# Generative Models for Fast (Calorimeter) Simulation

ACAT 2022

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Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

CLUSTER OF EXCELLENCE QUANTUM UNIVERSE

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

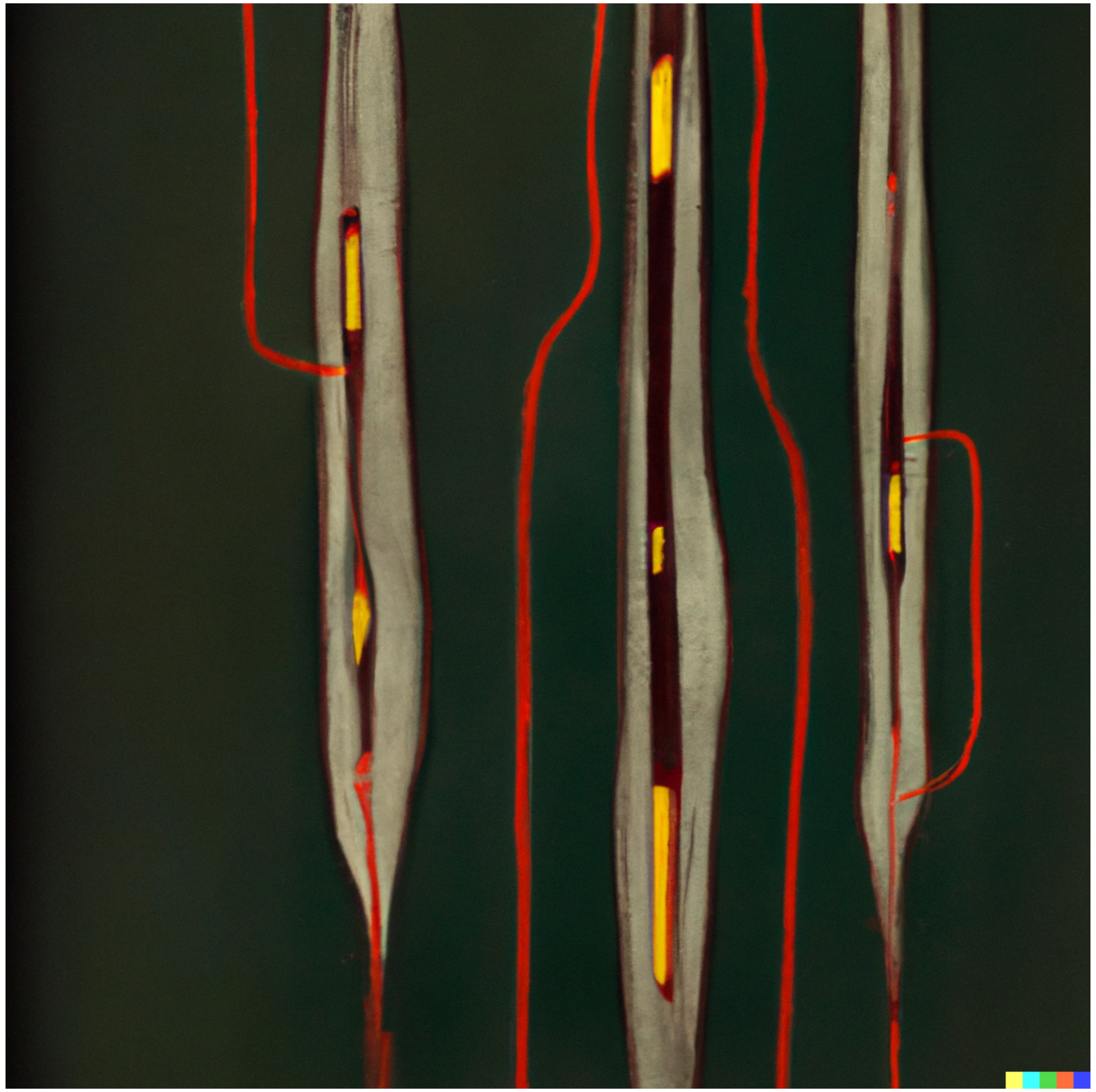
DESY.

# Generative Models

- Learn underlying distribution of data
- Produce realistic new samples
- Recently gained notoriety for AI art generation (Dall-E 2, Imagen, Midjourney)

GOOGLE IMAGEN AI

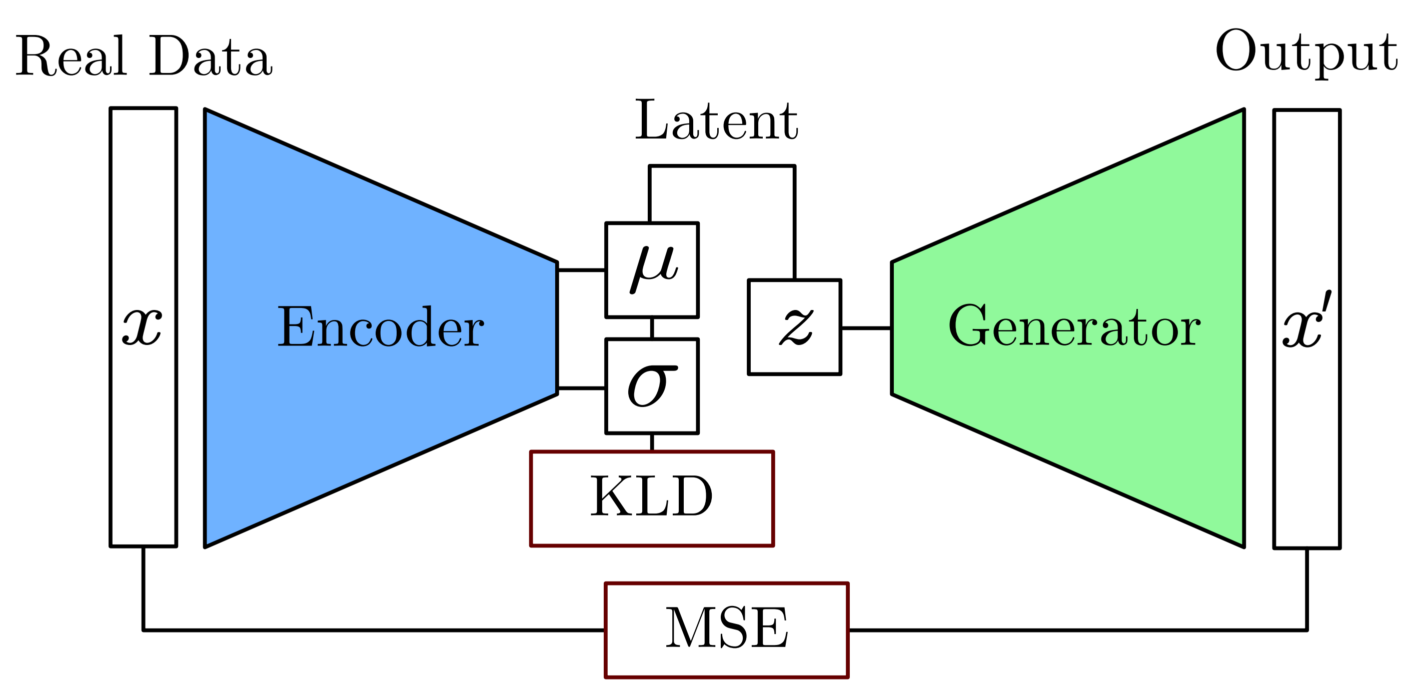
DALL·E 2



**plasma accelerators in the syle of Egon Schiele**, Dall-E 2

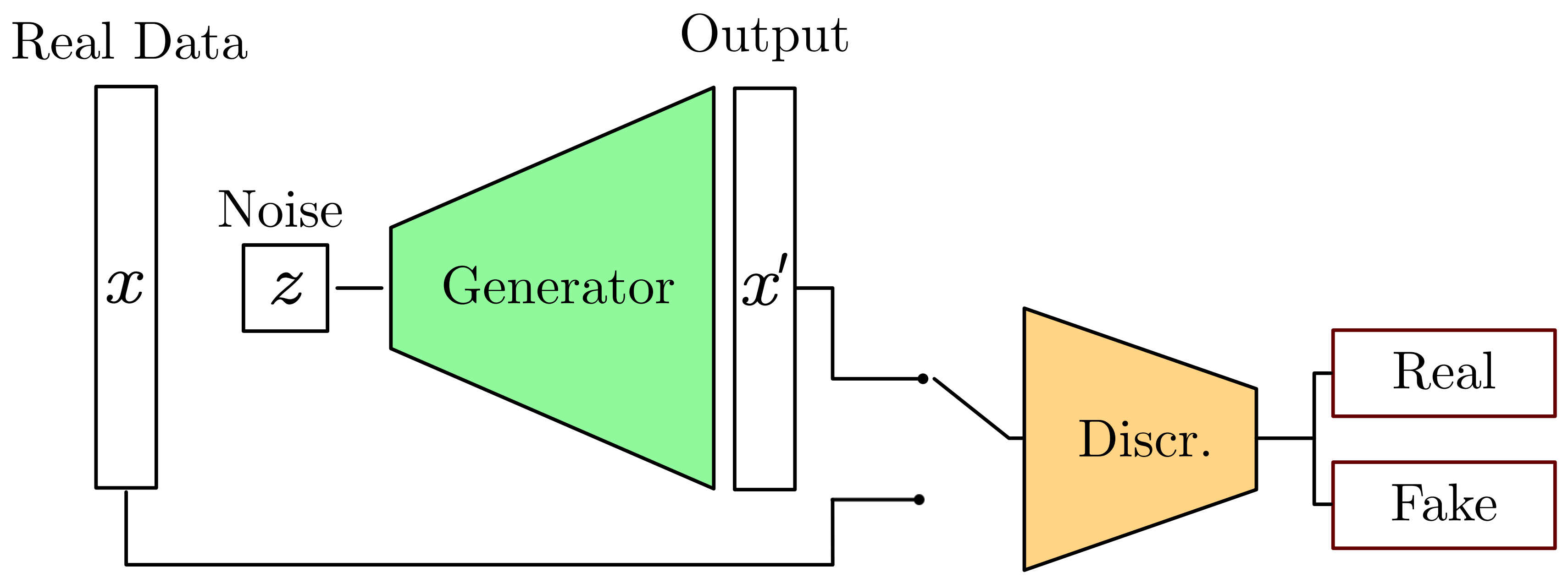
# Generative Model Types

## Variational Autoencoder (VAE)



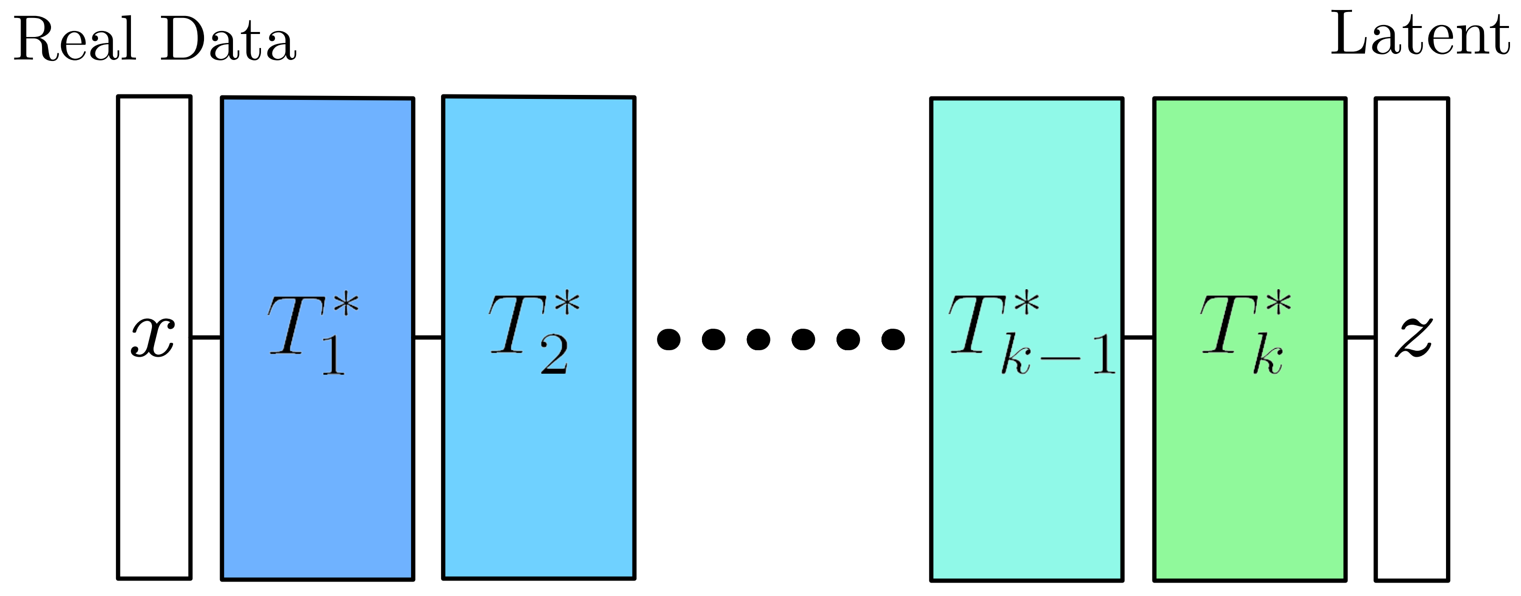

- Use encoder/decoder pair
- Map data to regular Gaussians
- Decoder generates samples

## Generative Adversarial Network (GAN)




- Use generator/discriminator pair
- Discriminator trains generator
- Generator produces samples

## Normalizing Flow




- Use invertible network
- Map data to regular gaussians
- Inverse generates samples

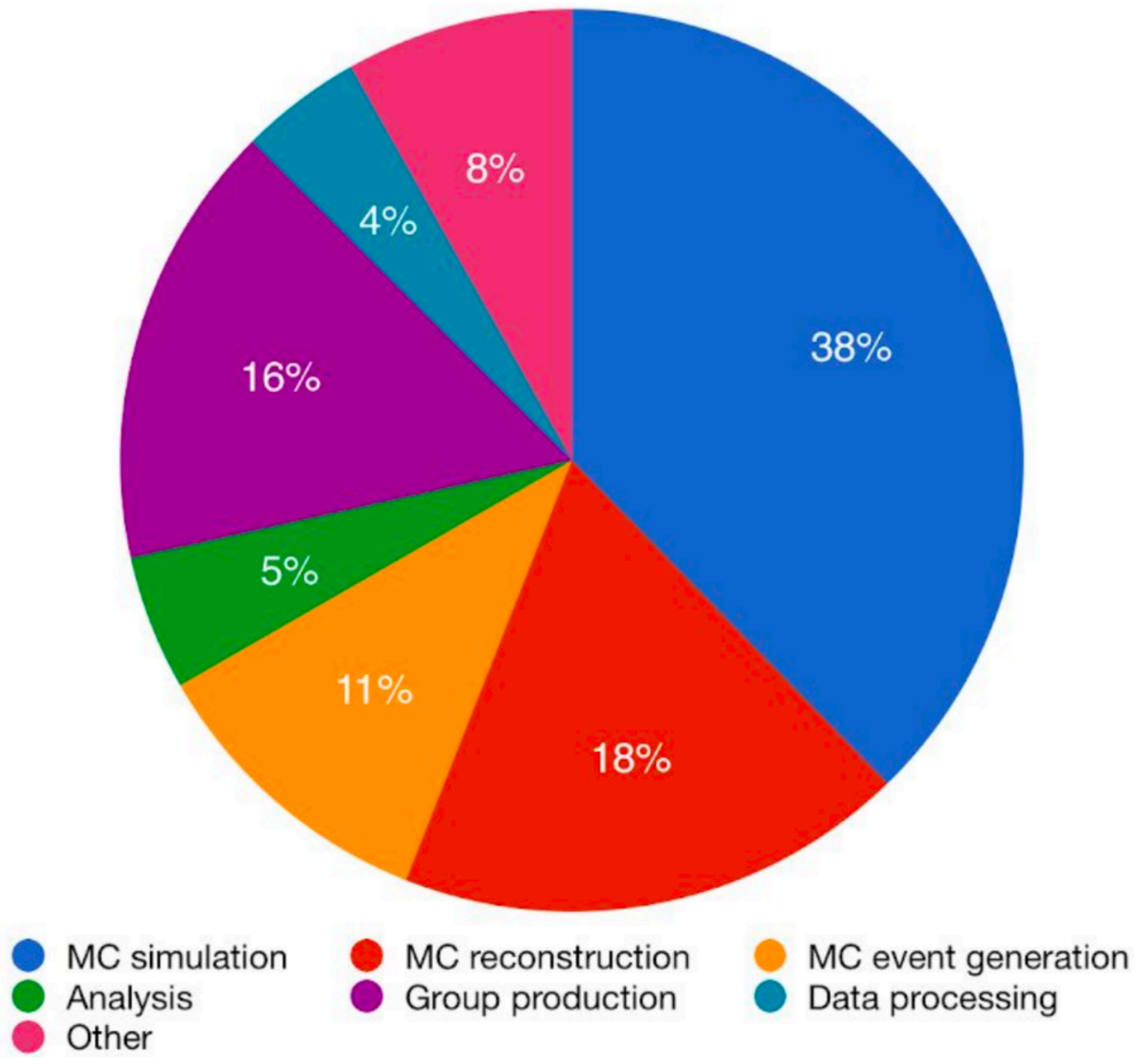
Additionally: diffusion models

DP. Kingma et al.: **An Introduction to Variational Autoencoders** (2019), 1906.02691

I. Goodfellow et al.: **Generative Adversarial Networks** (2014), 1406.2661

G. Papamakarios et al.: **Normalizing Flows for Probabilistic Modeling and Inference** (2019), 1912.02762

# Generative 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

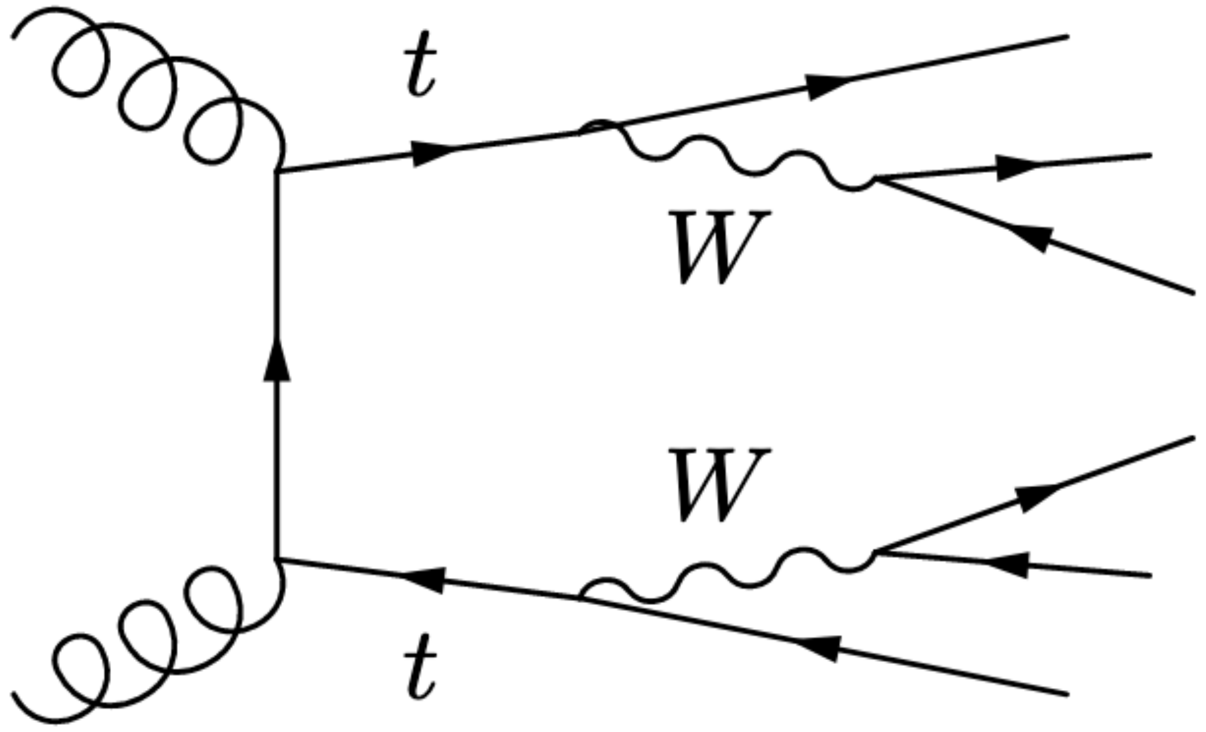
➔Significantly faster

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

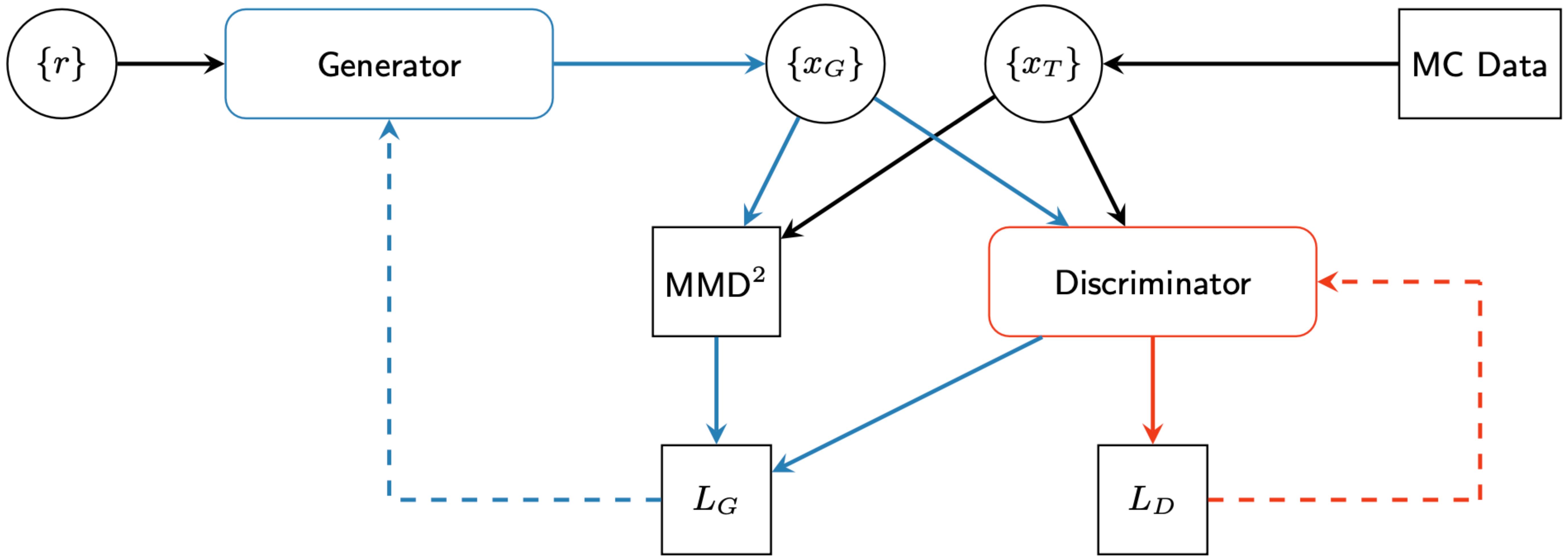
# Generative Simulation

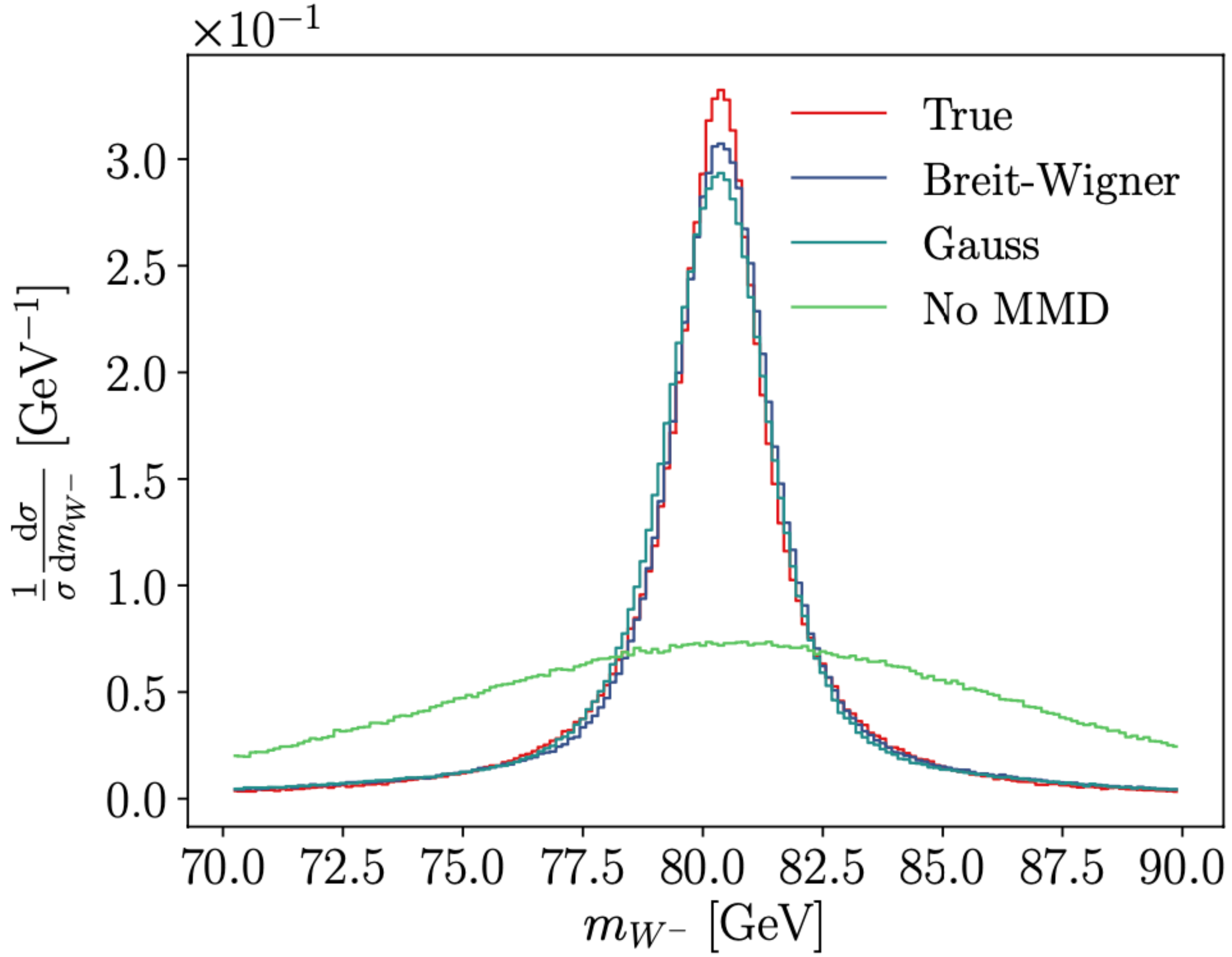
Low-dimensional
fixed structures



# Low-Dim Fixed Structure

- Generation of event 4-momenta, ordered list, O(10) dimensions
- Using GAN model with additional MMD loss for mass peaks

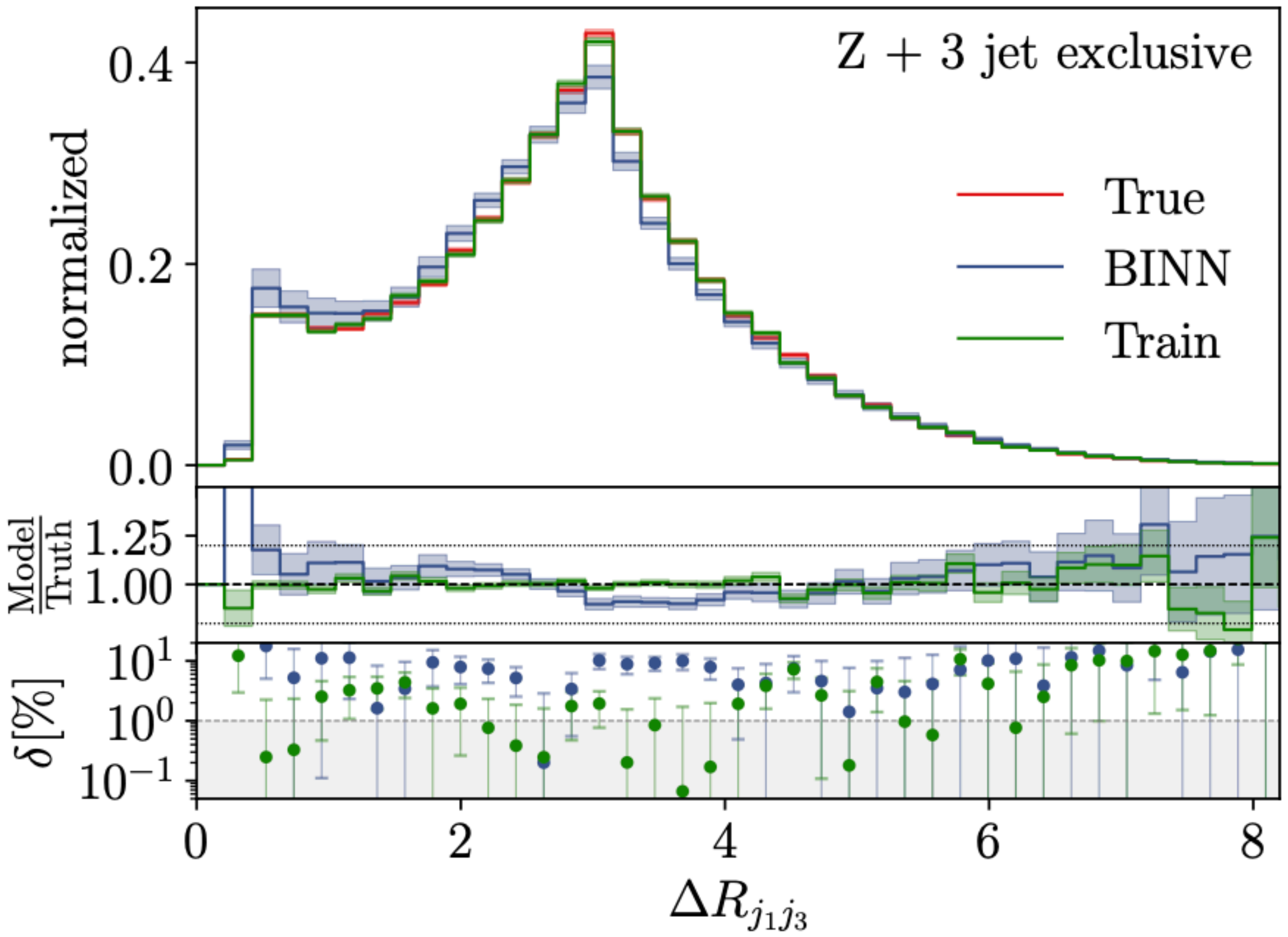


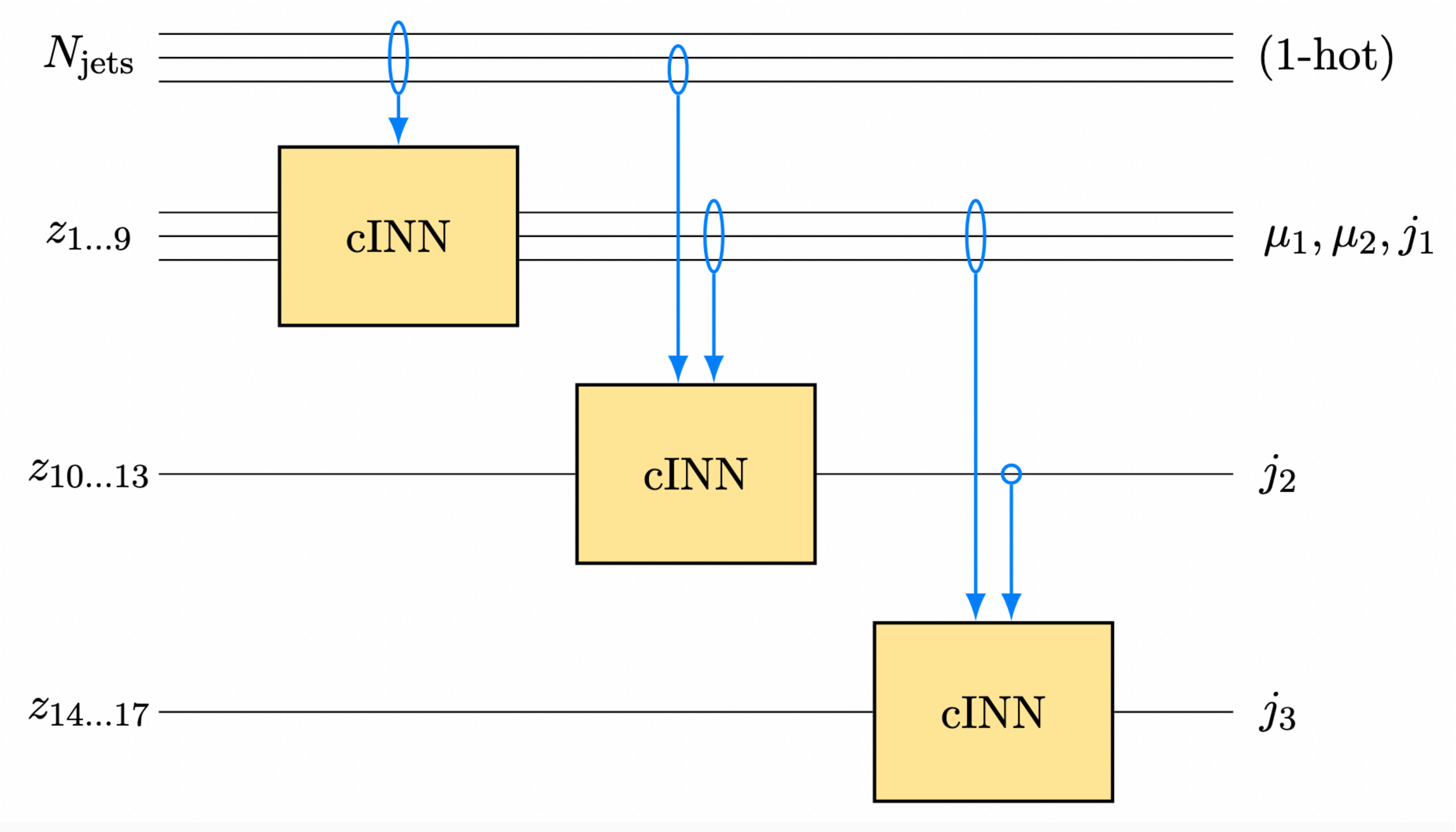




Butter et al.: **How to GAN LHC Events:** (2019), [1907.03764]

# Low-Dim Fixed Structure

- Normalizing flow approach improves precision
- Bayesian network enables uncertainty estimation

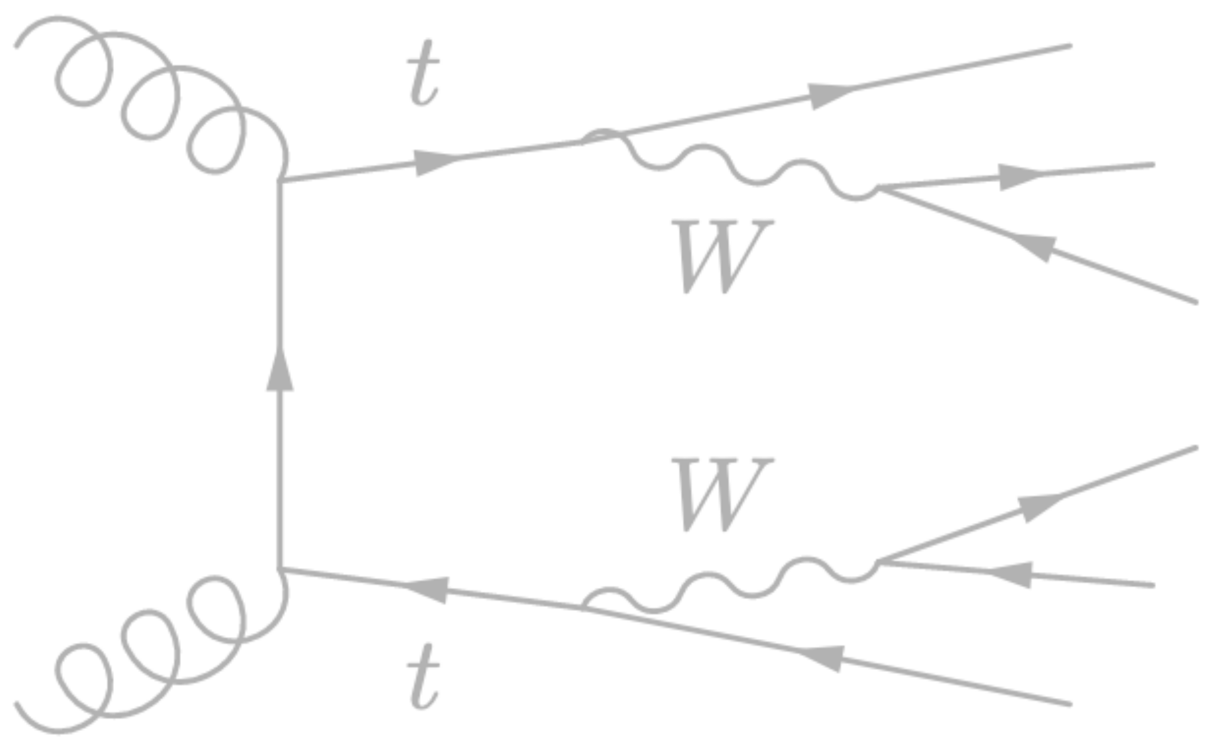


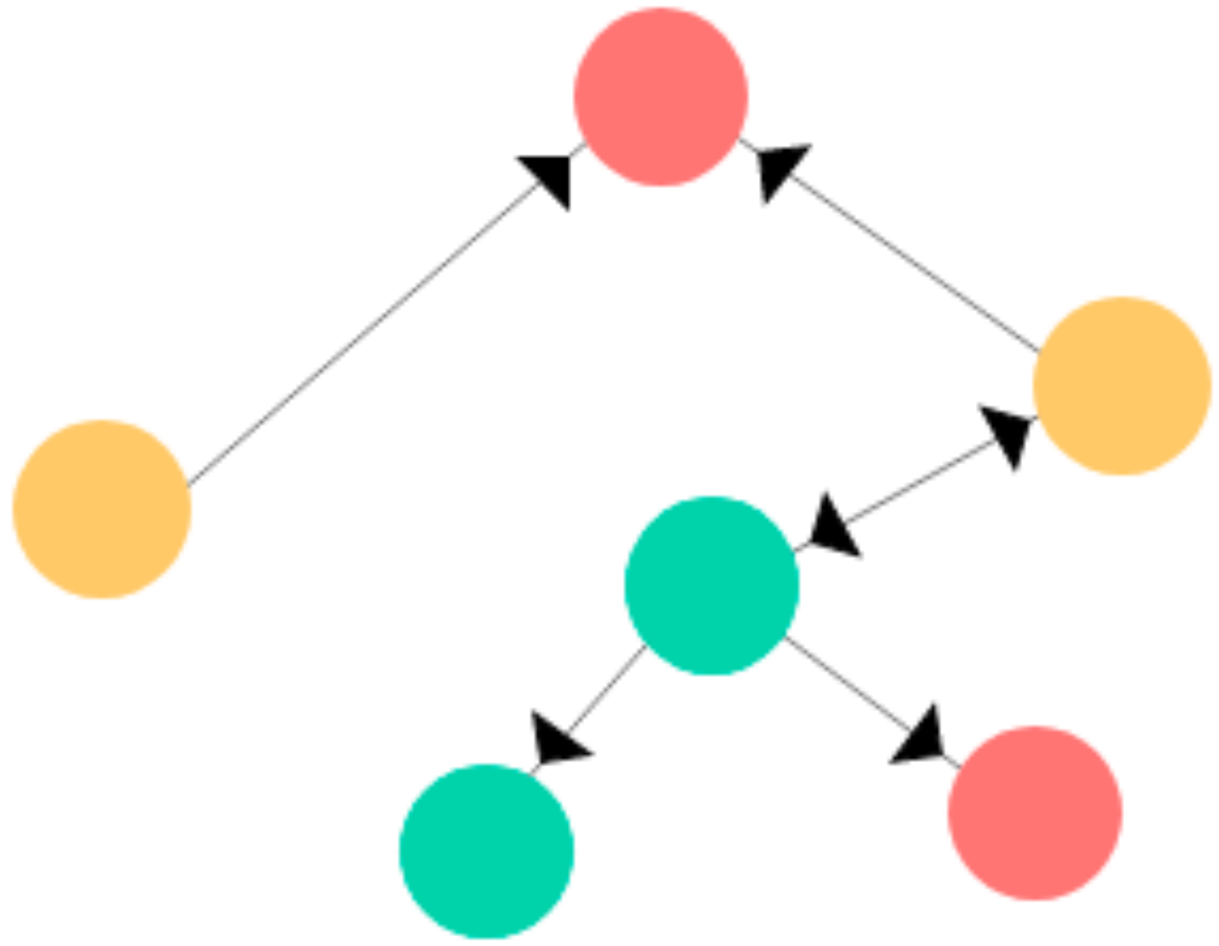

Butter et al.: **Generative Networks for Precision Enthusiasts** (2021), [2110.13632]

# Generative Simulation

Low-dimensional
fixed structures

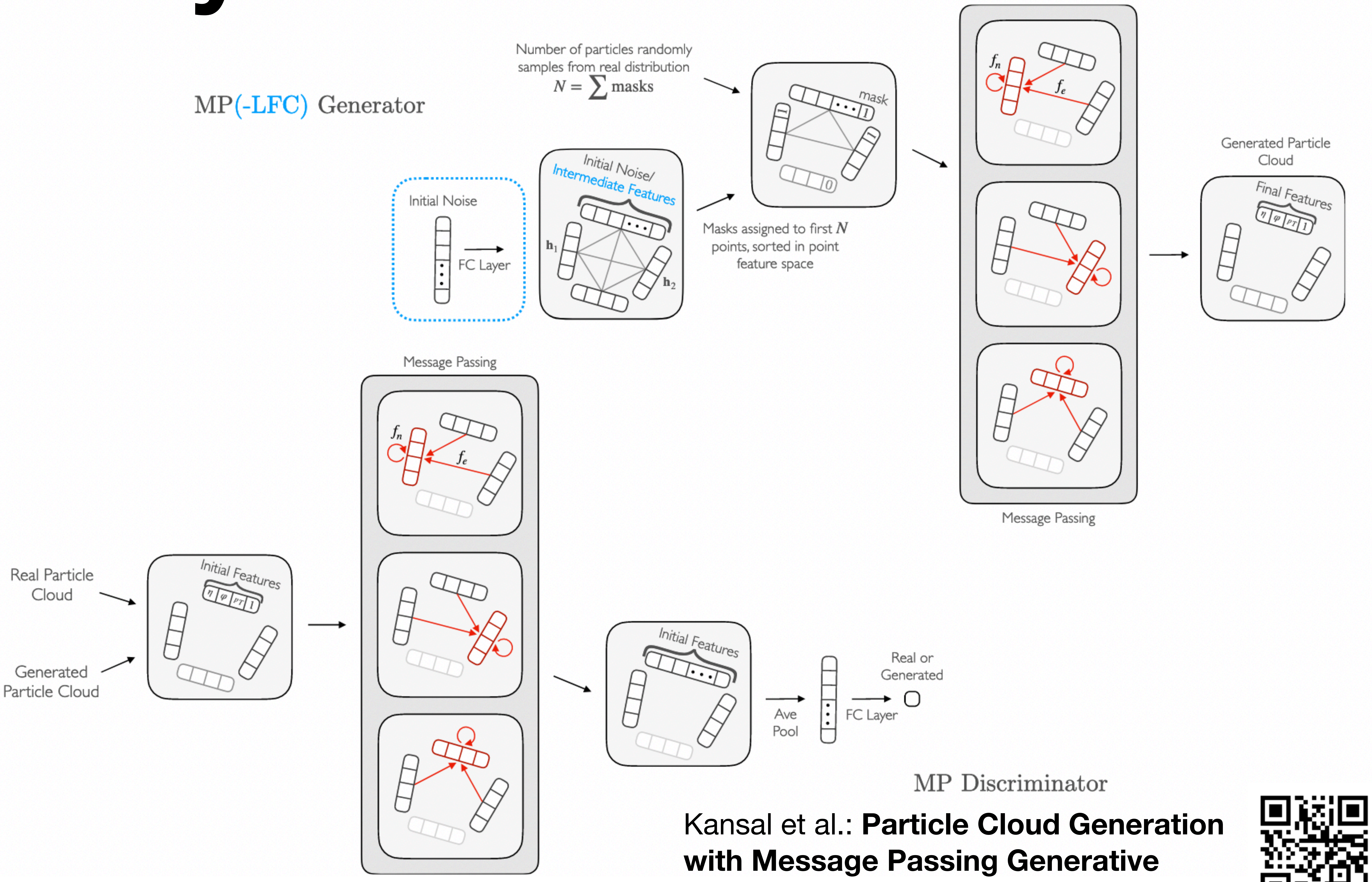



Low-dimensional
dynamic strutures



# Low-Dim Dynamic Structure

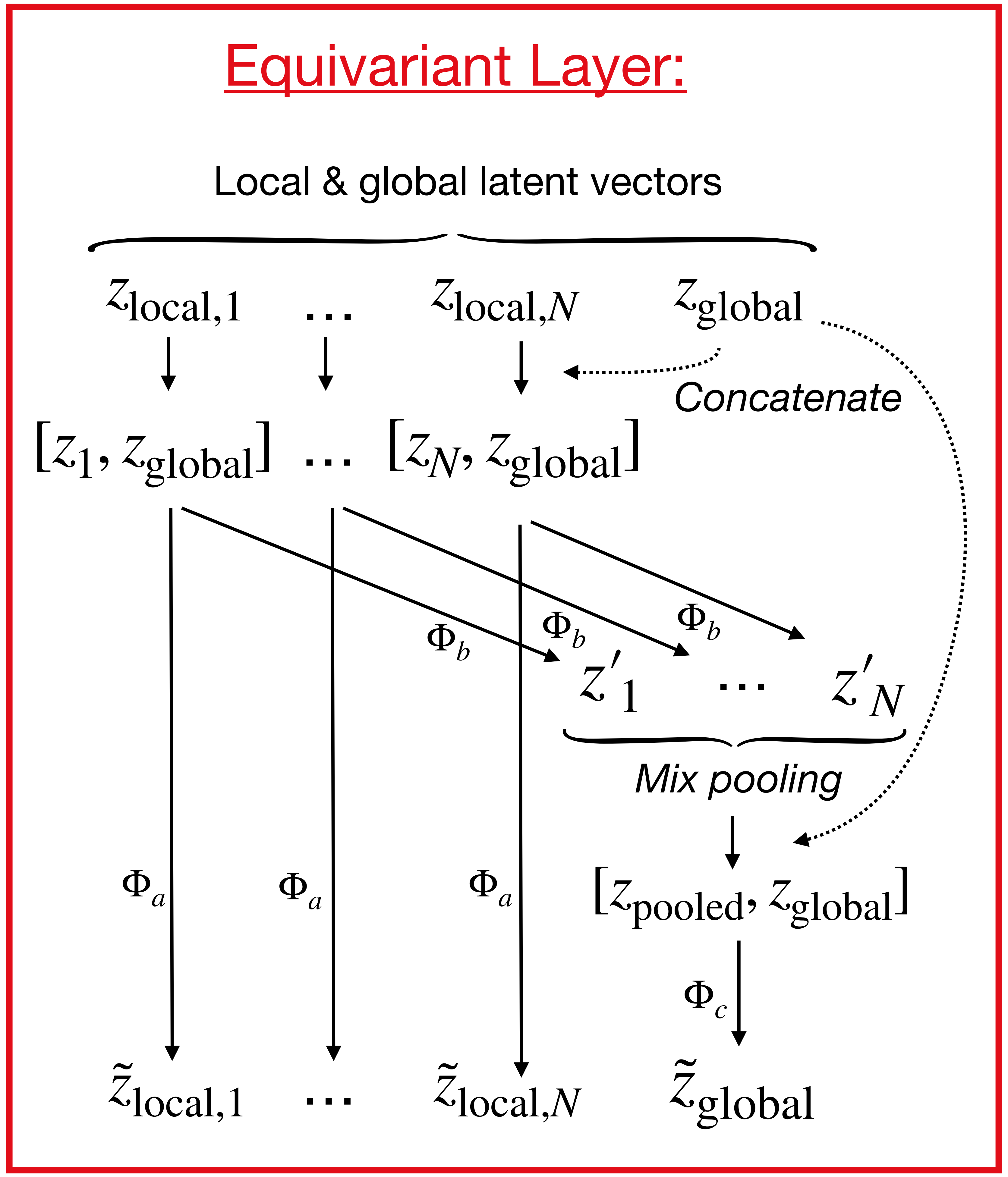
- Point-cloud/graph methods
- Enable variable output sizes
- Not bound to fixed geometries
- e.g. hadronization with message passing GANs

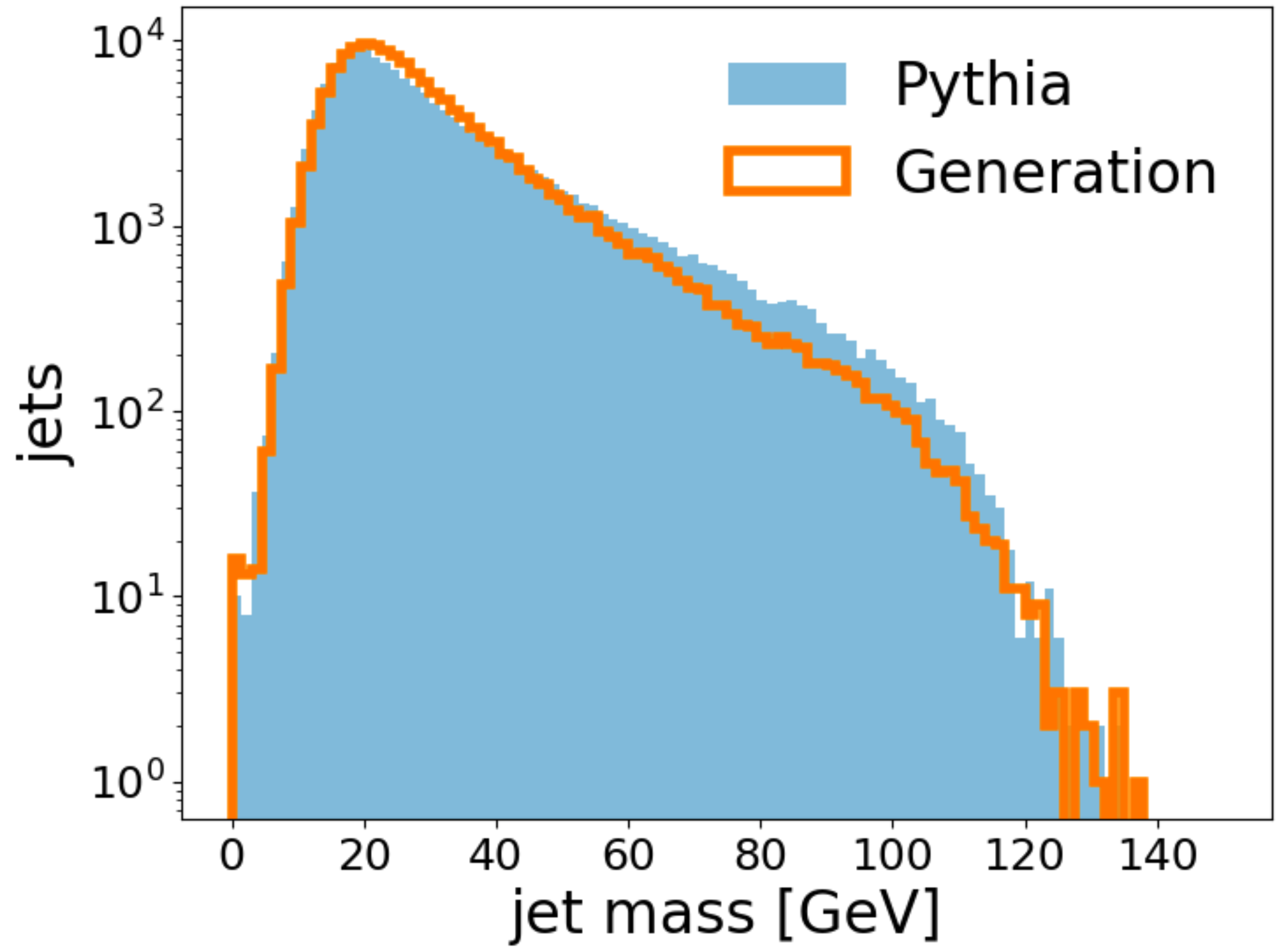


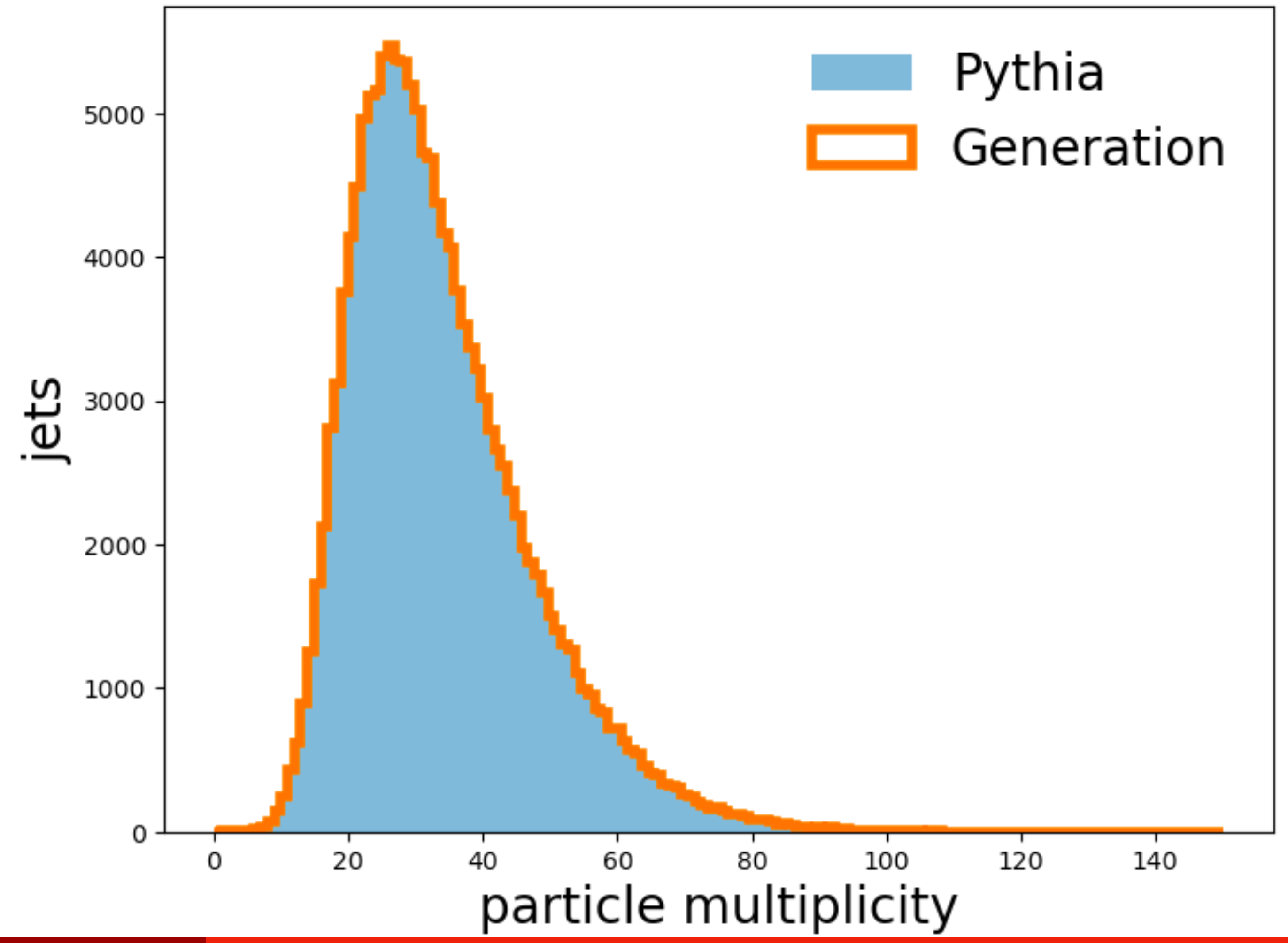

Kansal et al.: **Particle Cloud Generation with Message Passing Generative Adversarial Networks** (2021), [2106.11535](2106.11535)

# Low-Dim Dynamic Structure

- Deep set approach for jets simulation
- Permutation invariant setup
- More details: talk by E. Buhman @ML4jets 2022, next week

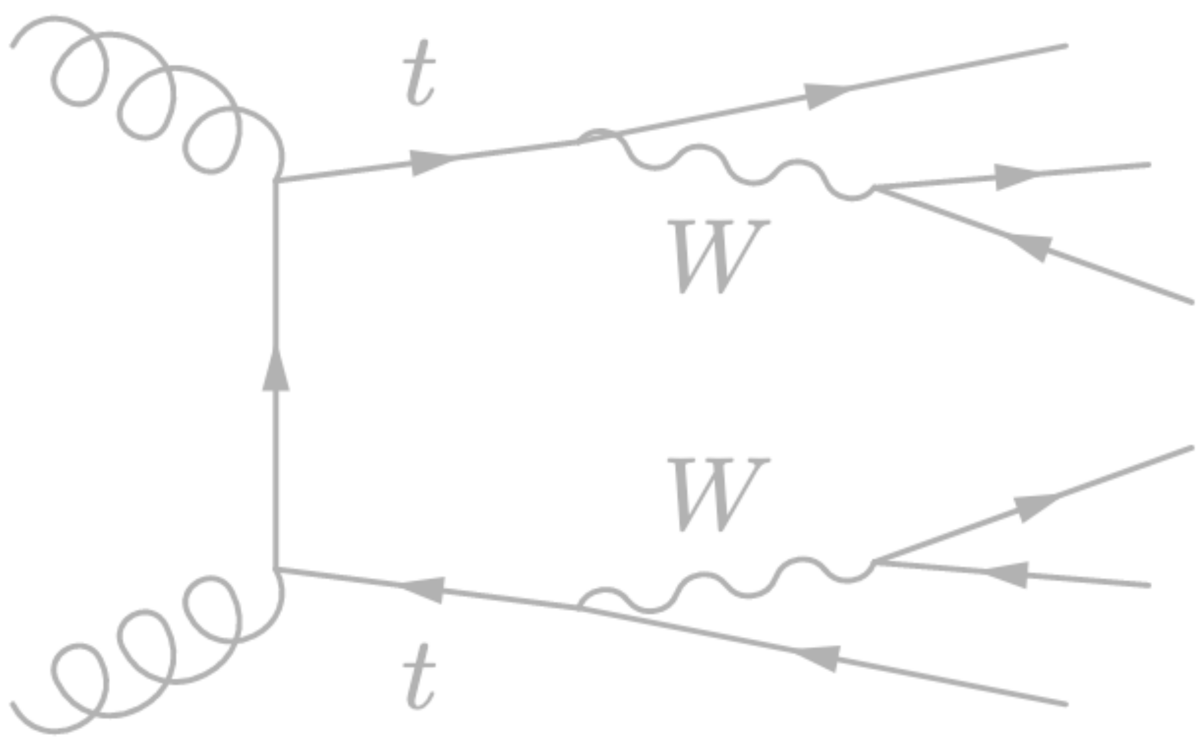


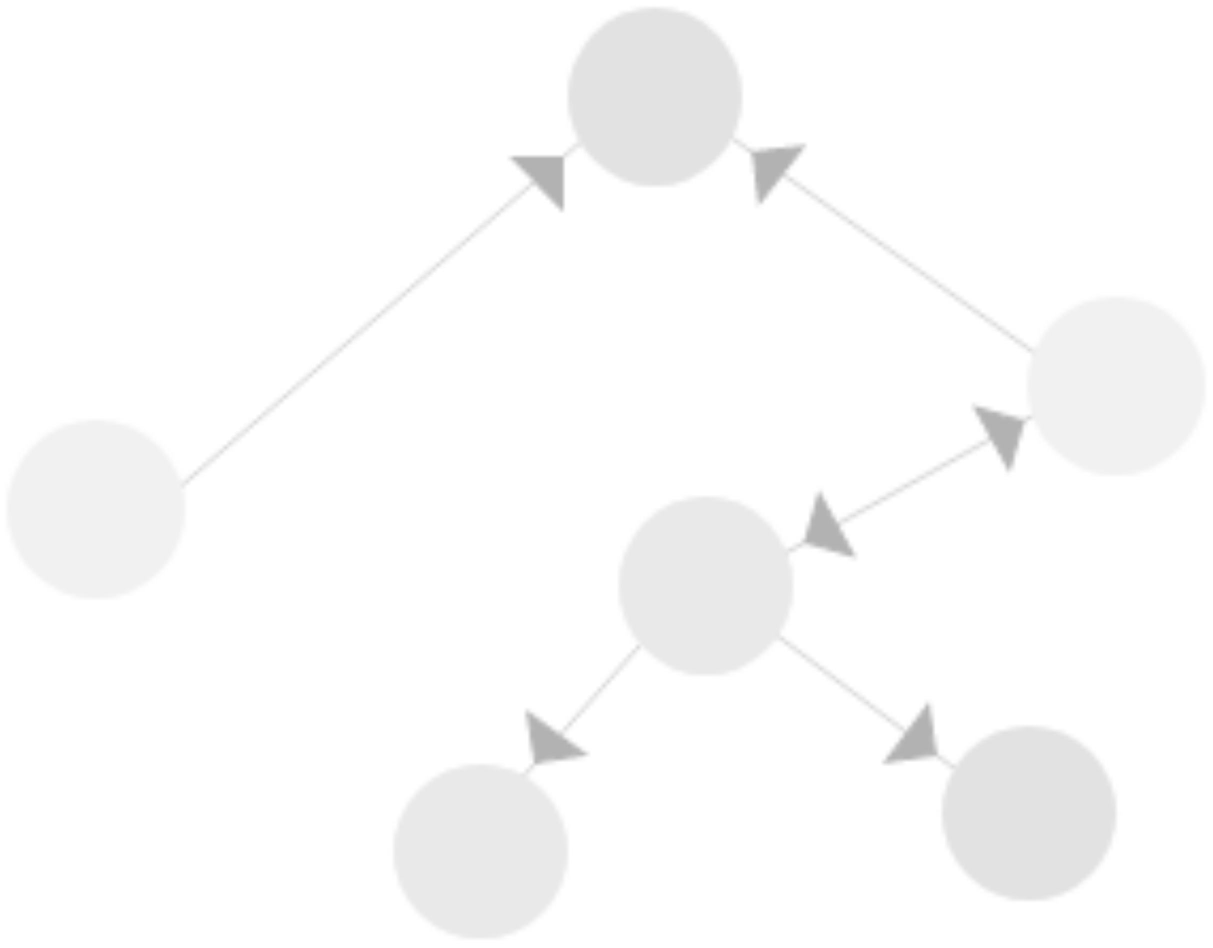



# Generative Simulation

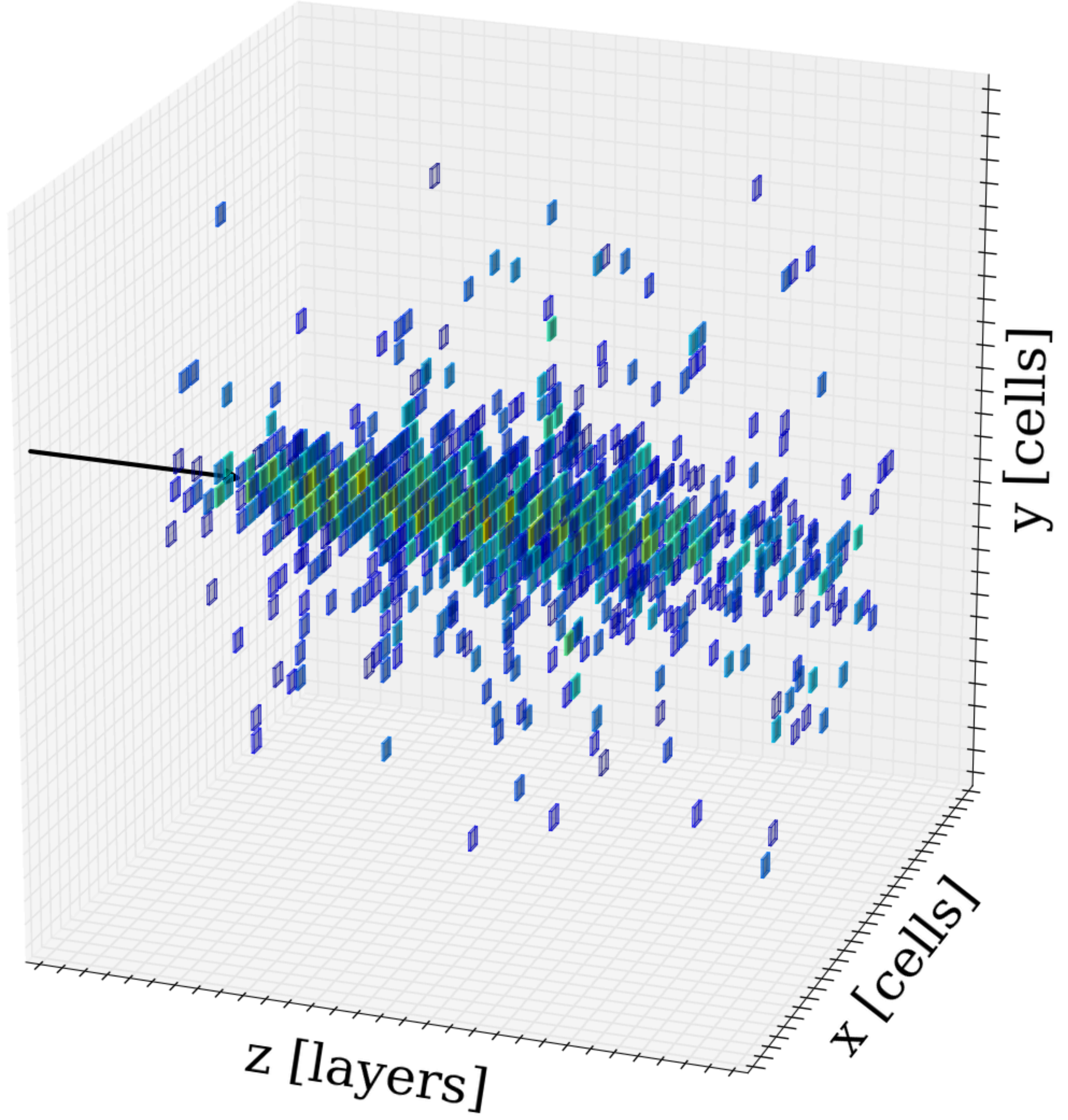
Low-dimensional fixed structures




Low-dimensional dynamic strutures

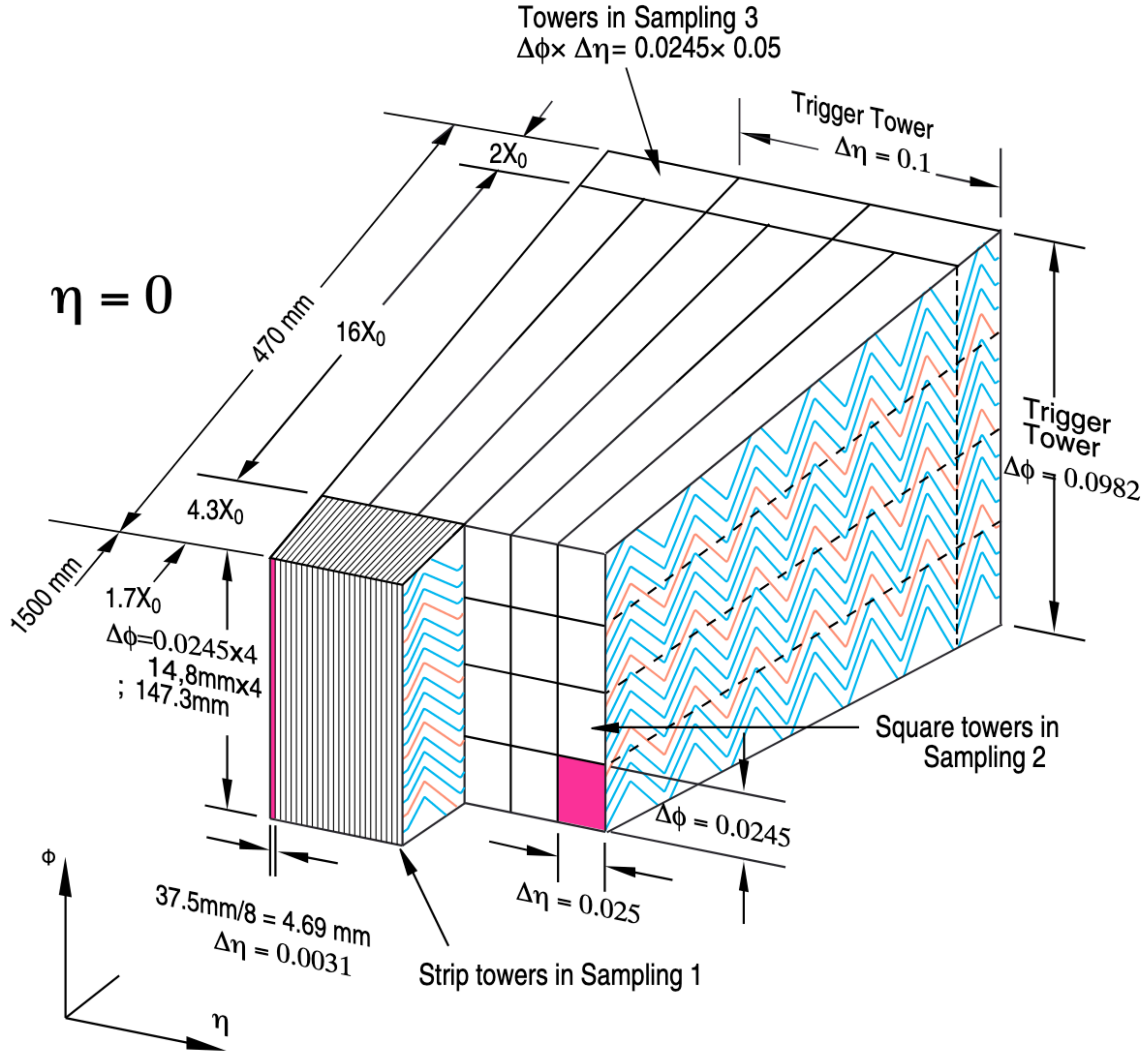


High-dimensional fixed structures



# High-Dim Fixed Structure

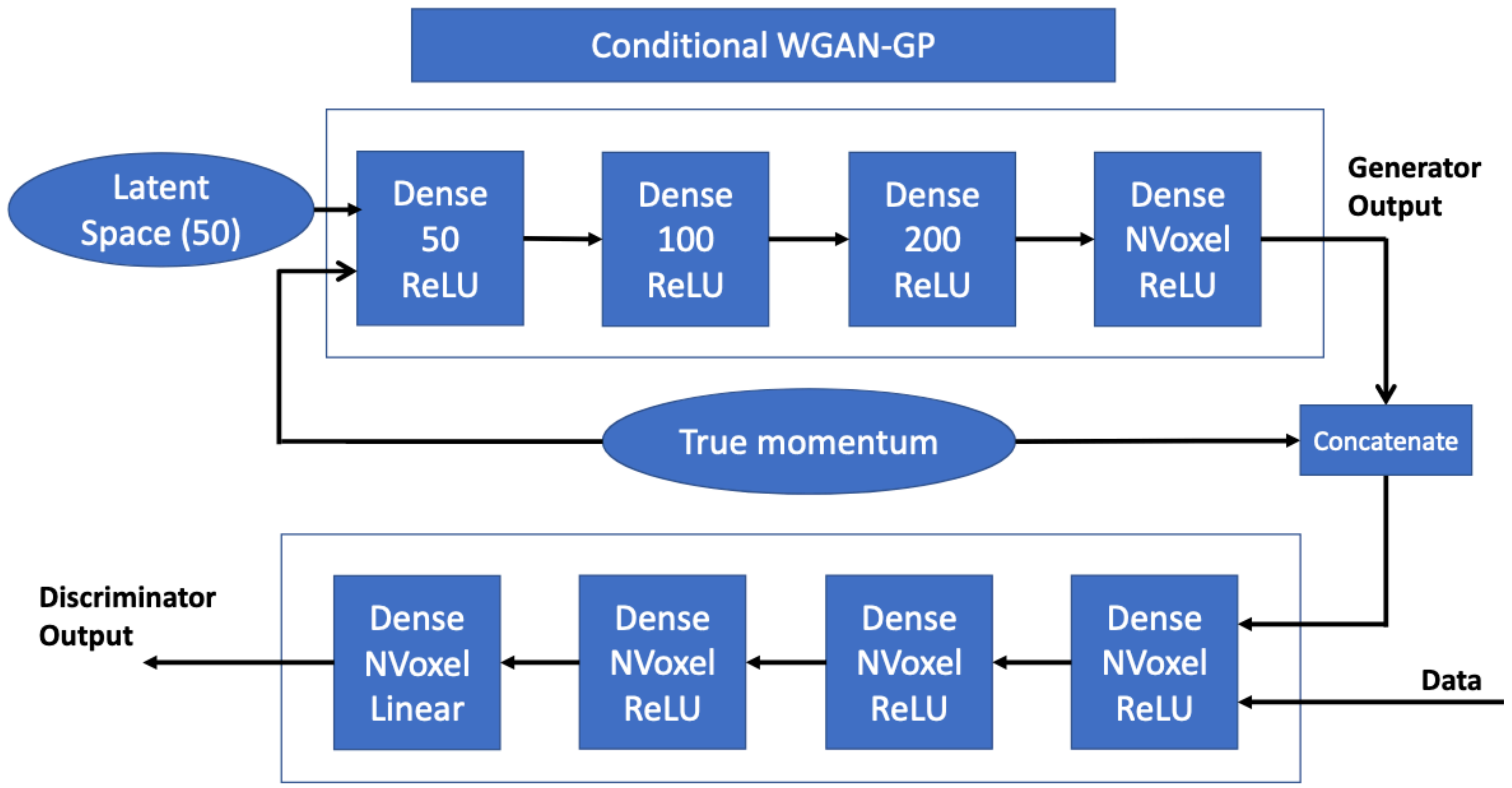
- Fixed output geometry O(100-10,000) dimensions
- Common in detector simulation, e.g. ATLAS FastCaloGAN
- Already in use for fast simulation of calorimeter showers

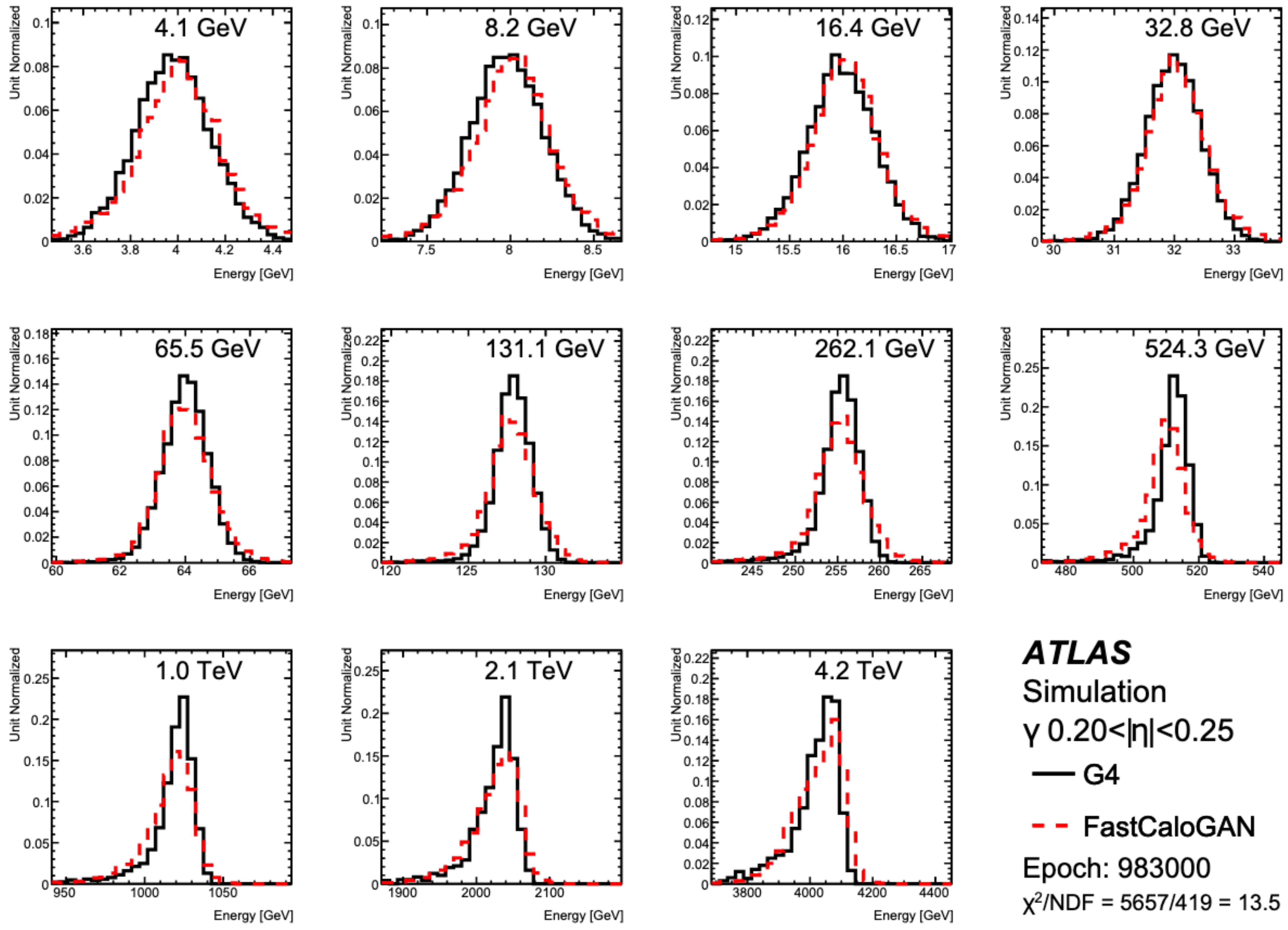



ATLAS Collaboration, **AtlFast3: the next generation of fast simulation in ATLAS** (2021), [2109.02551](2109.02551)

# High-Dim Fixed Structure

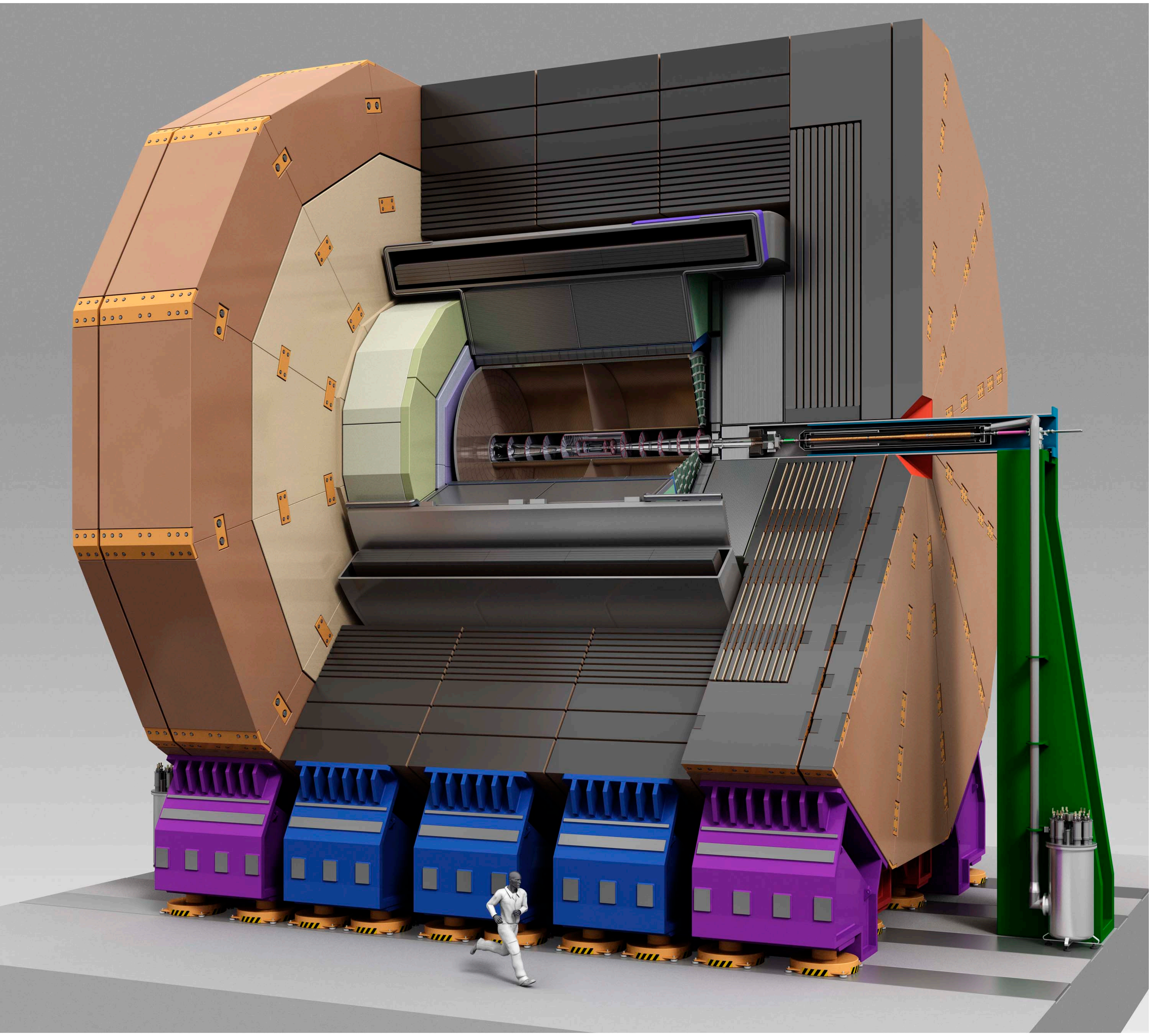
- ATLAS FastCaloGAN
- 300 total networks for particle types and $\eta$ slices



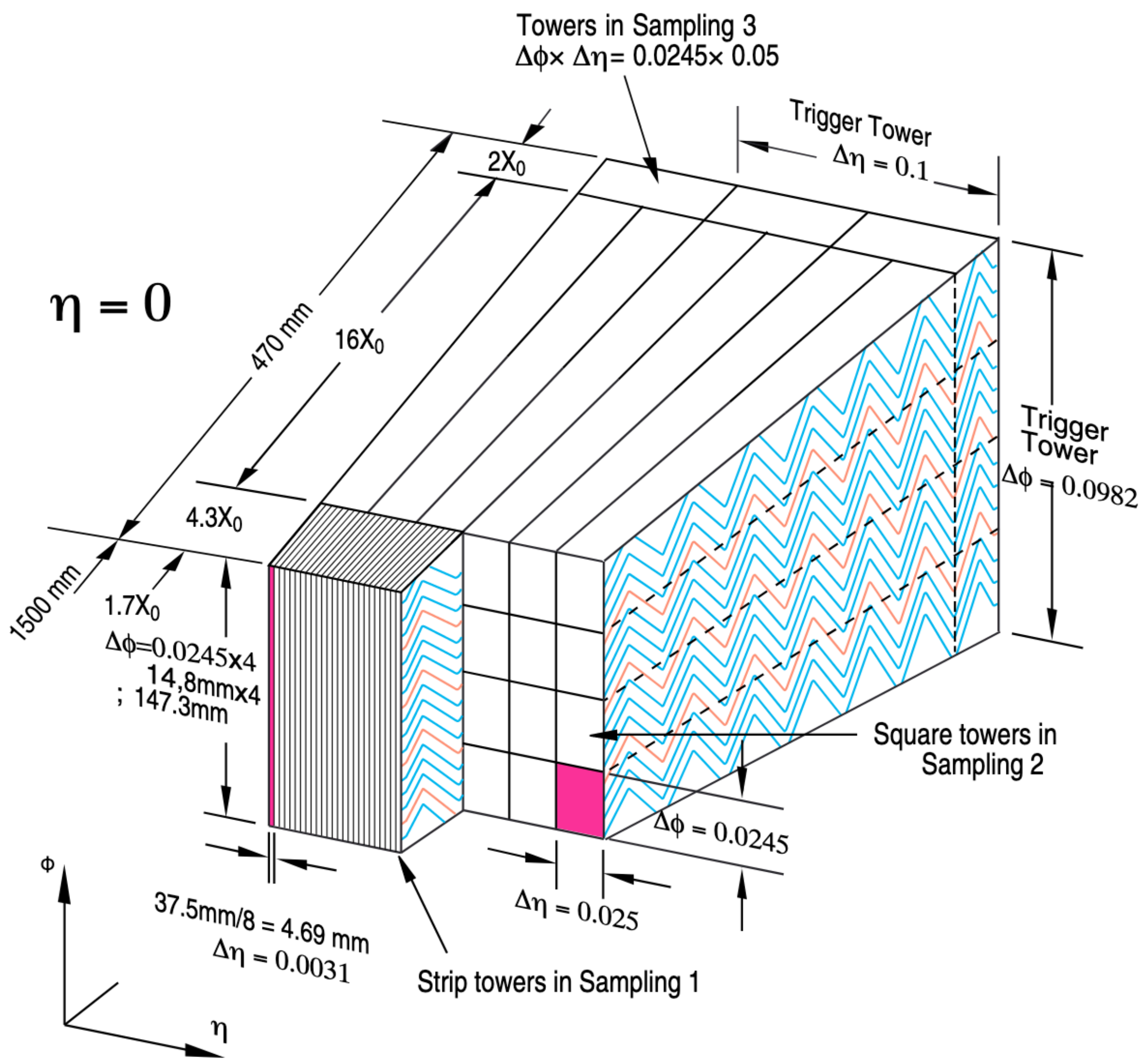

ATLAS Collaboration, **AtlFast3: the next generation of fast simulation in ATLAS** (2021), [2109.02551](https://arxiv.org/abs/2109.02551)

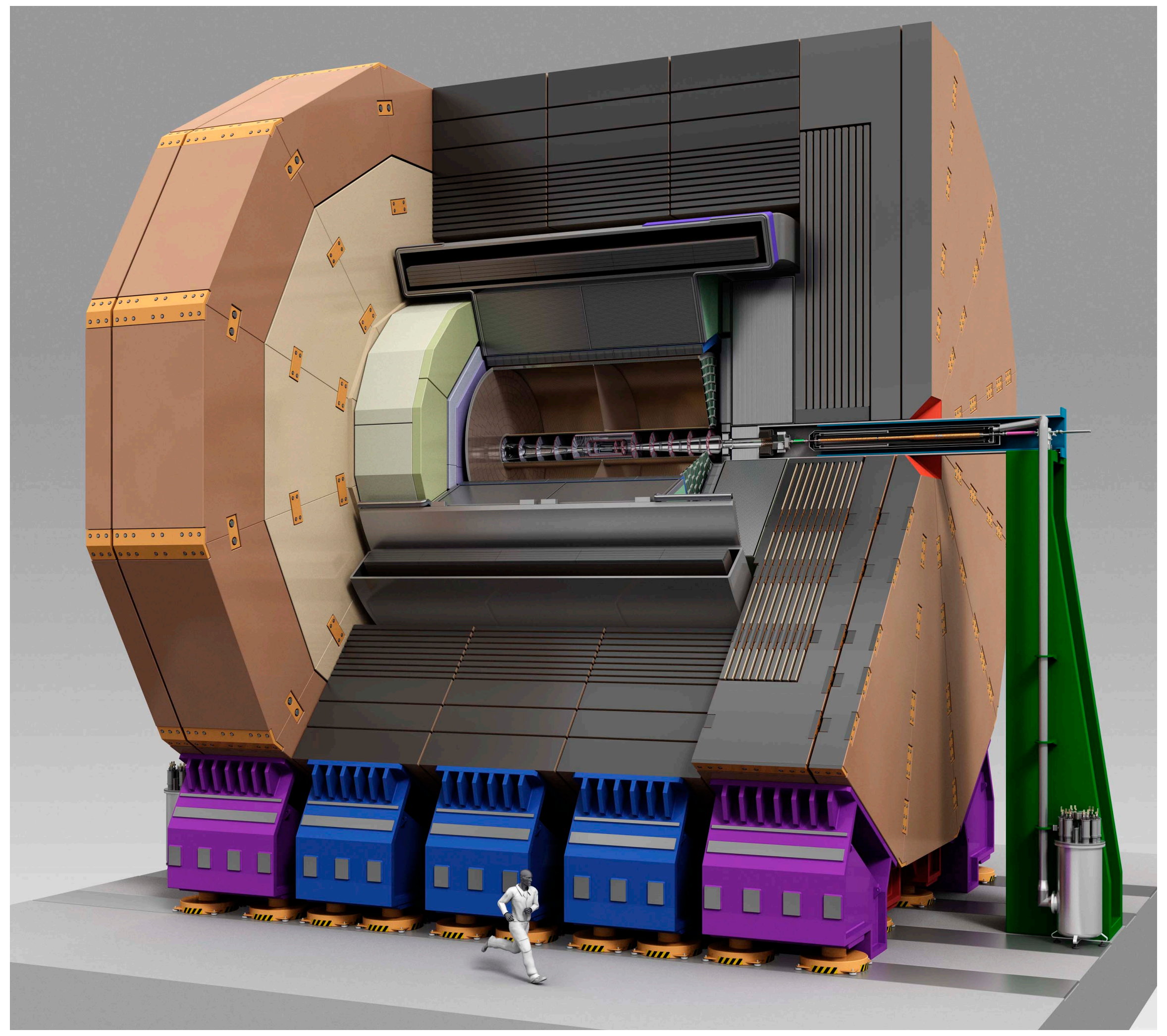
# ILD Calorimeters



- International Large Detector (ILD)
  - Proposed International Linear Collider
- ILD electromagnetic calorimeter
  - Active silicon, passive tungsten
  - 30 layers, 5mm x 5mm cells
- ILD hadronic calorimeter
  - Active scintillator, passive iron
  - 48 layers, 30mm x 30mm cells

# Calorimeter Simulation



## ATLAS ECAL

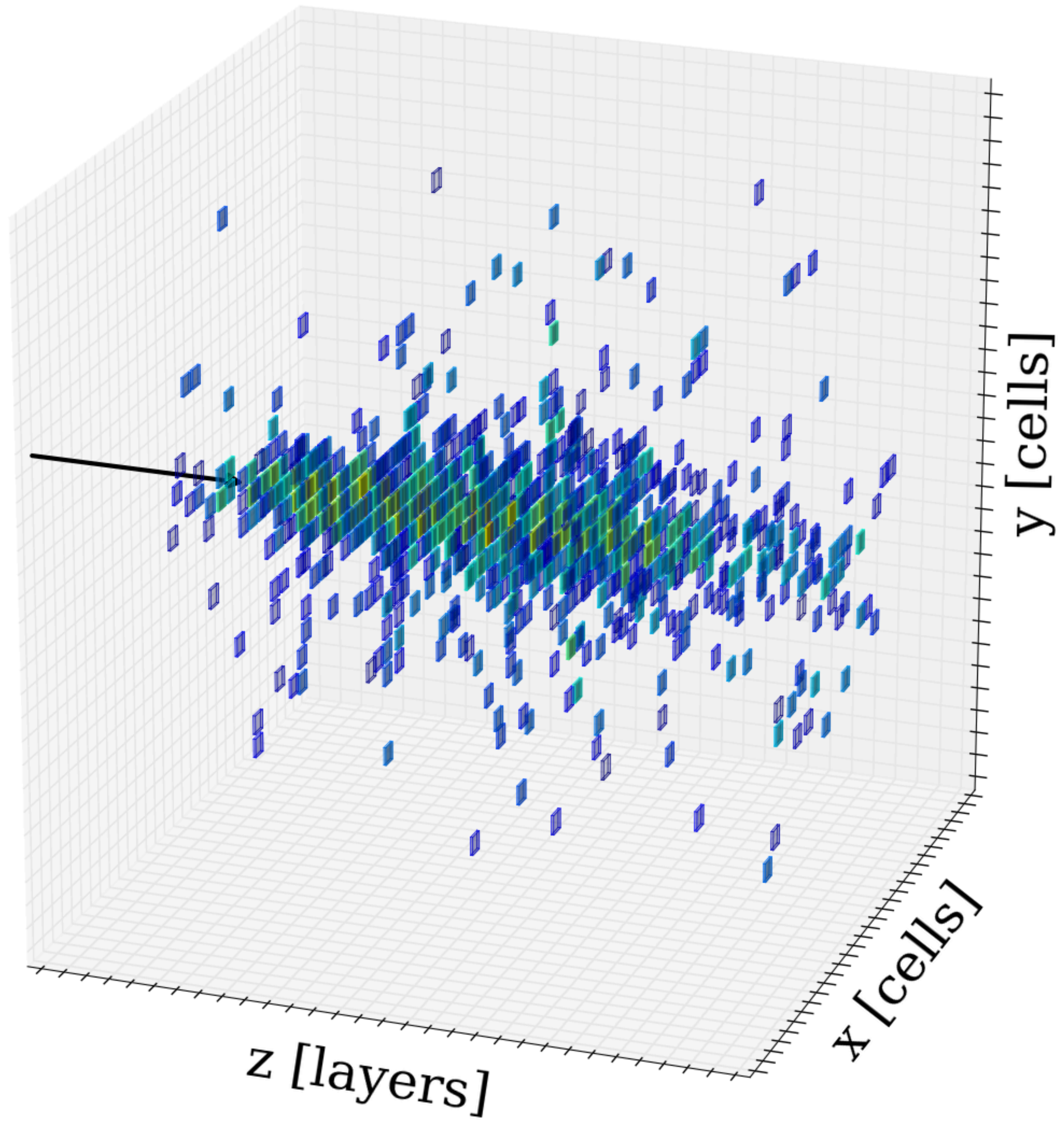
- 3 layers + pre-sampler
- 110,000 channels total
- 266 channel segments used in generative models

## ILD ECAL / HCAL

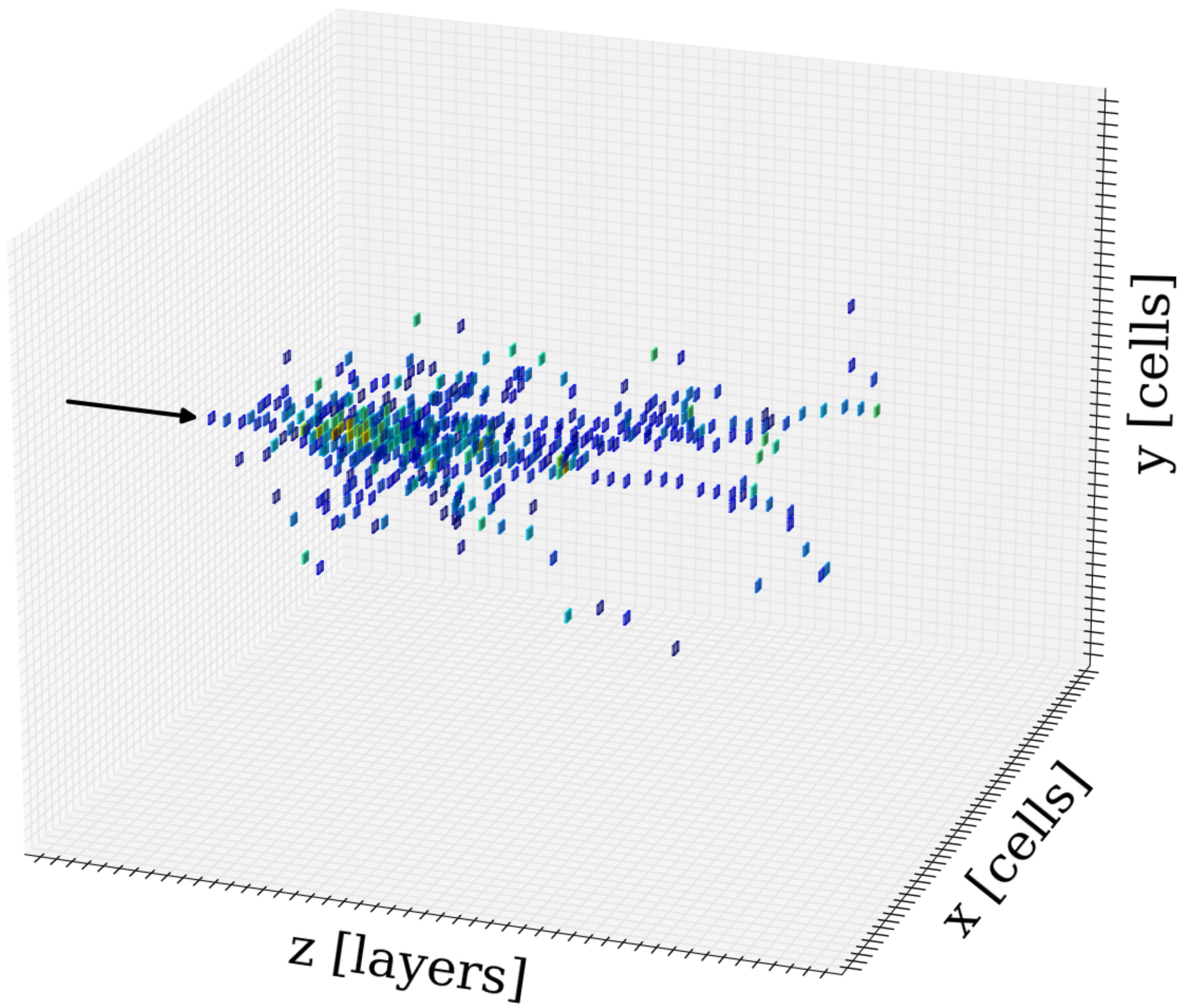
- 30 / 48 layers
- 100,000,000 / 8,000,000 total channels
- 27,000 / 30,000 channel segment using in generative models

# Shower Dataset

**Photon shower**




**Charged pion shower**




Training data:

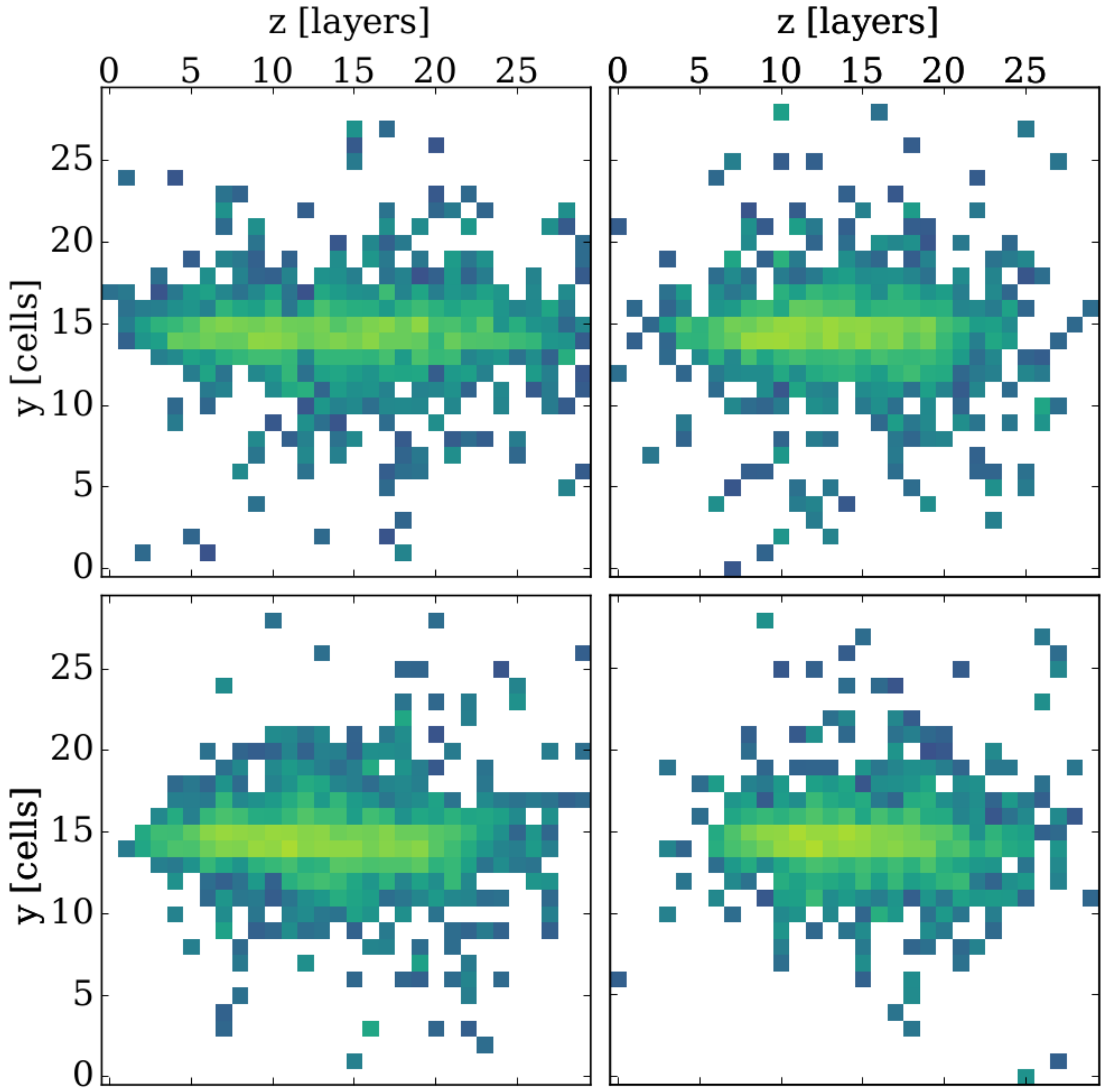
- Photons / charged Pions
- 1 million / 500k showers
- 10 to 100 GeV
- Fixed incident point & angle
- Project to grid
- 30×30×30 / 25×25×48

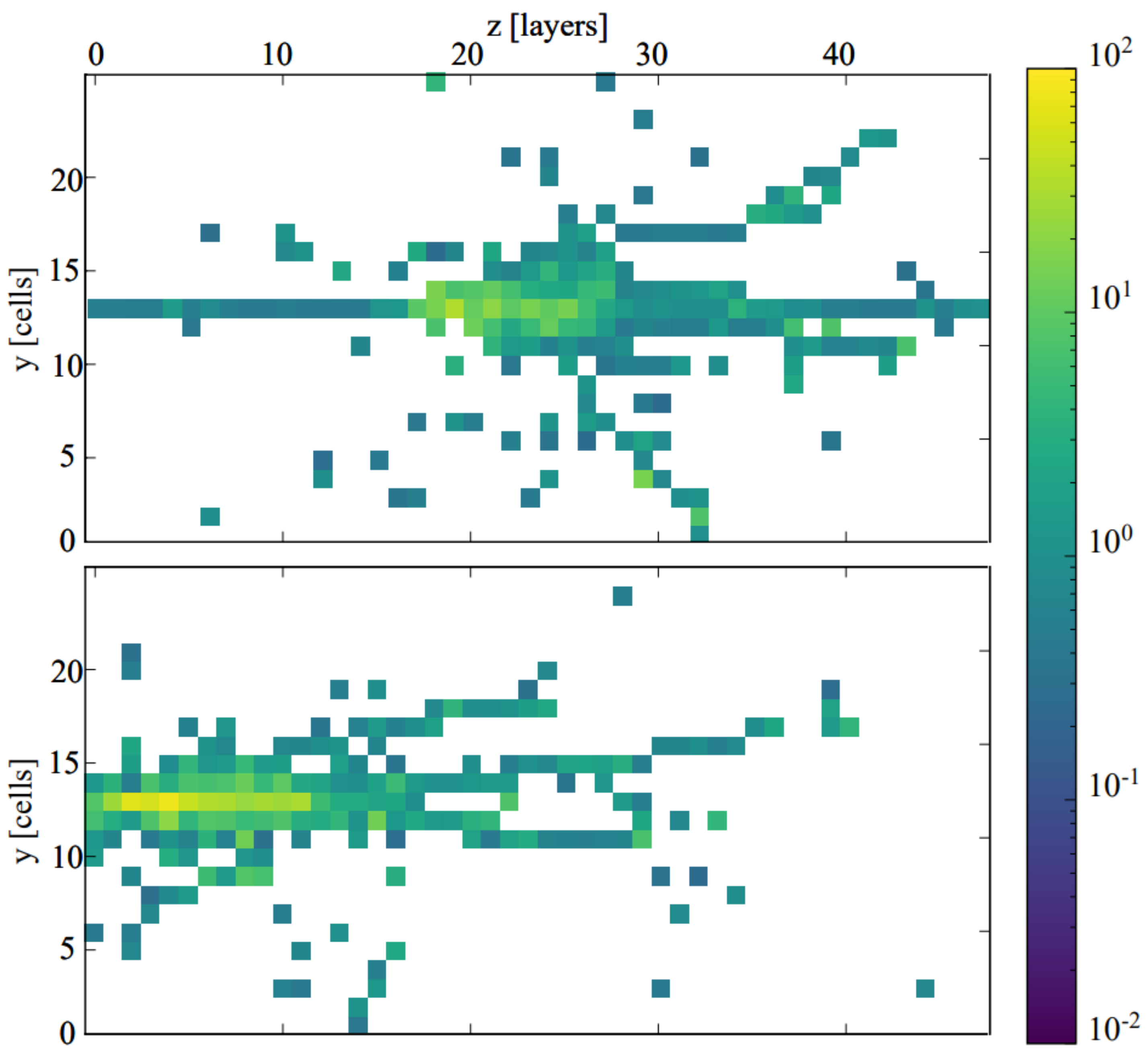
Buhmann et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed** (2020) 2005.05334

Buhmann et. al. **Hadrons, Better, Faster, Stronger:** (2021) 2112.09709

# Shower Dataset

**Photon showers** **Charged pion showers**




Pion showers significantly more complex

Training data:

- Photons / charged Pions
- 1 million / 500k showers
- 10 to 100 GeV
- Fixed incident point & angle
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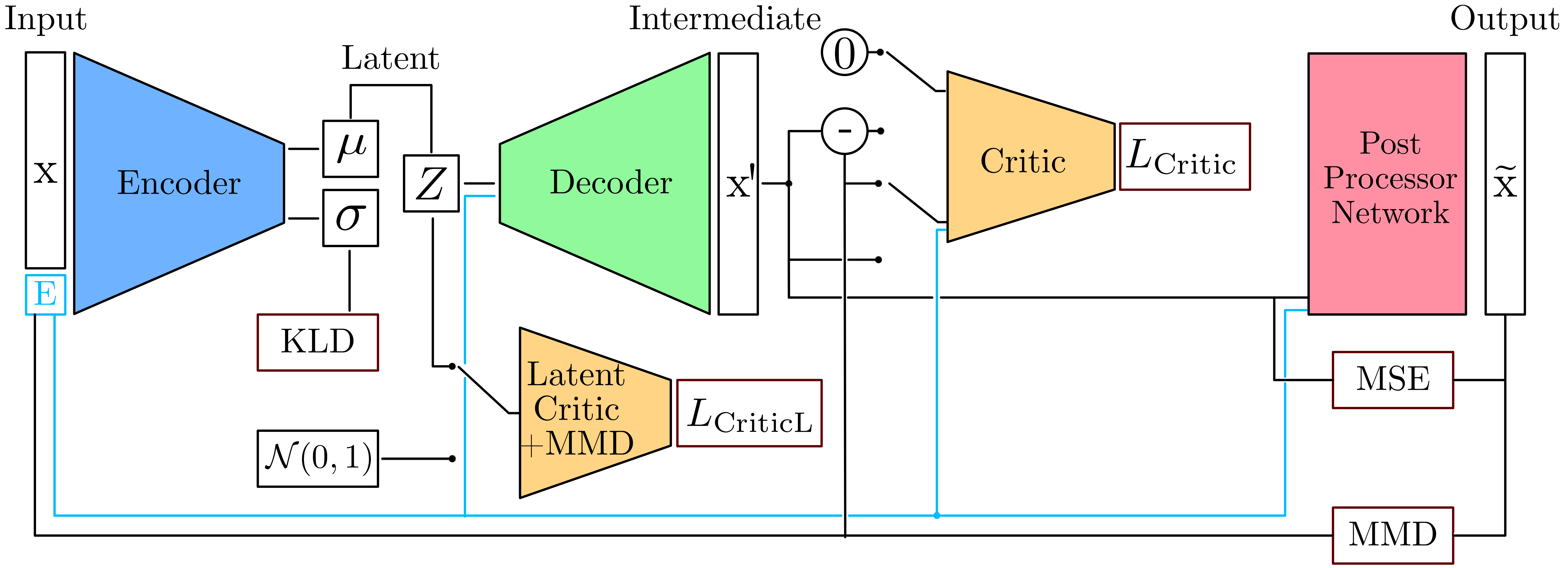
Buhmann et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed** (2020) [2005.05334]

Buhmann et. al. **Hadrons, Better, Faster, Stronger:** (2021) [2112.09709]

# Bounded Information Bottleneck Autoencoder

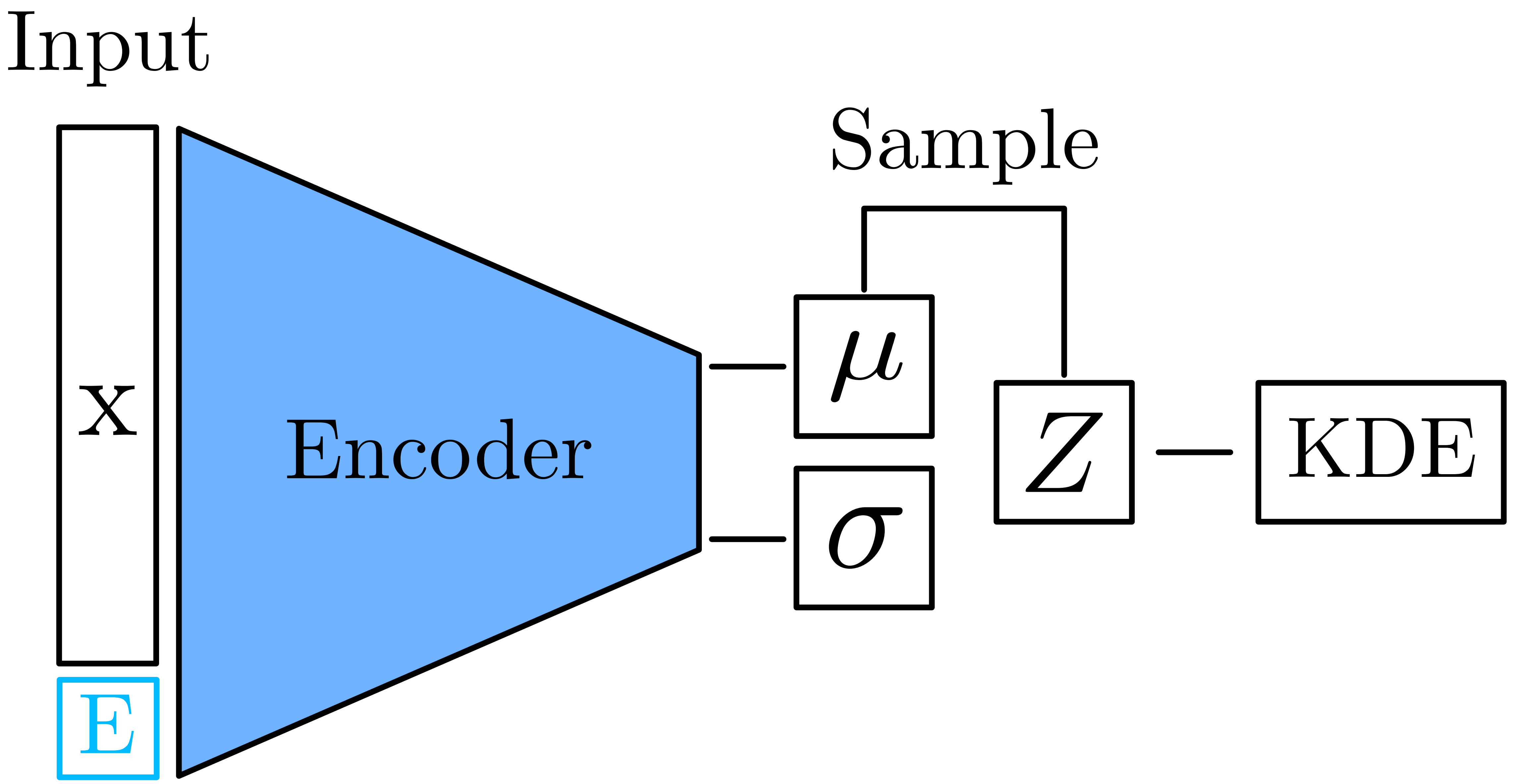


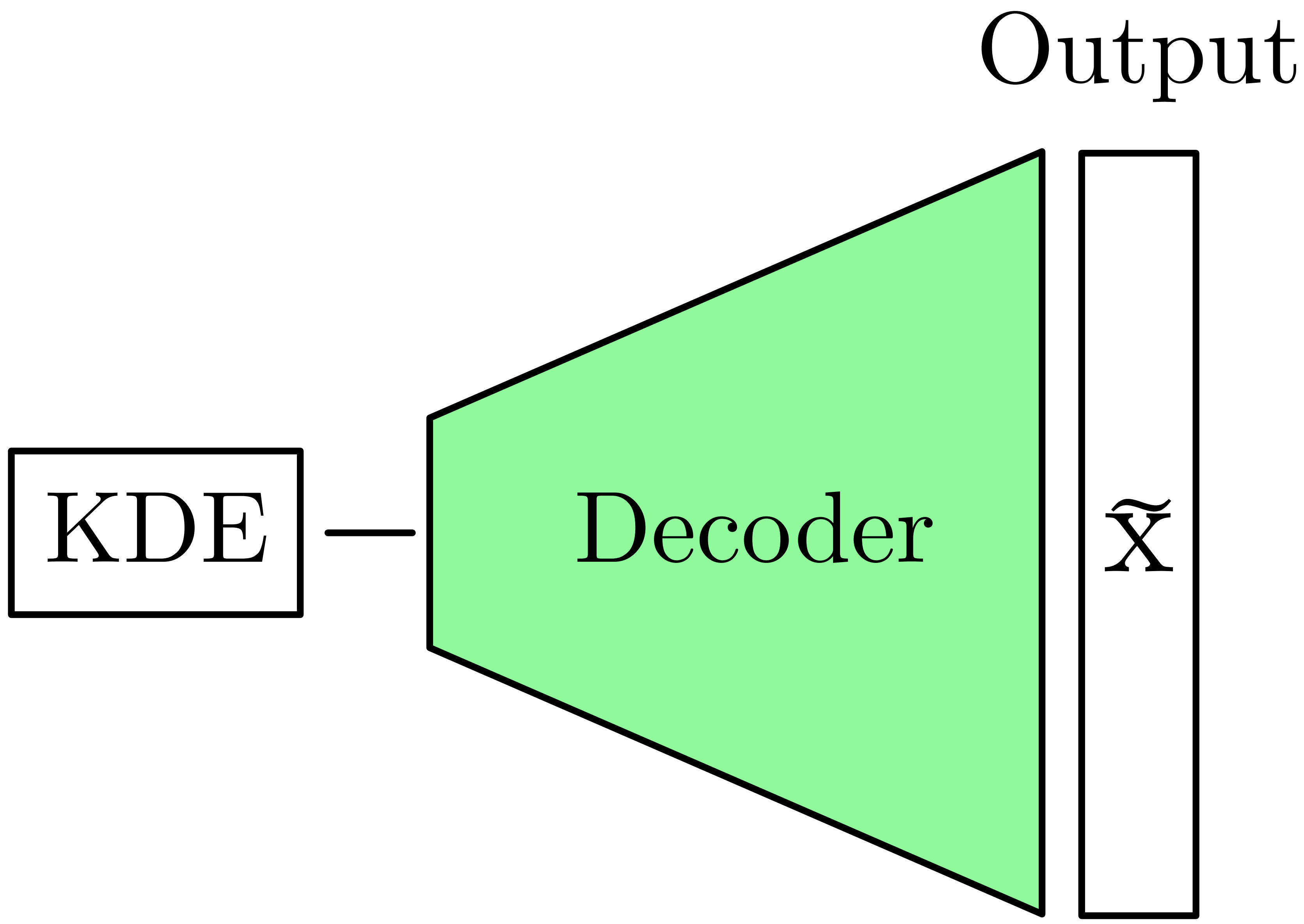

- Combines VAE and GAN approaches
- Final Post Processor network for fine tuning

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

# Kernel Density Estimation BIB-AE

- Encode real shower images
- Fit KDE to latent space
- Sample latent space from KDE for generation

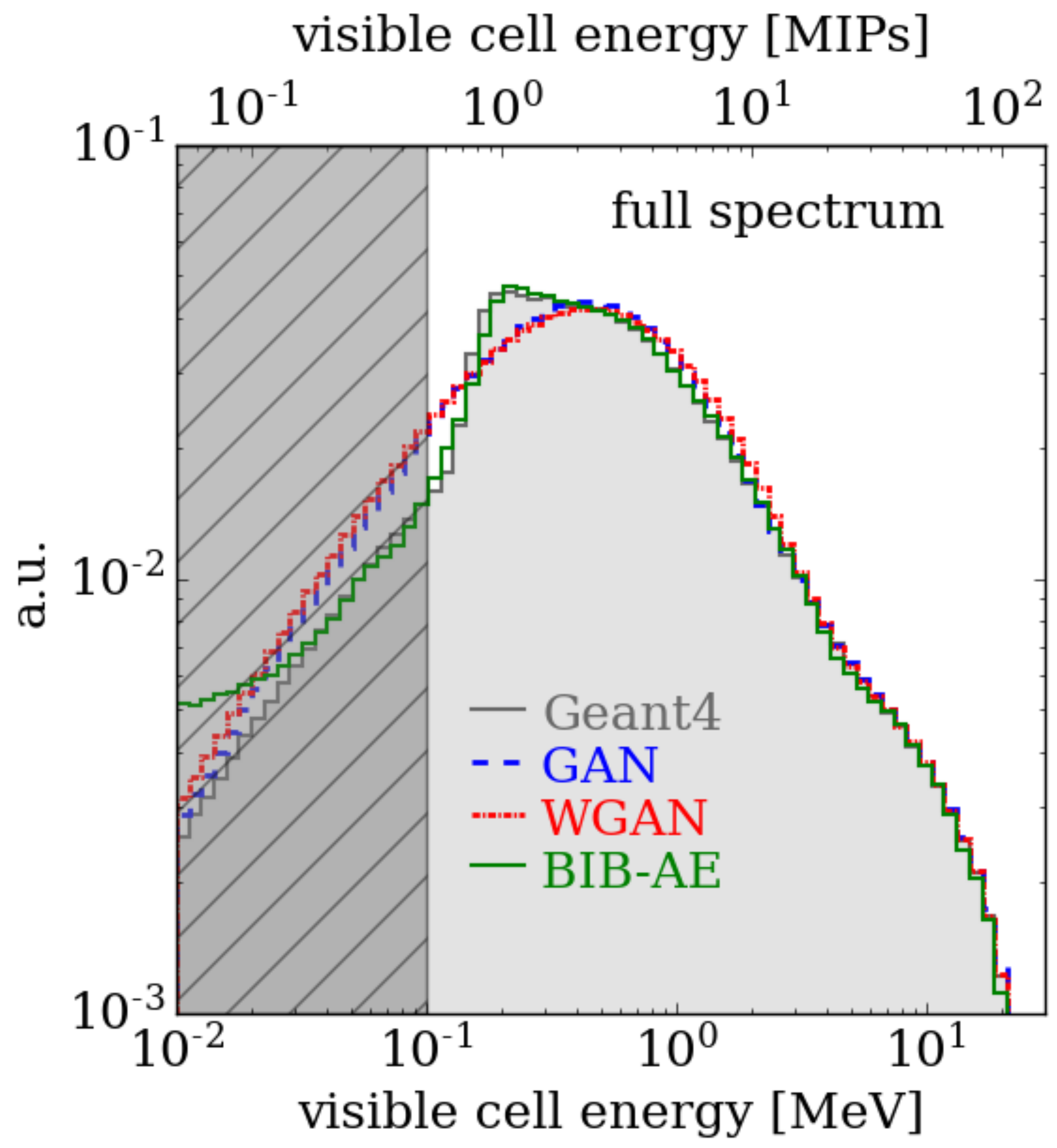


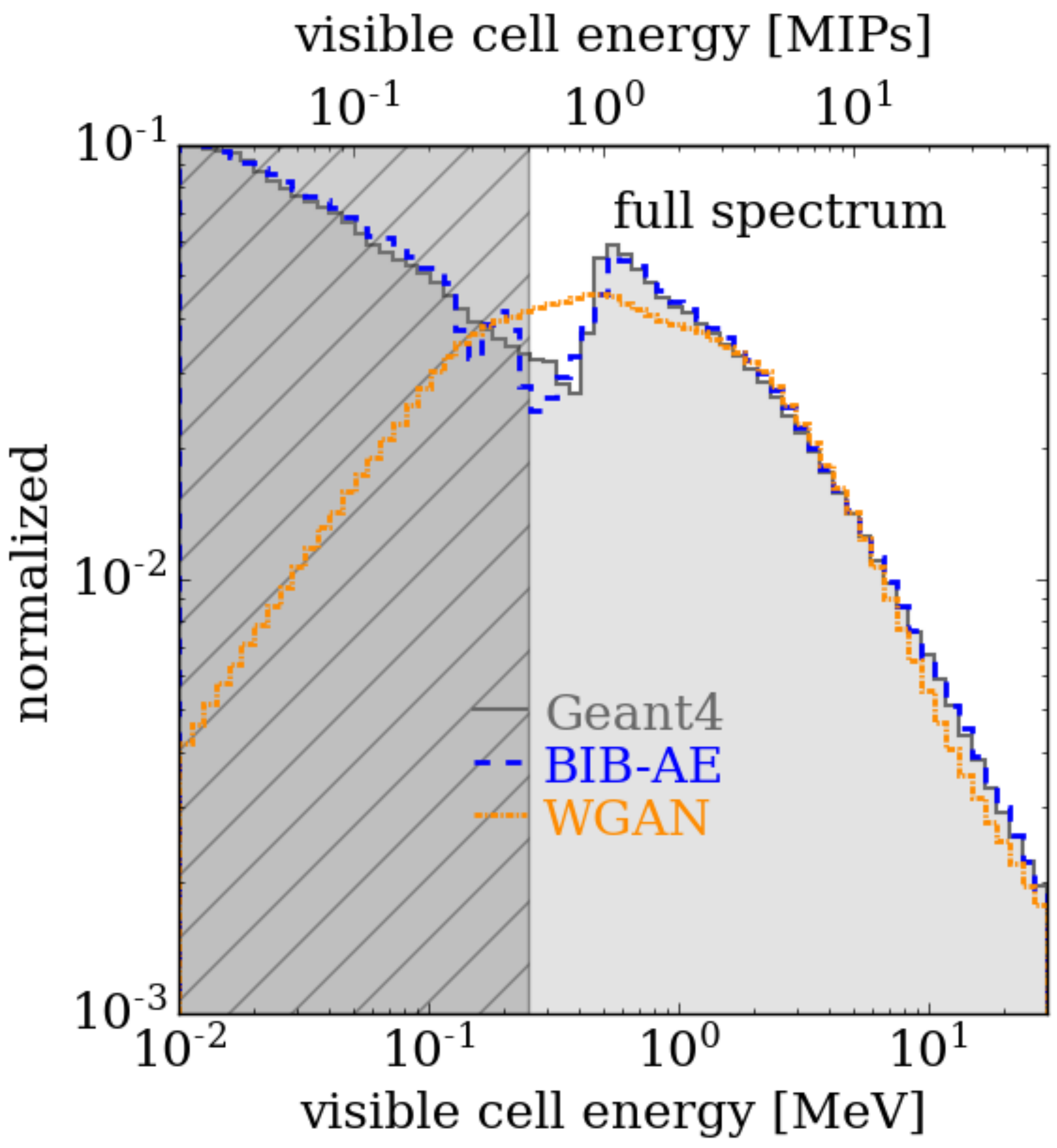

Buhmann et. al. **Decoding Photons: Physics in the Latent Space of a BIB-AE Generative Network:** (2021) [2102.12491]

# Cell Energy Spectrum

Photons

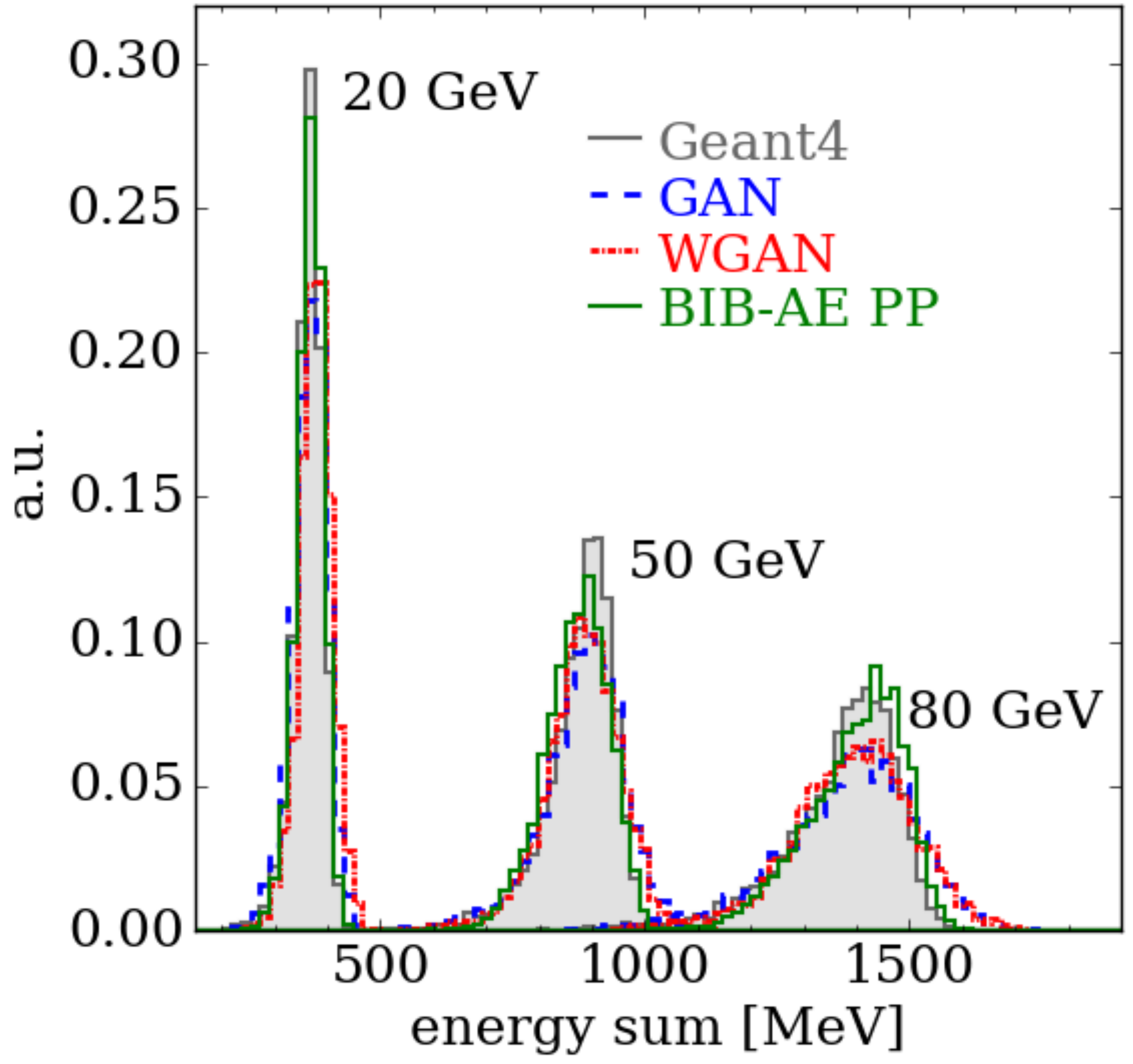



Pions

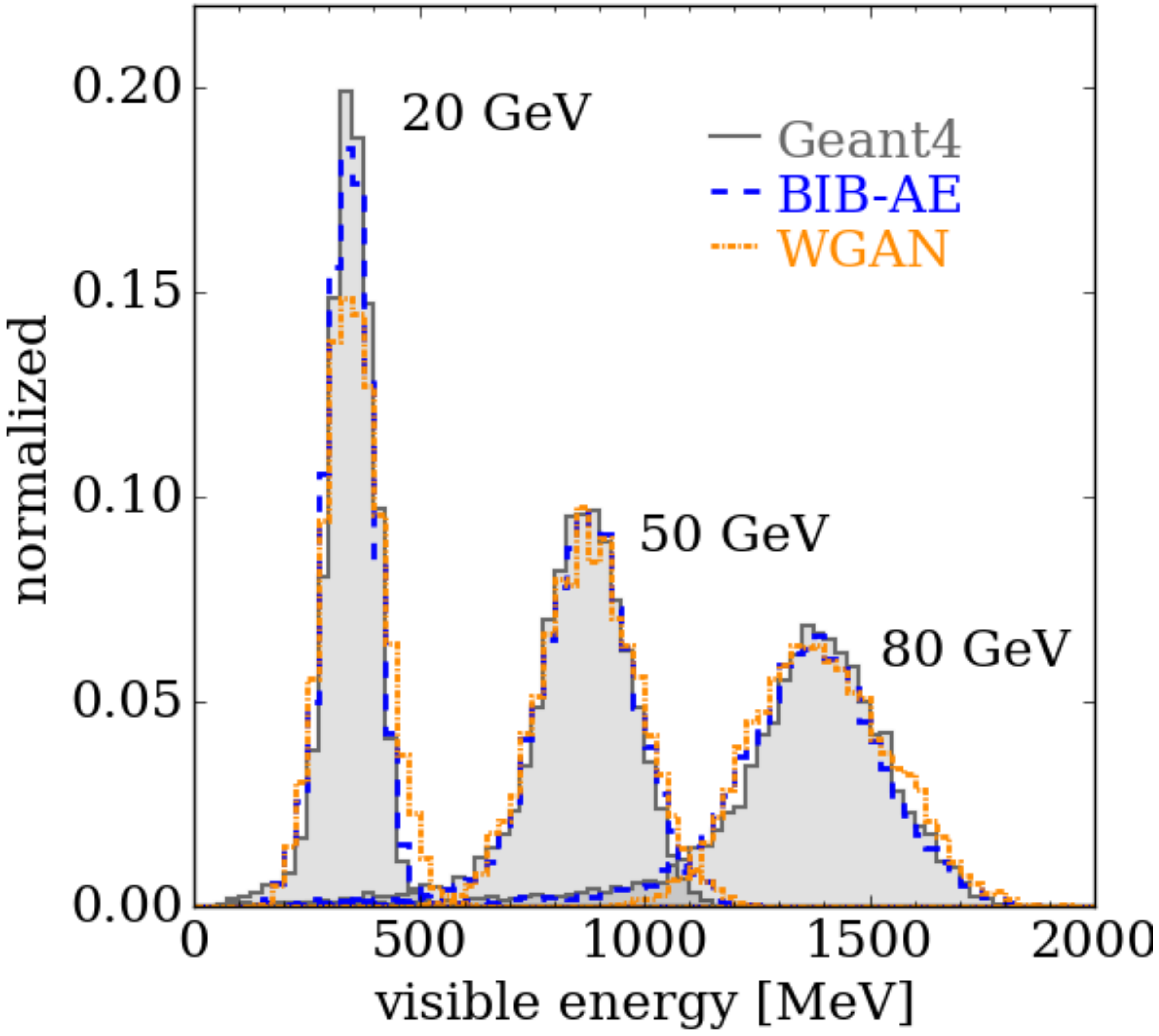


# Visible Energy Sum

Photons

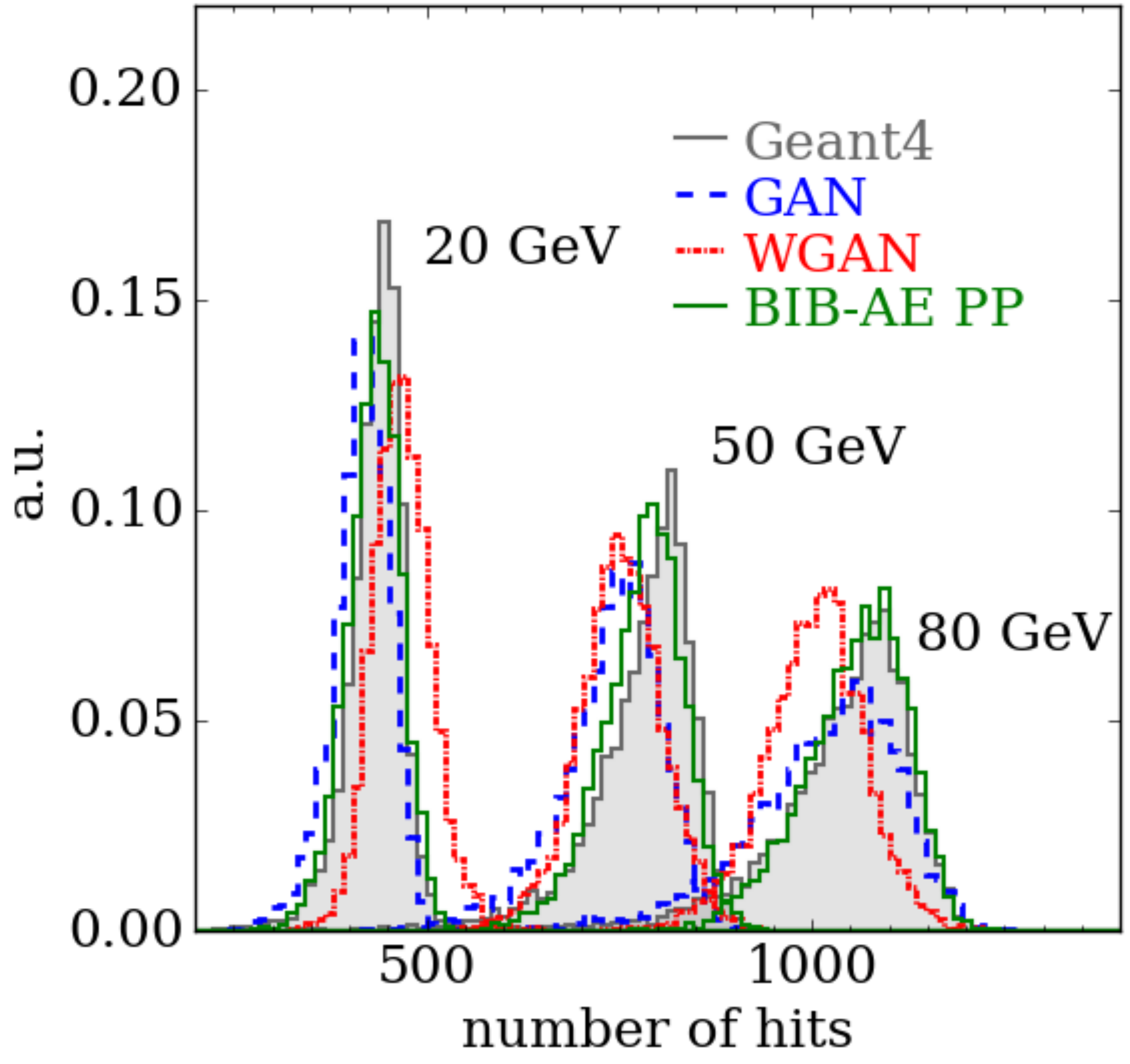



Pions

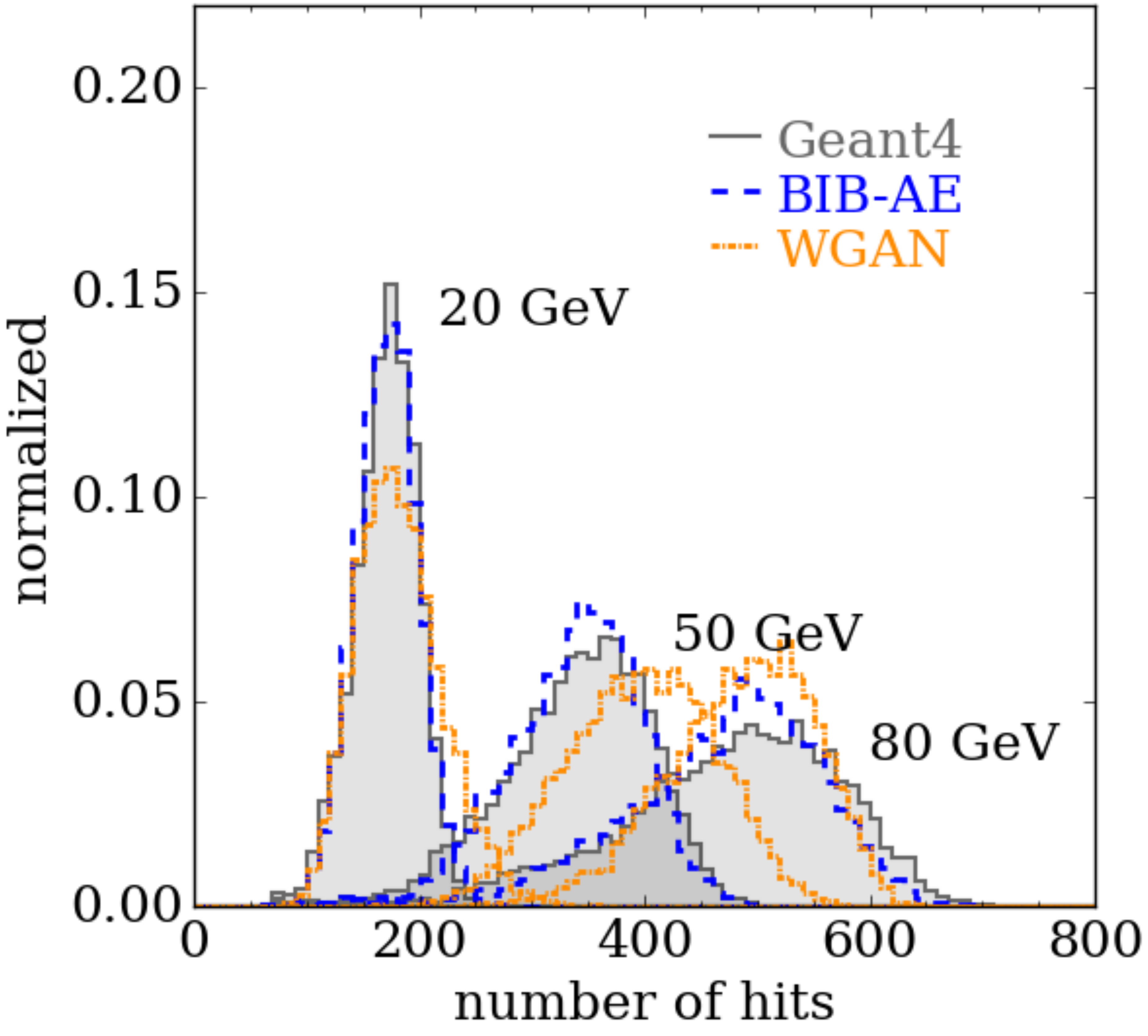


# Number of Hits

Photons




Pions



# Cell Energy Spectrum

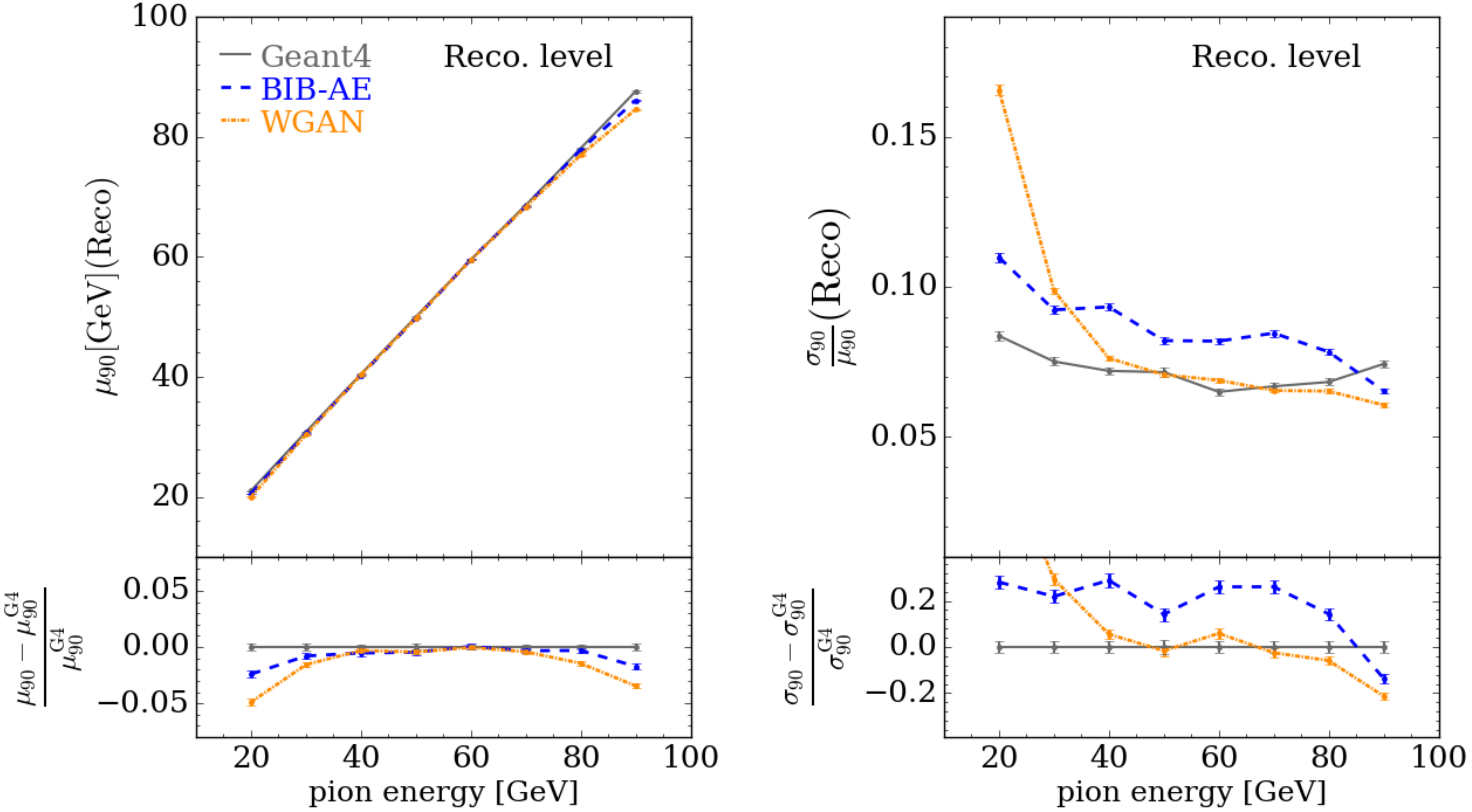
| Simulator | Hardware | Photons | Speedup | Pions | Speedup |
|---|---|---|---|---|---|
| GEANT4 | CPU | 4082±170 ms | - | 2684±125 ms | - |
| BIB-AE | CPU | 426.3±3.6 ms | x10 | 350.824±0.574 ms | x8 |
| WGAN | CPU | 57.99±0.18 ms | X70 | 47.923±0.089 ms | ×56 |
| BIB-AE | GPU | 1.42±0.01 ms | x2874 | 2.051±0.005 | ×1309 |
| WGAN | GPU | 3.34±0.01 ms | x1256 | 0.264±0.002 | x10167 |

Times for fastest evaluation batch sizes

Buhmann et al.: **Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speed** (2020) 2005.05334

Buhmann et. al. **Hadrons, Better, Faster, Stronger:** (2021) 2112.09709

# Pion Reconstruction Results



# Current Status

| Shower Type | Generative Simulation | Energy Conditioning | Angle Conditioning | Reconstruction |
|---|---|---|---|---|
| EM | ✓ | ✓ | + | ✗ |
| Hadronic | ✓ | ✓ | ✗ | ✓ |

✓ **: Done** + **: In progress** ✗ **: To be done**

# Angle Conditioning

- Need variable angles for practical application
- Conditioning on both photon shower angle and energy

# Angle Conditioning


- Additional angle input to BIB-AE and Post Processor network
- Replace latent KDE with conditional latent flow model

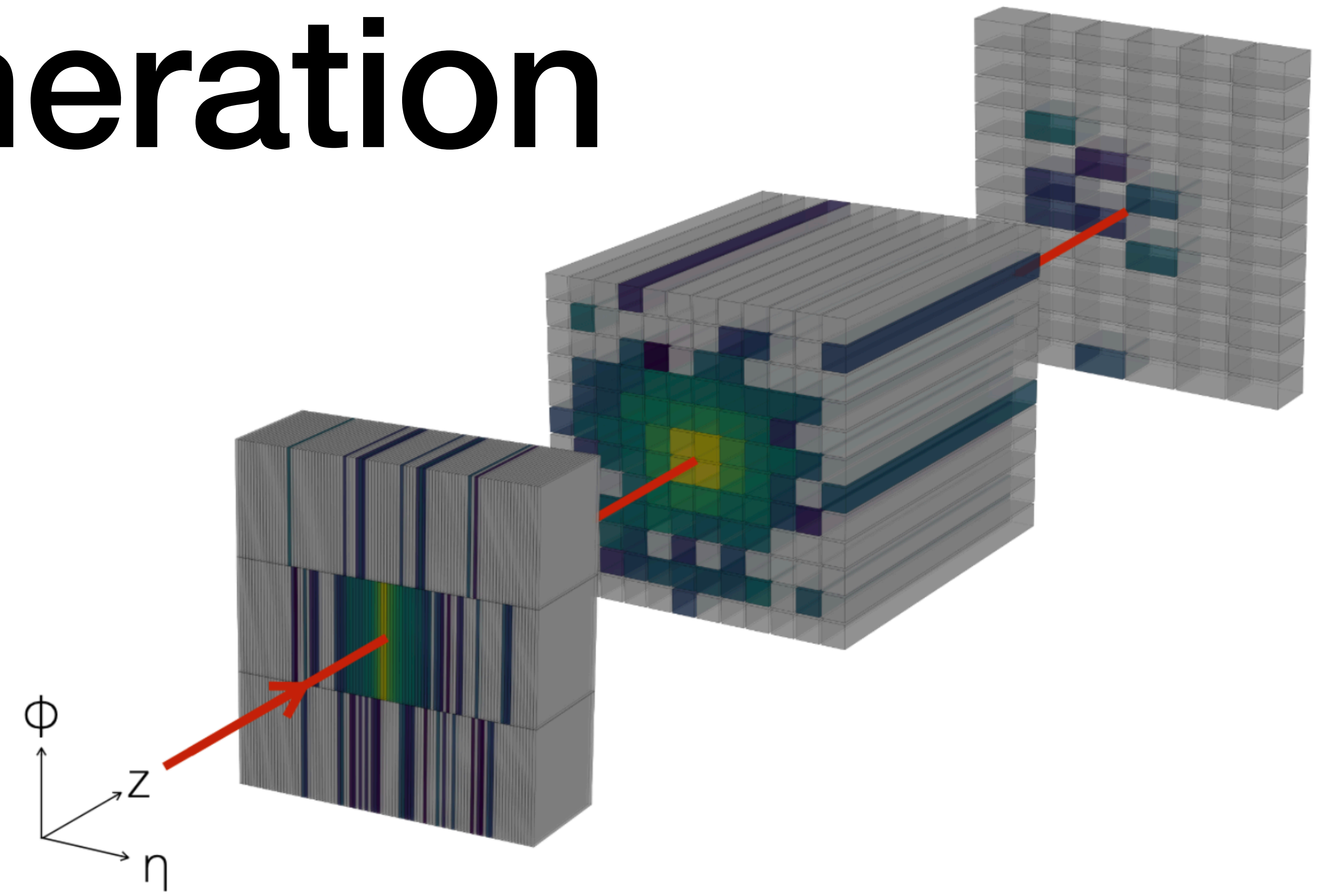
# Angle Conditioning

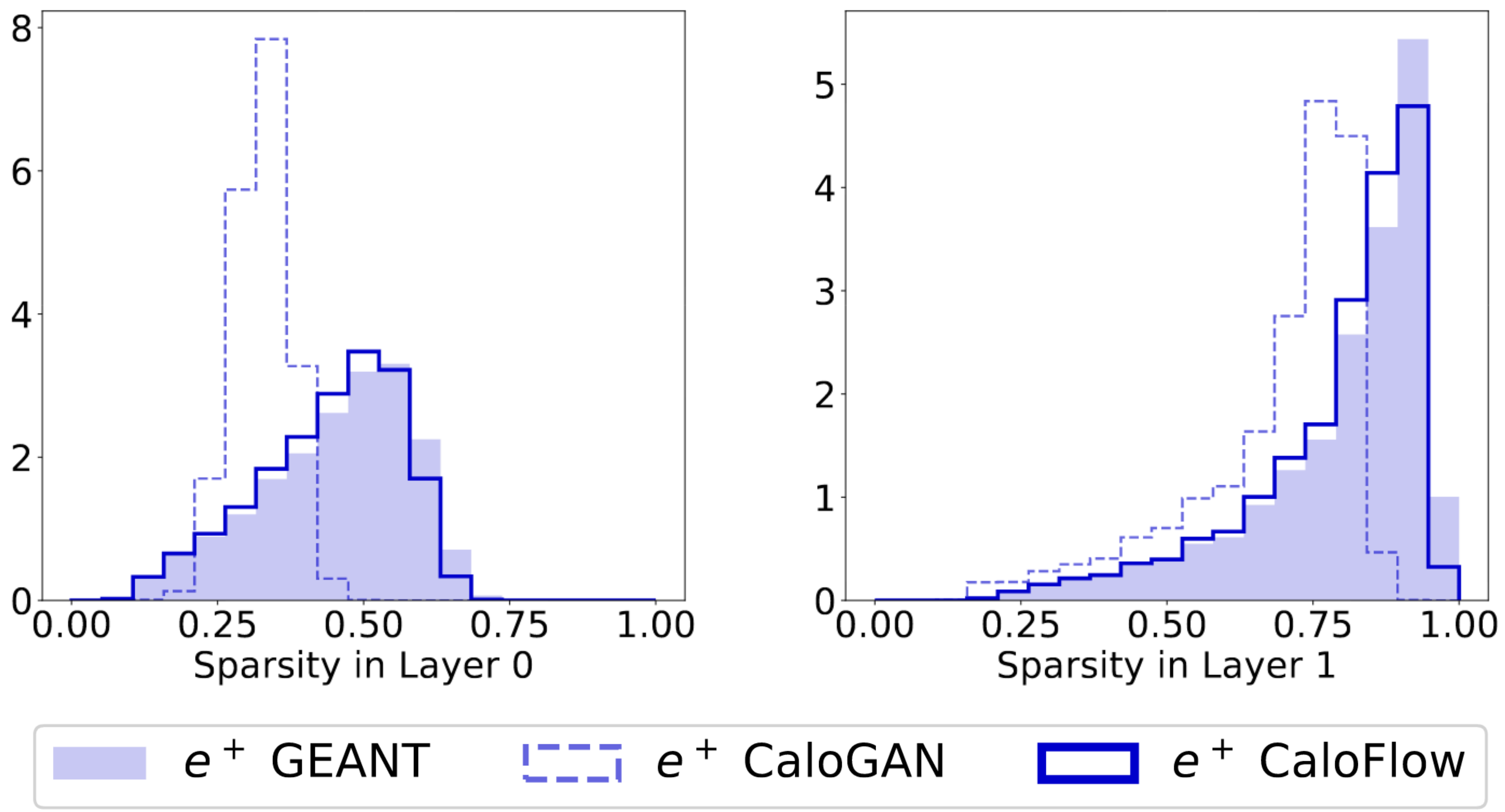
- Use PCA to reconstruct particle angle from shower
- BIB-AE accurately reproduces variety of  angles and energies

# Flow Based Generation

- CaloFlow:
  - Demonstration of flows on CaloGAN data set
  - 3 layers, ~500 dimensions total
  - Significant performance increase going from GAN to flow

➡ Test on scaled down version of ILD ECAL data set



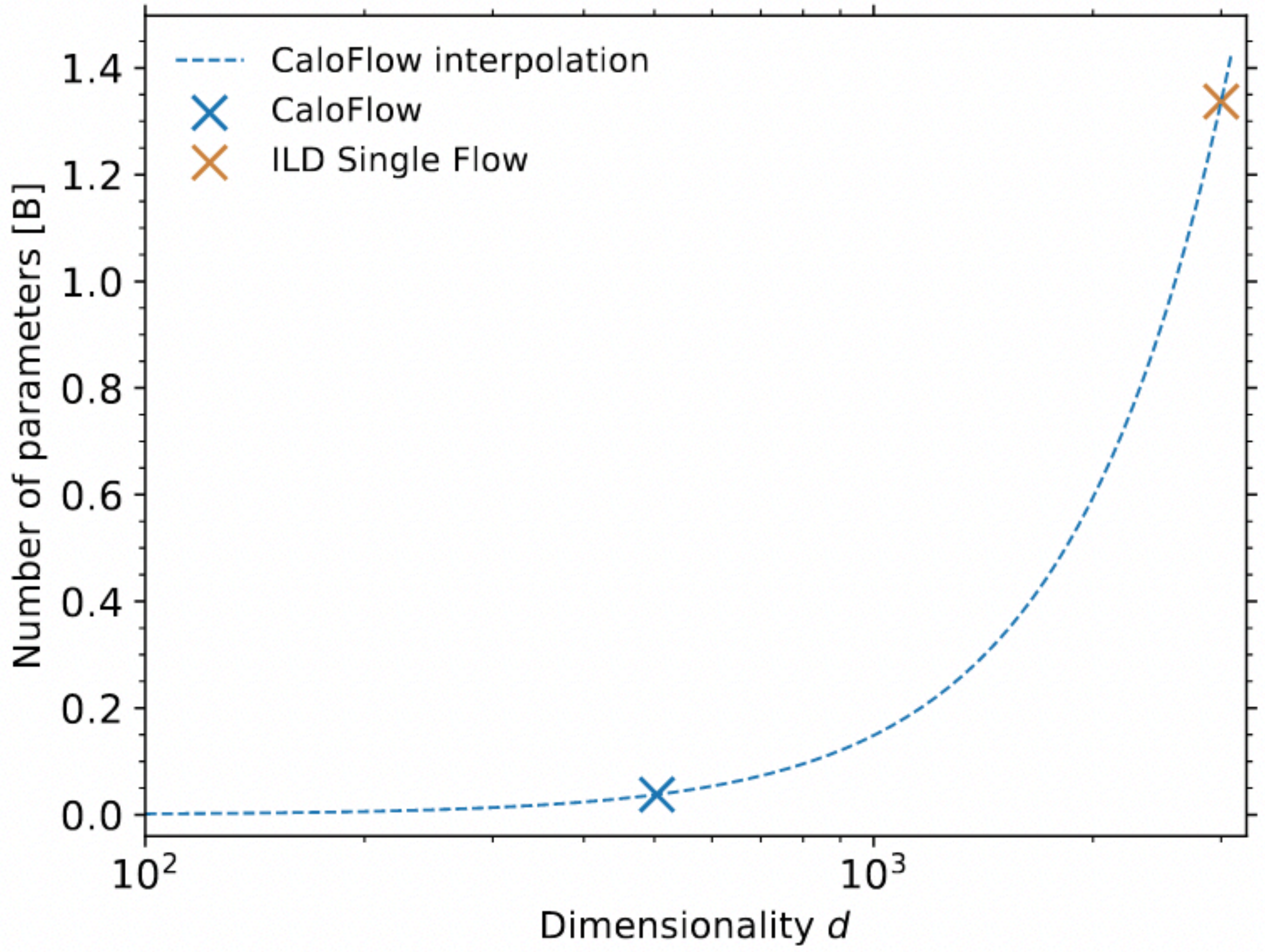

Krause et. al. **CaloFlow: Fast and Accurate Generation of Calorimeter Showers with Normalizing Flows:** (2021) [2106.05285](2106.05285)

# Number of Parameters

- Flow trained on all cells too large
- Alternate approach:
  - 30 flows, one per layer
  - Each flow conditioned on previous layers

➡ Parameters scale linear with number of calorimeter layers

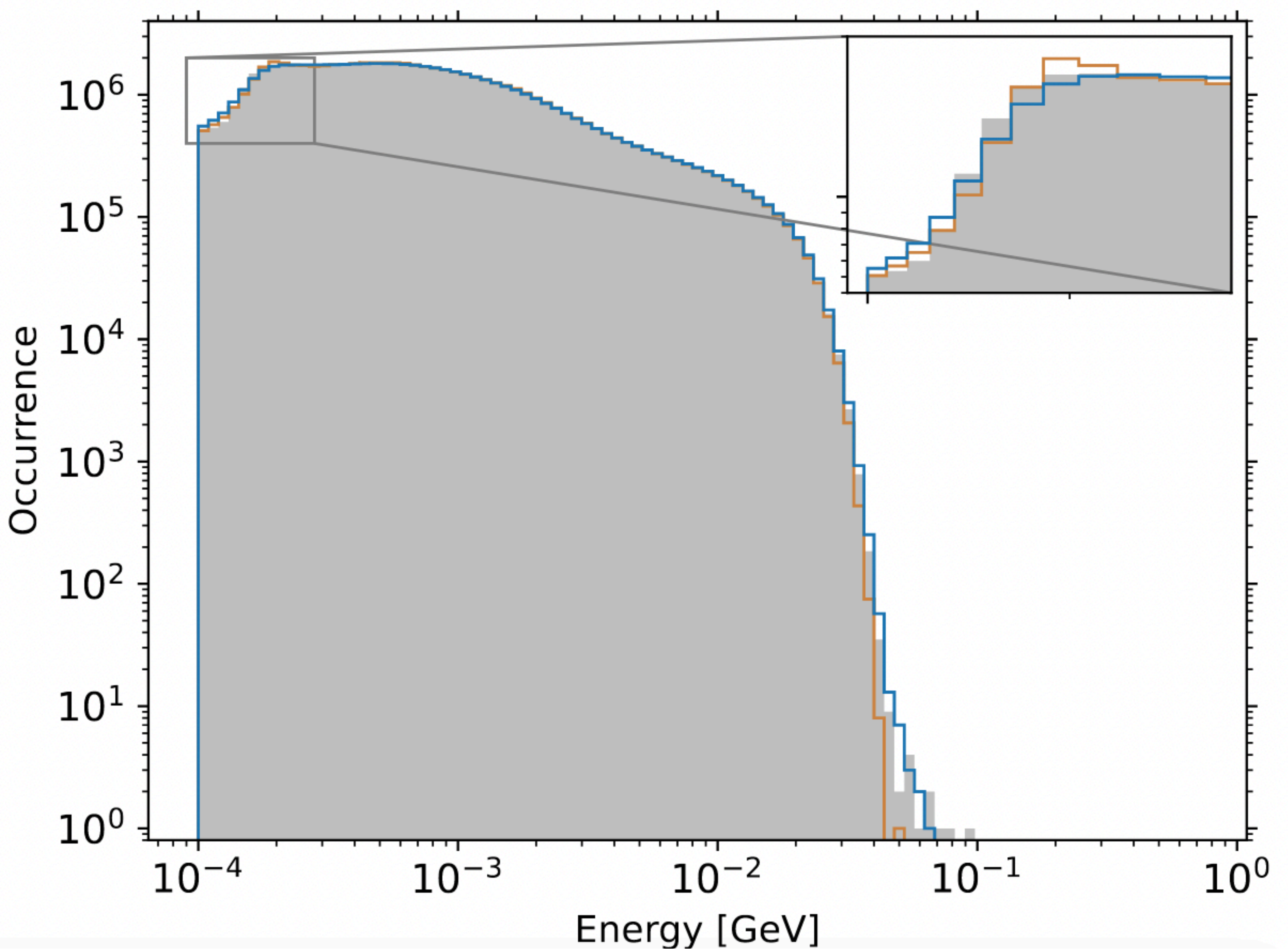
- Quickly generate full shower

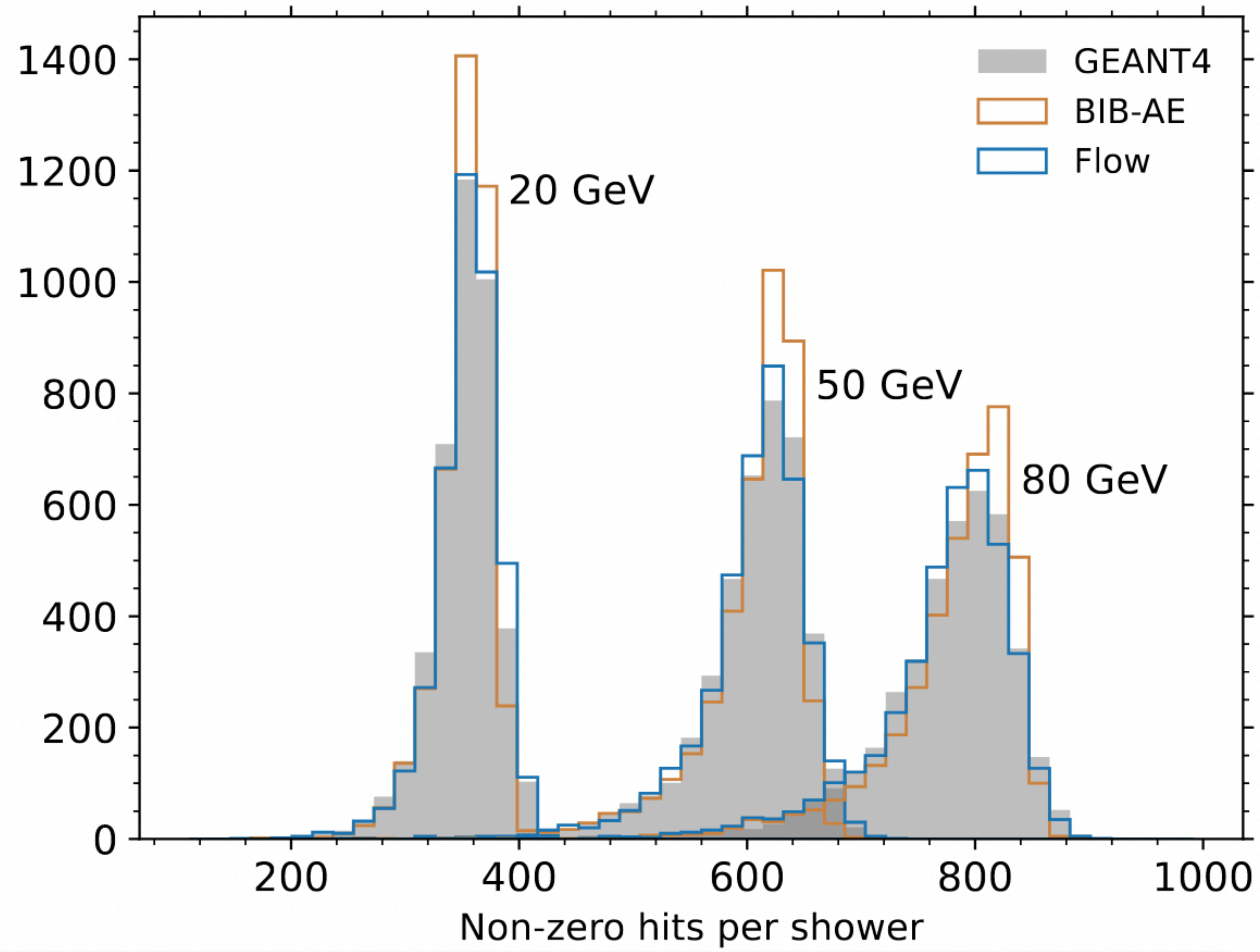



| Flow $i$ | Context features | Context shape |
|---|---|---|
| 0 | $E_0$, $E_{\text{inc}}$ | $[N, 2]$ |
| 1 | $I_0$, $E_1$, $E_{\text{inc}}$ | $[N, 102]$ |
| 2 | $I_1$, $I_0$, $E_2$, $E_{\text{inc}}$ | $[N, 202]$ |
| 3 | $I_2$, $I_1$, $I_0$, $E_3$, $E_{\text{inc}}$ | $[N, 302]$ |
| 4 | $I_3$, $I_2$, $I_1$, $I_0$, $E_4$, $E_{\text{inc}}$ | $[N, 402]$ |
| $\geq 5$ | $I_{i-1}$, $I_{i-2}$, $I_{i-3}$, $I_{i-4}$, $I_{i-5}$, $E_i$, $E_{\text{inc}}$ | $[N, 502]$ |

Work in process in collaboration with
Claudius Krause and David Shih

# Cell Spectrum and Number of Hits



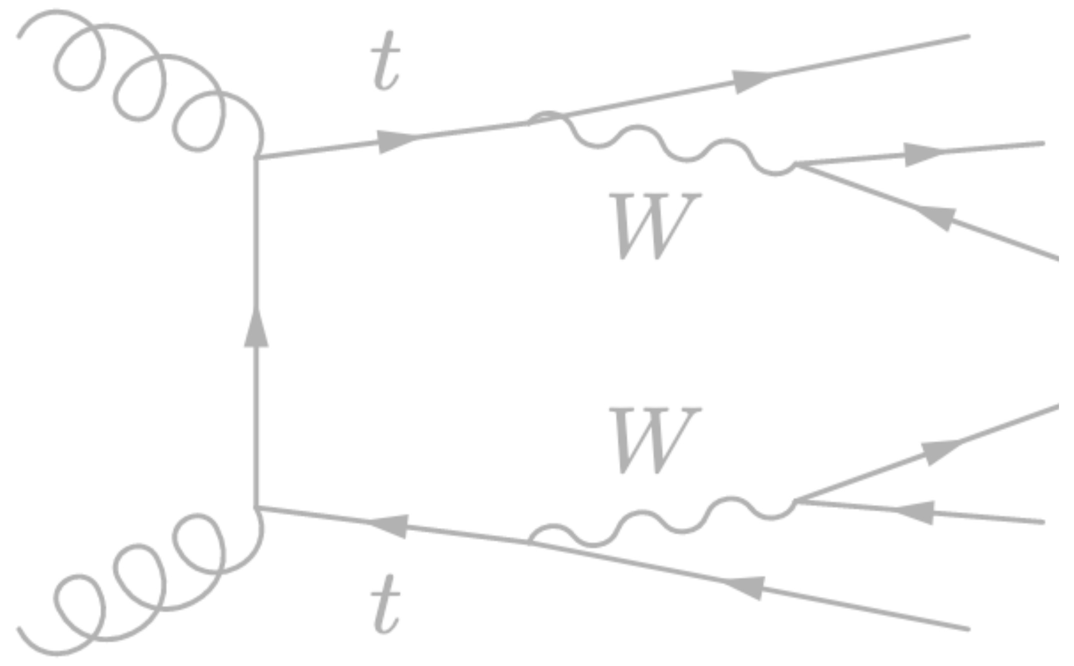



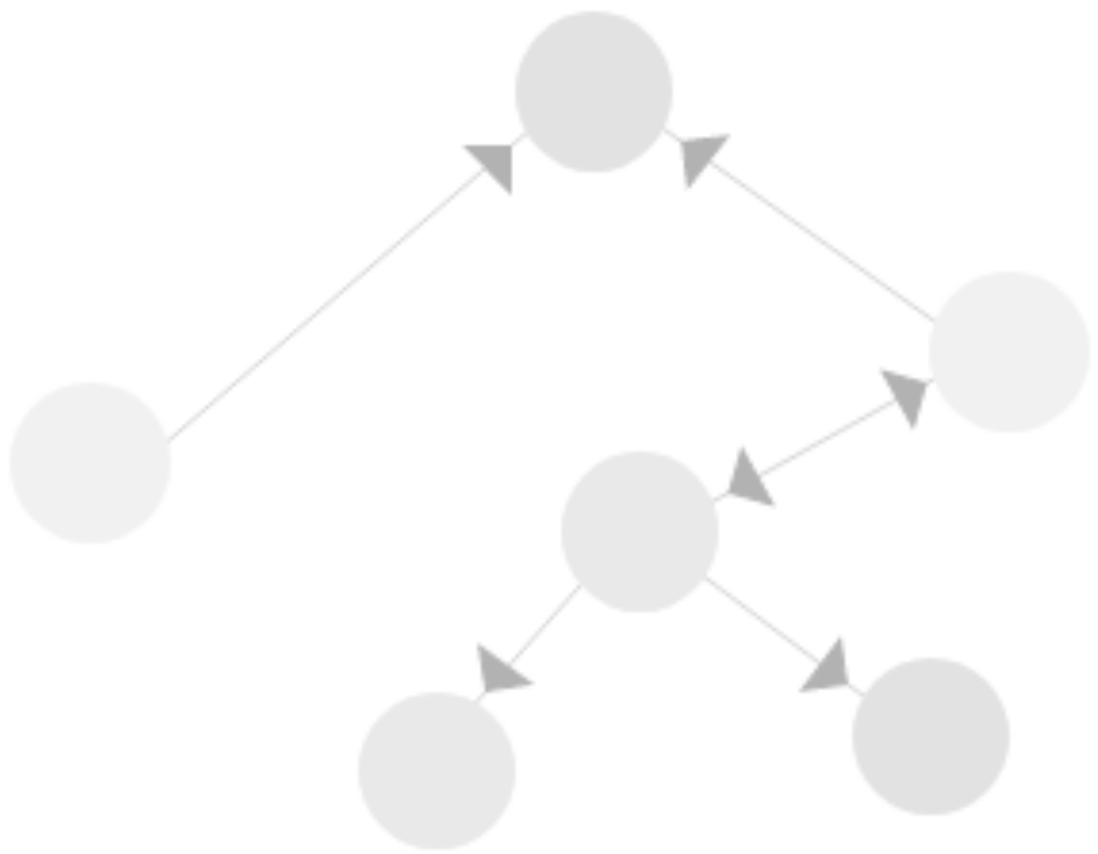

- Flow outperforms BIB-AE model

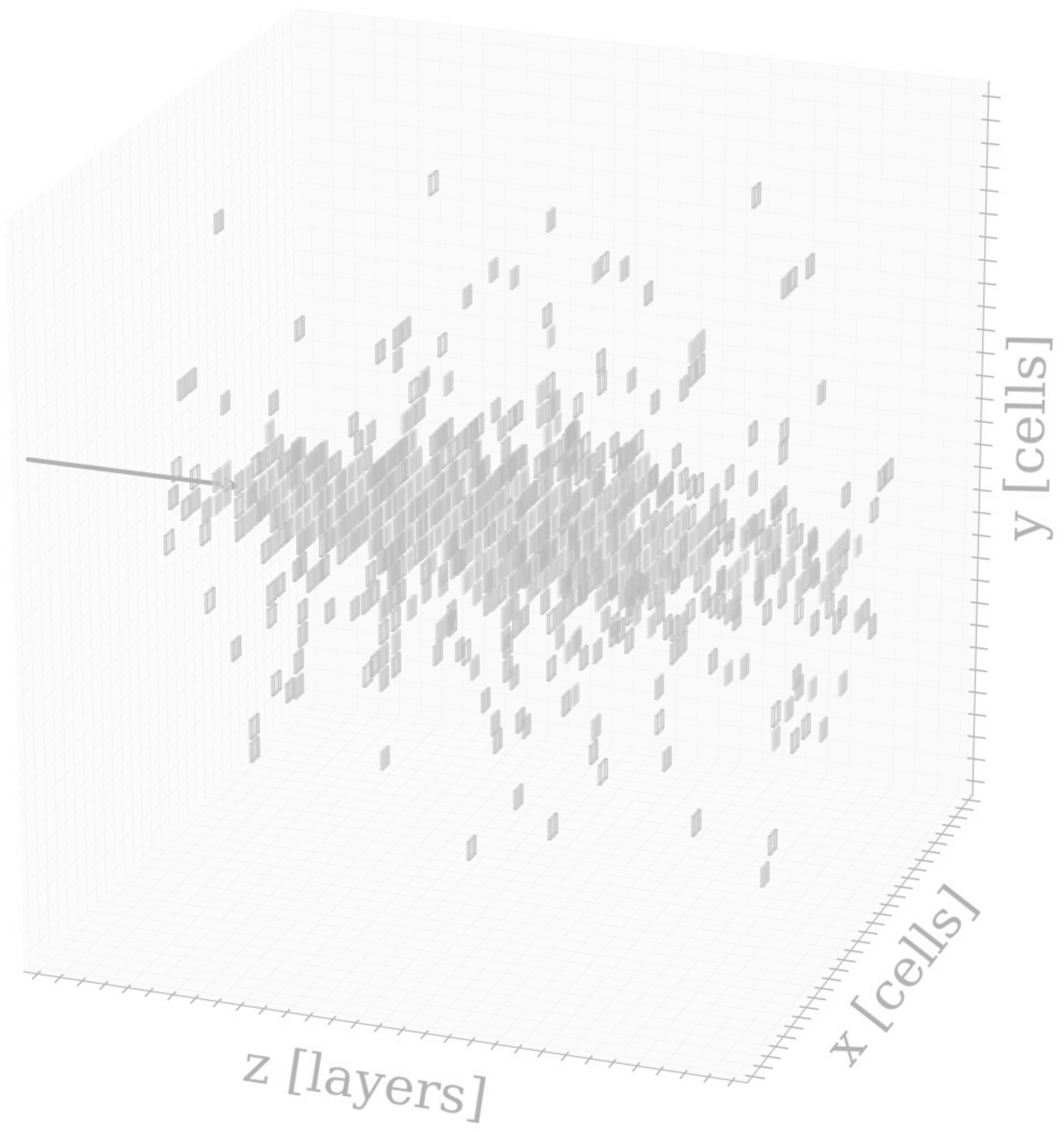
Work in process in collaboration with
Claudius Krause and David Shih

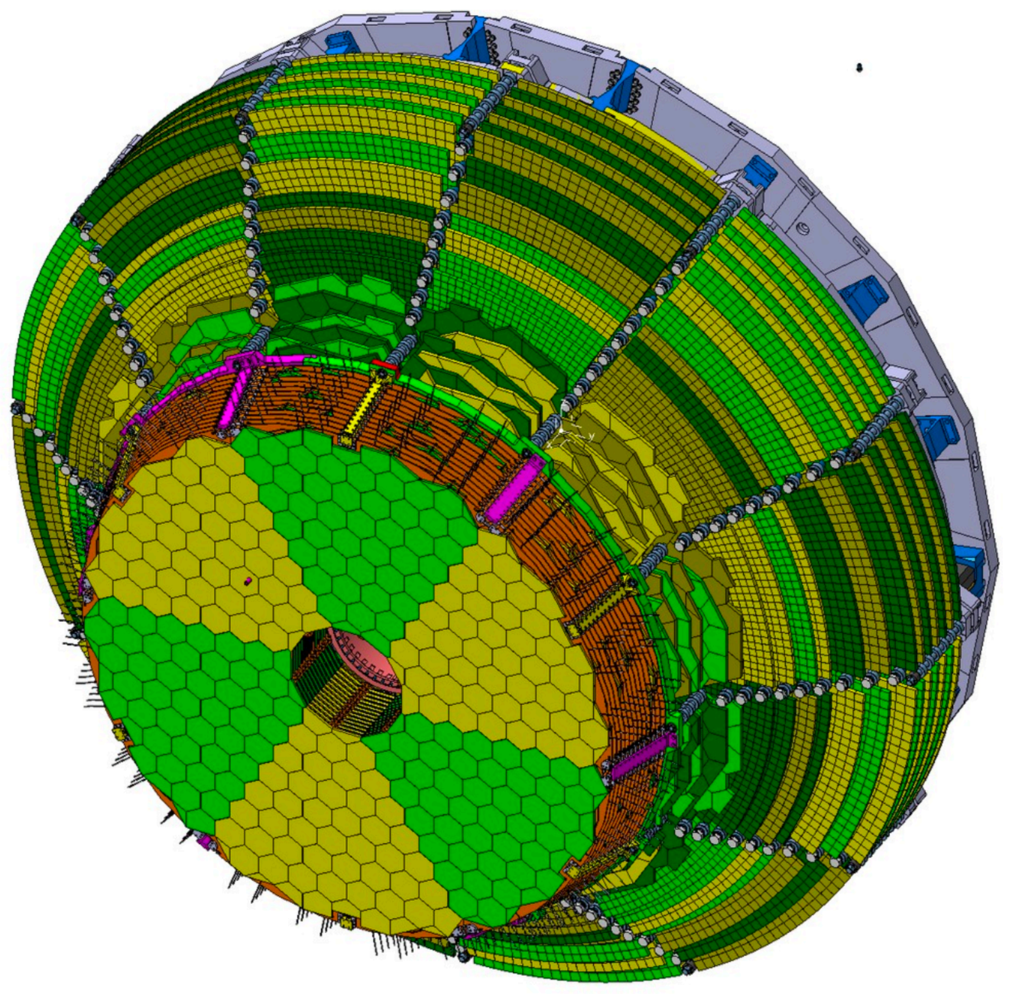
# Generative Simulation

| Low-dimensional fixed structures | Low-dimensional dynamic strutures | High-dimensional fixed structures | High-dimensional dynamic strutures |
| --- | --- | --- | --- |





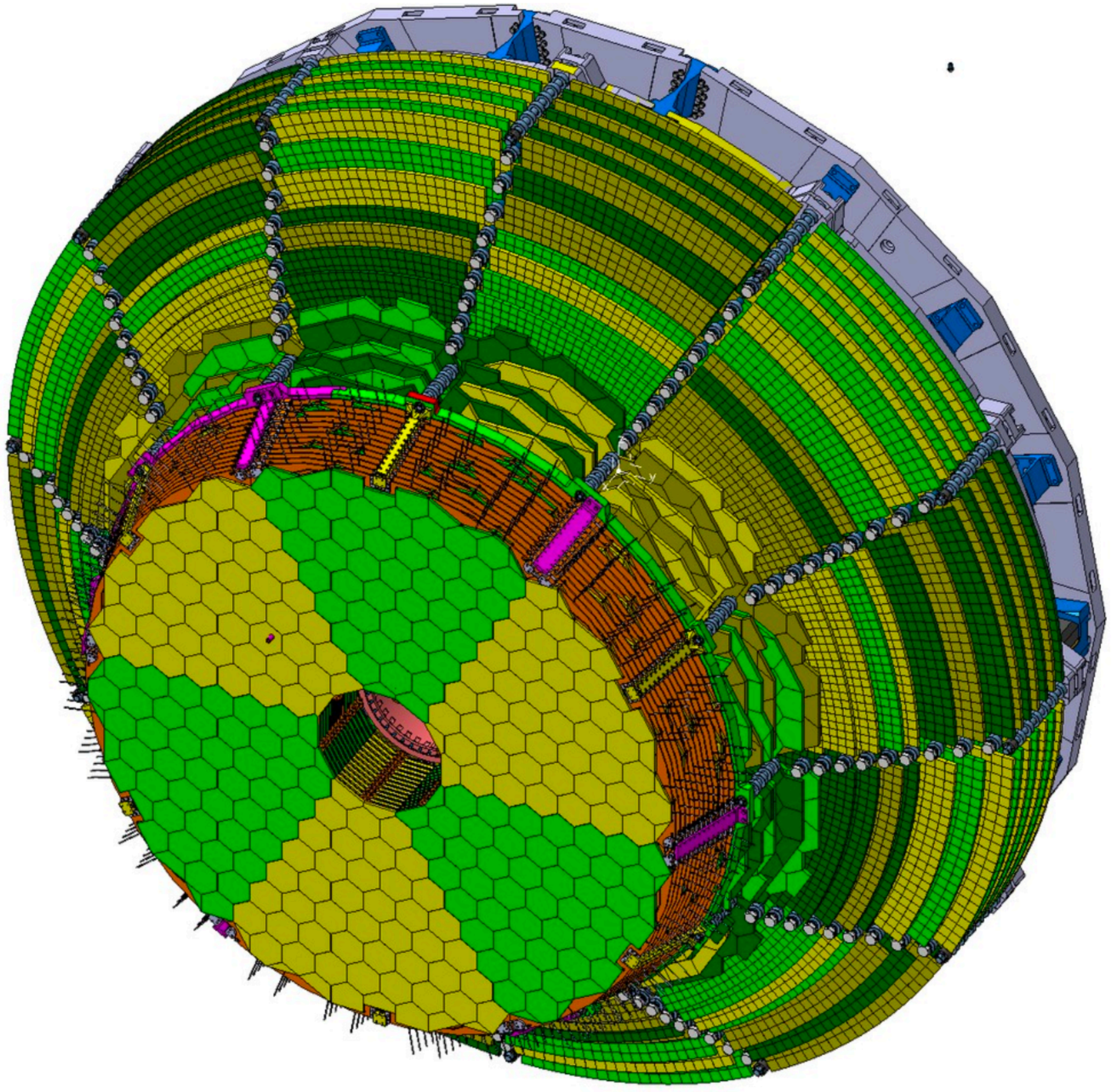
# High-Dim Dynamic Structure

- CMS HGCAL
  - Large number of channels

    ➔ Large network needed
  - Hexagonal cells

    ➔ Difficult to put in grid

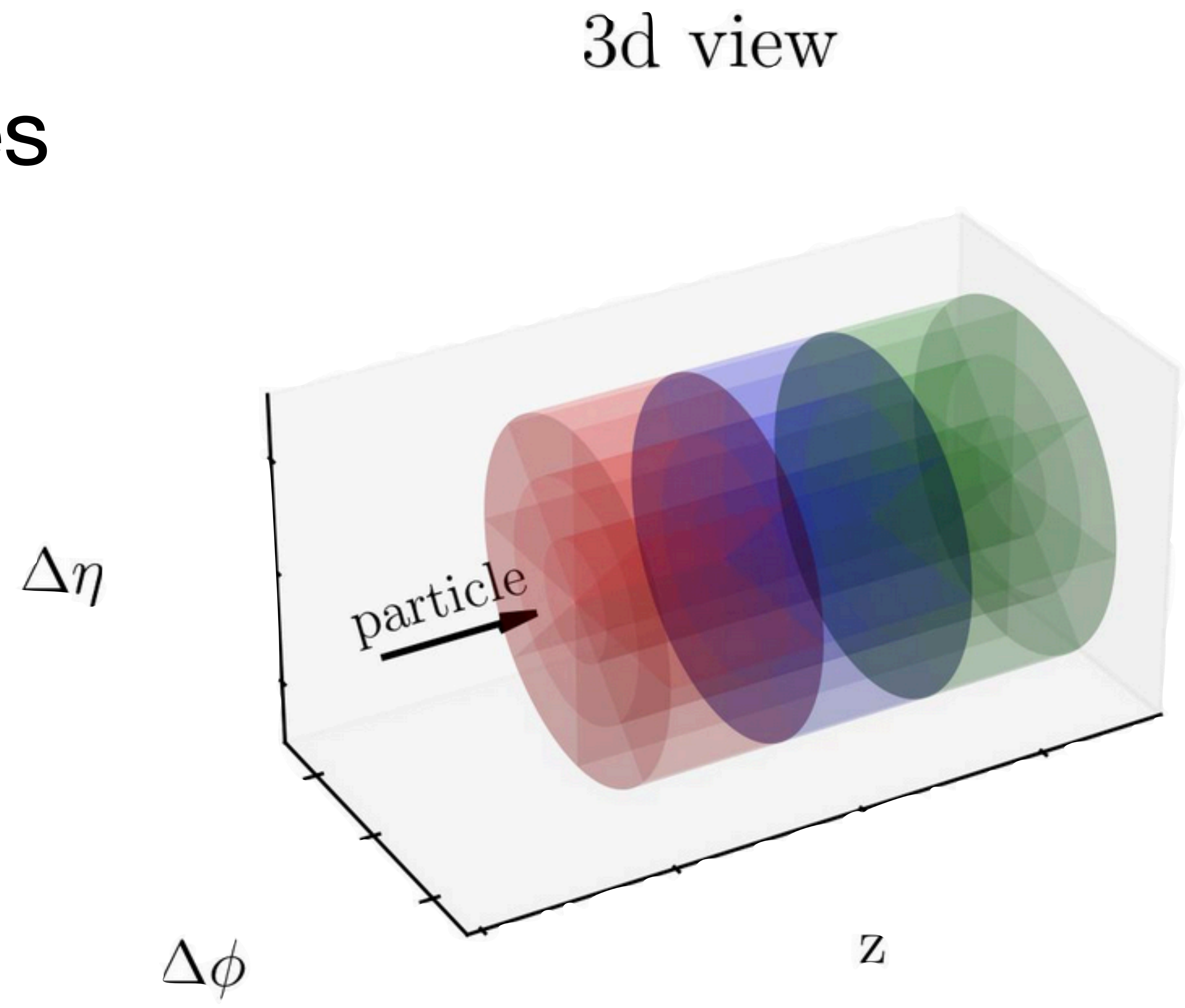
➔ Graph based high dimensional network
  - Work underway
  - Implementation challenging



CMS Collaboration, **The Phase-2 Upgrade of the CMS Endcap Calorimeter** (2017), [2293646](2293646)

# Fast Calorimeter Simulation Challenge 2022

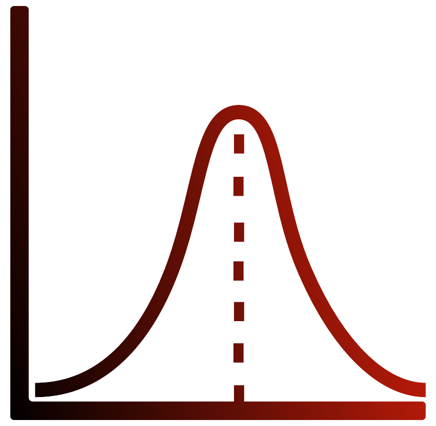
- Benchmarking for generative approaches
- 3 increasingly complex data sets based on ATLAS calorimeter simulation
- Results presented at ML4Jets 2022
- Next week at Rutgers (New Jersey)




**Fast Calorimeter Simulation Challenge:**
https://calochallenge.github.io/homepage/

# Generative Models: Use cases in Fundamental Physics

## Amplification of statistics



- Strong inductive bias of architectures help models to learn underlying manifold
- Powerful data augmentation technique

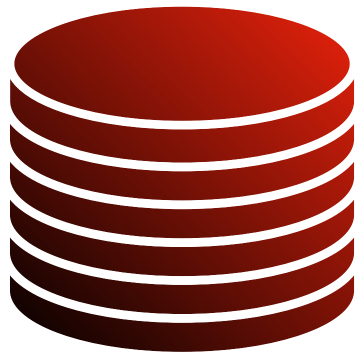
S Bieringer et al: Calomplification – The Power of Generative Calorimeter Models

A Butter et al: GANplifying Event Samples

J Kummer et al: Radio Galaxy Classification with wGAN-Supported Augmentation

[…]

## Amortised computation



- Minimisation of local computing resources by upfront central model training
- Storing model weights instead of data

M Paganini et al: CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks

EB, Sascha Diefenbacher et al: Getting High: High Fidelity Simulation of High Granularity Calorimeters with High Speeds

A Butter et al: Machine Learning and LHC Event Generation

[…]

## Generation from detector data

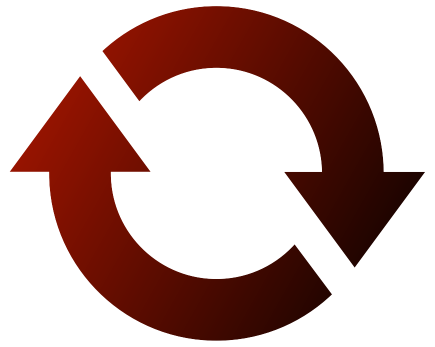
- Unsupervised training on real events instead of tuning Monte Carlo simulations
- I.e. for estimation of background densities

JN Howad et al: Learning to Simulate High Energy Particle Collisions from Unlabeled Data

A Hallin et al: Classifying Anomalies THrough Outer Density Estimation (CATHODE)

[…]

## Differentiable models



- Optimisation of experimental setup based on explicit data likelihood
- Backpropagation through analysis chain

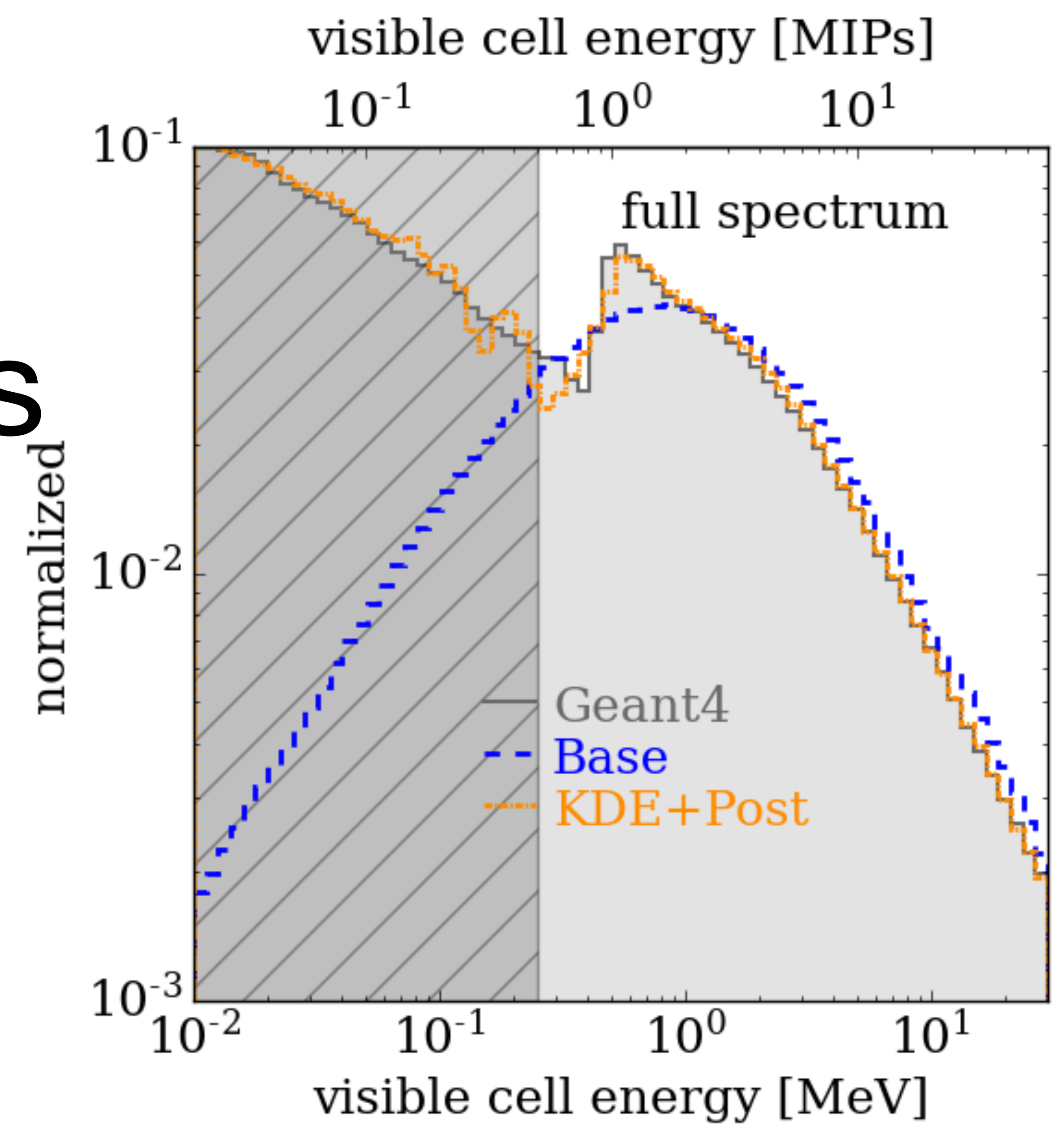
T Dorigo et al: Toward the End-to-End Optimization of Particle Physics Instruments with Differentiable Programming: a White Paper

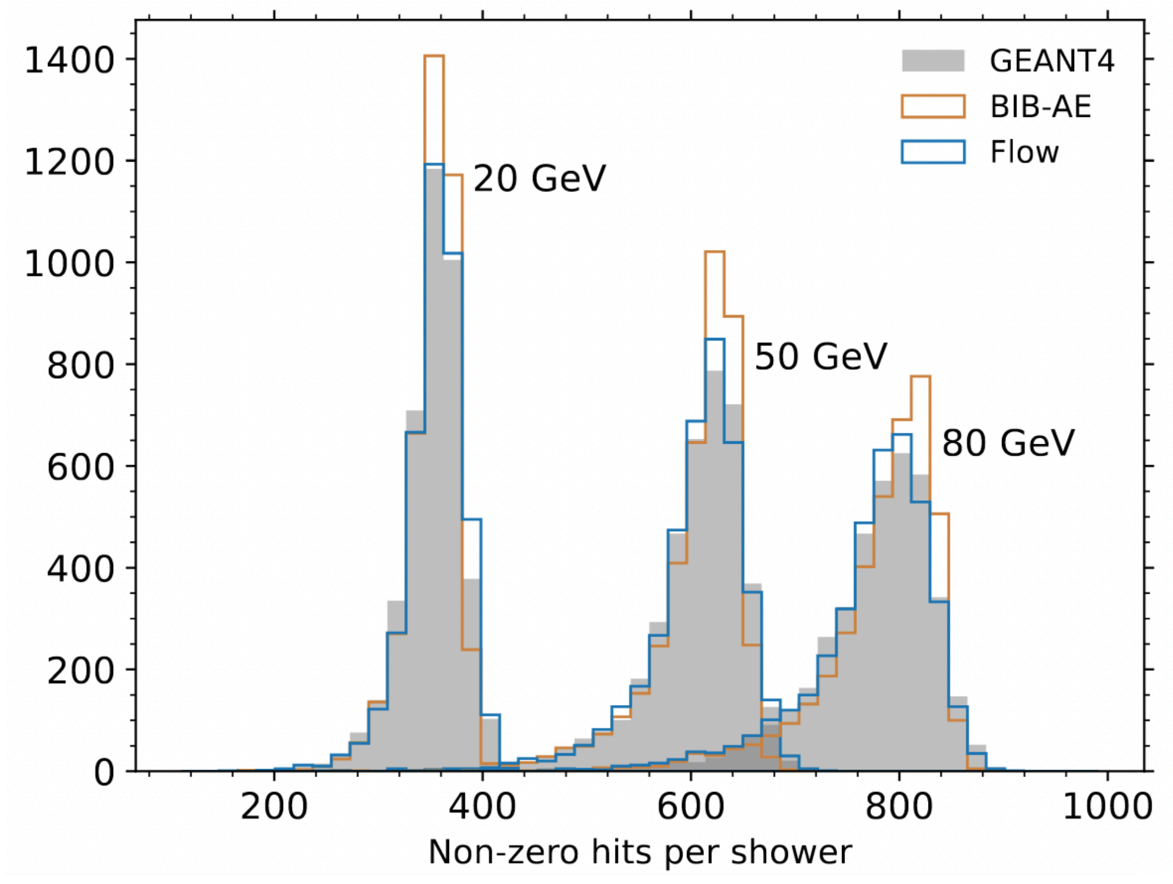
A Adelmann et al: New directions for surrogate models and differentiable programming for High Energy Physics detector simulation

[…]

# Conclusion

- Generative models growing field in particle physics
- Large range of potential applications
- Calorimeter simulation:
  - BIB-AE model accurately produces HG showers
  - Angle conditioning work in progress
  - Flow based models provide increased accuracy on smaller scale data

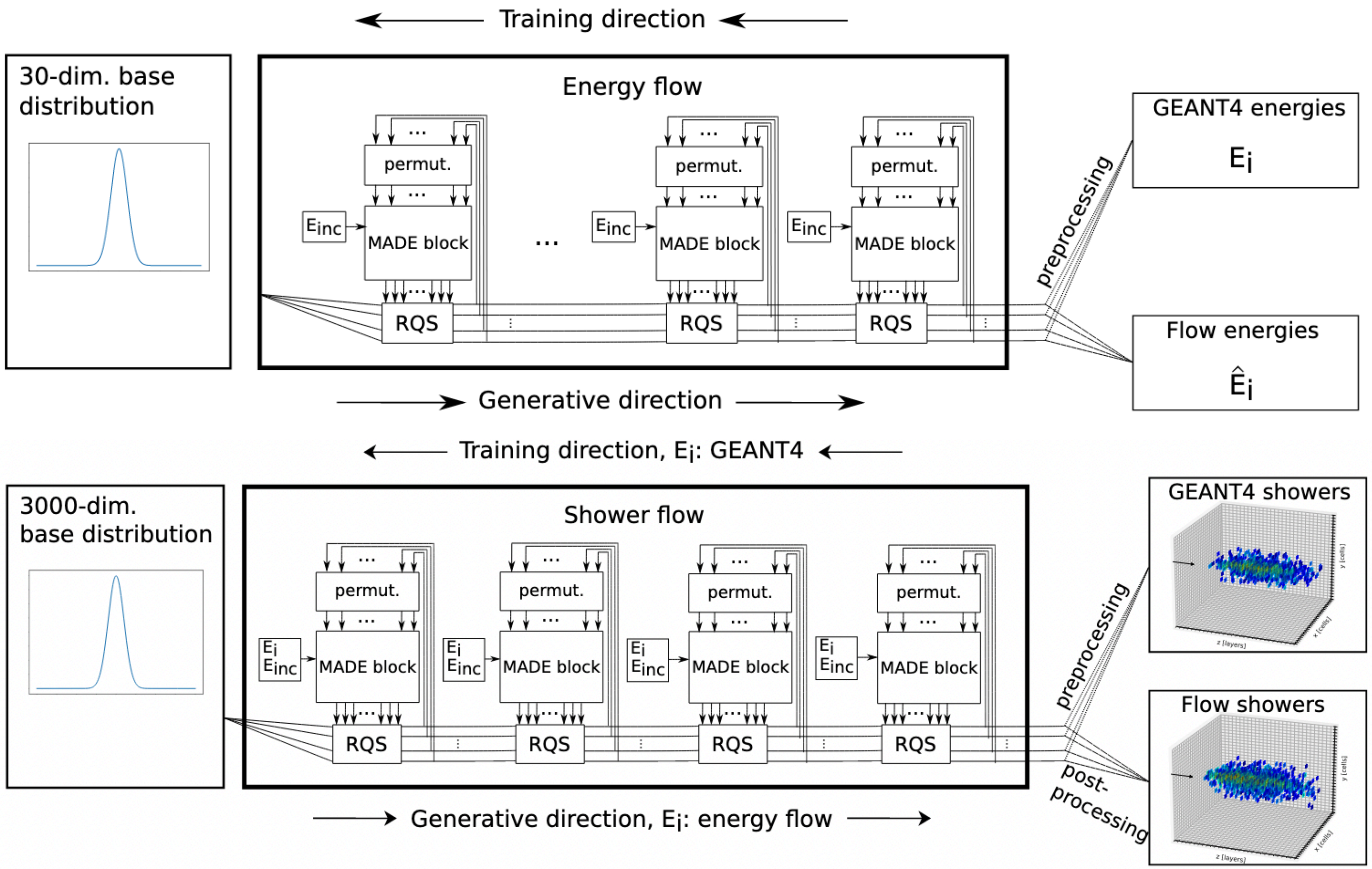


# Thank you

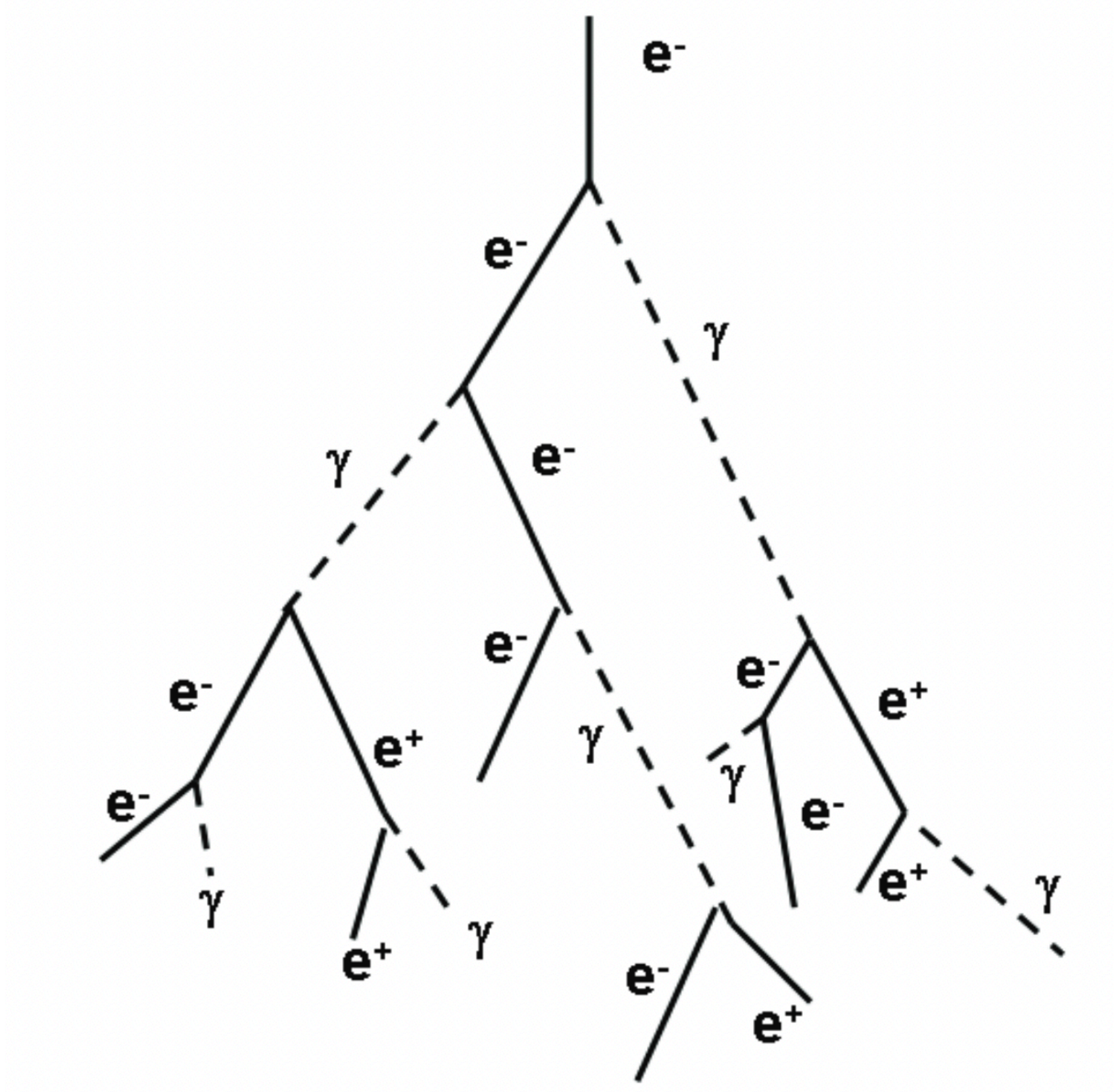
# ILD HG CaloFlow

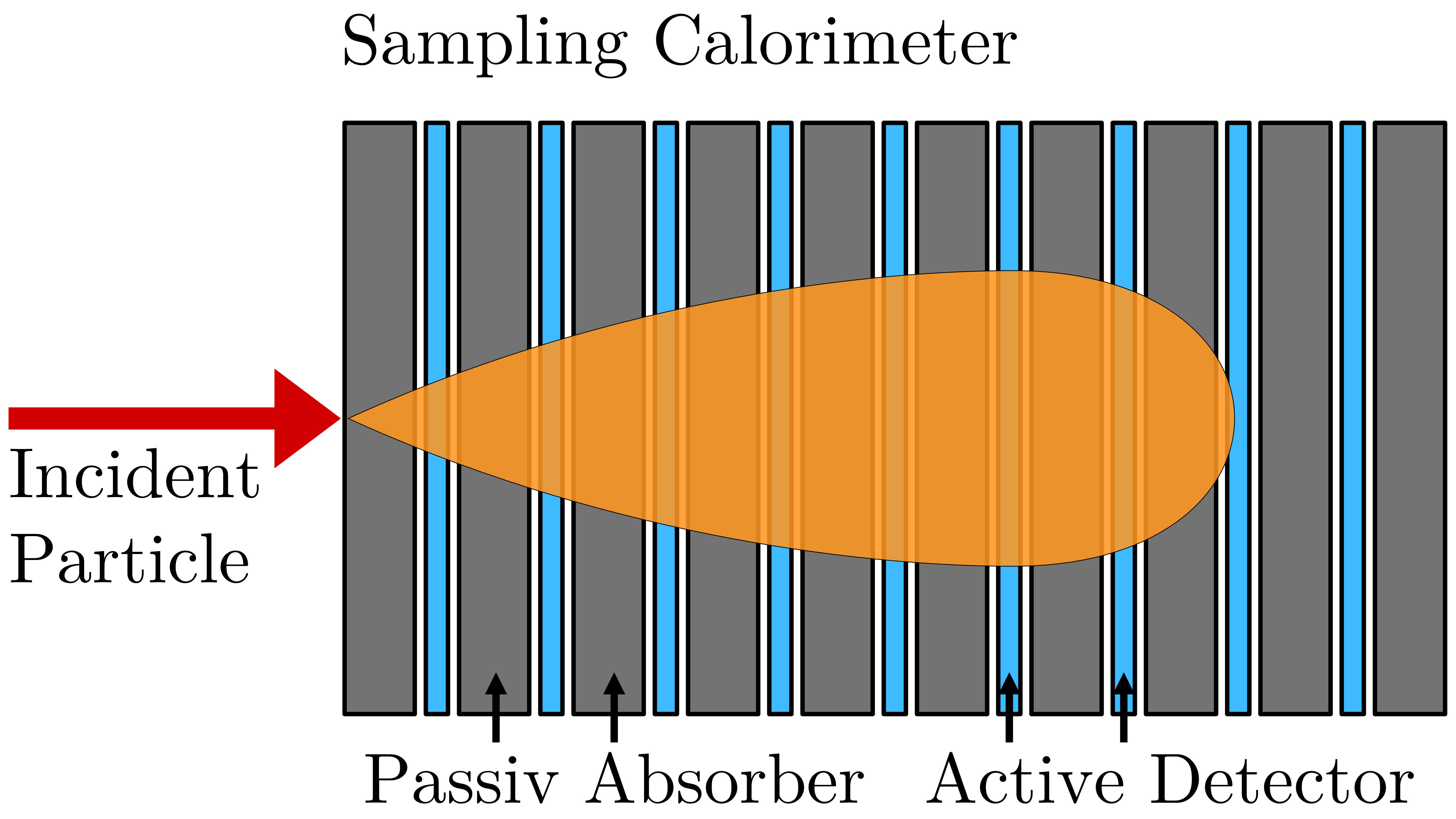
- CaloFlow method:
- Train Energy Flow
  - Generates energy per layer
- Train Shower Flow
  - Uses Energy Flow as conditioning




Krause et. al. **CaloFlow: Fast and Accurate Generation of Calorimeter Showers with Normalizing Flows:** (2021) 2106.05285

# Calorimeter Simulation




- Calorimeter shower:
  - Particle interacts with material
  - Cascade of secondary particles
- Sampling Calorimeter
  - Interspersed active and passive parts
  - Only active segments are recorded