Pay Attention to Mean Fields for Point Cloud Generation

ML4Jets - 6.10.2023

Artwork(s) by DALL – E · 3

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DESY.

Generative Modelling for Detector Simulation

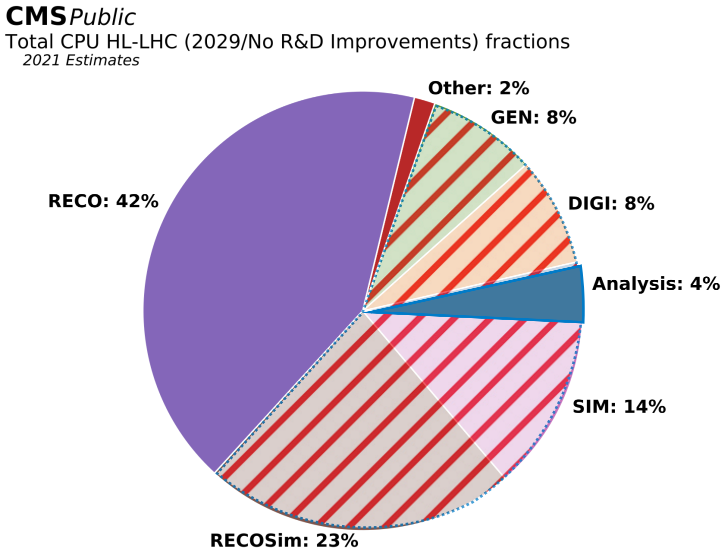
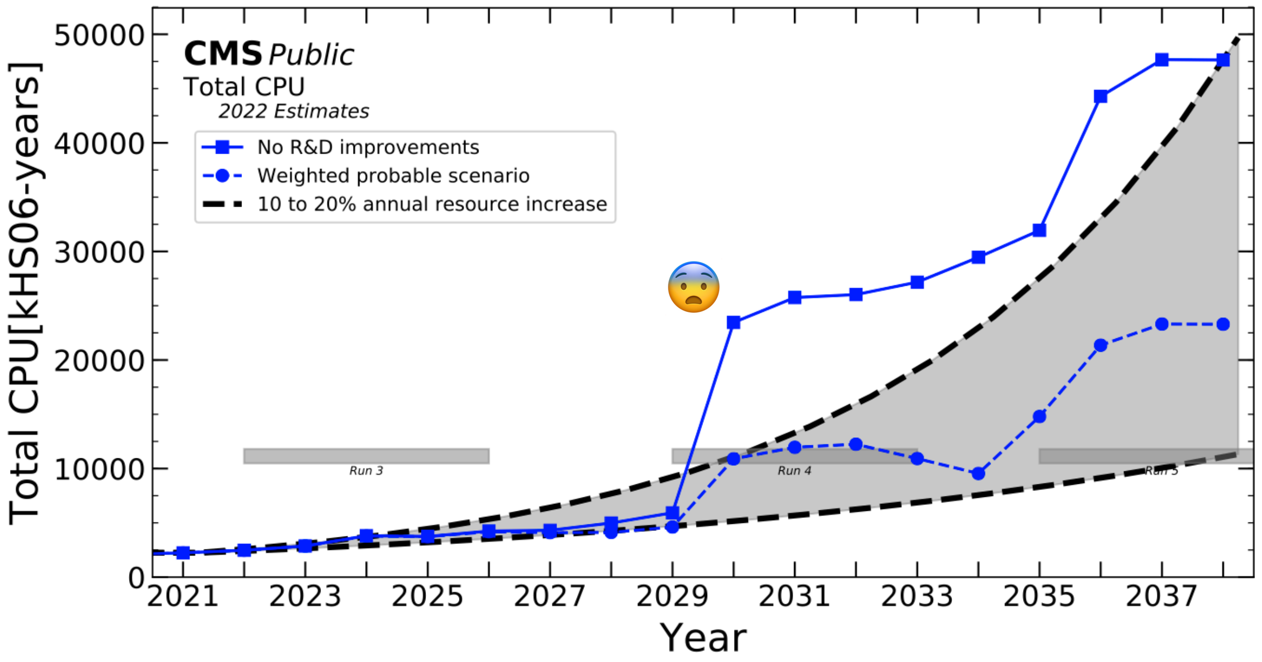
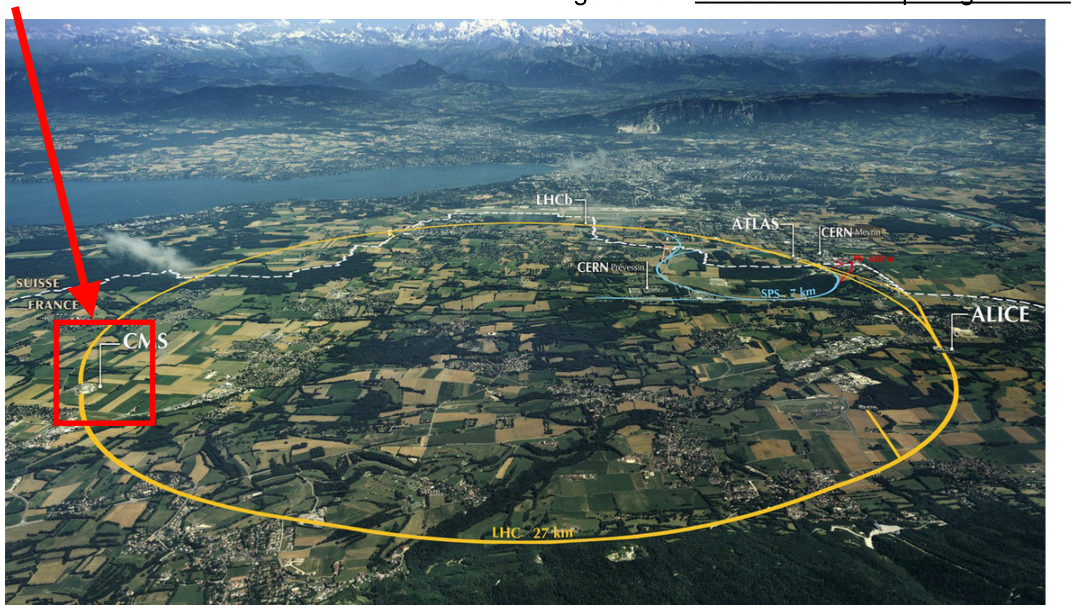


Figure from CMS Offline Computing Results

- Rely on experiment simulation in High Energy Physics (Digital Twin)
- Classically generated with Monte Carlo simulation
  → slow and computing intense
- Already > 50 % of computing budget
- Coming High Luminosity upgrades makes MC approach challenging



CMS Experiment



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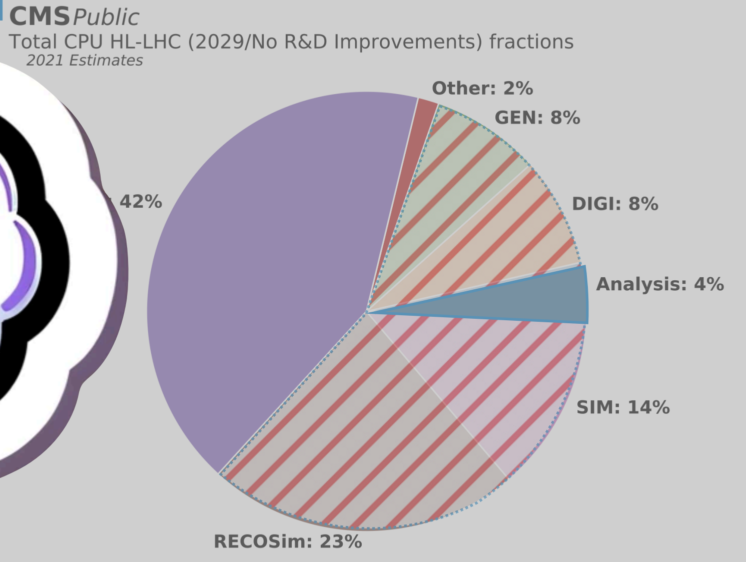

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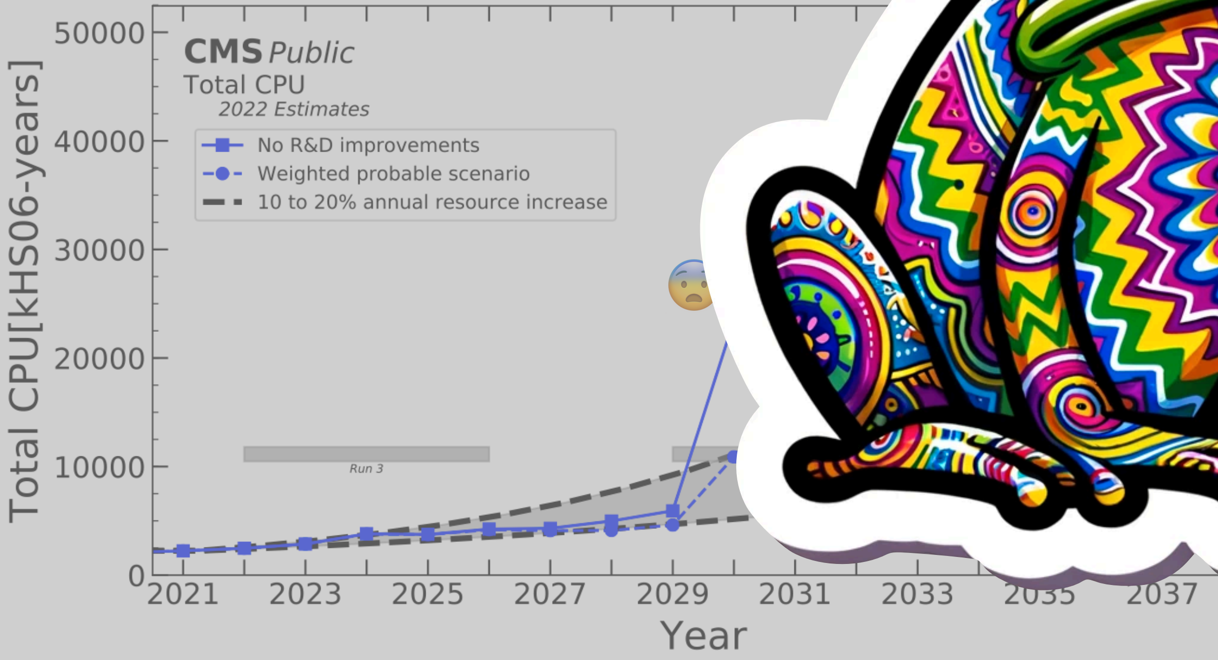


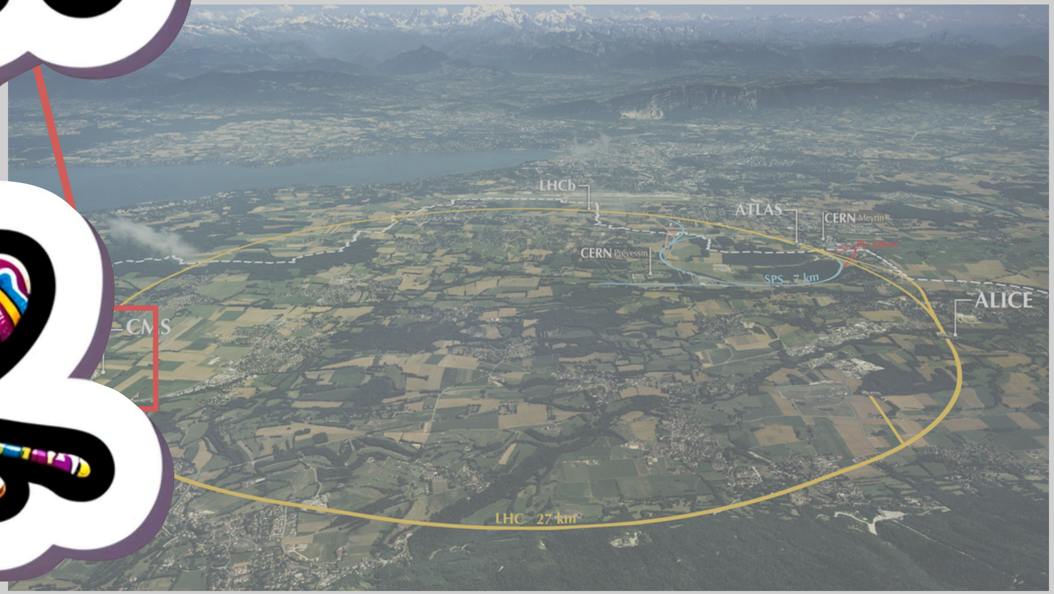


Figure from CMS Offline Computing Results

Point Clouds, their Symmetries

- Most natural representation of collider data
- Handles sparsity
- Detector independent
- Point clouds are permutation invariant → Use permutation-equivariant aggregations

[1]: Kansal et al., Particle Cloud Generation with Message Passing Generative Adversarial Networks
[2]: Krause et al., CaloChallenge

Point Clouds, their Symmetries and Requirements

- Most natural representation of collider data
- Handles sparsity
- Detector independent
- Point clouds are permutation invariant → Use permutation-equivariant aggregations

- Aggregations should scale **linearly** with point cloud cardinality [3]
  → otherwise memory goes 👋🏻 → already a problem at 150 points on one GPU
  → Showstopper for (Self-Attention-based) model I presented at last ML4Jets from scaling from 30 to 150 particles
- Datasets for point clouds: (JetNet [1], preprocessed CaloChallenge [2])

[1]: Kansal et al., Particle Cloud Generation with Message Passing Generative Adversarial Networks
[2]: Krause et al., CaloChallenge
[3]: Kaech et al., Point Cloud Generation using Transformer Encoders and Normalising Flows

Building a permutation equivariant model

- Universal approximation for functions from **Deep Sets** [1]: Sum pooling latent representation of particles:

$$z = \sum_{i=1}^{N} \Phi(x_i)$$

  - Disclaimer: latent space dimension $=$ max set cardinality $\times$ features per point
  - **EPiC**-GAN [2] by Buhmann et al. first to use equivariant architecture to obtain promising results on Jetnet150

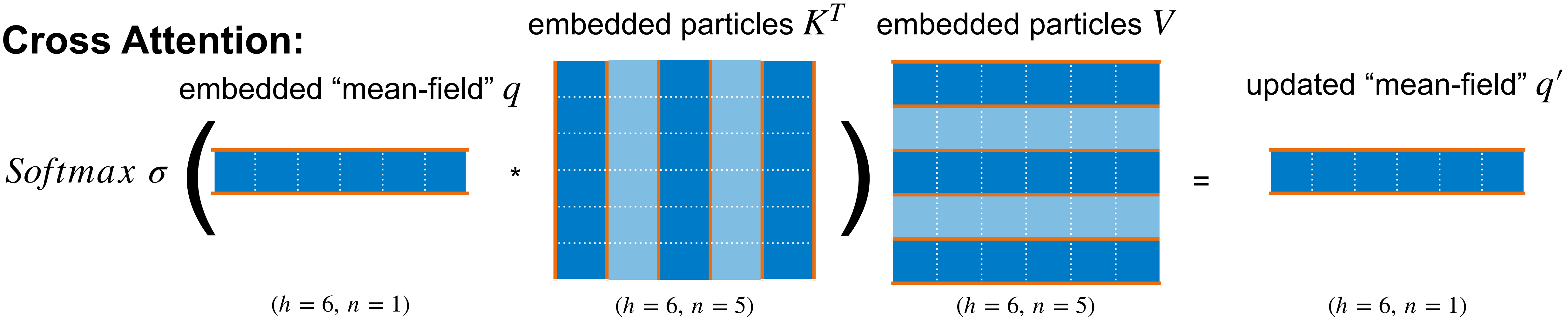
  $\rightarrow$ used combination of sum and mean pooling to update global latent state of jet given which particles are conditionally independent $\rightarrow$ scales $O(n)$

- But I really wanted to keep Attention! - Attention is permutation-equivariant, although most commonly known from (sequential) NLP

[1]: Wagstaff et al., On the Limitations of Representing Functions on Sets
[2]: Buhmann et al., EPiC-GAN: Equivariant Point Cloud Generation for Particle Jets

Cross Attention to the rescue

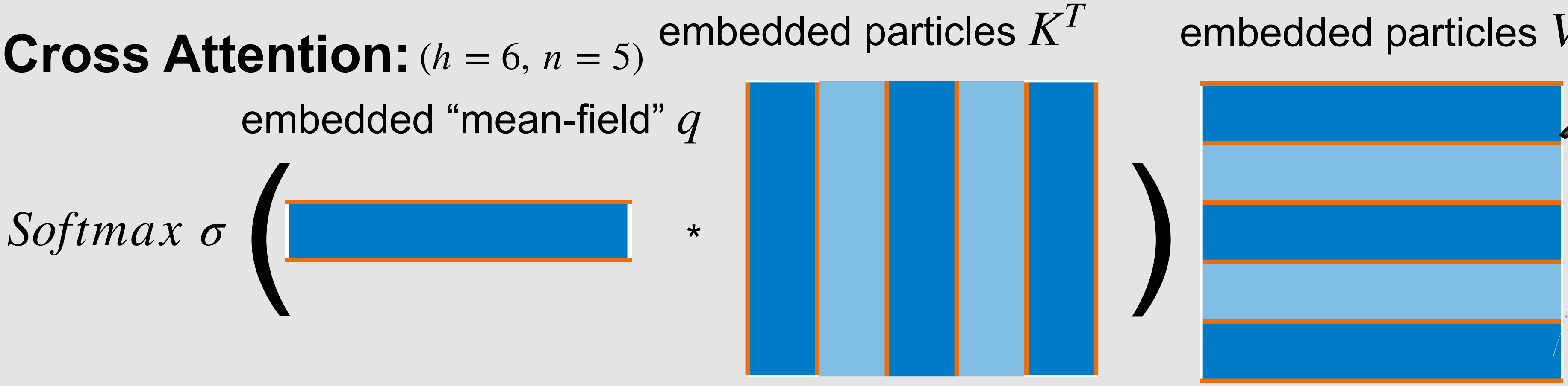
Cross Attention:



$$q' = \sigma\left(\frac{qK^T}{\sqrt{h}}\right) V$$

Similar to Sum-Pooling but more General

Cross Attention: $(h = 6,\ n = 5)$

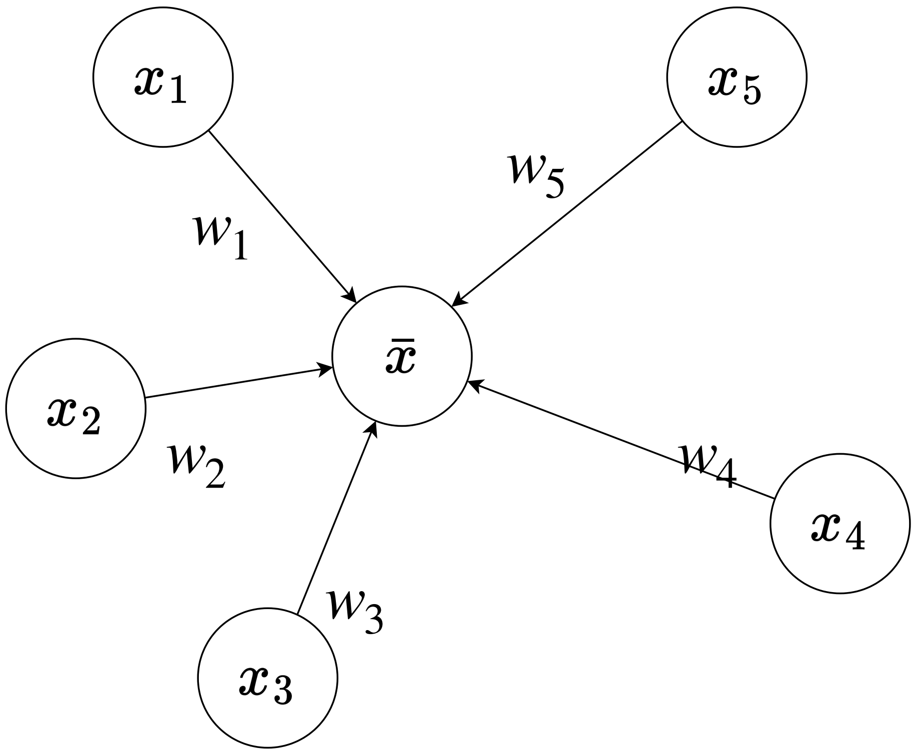


- “Mean-field” $q \in \mathbb{R}^{1\times h}$, h hidden dimension
- K: n embedded particles $K = (W_K x)^T$, $x \in \mathbb{R}^{n\times 4}$, $W_K \in \mathbb{R}^{h\times n}$
- V: n embedded particles, $V = W_V x$, $x \in \mathbb{R}^{n\times 4}$, $W_V \in \mathbb{R}^{h\times n}$

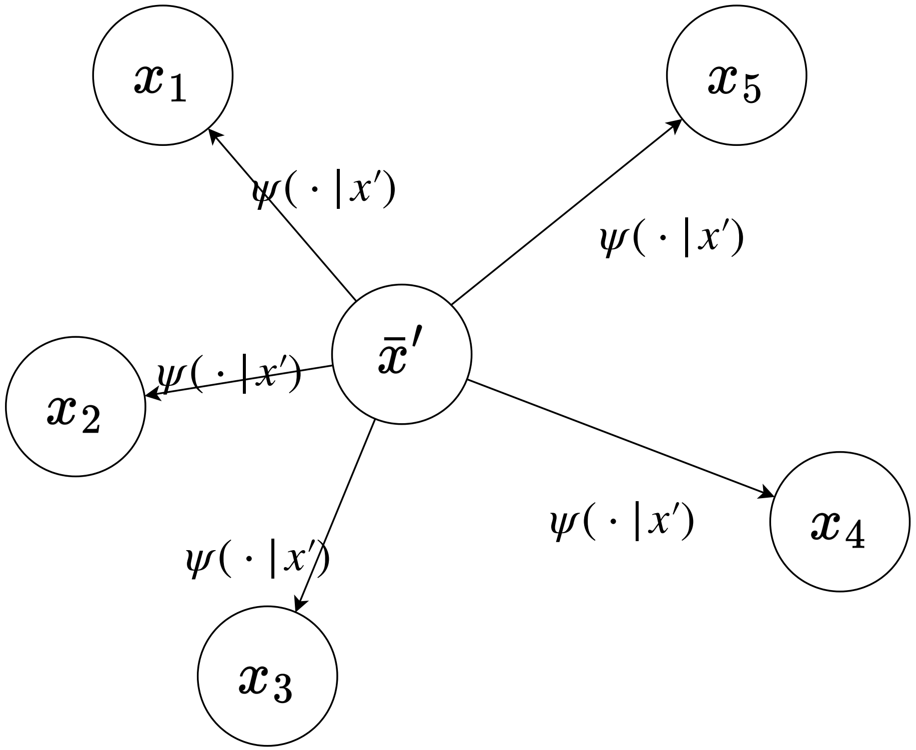
$$\bar{\mathbf{x}}' = \sigma\left((\mathbf{q} \cdot K)/\sqrt{h}\right) V = \sum_{i=1}^{n} w_i W_V \mathbf{x}_i$$

Mean-Field Aggregation

- Introduce "artificial" mean-field $\bar{x}$: proxy for particle-particle interaction
- Particles update mean-field via cross-attention, mean-field concatenated to particles
- Computation scales with $O(n)$



$\longrightarrow$



The Missing Piece

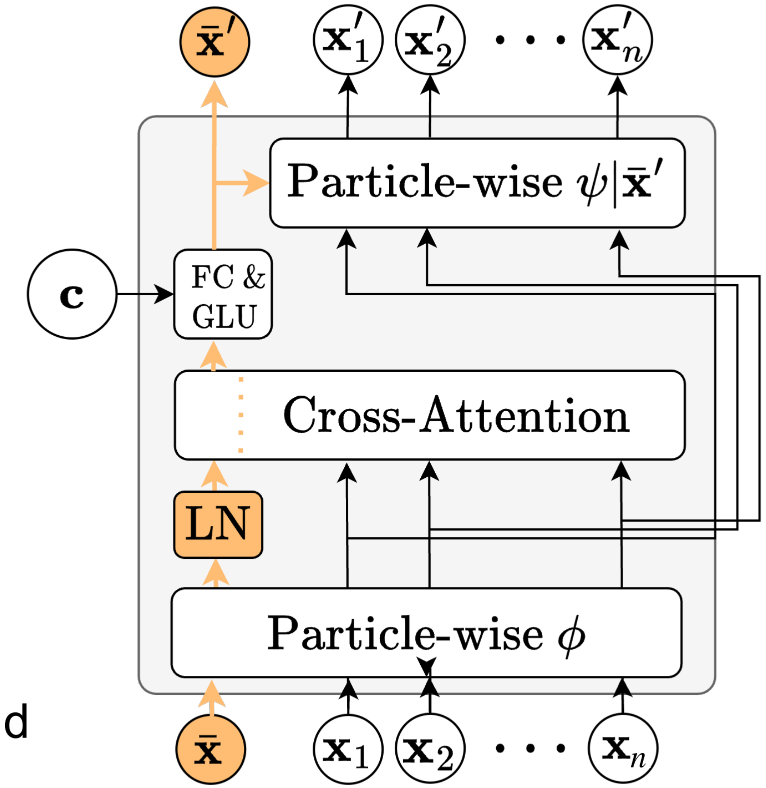
- Although having found a fancy aggregation results were still not acceptable for higher set cardinalities
- Model performs very well up to 50 particles - then stops working
- Why does EPiC-GAN work and my model does not? 😢
- Also is mean and sum pooling not very similar?

The Missing Piece

- Although having found a fancy aggregation results were still not acceptable for higher set cardinalities
- Model performs very well up to 50 particles - then stops working
- Why does EPiC-GAN work and my model does not? 🥲
- Also is mean and sum pooling not very similar?
  - Only difference: the **number of constituents** n!
  - Also: My model is **agnostic** of the number of constituents!

Main Architecture Block

- Architecture motivated by Transformer Encoder architecture used on JetNet 30 [1]
- IN: embedded particles $x_i \in \mathbb{R}^l$, embedded mean-field $\bar{x} \in \mathbb{R}^l$, OUT: embedded particles $x_i \in \mathbb{R}^l$, embedded mean-field $\bar{x} \in \mathbb{R}^l$
  1. Particle-wise ϕ mapping from latent dimension $\mathbb{R}^l \rightarrow \mathbb{R}^h$
  2. Layer Norm applied to mean-field
  3. Multi Headed Cross-Attention between mean-field and particles
  4. Cloud multiplicity & incoming energy (only for CaloChallenge) conditioned fully-connected layer updates mean-field
  5. Particle-wise FC ψ conditioned on mean-field updates particles
- **Permutation-equivariant**
- Not shown here: residual connection between in/out particles & mean-field



[1] Kaech et al., Point Cloud Generation using Transformer Encoders and Normalising Flows

GAN Training

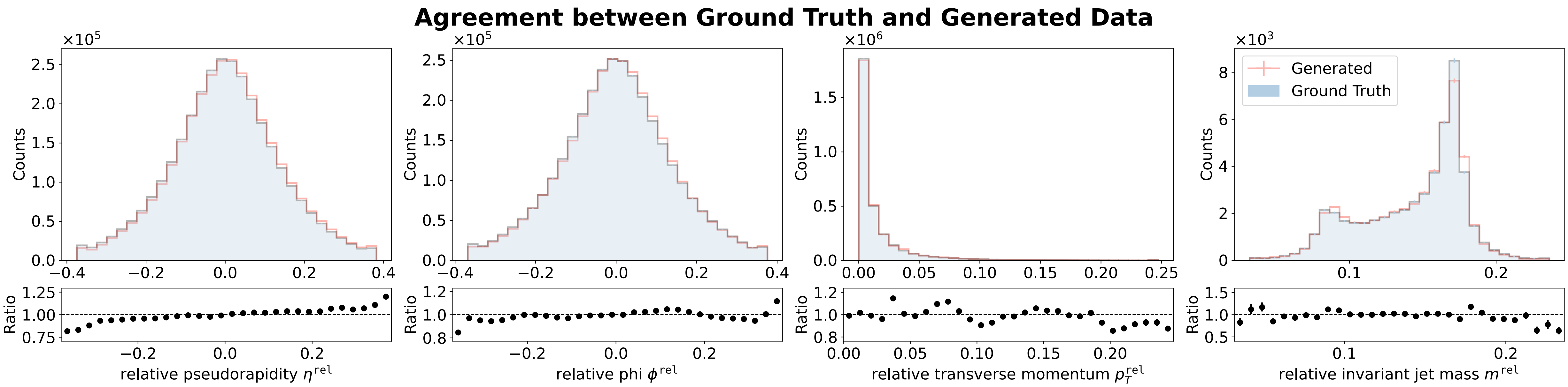
- WGAN GP Loss: $\begin{cases} L_C = -C(x_{real}) + C(x_{gen}) + GP & \text{Critic} \\ L_G = -C(G(z)) & \text{Generator} \end{cases}$
- Gradient Penalty: $GP = (\nabla_{\hat{x}}(C(\hat{x}) - 1)^2, \begin{cases} \hat{x} = \lambda x_{real} + (1-\lambda)x_{gen} \\ \lambda \sim U(0,1) \end{cases}$

  → Only interpolate between same sized clouds
- Deep Mean-field Matching: Generator L2 loss between mean-field in last critic layer for real and fake showers

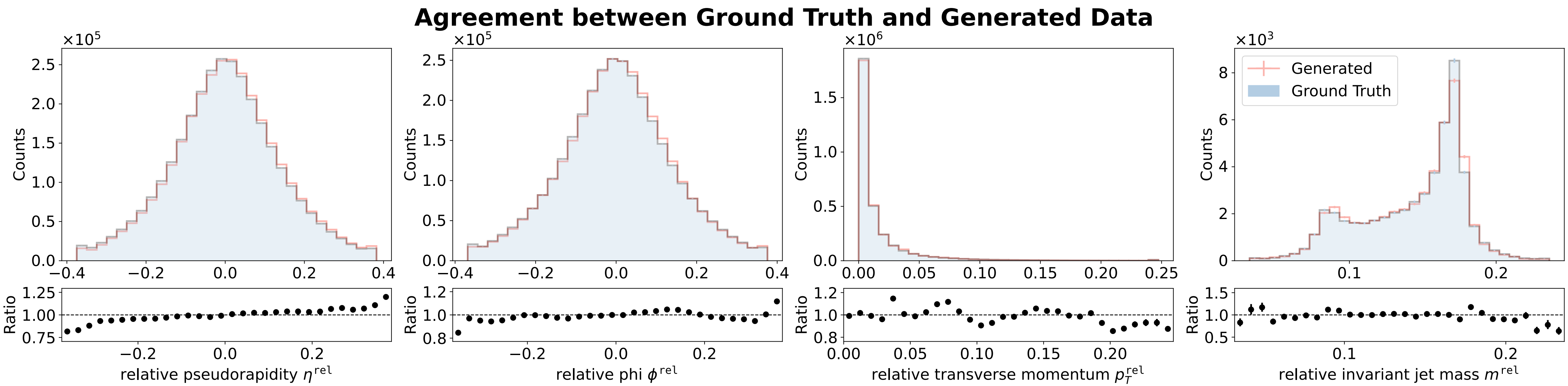
$$L_{MF} = \left| \bar{x}'_{fake} - \bar{x}'_{real} \right|^2$$

- Hence the name: **M**atching **D**eep **M**ean-fields **A**ttentive (**MDMA**) GAN

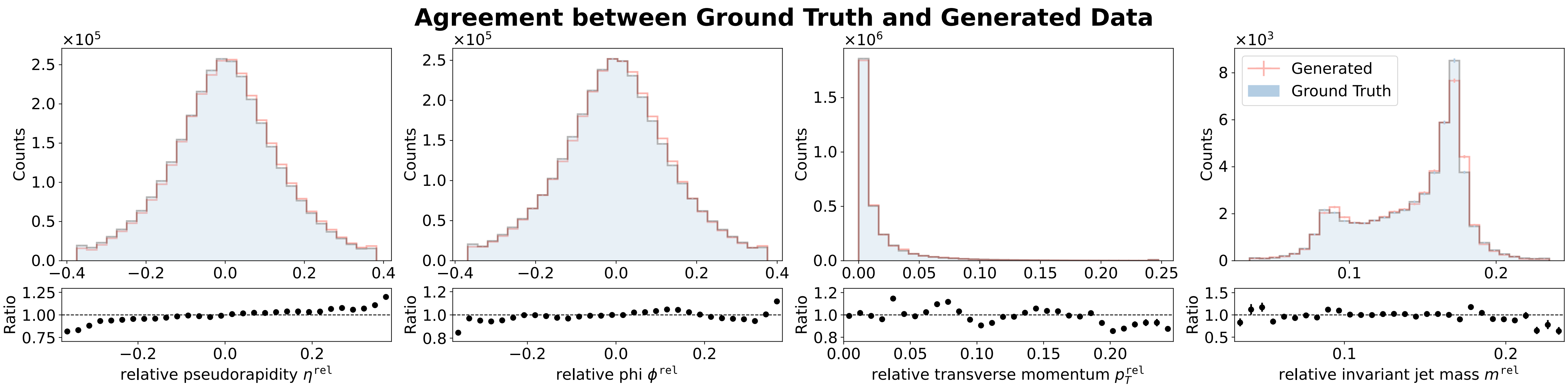
Results: Top-quark JetNet150



Results: Top-quark JetNet150



Results: JetNet150 - quantitative Results

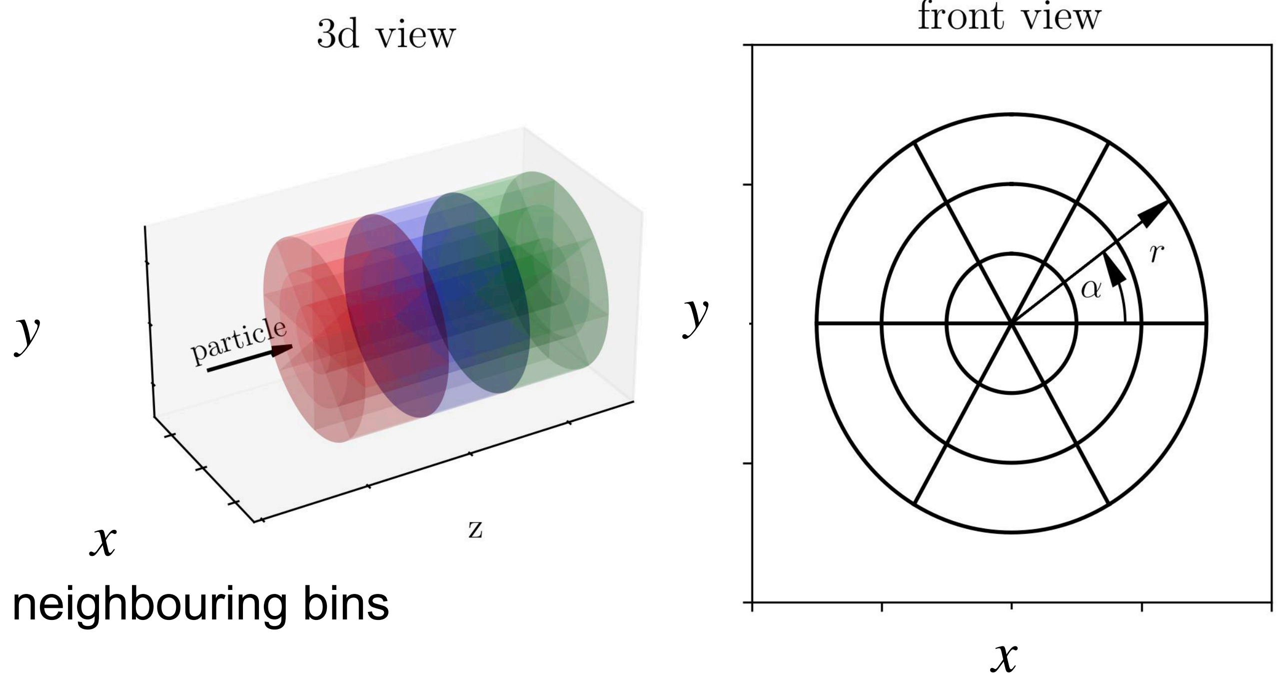


Jet Class	Model	$W_1^M (\times 10^3)$	$W_1^P (\times 10^3)$	$W_1^{EFP} (\times 10^5)$	$KPD (\times 10^4)$	$FPD (\times 10^4)$
Light Quark	EPiC	$\mathbf{0.5 \pm 0.1}$	1.25 ± 0.09	0.81 ± 0.16	-0.0 ± 0.1	5 ± 1
	MDMA	0.7 ± 0.1	$\mathbf{0.37 \pm 0.05}$	0.82 ± 0.14	-0.05 ± 0.07	$\mathbf{3.8 \pm 0.8}$
	IN	0.5 ± 0.1	0.15 ± 0.04	0.59 ± 0.16	-0.0 ± 0.2	3 ± 2
Gluon	EPiC	0.5 ± 0.1	1.13 ± 0.04	$\mathbf{0.93 \pm 0.14}$	0.06 ± 0.05	4.2 ± 0.7
	MDMA	0.5 ± 0.1	$\mathbf{0.27 \pm 0.02}$	1.12 ± 0.13	$\mathbf{-0.05 \pm 0.03}$	$\mathbf{1.4 \pm 0.5}$
	IN	0.6 ± 0.2	0.048 ± 0.009	0.79 ± 0.24	-0.1 ± 0.1	3.2 ± 0.8
Top Quark	EPiC	0.69 ± 0.08	0.65 ± 0.03	2.67 ± 0.39	1.7 ± 1.0	22 ± 1
	MDMA	$\mathbf{0.57 \pm 0.09}$	$\mathbf{0.10 \pm 0.02}$	$\mathbf{2.12 \pm 0.64}$	$\mathbf{-0.0 \pm 0.2}$	$\mathbf{5.3 \pm 0.9}$
	IN	0.42 ± 0.09	0.12 ± 0.04	1.22 ± 0.32	-0.1 ± 0.2	1.2 ± 0.6

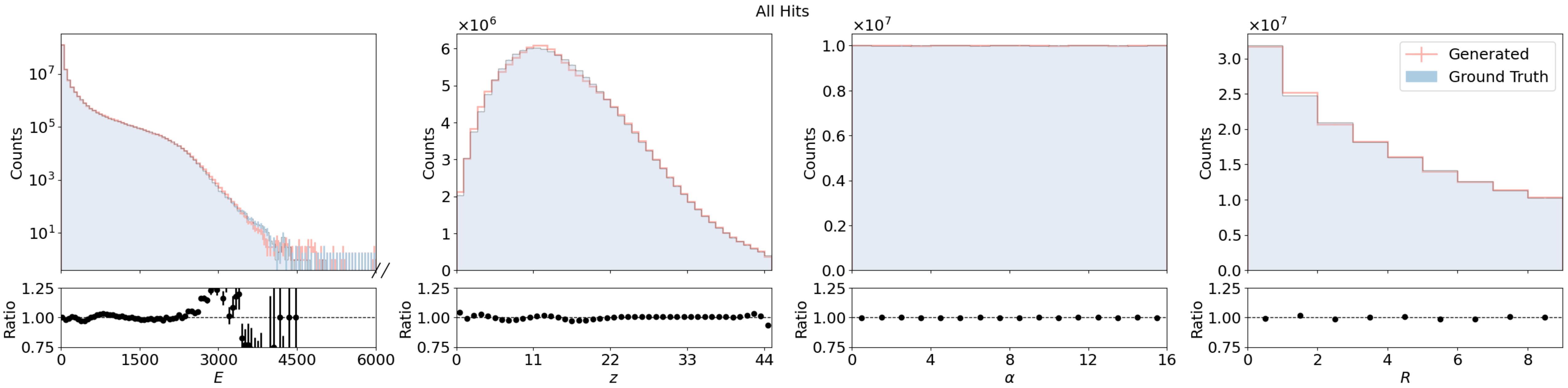
Best written in **bold**

Conclusion: **MDMA** is quite **EPiC** as well

Results: CaloChallenge



- Points: voxels with $E > 0$
- Coordinates: (z, α, R) index
- Dequantisation: Random noise interpolating between neighbouring bins



Classifier Metric, Detector Response & Cross Section

<u>Dataset 2</u>

High-level classifier:

AUC: 0.89

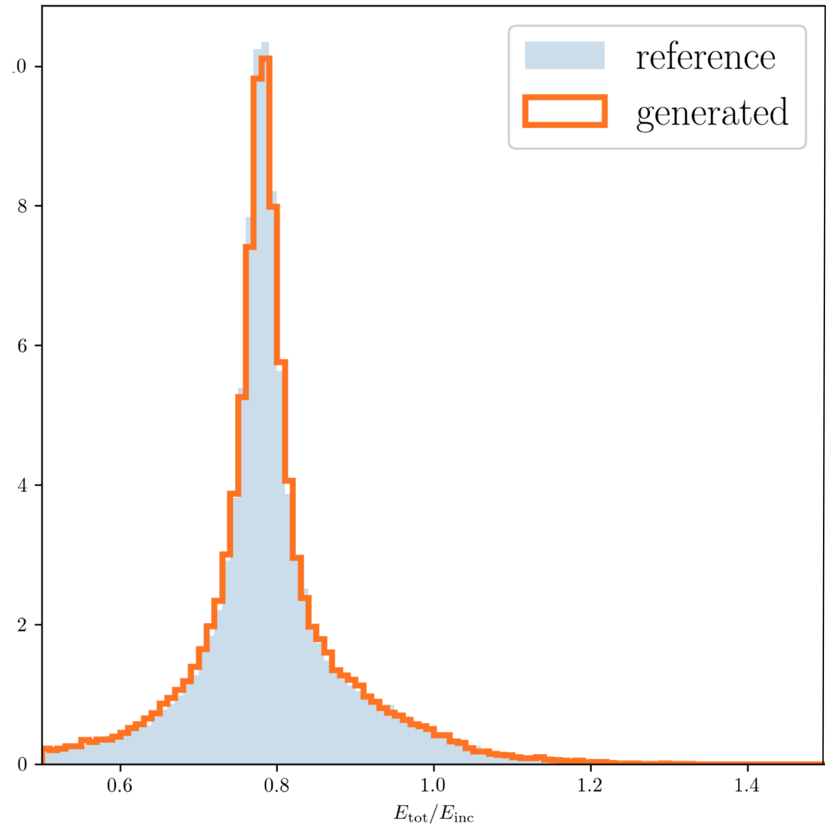
JSD: 0.39

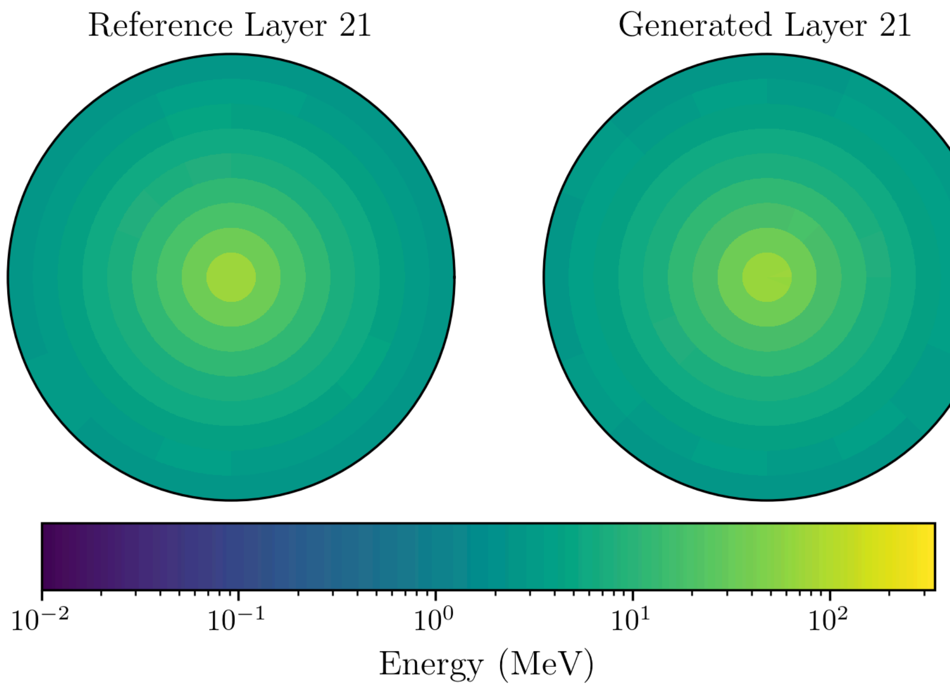
Low-Level classifier:

AUC: 0.97

JSD: 0.71

Target: AUC=0.5





But wait there's more

GANs are Dead - let's Match Flows on MDMA

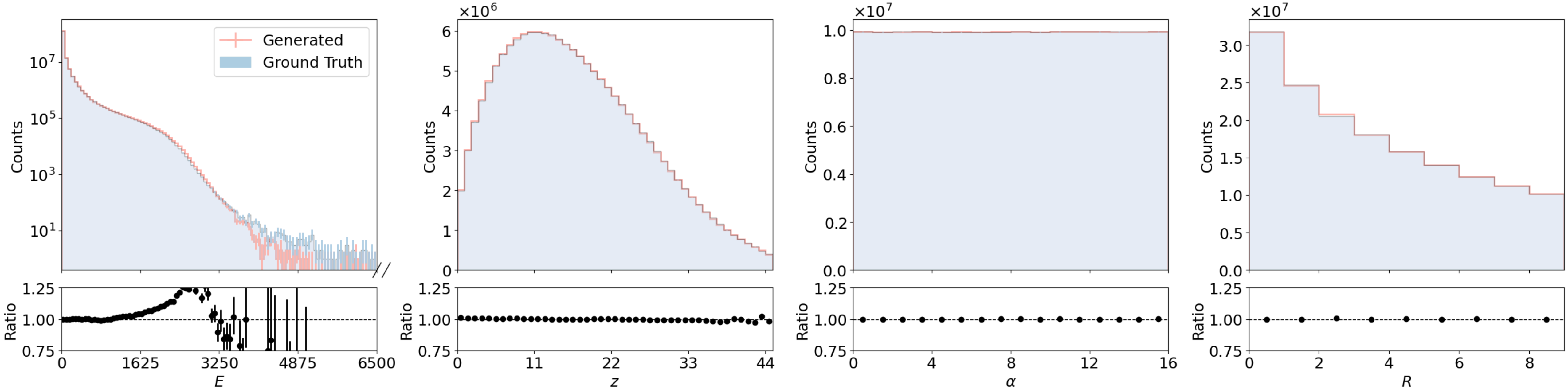
Based on work from Erik Buhmann, Cedric Ewen, Anatoli Karol and Gregor Kasieczka

- Flow Matching [1] novel generative framework, recently proposed for JetNet150 by Buhmann et al. [2]
- They used the EPiC block → replace it with MDMA-block
- Works out of the Box on JetNet150 → never spend months of GPU time on hyperparameter optimisation again!

[1]: Lipman et al., Flow Matching for Generative Modeling
[2]: Buhmann et al., EPiC-ly Fast Particle Cloud Generation with Flow-Matching and Diffusion

Promising First Results on CaloChallenge

Downside: it is a lot slower but please don't ask



<u>Dataset 2</u>
High-level classifier:
AUC: 0.69
JSD: 0.08
Low-level classifier:
AUC: 0.90
JSD: 0.47

Promising First Results on CaloChallenge

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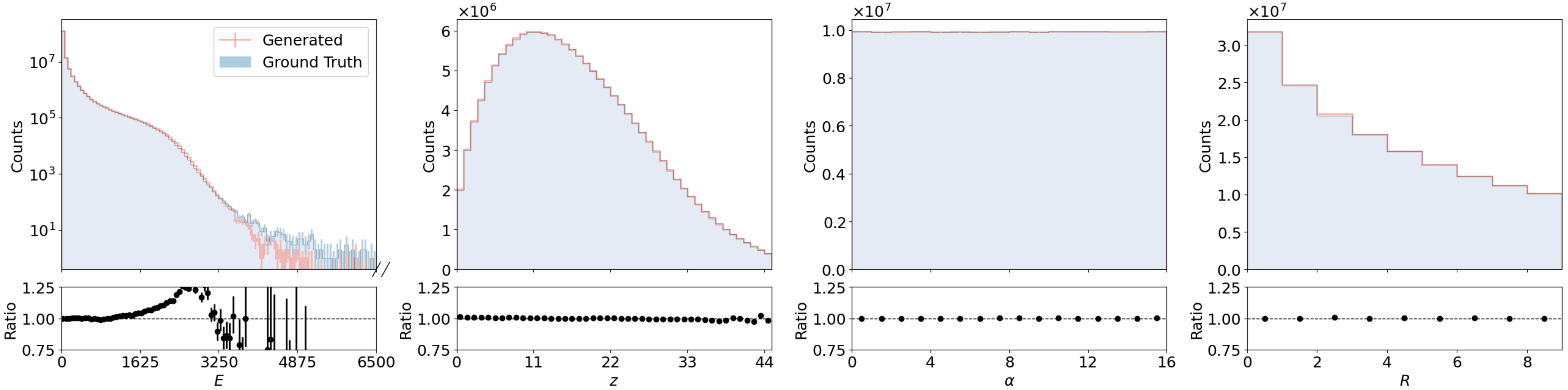

Generation Time:

670 μs→ 270 ms

GAN Results		Flow Matching
High-level classifier:		High-level classifier:
AUC: 0.89		AUC: 0.69
JSD: 0.39	→	JSD: 0.08
Low-level classifier:		Low-level classifier:
AUC: 0.97		AUC: 0.94
JSD: 0.71		JSD: 0.57

Promising First Results on CaloChallenge

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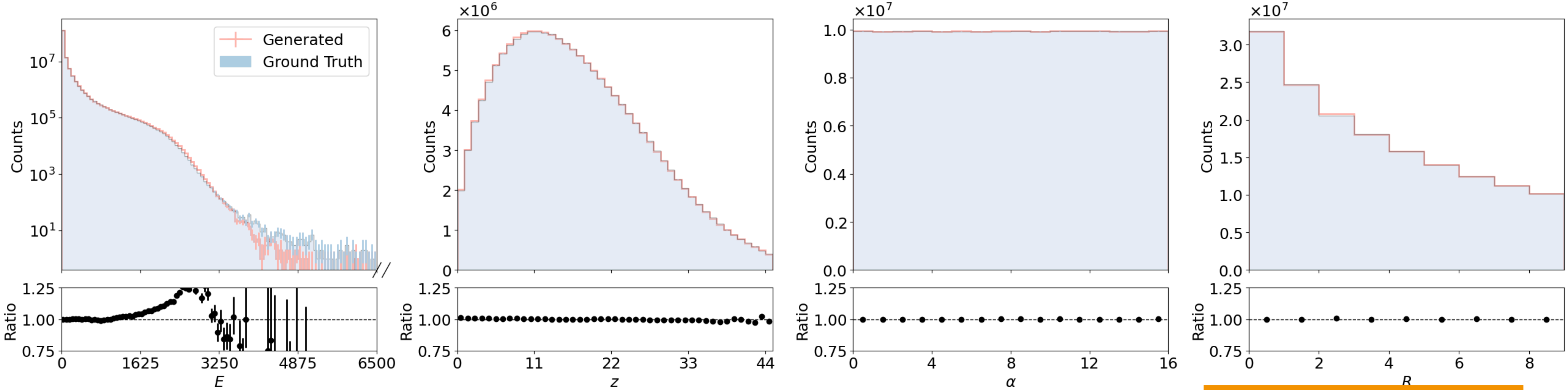

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JSD: 0.57

→

Shifting Double Hits
High-level classifier:
AUC: 0.69
JSD: 0.08
Low-level classifier:
AUC: 0.90
JSD: 0.47

See Moritz's Scham talk:
caloutils (Thursday)

Conclusion

- Point Clouds representation of choice for colliders (sparsity, geometry independent)
- Model using attention-based aggregation mechanism that scales linearly
- Linear scaling achieved by proxying particle-particle interactions by mean-field interaction
- Attention sounds complicated - inherently in our case just a weighted sum
- Results presented for 2 datasets: JetNet150-Top and CaloChallenge Dataset 2
- Although main building block was designed for GAN also works with Flow Matching → improves results on CaloChallenge Dataset 2
- Albeit Flow Matching orders slower, a lot more pleasurable to work with - speed up also possible!

Questions?

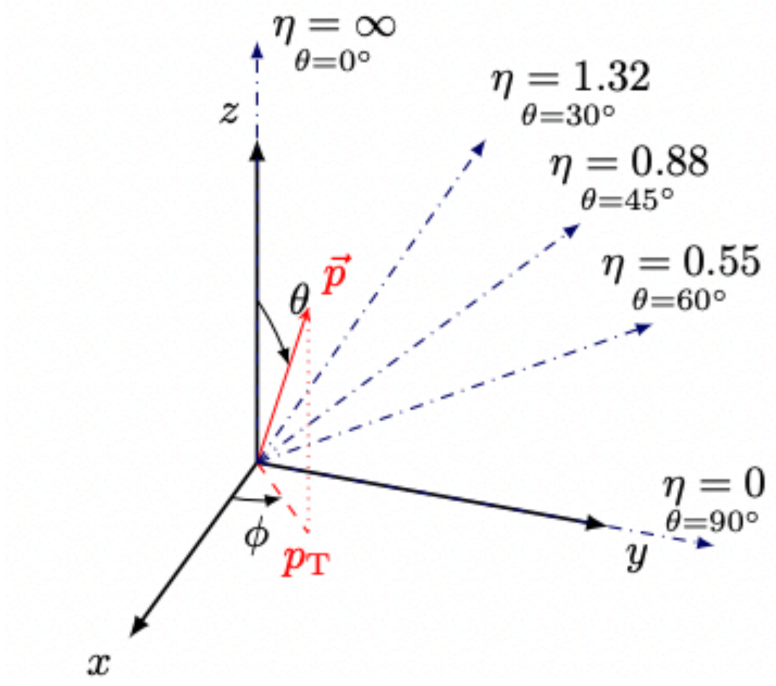
JetNet

JetNet [1] Datasets

- Jets: unordered sprays of particles
- Particles: tuples of $(\eta^{\mathrm{rel}}, \phi^{\mathrm{rel}}, p_T^{\mathrm{rel}})$ relative to jet axis
- Constrained to max 150 particles/jet

  → Goal: generate $\boldsymbol{X} = \left\{ \left(\eta_{(i)}^{\mathrm{rel}}, \phi_{(i)}^{\mathrm{rel}}, p_{T,(i)}^{\mathrm{rel}} \right) \right\}_{(i \leq n)} \sim p_{data}(\boldsymbol{X})$

- Invariant jet mass: $m_{rel}{}^2 = \left(\sum_{i=1}^{n} |\boldsymbol{p}_i| \right)^2 - \left(\sum_{i=1}^{n} \boldsymbol{p}_i \right)^2$
- Size $\sim 178'000$ Samples
- 70% used for training
- Benchmarking possible



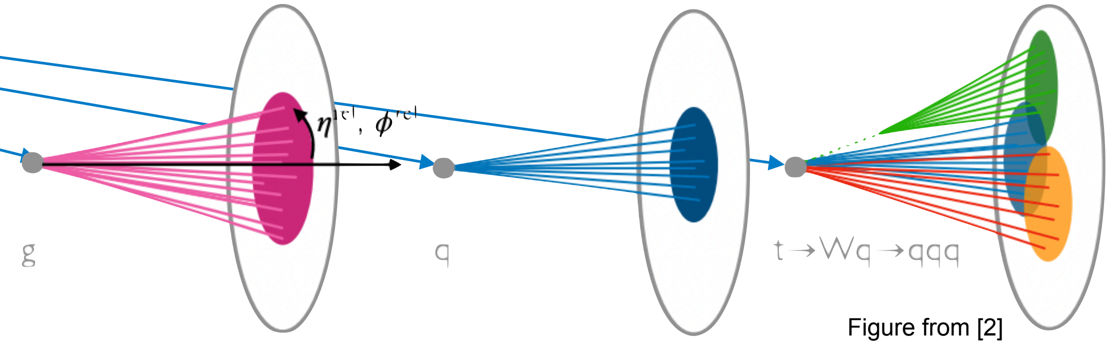


Figure from [2]

[1] Kansal et al, JetNet, PyPi
[2] Kansal et al., Particle Cloud Generation with Message Passing Generative Adversarial Networks, arxiv.org/abs/2106.11535

Point Cloud Representation of Collider Data

- Handle sparsity in the detector by representing hits as Point Cloud [1]
- Reduces batch dimension to (batch size,~4k hits,4) → fits on one GPU
- Model learns physics ~decoupled of detector geometry
- Mapping detector cells to point clouds:

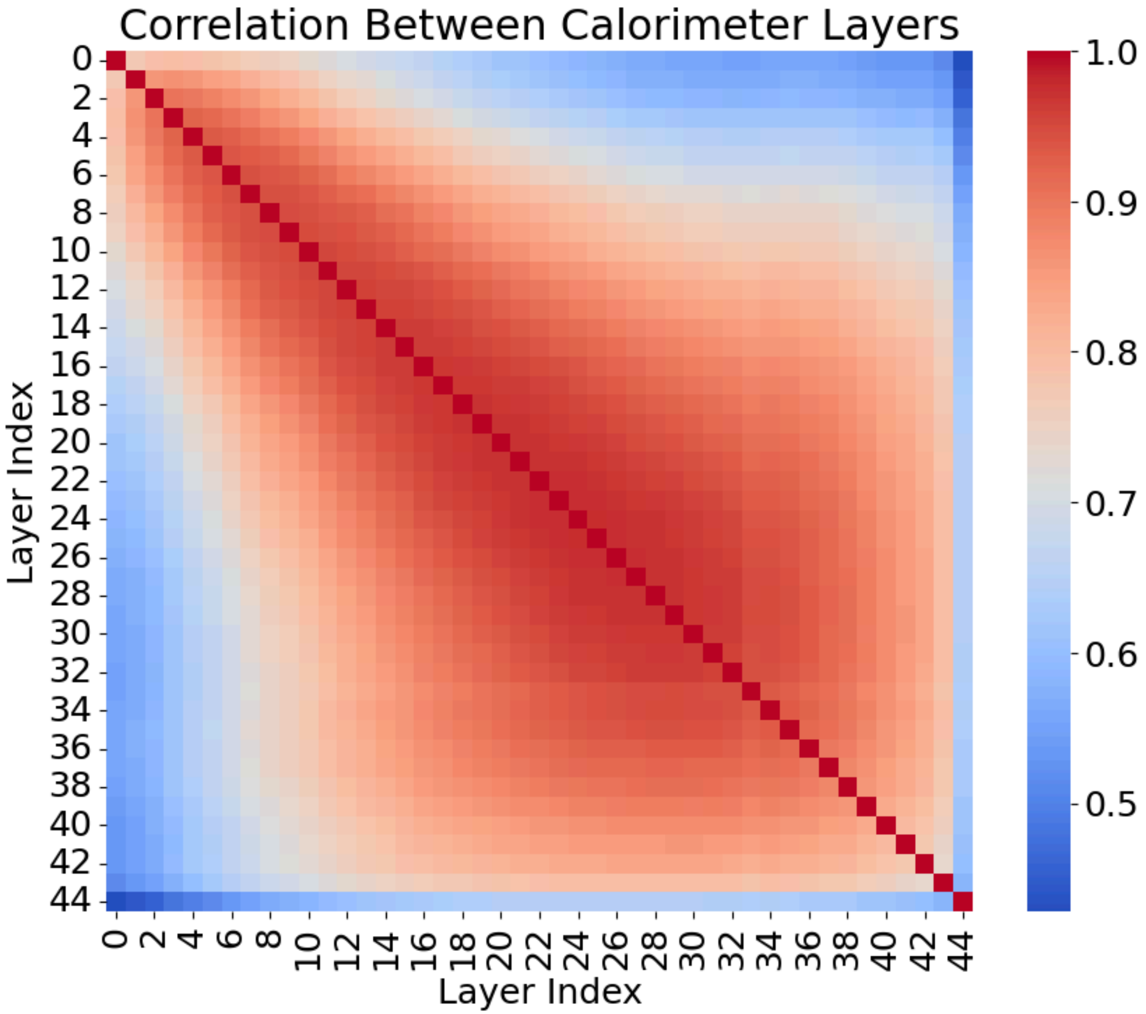
```
hits=detector[E>0]
for coordinate  in (z, alpha, R):
    for cellnumber in enumerate(cells):
            coordinate(cellnumber) x=cellnumber + DQ(0,1)
    x=MinMaxScaler(x)
    x=Logit(x)
    x=StandardScale(x)
for hit in hits:
    E(hit)=BoxCoxTransform(E(hit))
```

- Gives about Gaussian distribution for different variables (except α)
- α periodcity → problematic
- Volume of space **not** respected in particle cloud definition

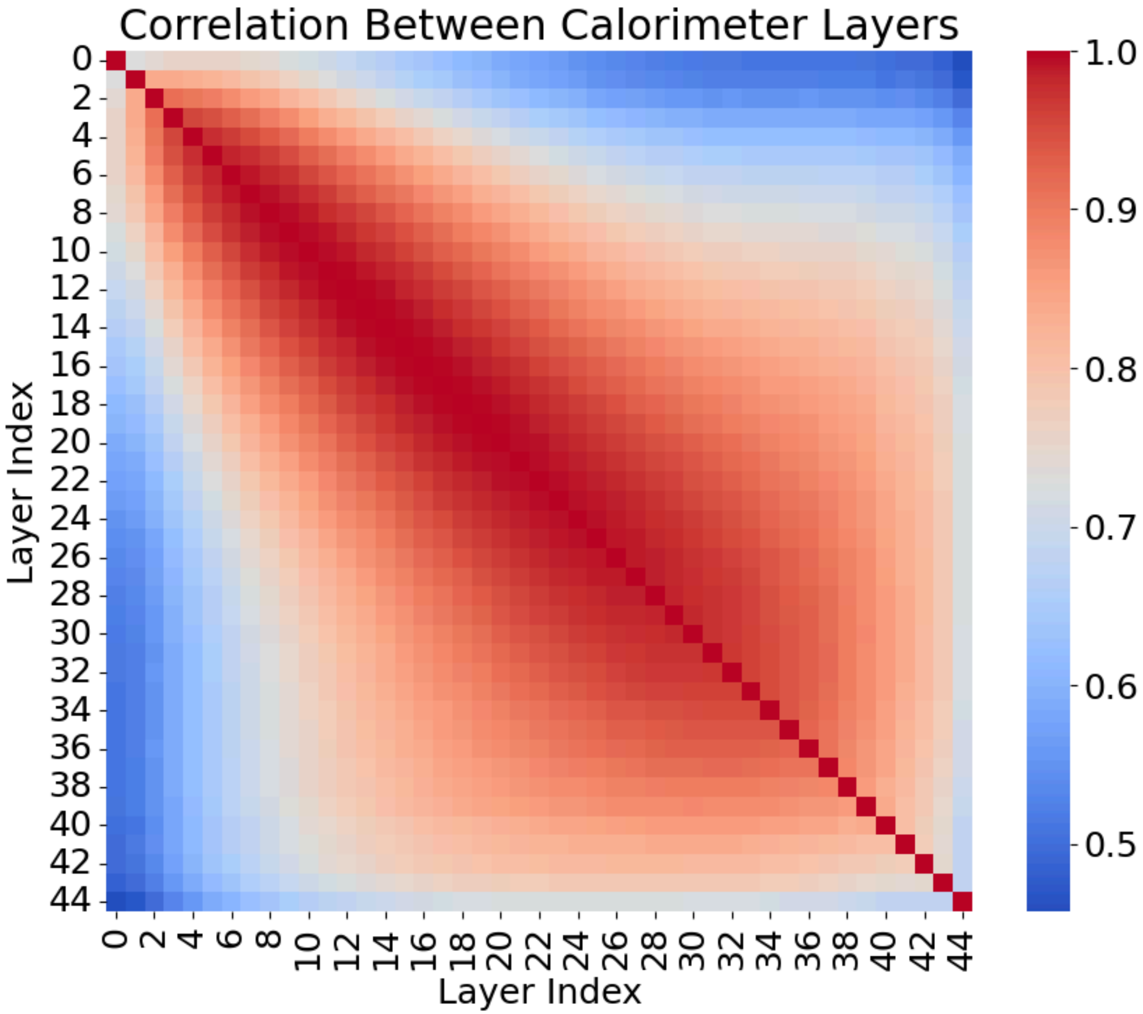
[1] Simon Schnake et al., 2022

CaloChallenge Correlation between Layers

Generated

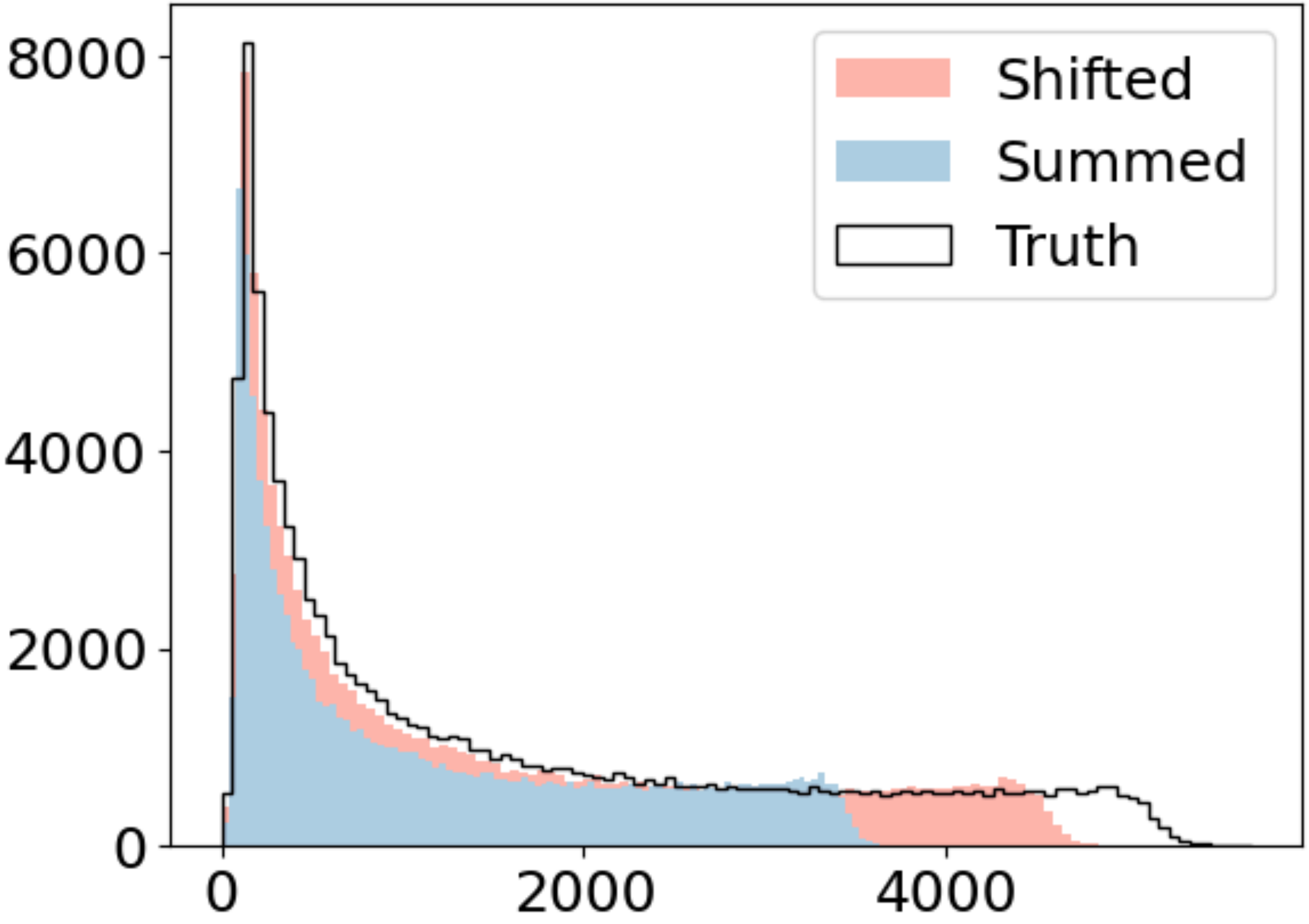


Ground Truth

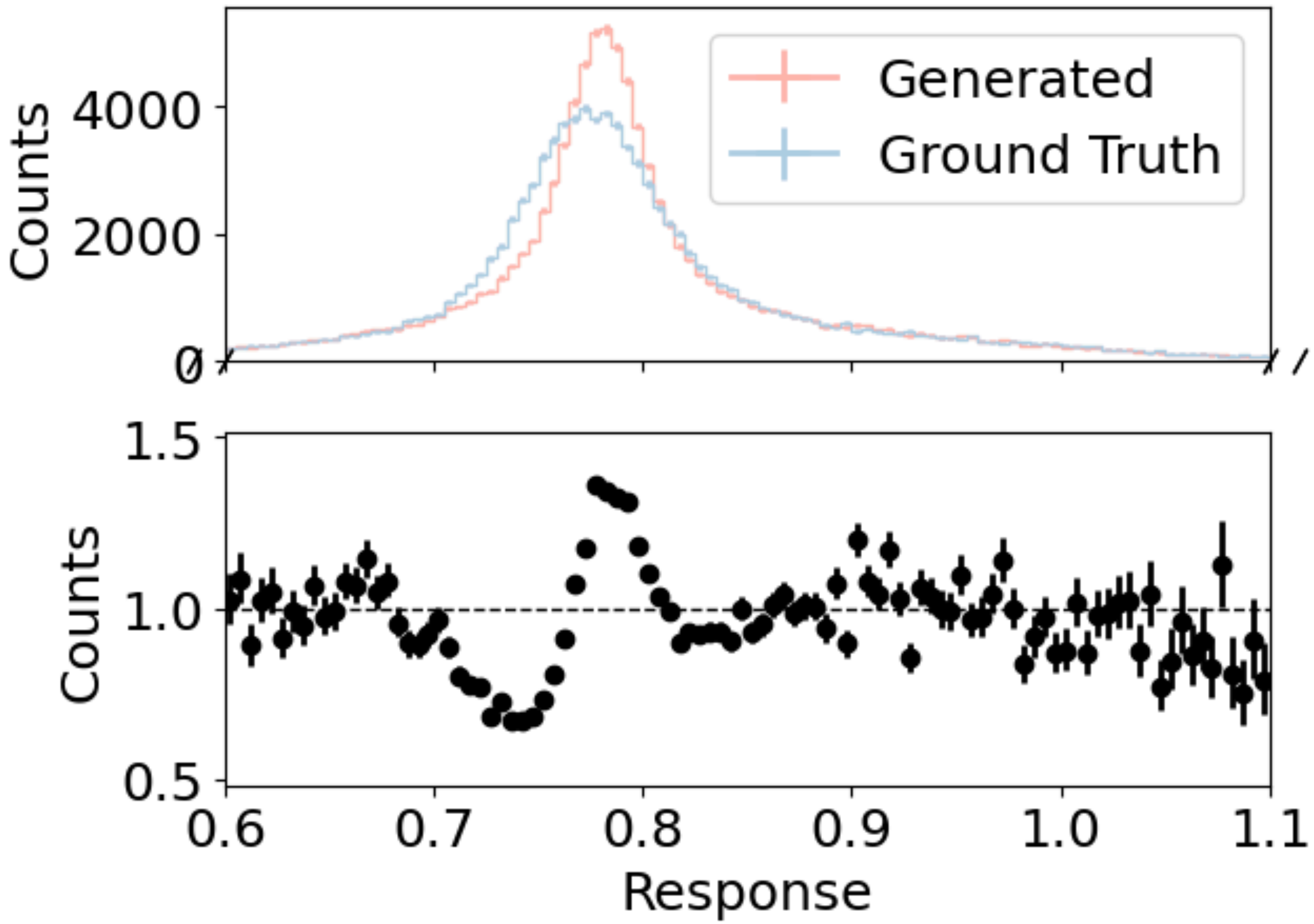


Double Hits

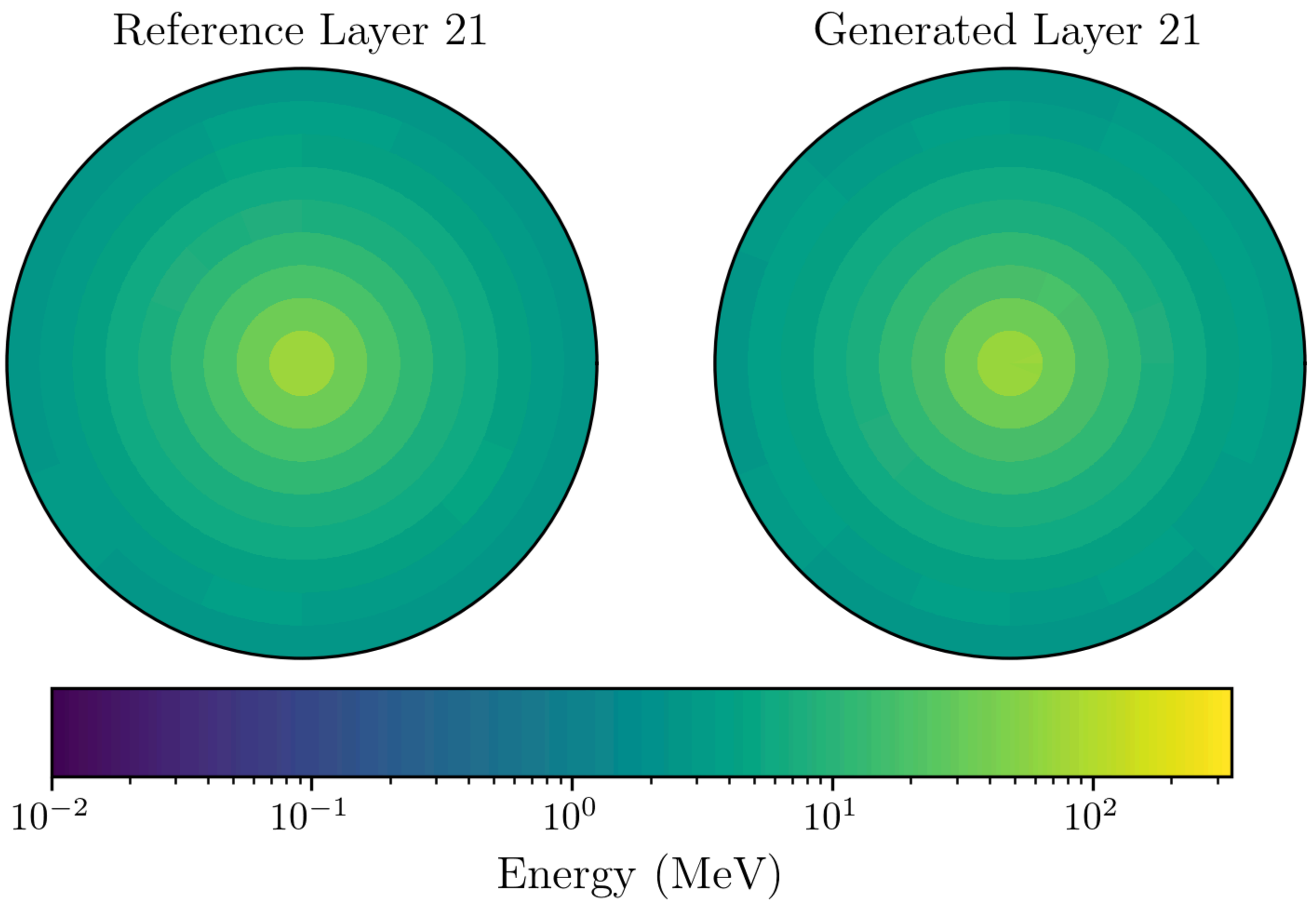
- Multiple hits can get assigned to same detector cell
- Simplest approach: just summing energies
- Check Moritz Schams presentation about our repository *caloutils* for a more sophisticated approach!



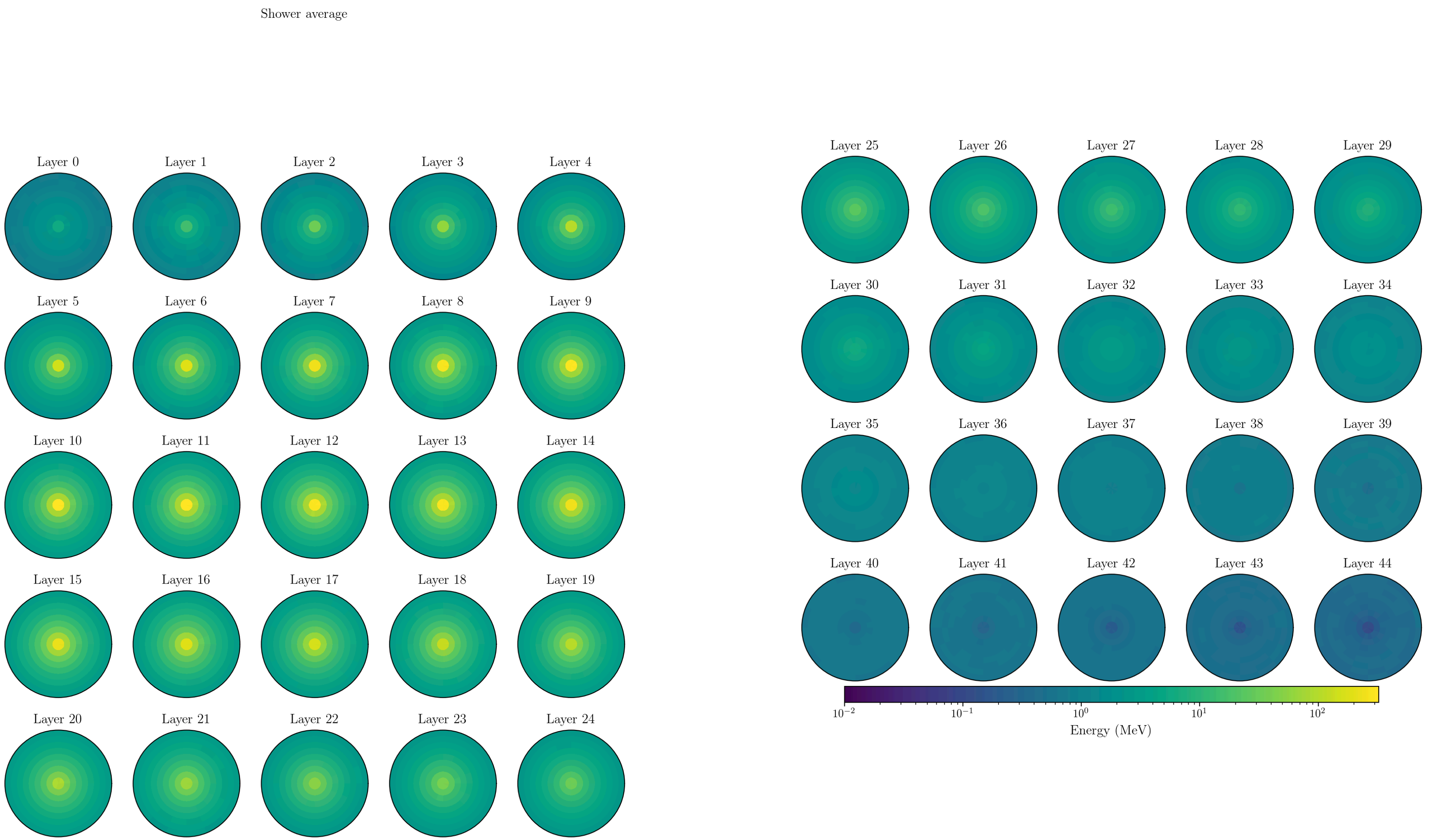
Todo: Improve Incoming Energy Conditioning



Energy Per Layer



All Layers


Shower average
Layer 0
Layer 1
Layer 2
Layer 3
Layer 4
Layer 5
Layer 6
Layer 7
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Layer 9
Layer 10
Layer 11
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Layer 14
Layer 15
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Layer 39
Layer 40
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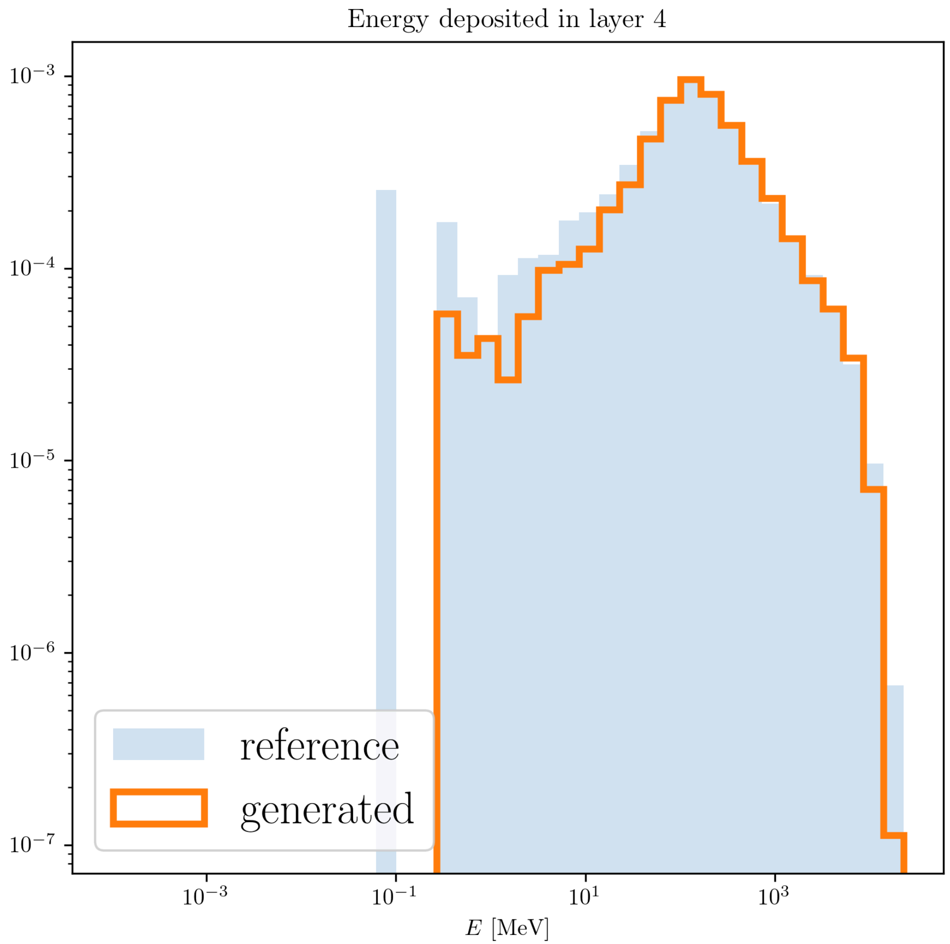
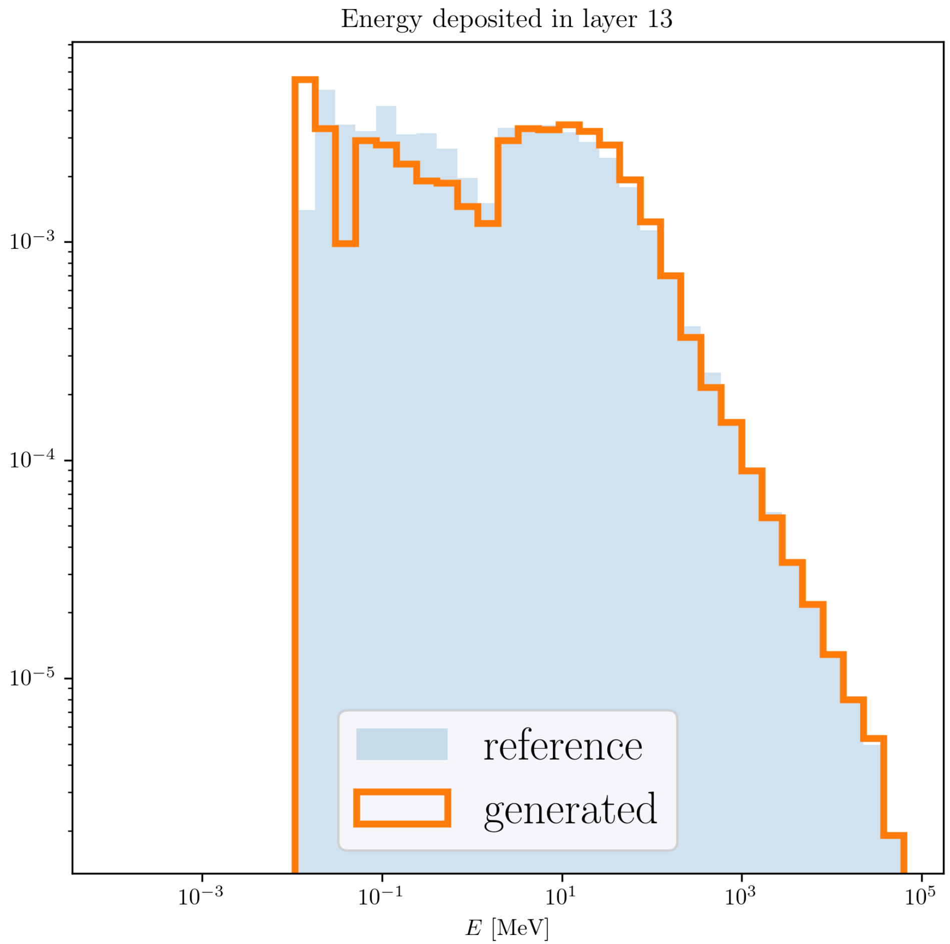
Layer 42
Layer 43
Layer 44
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Energy (MeV)

Energy Deposition per Layer





Center of Energy