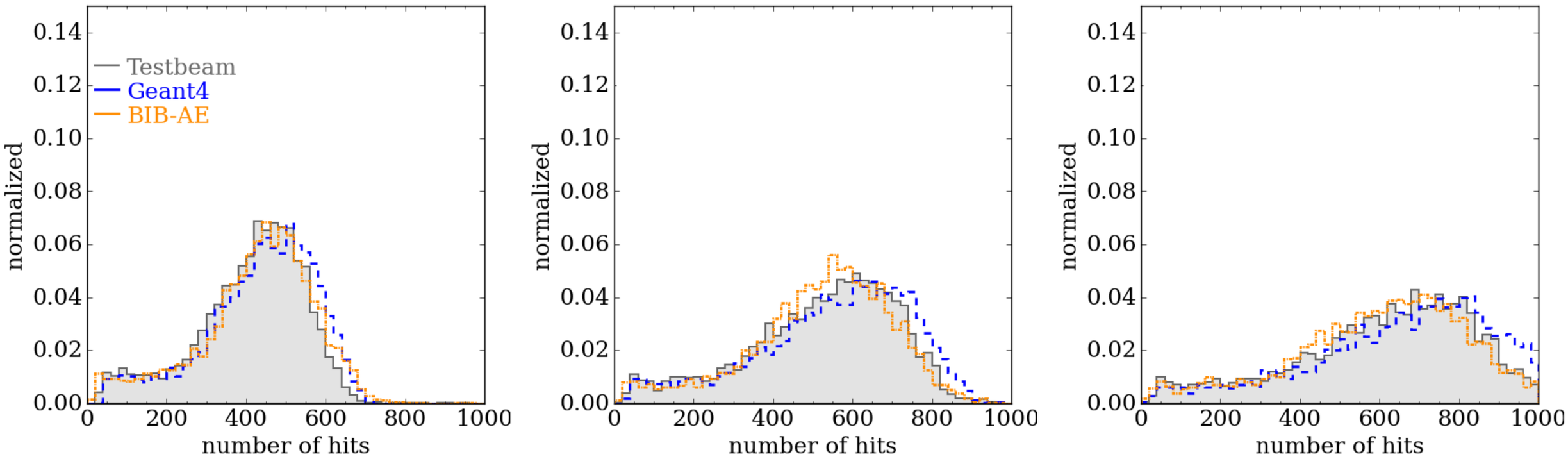


160GeV



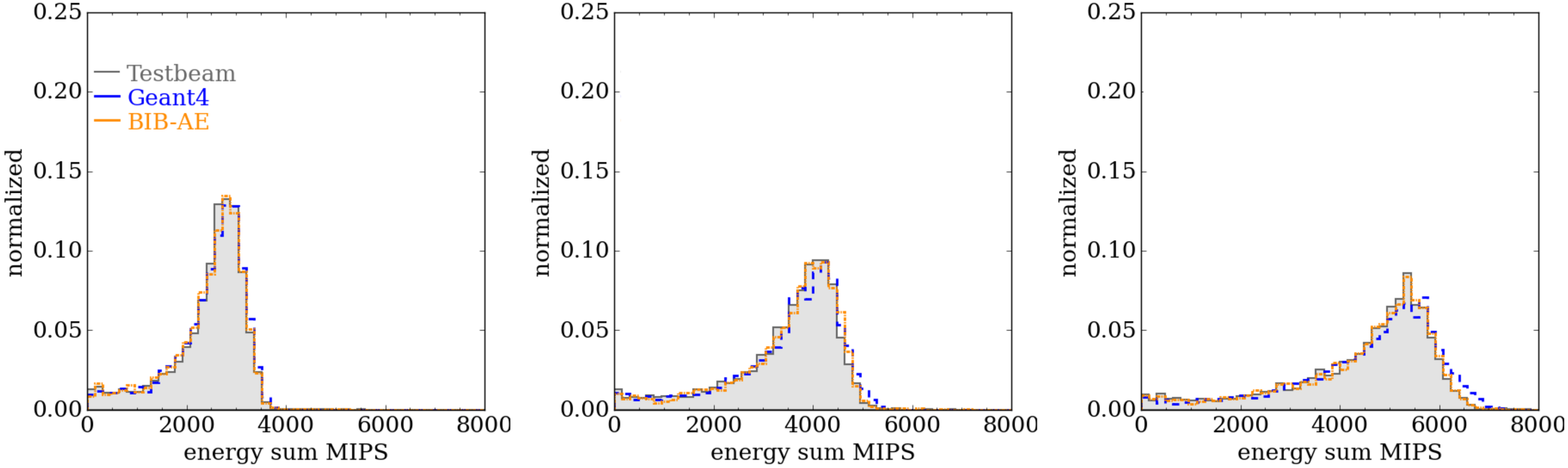
Number of Hits

80GeV **120GeV** **160GeV**



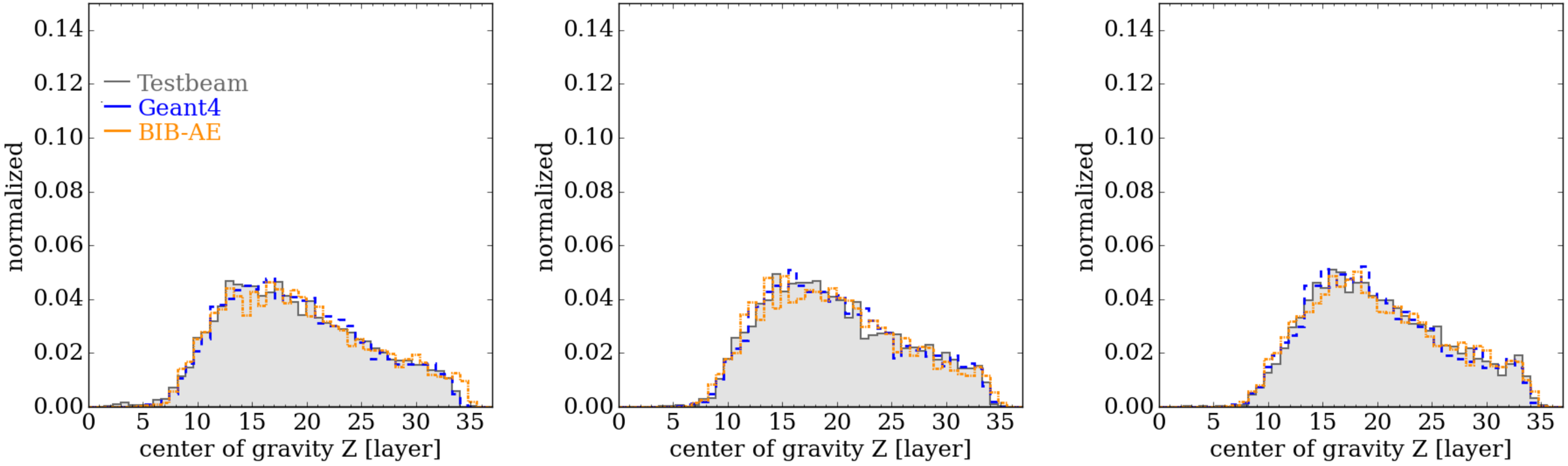
Visible Energy Sum

80GeV **120GeV** **160GeV**



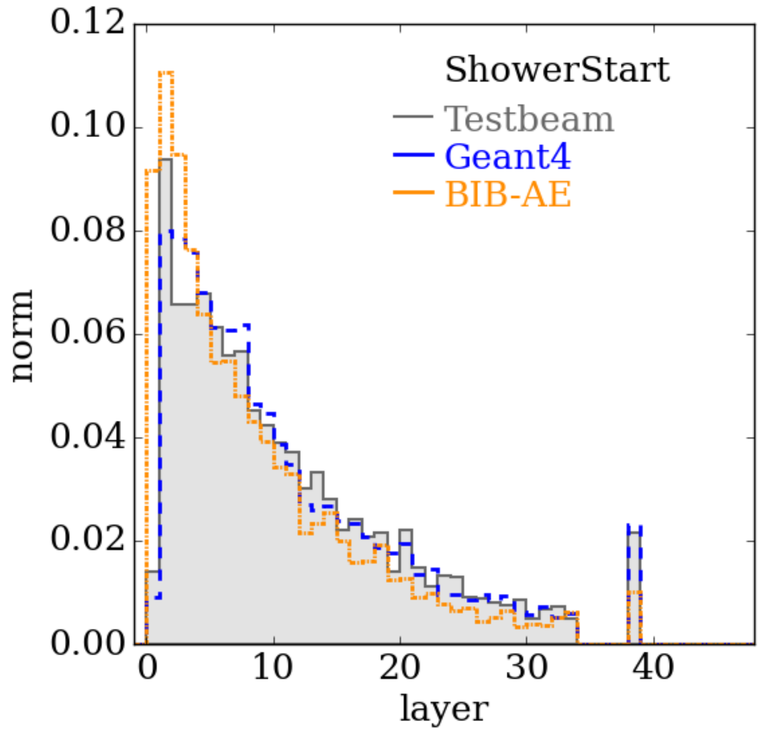
Center of Gravity along Trajectory

80GeV **120GeV** **160GeV**

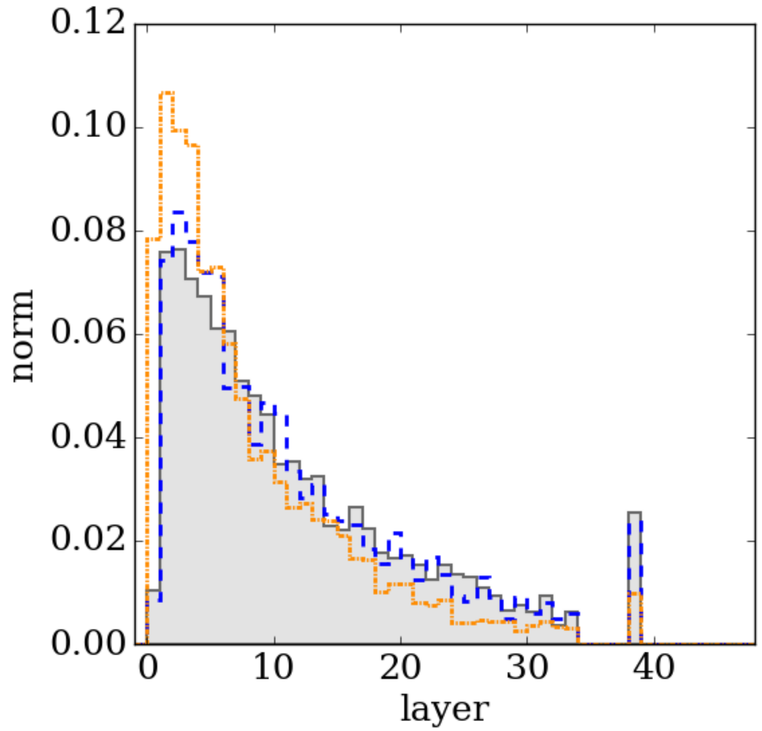


Shower Start Layer

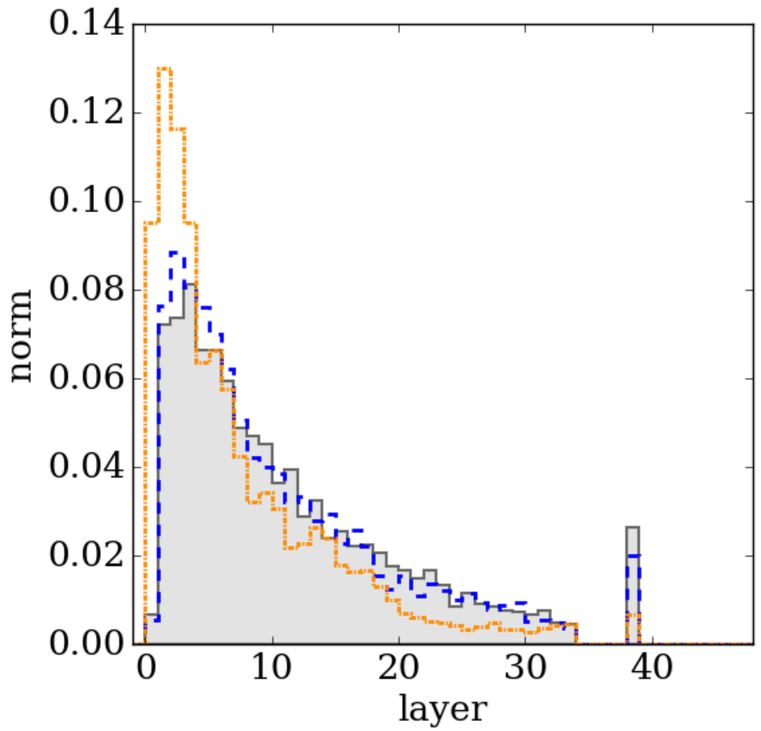
80GeV



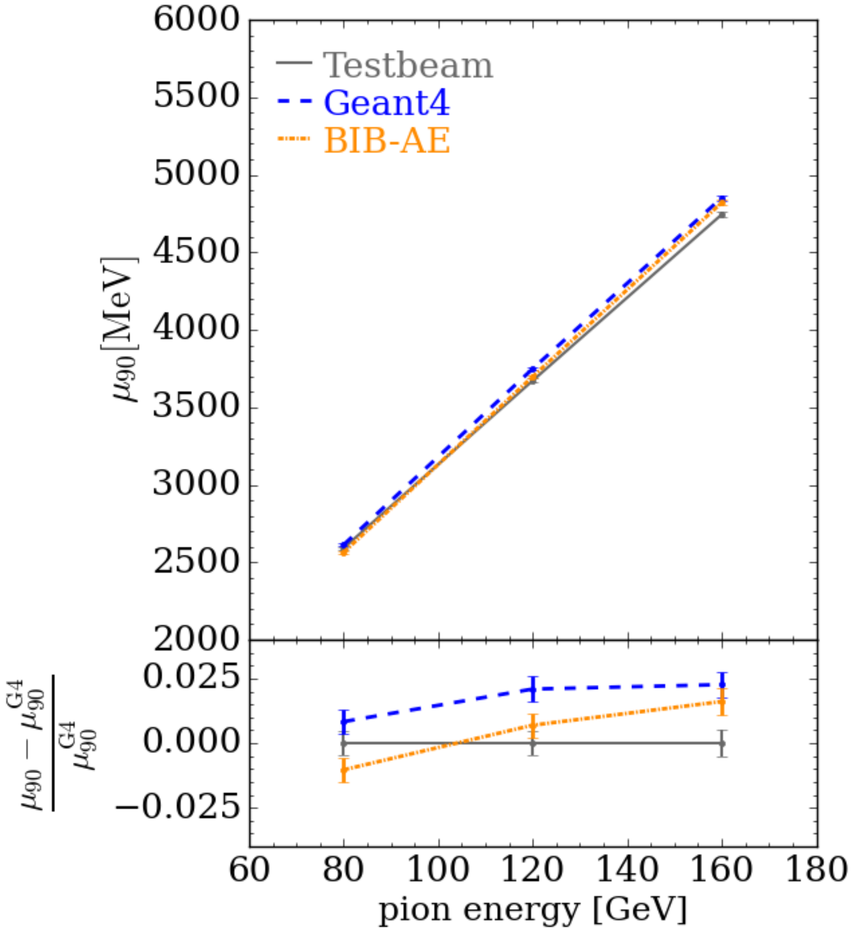
120GeV

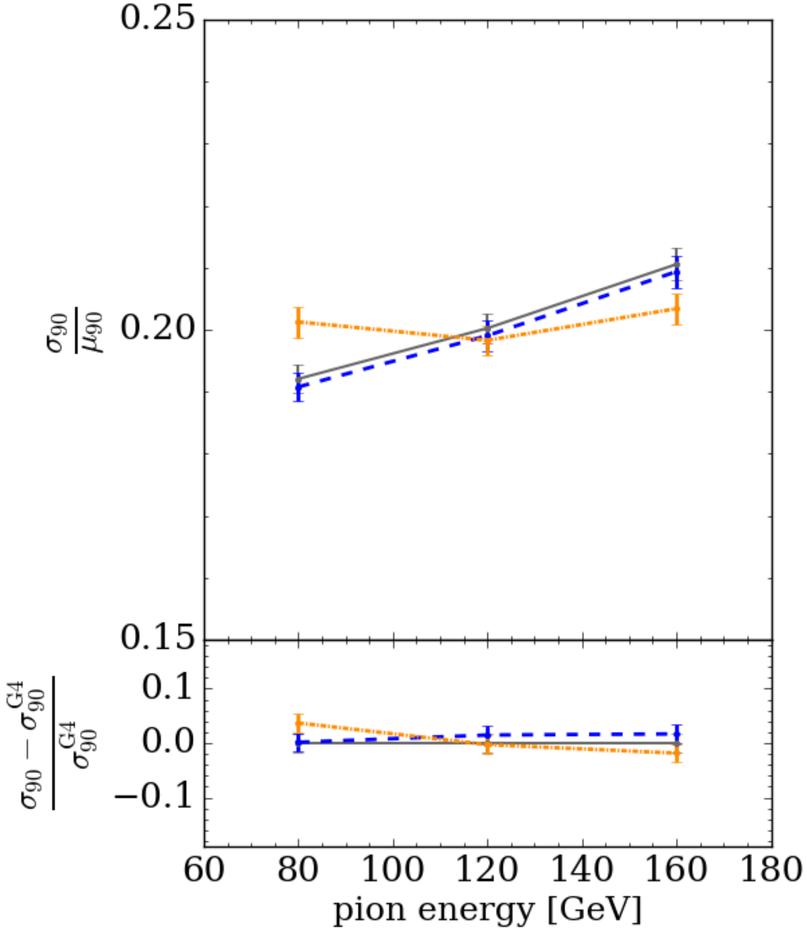


160GeV



Linearity and Resolution





Correlations

Testbeam

	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	1.00											
$m_{1,y}$	-0.13	1.00										
$m_{1,z}$	-0.04	-0.11	1.00									
$m_{2,x}$	-0.10	0.23	-0.19	1.00								
$m_{2,y}$	0.06	0.16	-0.21	0.64	1.00							
$m_{2,z}$	0.06	0.06	-0.46	0.32	0.36	1.00						
E_{vis}	0.04	-0.03	-0.63	-0.09	-0.08	0.12	1.00					
E_{inc}												
n_{hit}	0.05	0.00	-0.65	0.28	0.35	0.45	0.76		1.00			
E_1/E_{vis}	0.04	0.10	-0.93	0.18	0.19	0.49	0.48		0.53	1.00		
E_2/E_{vis}	-0.01	-0.05	0.44	-0.10	-0.10	-0.39	0.04		-0.05	-0.71	1.00	
E_3/E_{vis}	-0.04	-0.07	0.80	-0.13	-0.15	-0.23	-0.72		-0.69	-0.57	-0.17	1.00

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}
$m_{1,x}$	1.00											
$m_{1,y}$	-0.17	1.00										
$m_{1,z}$	-0.12	-0.10	1.00									
$m_{2,x}$	-0.36	0.42	-0.15	1.00								
$m_{2,y}$	-0.32	0.36	-0.14	0.84	1.00							
$m_{2,z}$	0.02	0.19	-0.39	0.30	0.36	1.00						
E_{vis}	0.27	-0.14	-0.60	-0.26	-0.25	0.07	1.00					
E_{inc}												
n_{hit}	0.21	-0.03	-0.67	0.00	0.11	0.51	0.70		1.00			
E_1/E_{vis}	0.14	0.10	-0.94	0.12	0.10	0.40	0.48		0.55	1.00		
E_2/E_{vis}	-0.09	-0.08	0.49	-0.06	-0.04	-0.31	-0.00		-0.10	-0.74	1.00	
E_3/E_{vis}	-0.11	-0.06	0.80	-0.11	-0.11	-0.22	-0.70		-0.70	-0.59	-0.11	1.00

Correlations

Testbeam - Geant4

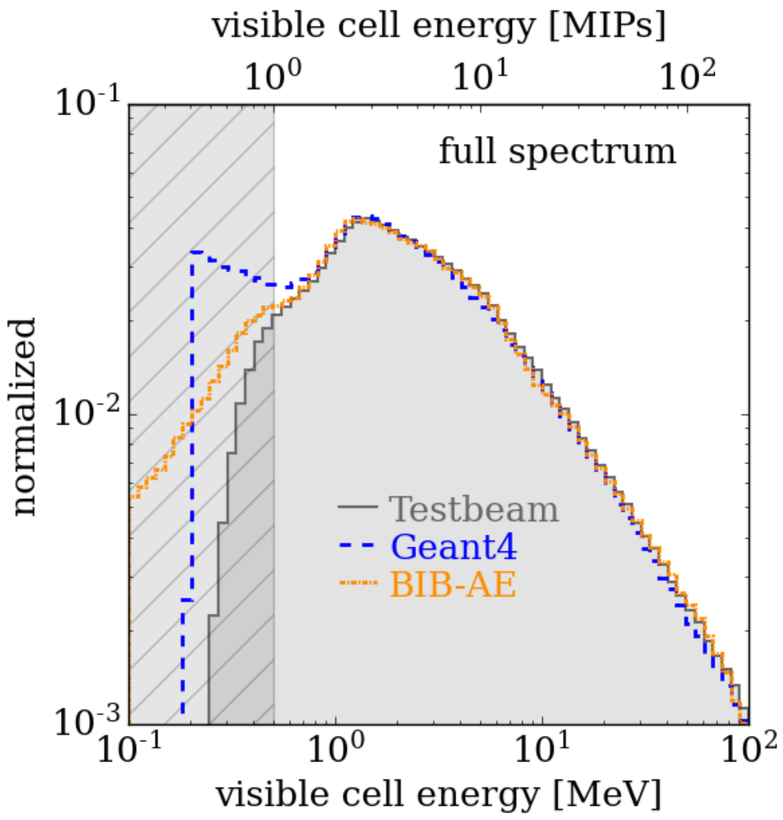
	$m_{1,x}$	$m_{1,y}$	$m_{1,z}$	$m_{2,x}$	$m_{2,y}$	$m_{2,z}$	E_{vis}	E_{inc}	n_{hit}	E_1/E_{vis}	E_2/E_{vis}	E_3/E_{vis}
$m_{1,x}$	0.00											
$m_{1,y}$	-0.08	0.00										
$m_{1,z}$	-0.08	-0.03	0.00									
$m_{2,x}$	-0.14	0.24	-0.11	0.00								
$m_{2,y}$	-0.04	0.14	-0.09	0.11	0.00							
$m_{2,z}$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

Testbeam - 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											
$m_{1,y}$	0.03	0.00										
$m_{1,z}$	0.06	0.05	0.00									
$m_{2,x}$	0.20	-0.16	-0.07	0.00								
$m_{2,y}$	0.26	-0.18	-0.07	-0.19	0.00							
$m_{2,z}$	0.00	-0.16	-0.01	-0.02	-0.04	0.00						
E_{vis}	-0.17	0.06	0.00	0.19	0.18	-0.06	0.00					
E_{inc}												
n_{hit}	-0.16	-0.03	0.04	0.28	0.23	-0.15	0.05		0.00			
E_1/E_{vis}	-0.08	-0.05	0.00	0.07	0.09	0.04	-0.01		-0.05	0.00		
E_2/E_{vis}	0.06	0.04	0.00	-0.04	-0.08	-0.09	0.00		0.03	-0.00	0.00	
E_3/E_{vis}	0.05	0.03	-0.00	-0.05	-0.04	0.06	0.00		0.03	0.01	-0.00	0.00

Conclusion

- First time training generative model on real measurement data
  - Generative model surpasses Geant4 accuracy for some observables
  - Significantly faster than Geant4
- Work ongoing to improve model
- Very exciting results already



Thank you