



Accelerating Science

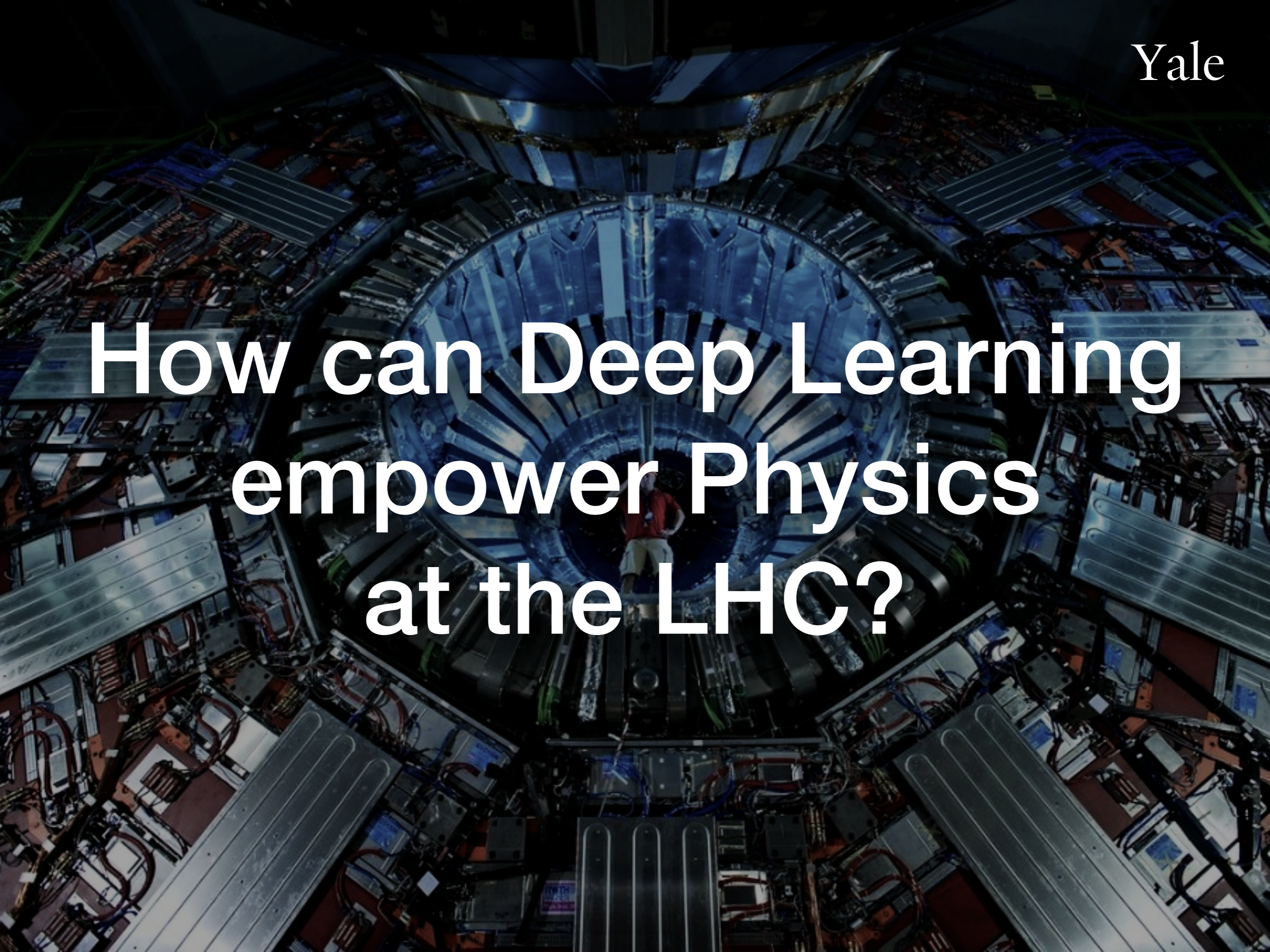
with Deep Learning

Michela Paganini

Yale

 [mickypaganini](#)

# How can Deep Learning empower Physics at the LHC?



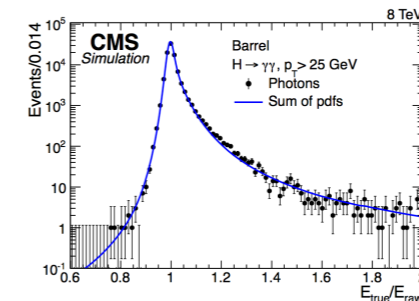
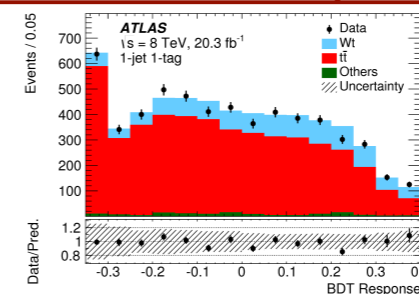
- Lots of convenient, but minor improvements across all aspects of the experiments

## How Does Machine Learning Fit In?

15

from M. Kagan

- In analysis:**
  - Classifying signal from background, especially in complex final states
  - Reconstructing heavy particles and improving the energy / mass resolution
- In reconstruction:**
  - Improving detector level inputs to reconstruction
  - Particle identification tasks
  - Energy / direction calibration
- In the trigger:**
  - Quickly identifying complex final states
- In computing:**
  - Estimating dataset popularity, and determining how number and location of dataset replicas



ATLAS Simulation  
 Tau Particle Flow  
 Diagonal fraction: 74.7%

| Reconstructed decay mode          | $Z/\gamma^* \rightarrow \tau\tau$ | $3h^1 \geq 1\pi^0$ | $3h^2$ | $h^1 \geq 2\pi^0$ | $h^1 \pi^0$ | $h^1$ |
|-----------------------------------|-----------------------------------|--------------------|--------|-------------------|-------------|-------|
| $Z/\gamma^* \rightarrow \tau\tau$ | 56.6                              | 5.3                | 3.6    | 2.5               | 0.2         | 0.2   |
| $3h^1 \geq 1\pi^0$                | 40.2                              | 92.5               | 0.3    | 0.6               | 0.2         | 0.2   |
| $3h^2$                            | 0.4                               | 0.1                | 35.4   | 6.0               | 0.4         | 0.4   |
| $h^1 \geq 2\pi^0$                 | 2.5                               | 0.9                | 56.3   | 74.8              | 9.4         | 9.4   |
| $h^1 \pi^0$                       | 0.3                               | 1.2                | 4.3    | 16.0              | 89.7        | 89.7  |
| $h^1$                             | 0.3                               | 0.3                | 1.2    | 4.3               | 16.0        | 89.7  |

Generated decay mode

- But nothing has really stood out as a major game-changer until...

# CaloGAN:

Simulating 3D High Energy Particle  
Showers in Multi-Layer EM Calorimeters  
with Generative Adversarial Networks

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Michela Paganini

with Luke de Oliveira, Ben Nachman



THEORY

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\Psi}\not{D}\Psi + h.c. \\ & + \bar{\Psi}_i \gamma_{ij} \Psi_j \phi + h.c. \\ & + |\mathcal{D}_\mu \phi|^2 - V(\phi) \end{aligned}$$

HARD  
INTERACTIONS (ME  
CALCULATIONS)

PARTON  
SHOWERING &  
HADRONIZATION

Geant 4

DETECTOR SIM. &  
MATERIAL  
INTERACTIONS

DIGITIZATION

...



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \bar{\psi}_i \gamma_{ij} \psi_j \phi + h.c. + \frac{1}{2} \partial_\mu \phi^2 - V(\phi)$$

**CaloGAN**

**Geant 4**

THEORY

HARD INTERACTIONS (ME CALCULATIONS)

PARTON SHOWERING & HADRONIZATION

DETECTOR SIM. & MATERIAL INTERACTIONS

DIGITIZATION

...



# Motivation and Challenges

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## Full Simulation is slow

Detector simulation can take  $O(\text{min}/\text{event})$ , and ME calculations to high order in perturbation can compete for total generation time

## Petabytes of Simulated Data

Large amounts of simulated data needs to be stored and transferred

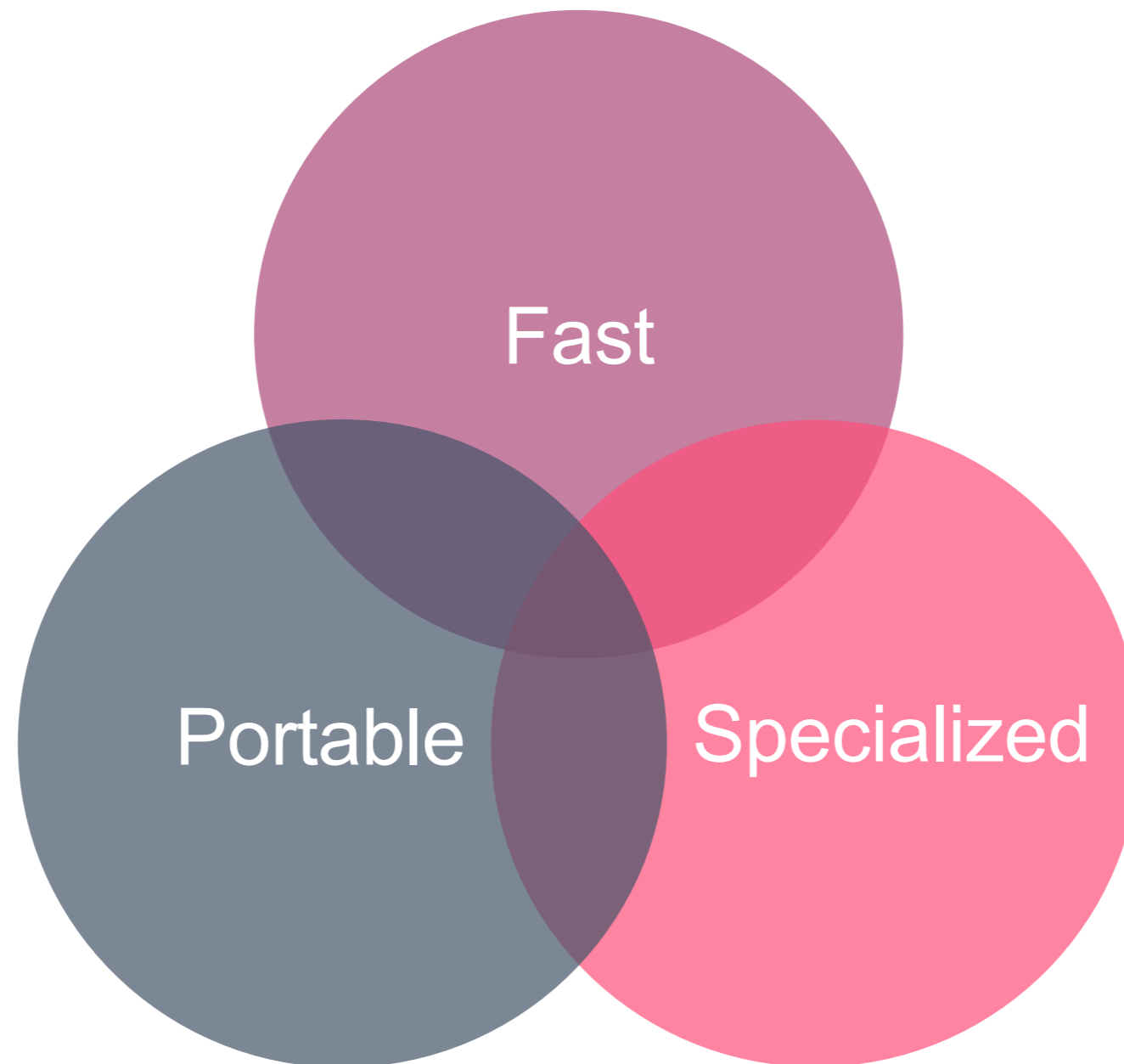
Time

## Fast Simulation is inaccurate

Current fast simulation techniques are not always precise enough to describe all fluctuations correctly

Disk Space

Non-Trivial Distributions





## 1. “Fast Simulation”:

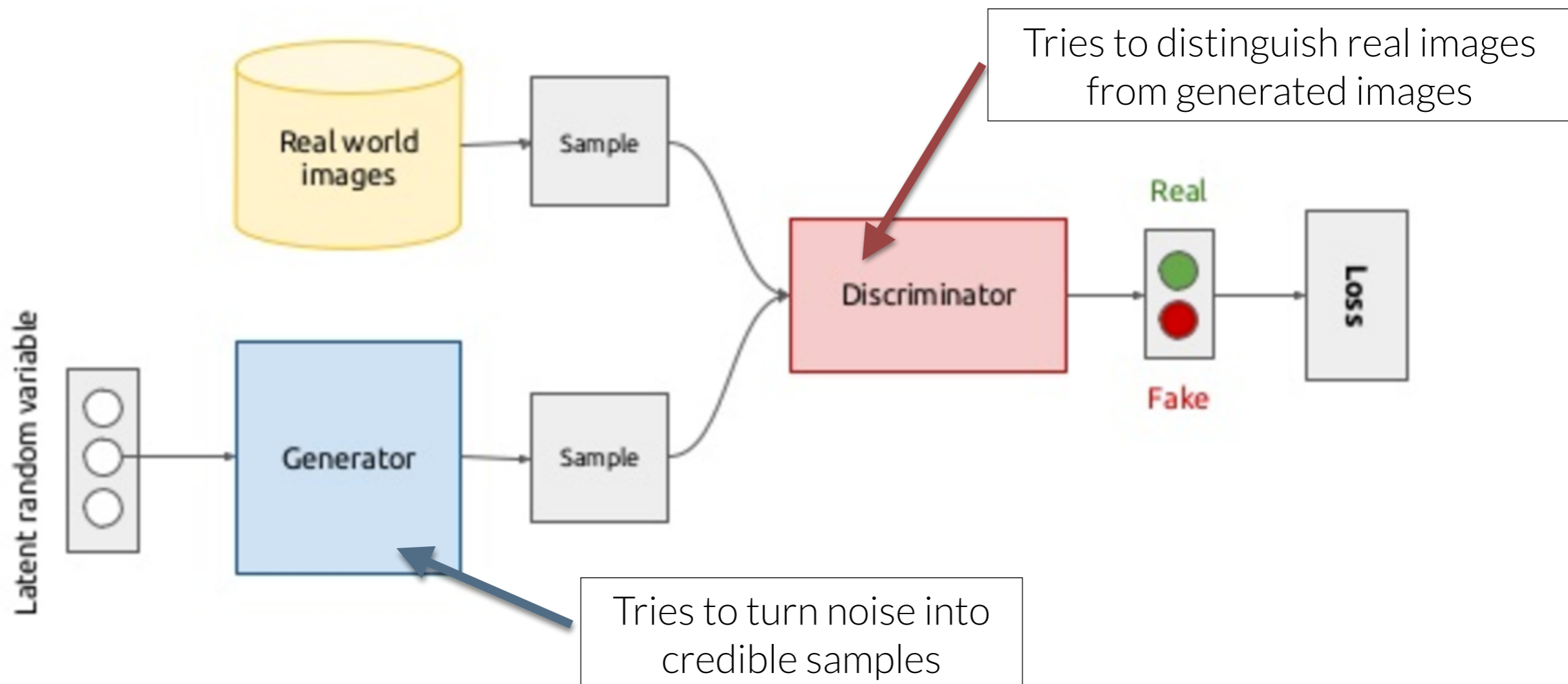
- Parametrized showers, frozen showers, ...
- Not accurate or fast enough

## 2. **Deep Learning** approaches:

- Variational Auto-Encoders, Autoregressive Models, **Generative Adversarial Networks**, ...

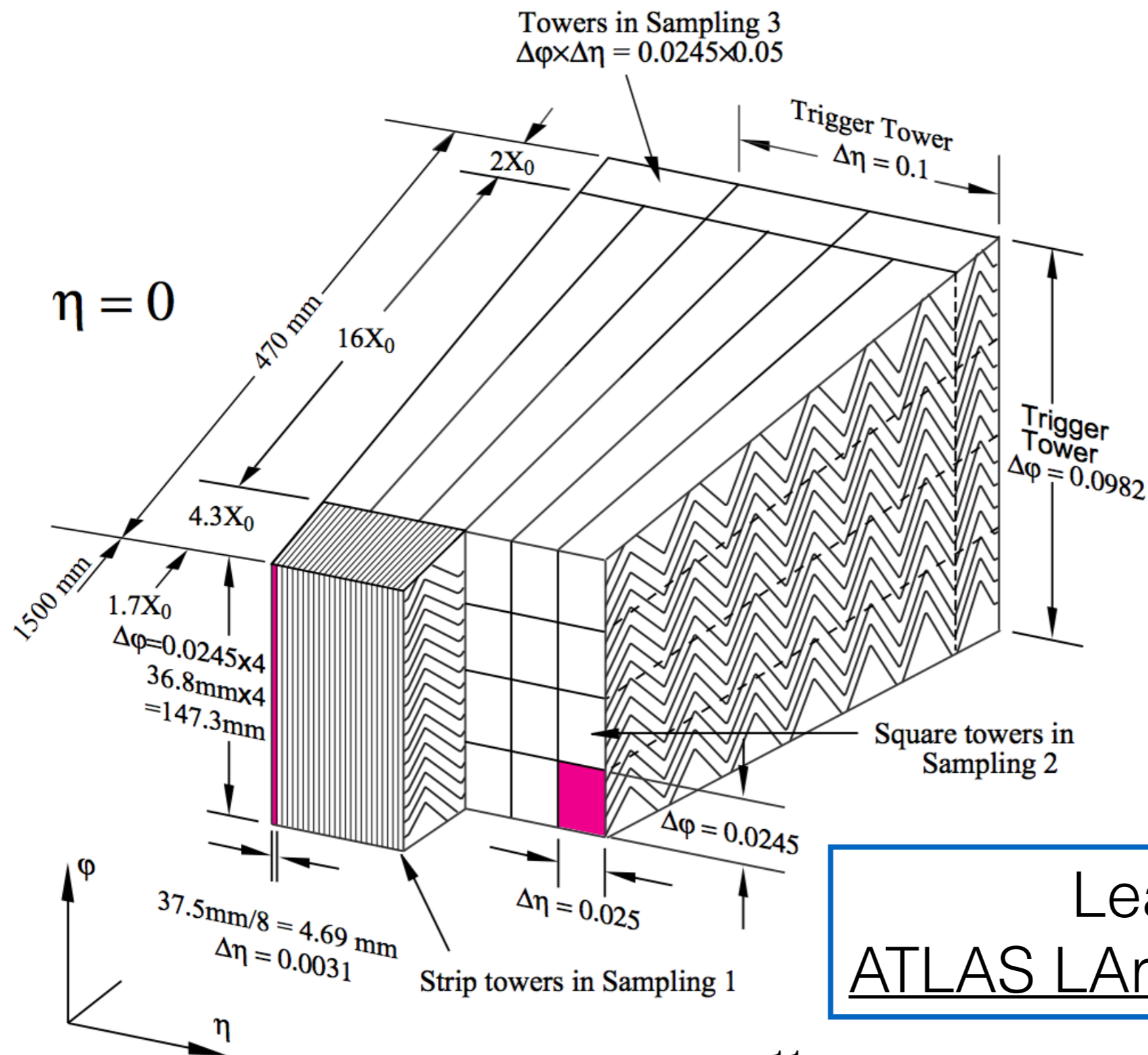
## Generative Adversarial Networks (Goodfellow et al., 2014):

- Two player non-cooperative game between two deep neural networks, the Generator and the Discriminator



# ATLAS EM Calorimeter

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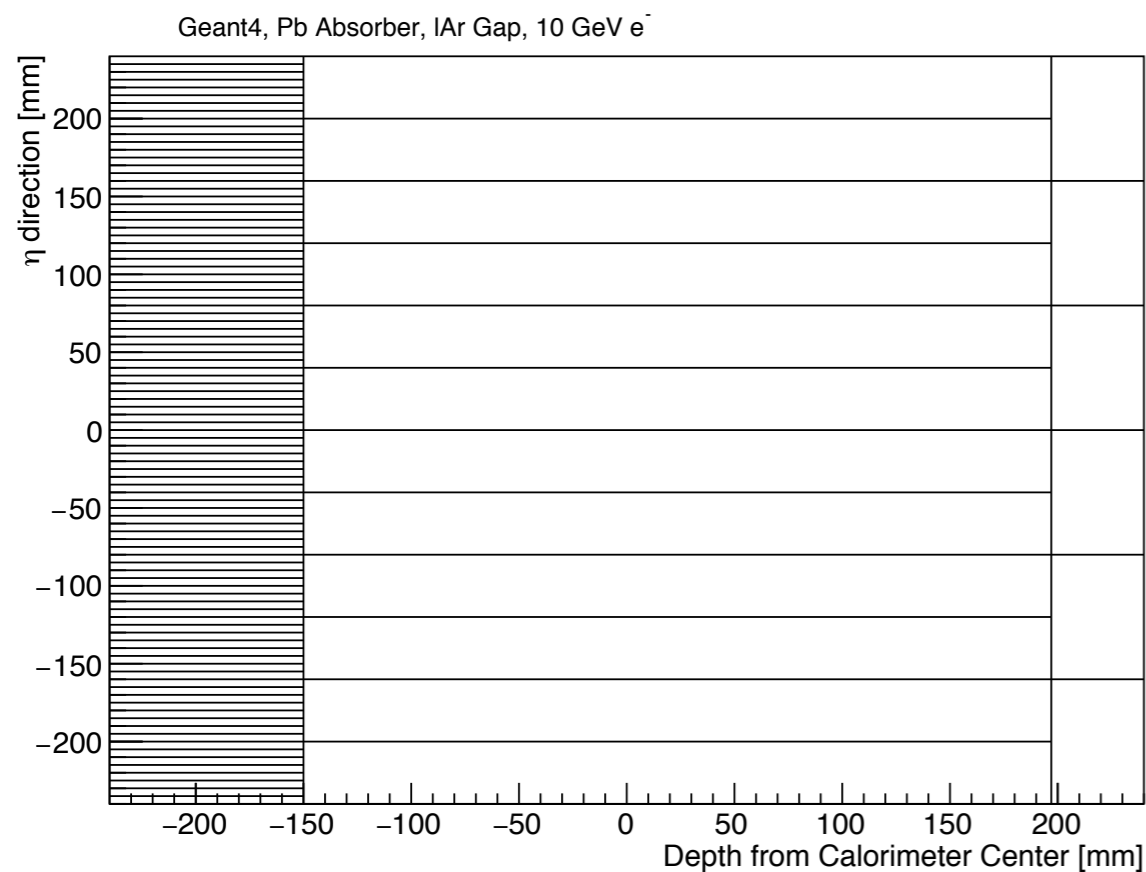
Learn more:  
[ATLAS LAr Calorimeter TDR](#)

# Shower Images

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- EM calorimeter drawing inspiration from the ATLAS geometry.
- Built with GEANT4.

- Heterogeneous longitudinal segmentation into **3 layers**.
- **Irregular granularity** in eta and phi.
- Sequence of alternating lead and liquid argon sublayers.

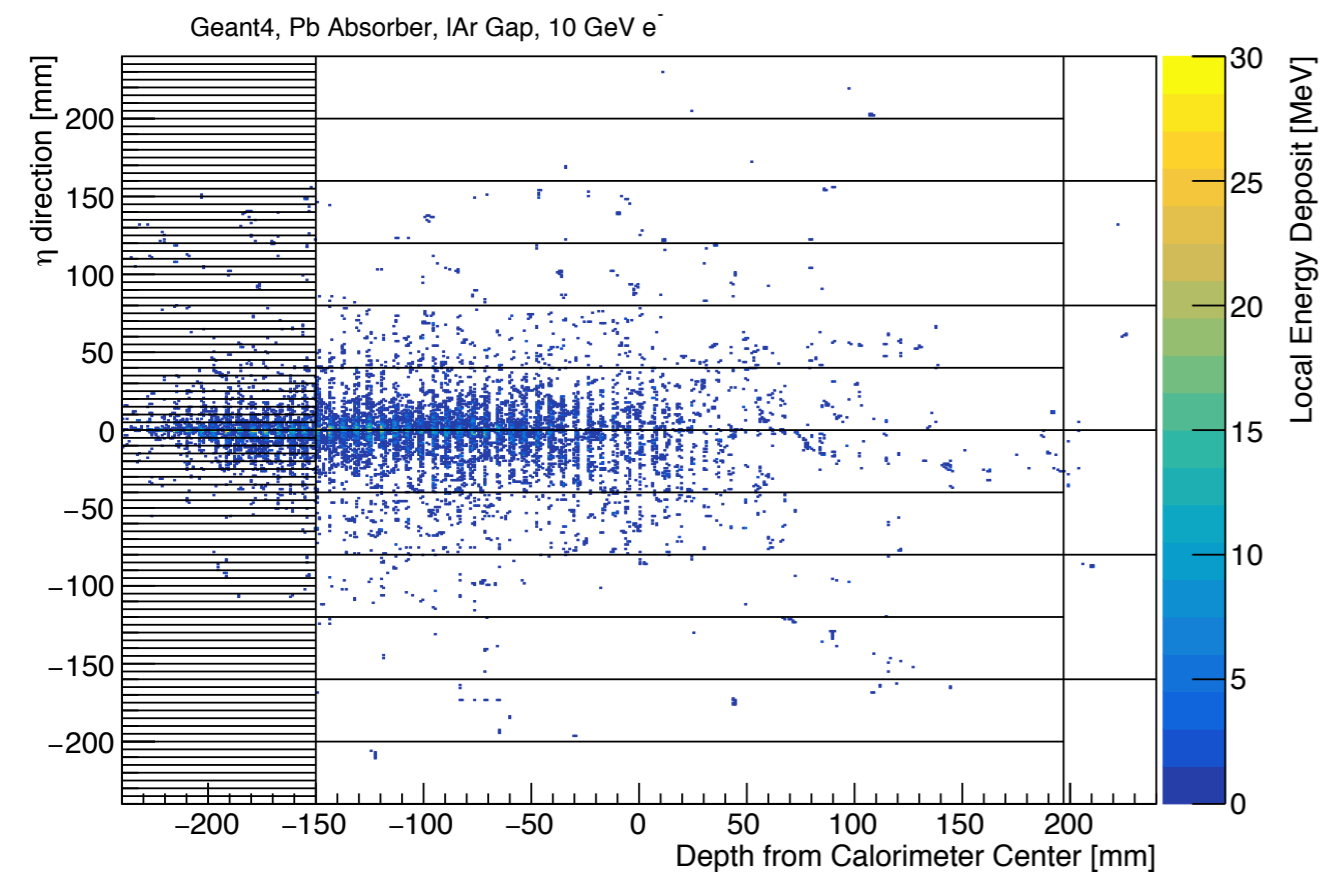


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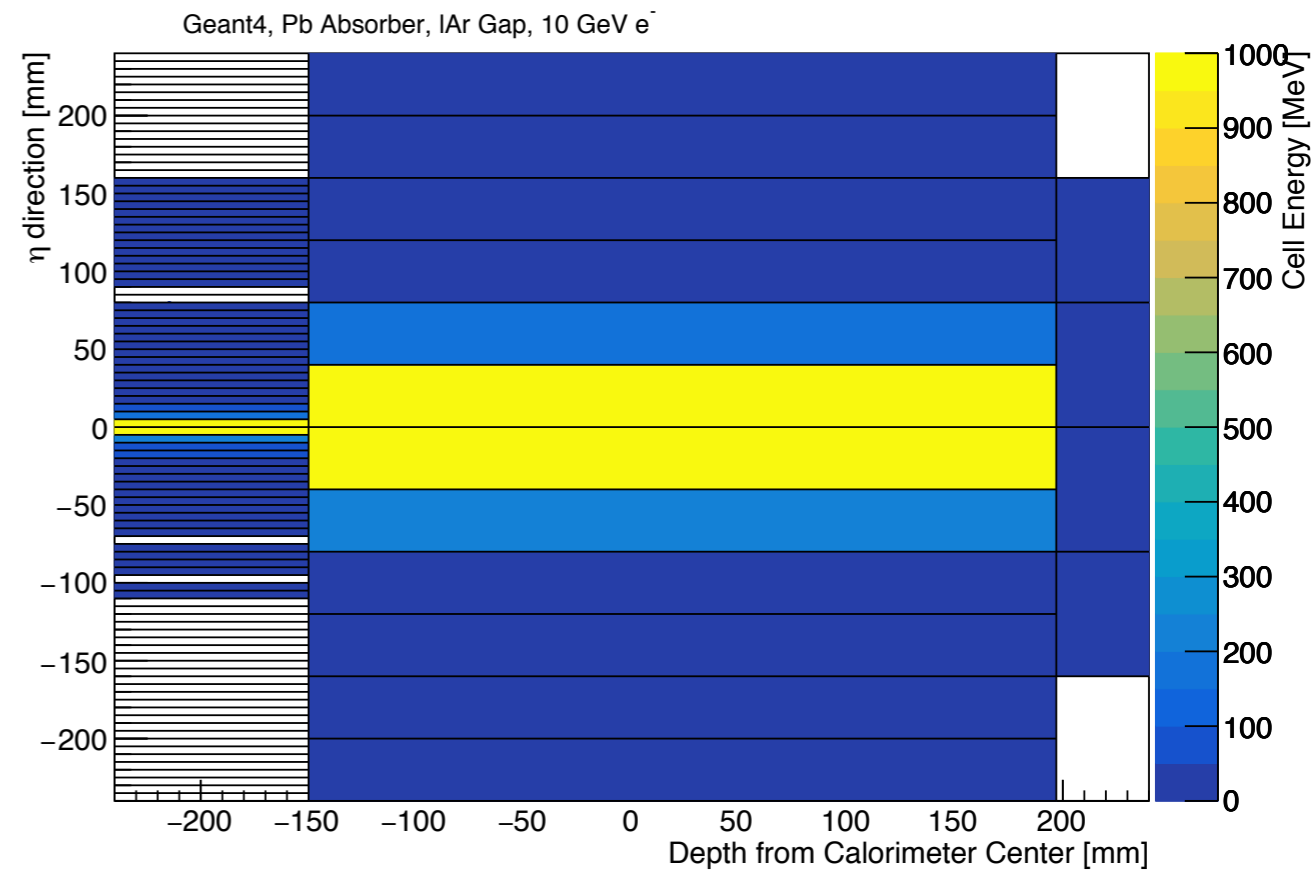
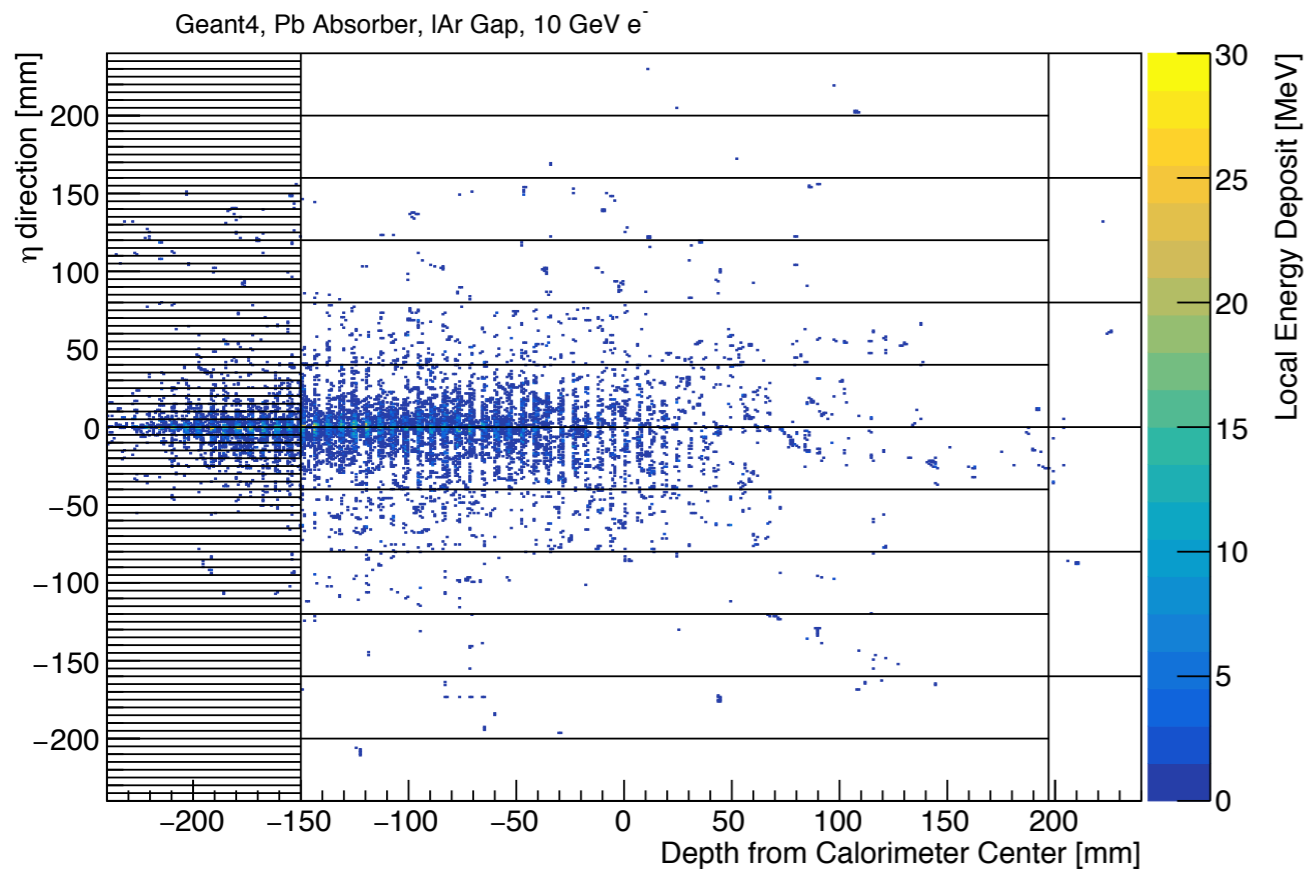


Simulated showers of  $e^+$ ,  $\pi^+$  and  $\gamma$  incident  $\perp$  to the center of the detector with uniform energy in [1, 100] GeV

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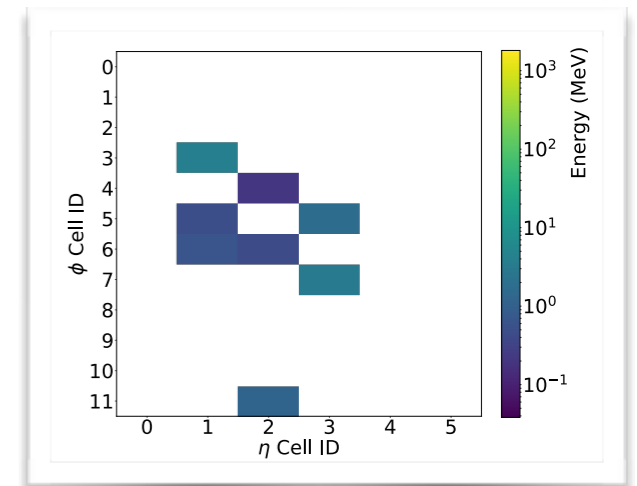
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# Shower Images

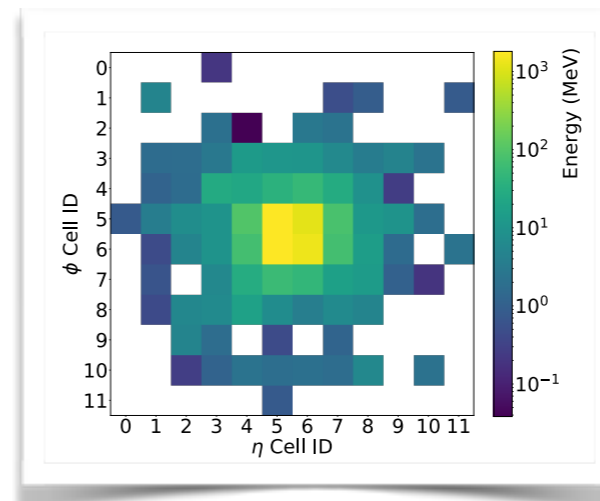
Yale

- Energy depositions in each layer as a **2D image**

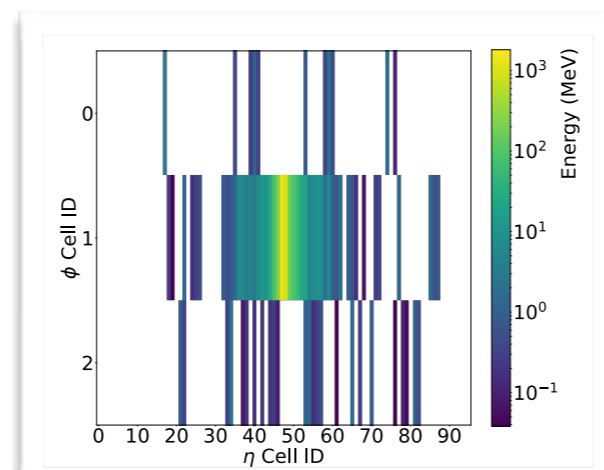
| Layer | $z$ segmentation [mm] | $\eta$ segmentation [mm] | $\phi$ segmentation [mm] |
|-------|-----------------------|--------------------------|--------------------------|
| 0     | 90                    | 5                        | 160                      |
| 1     | 347                   | 40                       | 40                       |
| 2     | 43                    | 80                       | 40                       |



12x6

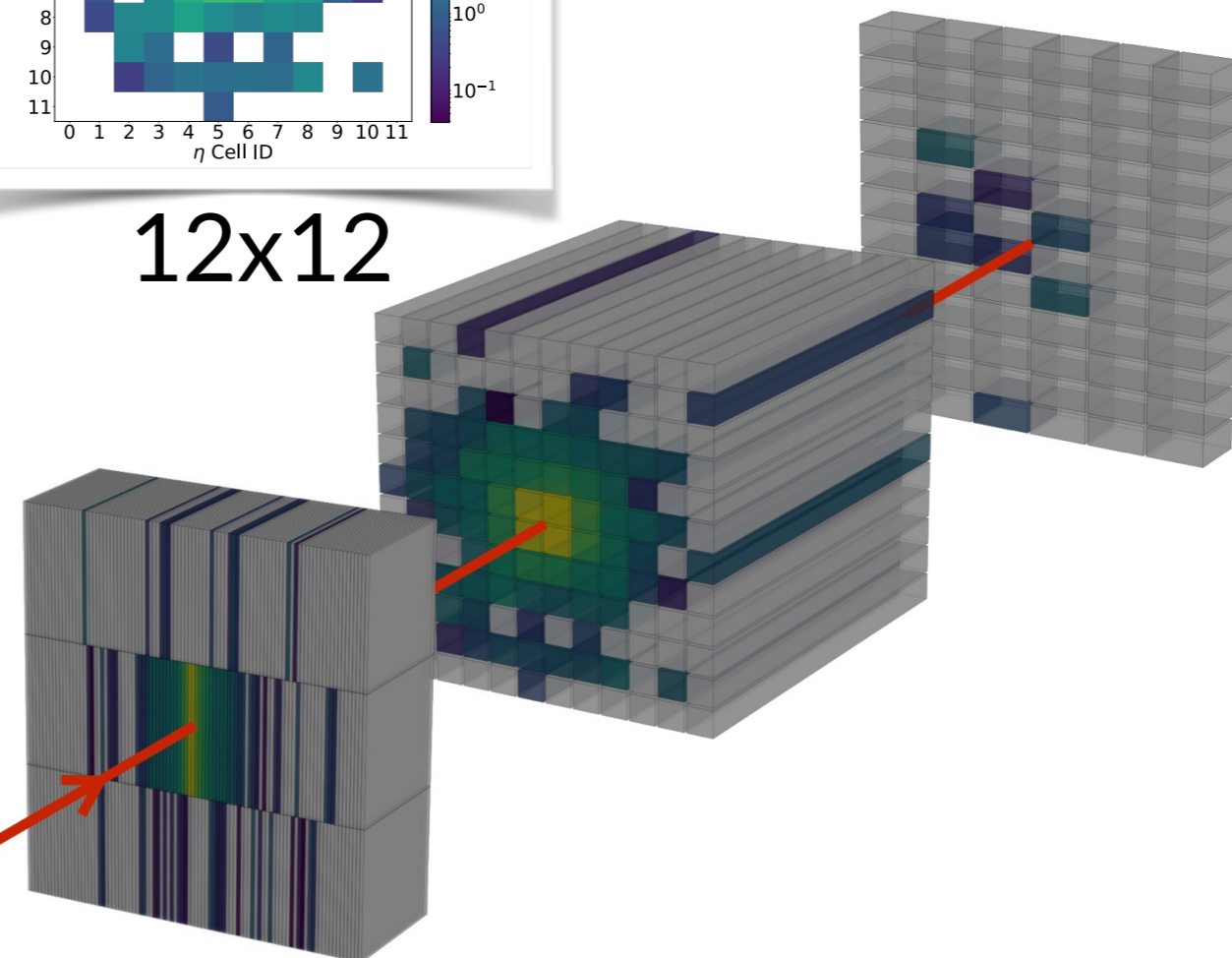
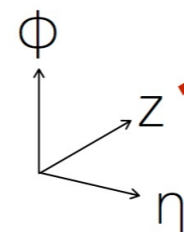


12x12



3x96

- Goal: generate this fixed representation



# Qualitative Performance (1)

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- Average shower images per calorimeter layer

$e^+$

$\gamma$

$\pi^+$

GEANT

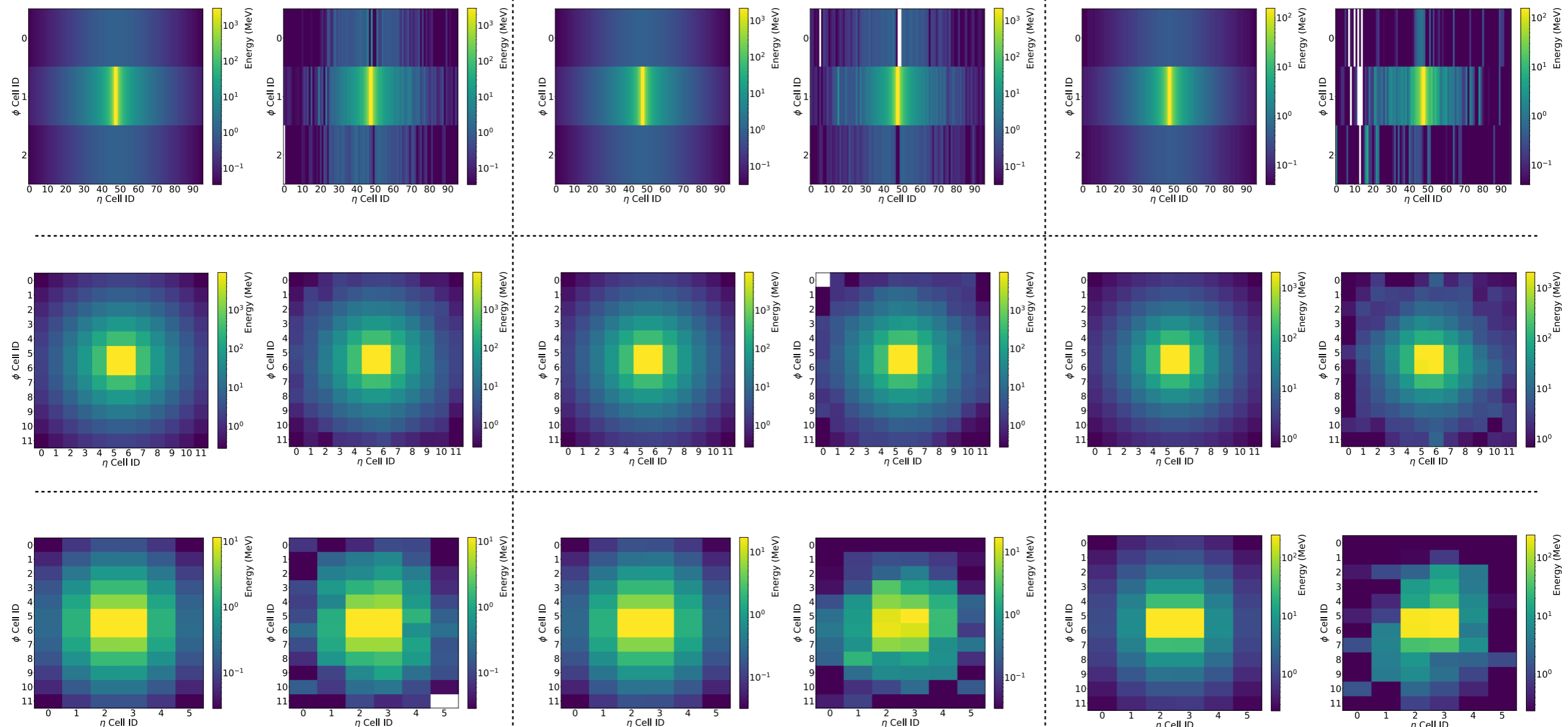
GAN

GEANT

GAN

GEANT

GAN





# Qualitative Performance (2)

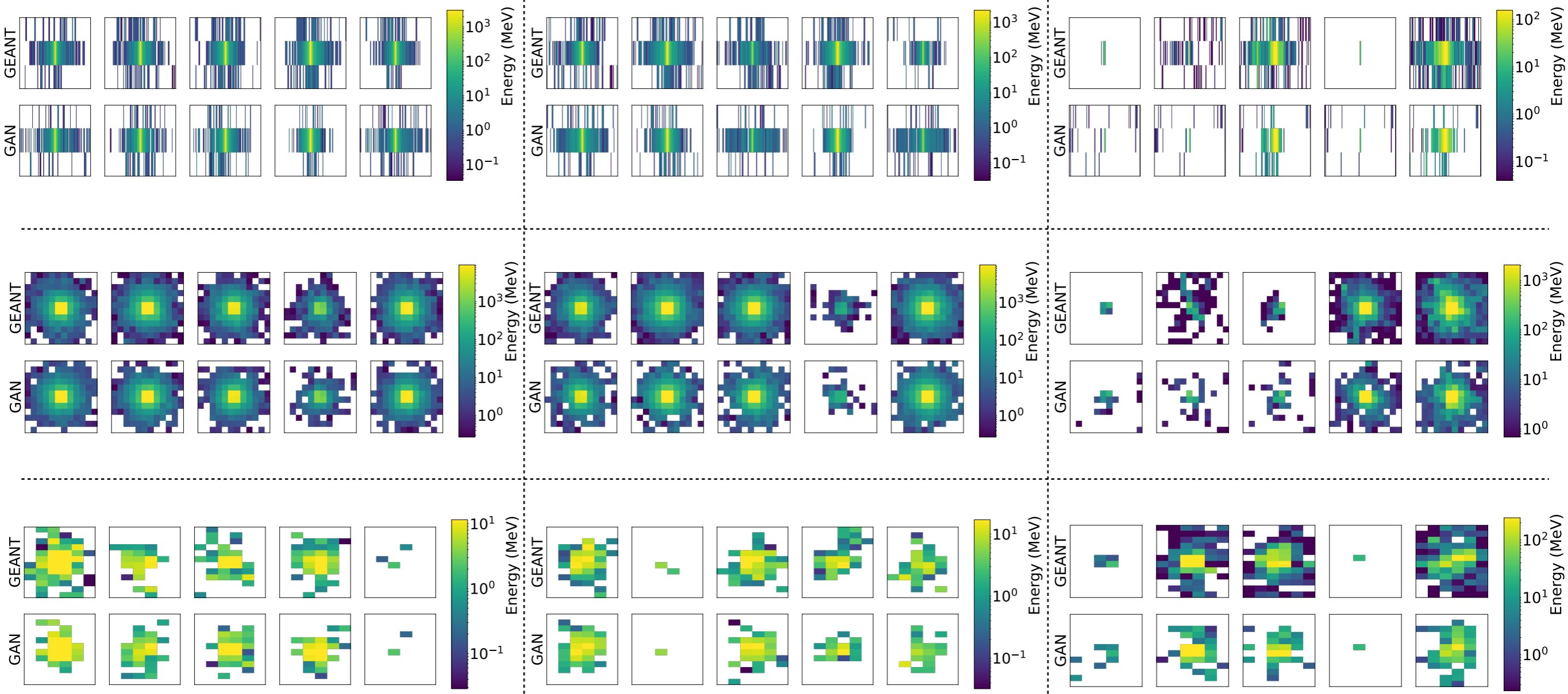
Yale

- 5 random shower images and their nearest GAN-generated neighbor

$e^+$

$\gamma$

$\pi^+$



# Qualitative Performance (2)

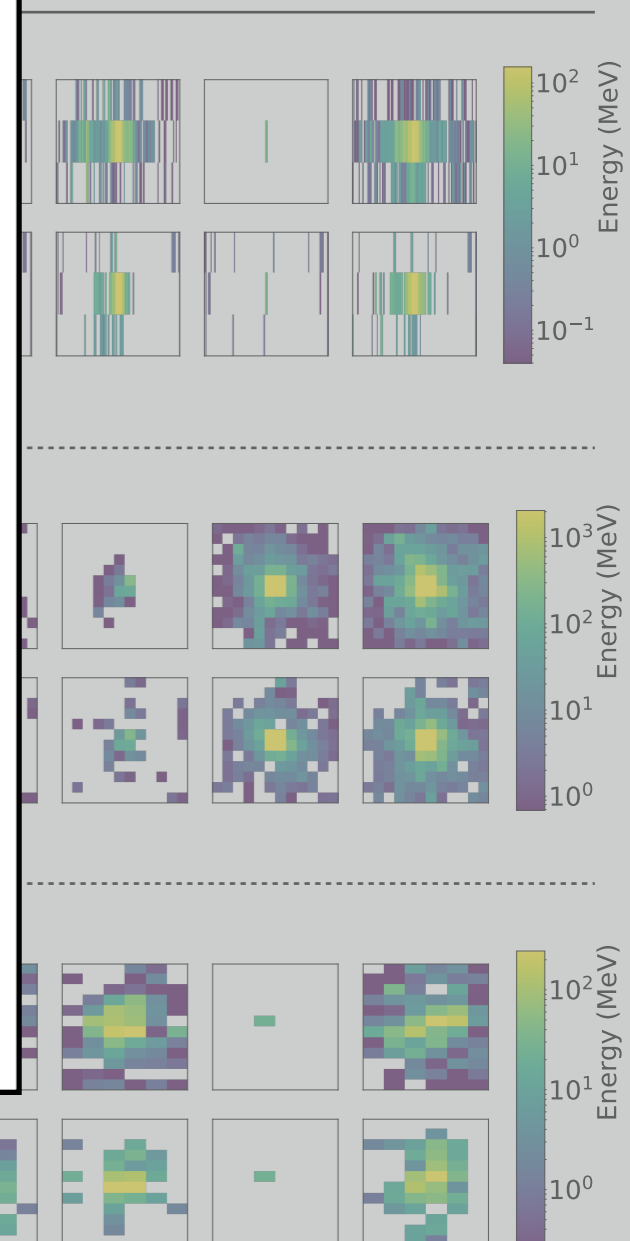
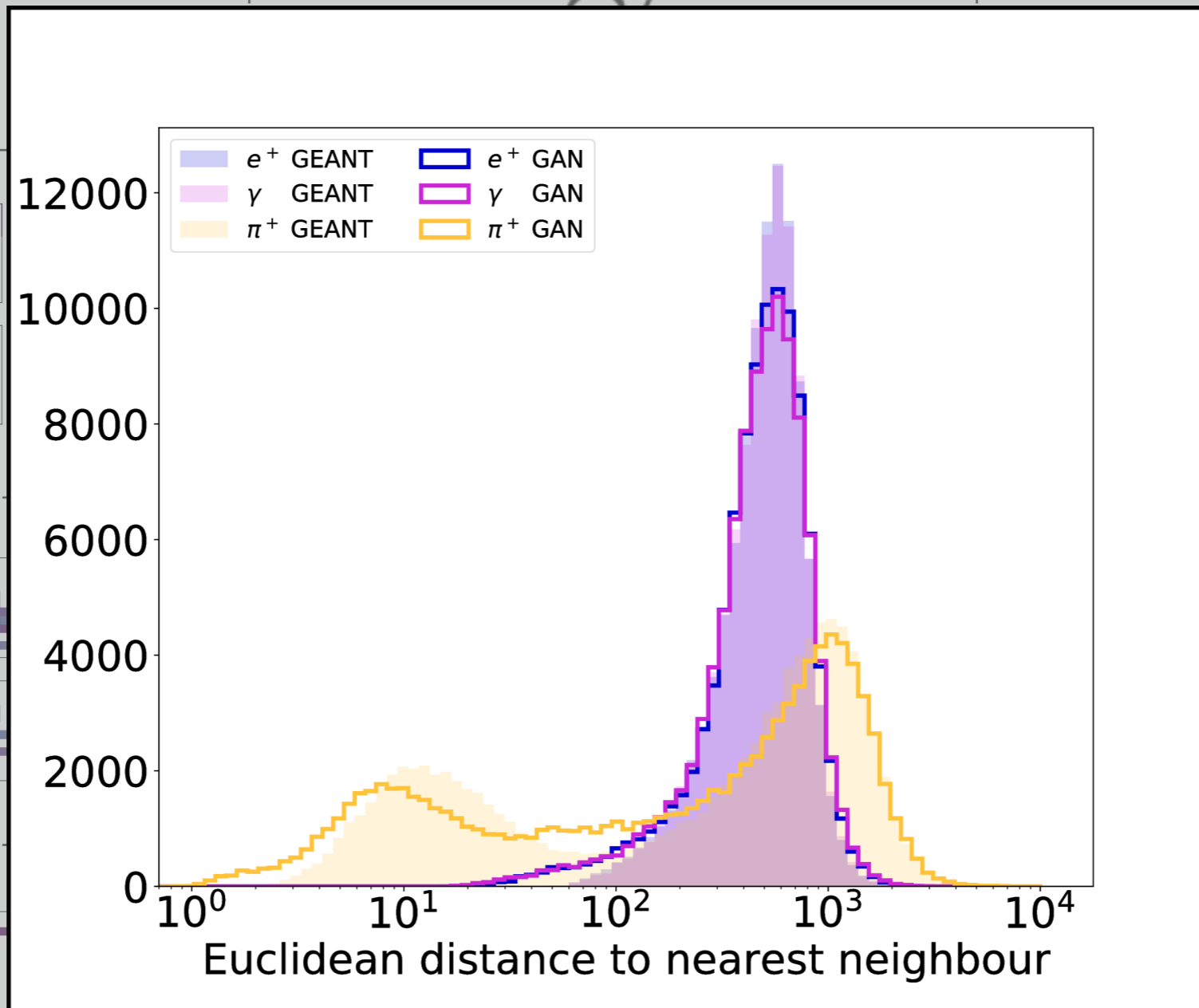
Yale

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$e^+$

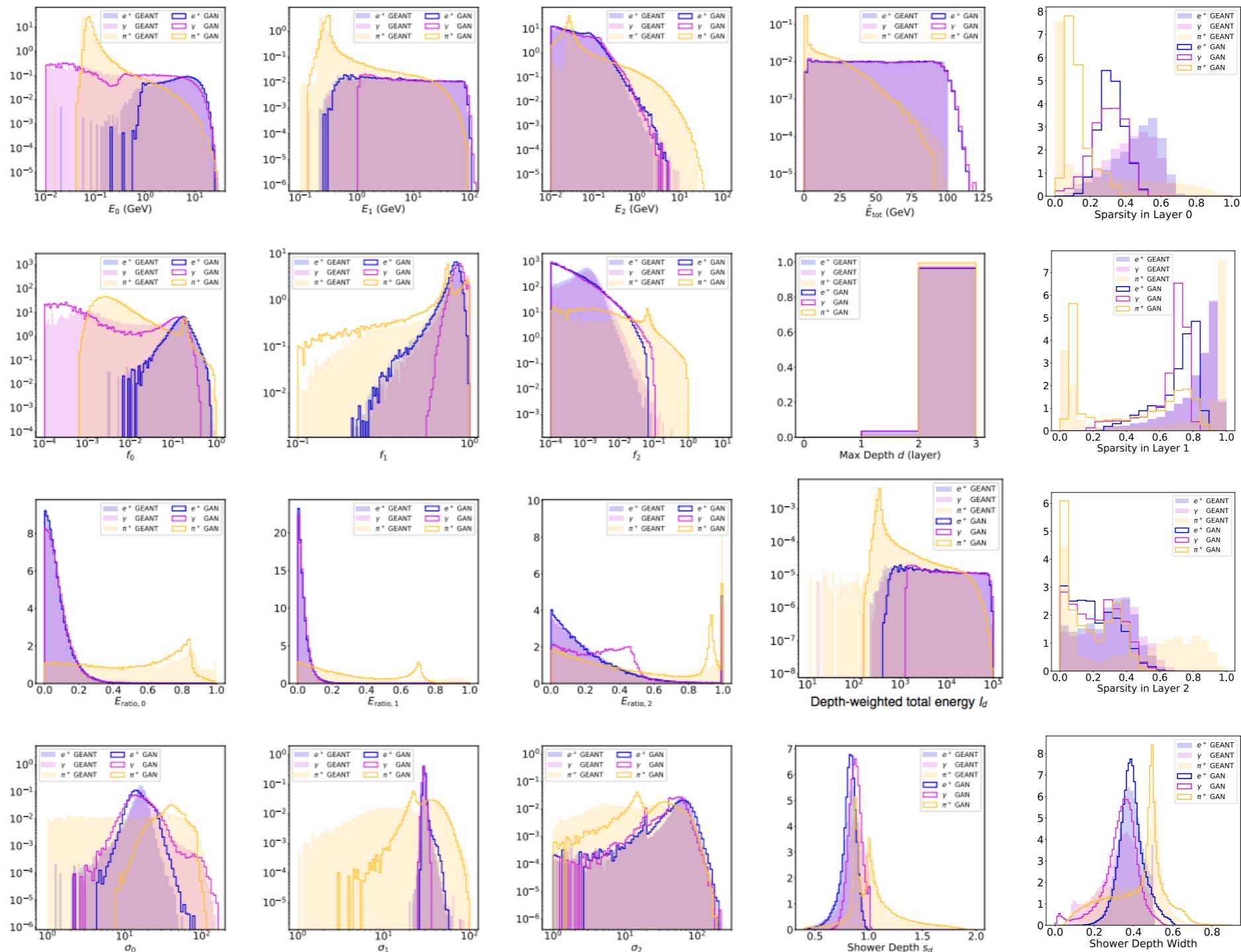
$\gamma$

$\pi^+$



# Shower Shapes

Check: does the GAN recover the true data distribution as projected onto a set of meaningful 1D manifolds?






Compared to single core sequential GEANT 4 simulation, can obtain an evaluation time speed **~100,000x** when evaluating GAN on GPU

| Generation Method | Hardware | Batch Size | milliseconds/shower |
|-------------------|----------|------------|---------------------|
| GEANT4            | CPU      | N/A        | 1772                |
| CALOGAN           | CPU      | 1          | 13.1                |
|                   |          | 10         | 5.11                |
|                   |          | 128        | 2.19                |
|                   |          | 1024       | 2.03                |
|                   | GPU      | 1          | 14.5                |
|                   |          | 4          | 3.68                |
|                   |          | 128        | 0.021               |
|                   |          | 512        | 0.014               |
|                   |          | 1024       | 0.012               |

GEANT 4 generation time grows with energy,  
GAN generation time is constant

- Main point: **we have a working solution!** [arXiv:1705.02355](https://arxiv.org/abs/1705.02355)
- Problem we are trying to tackle: accurate, fast calo simulation

- Emphasis on **reproducibility**: **contribute!**

| Data   | Code   |
|--|--|
| <p data-bbox="751 1234 1223 1291">DOI <a href="https://doi.org/10.17632/pvn3xc3wy5.1">10.17632/pvn3xc3wy5.1</a></p> <p data-bbox="159 1373 1805 1508">  <b>MENDELEY DATA</b></p> | <p data-bbox="1854 1210 2617 1291"><a href="https://github.com/hep-lbdl/CaloGAN">github.com/hep-lbdl/CaloGAN</a></p> <p data-bbox="1931 1324 2189 1549"></p> <p data-bbox="2343 1336 2535 1549"></p> |

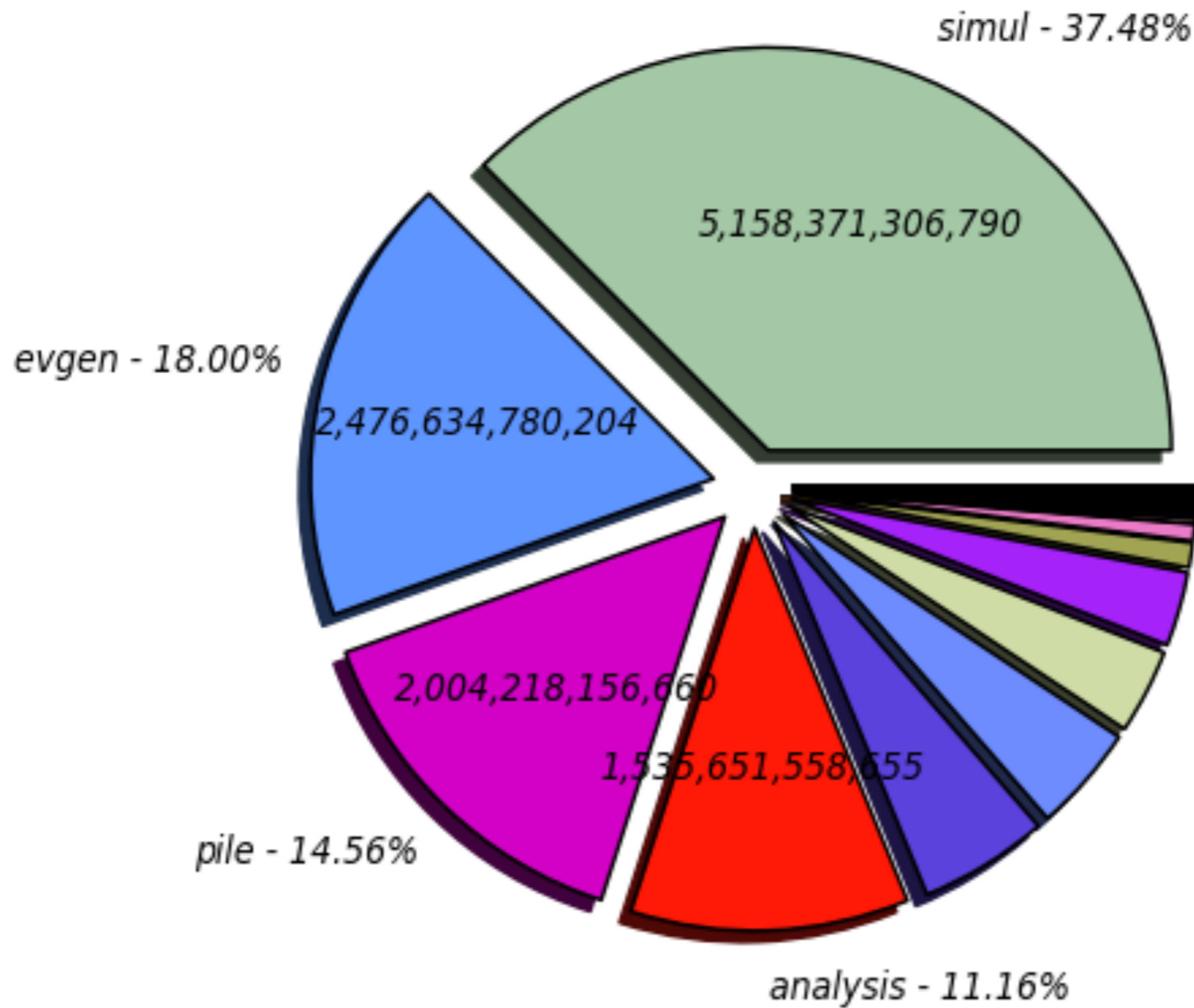
- Goal: getting this to work in ATLAS/GEANT in the not-so-distant future

Backup

# Grid Utilization

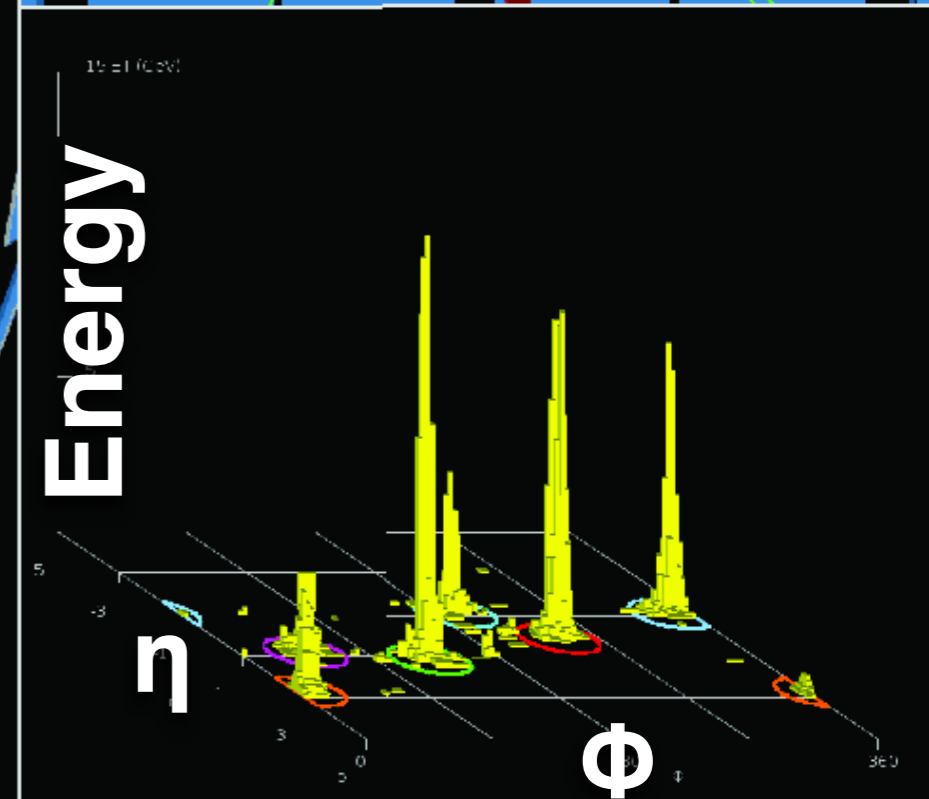
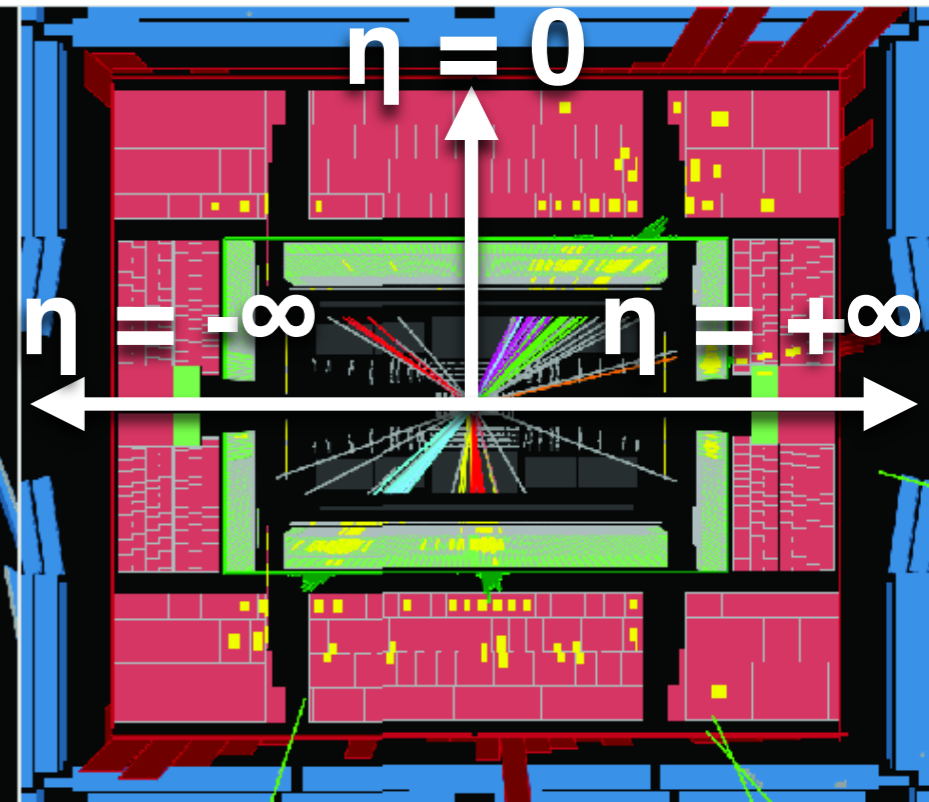
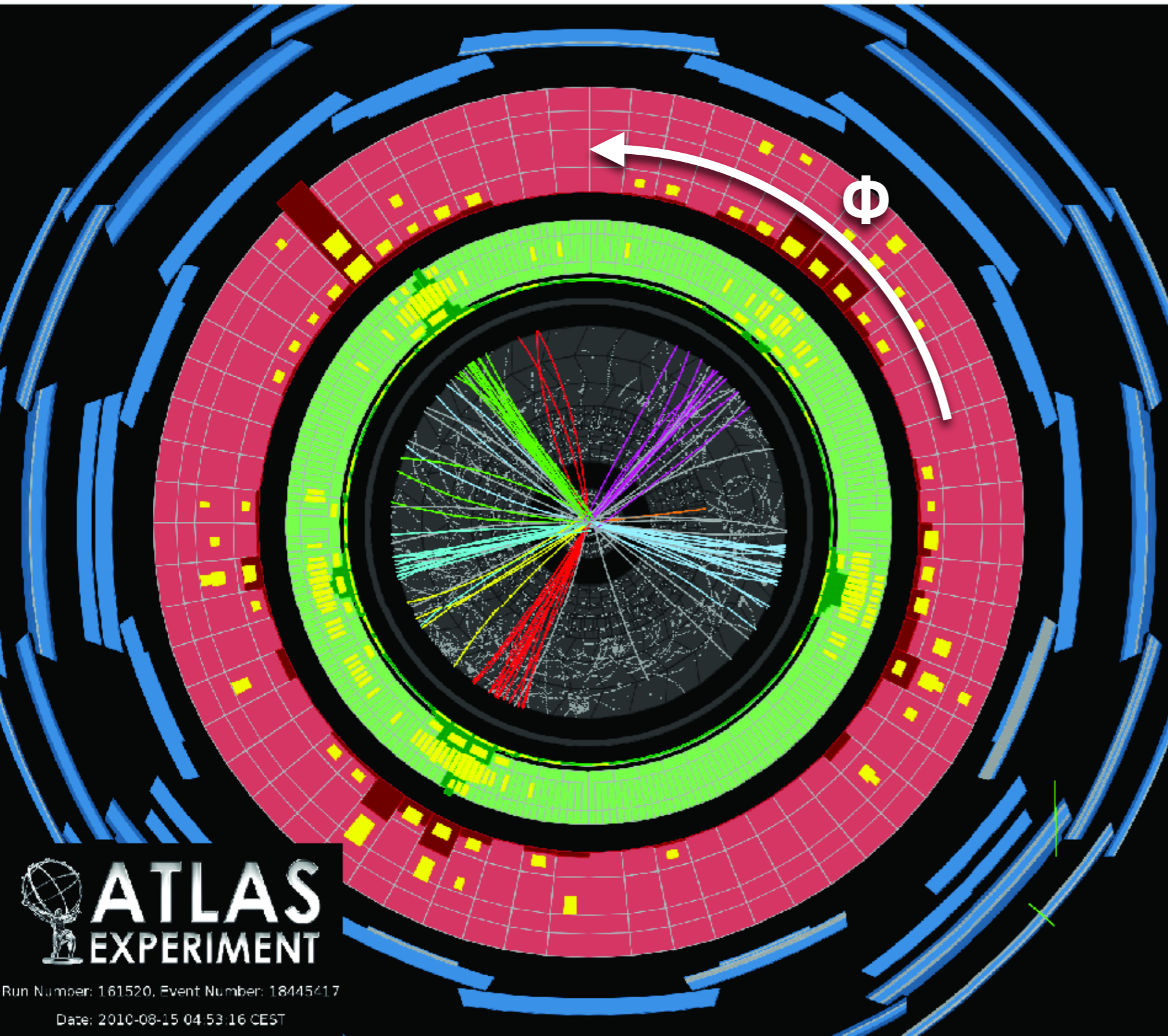


Wall Clock consumption All Jobs in seconds (Sum: 13,762,344,233,098)



# Events in ATLAS

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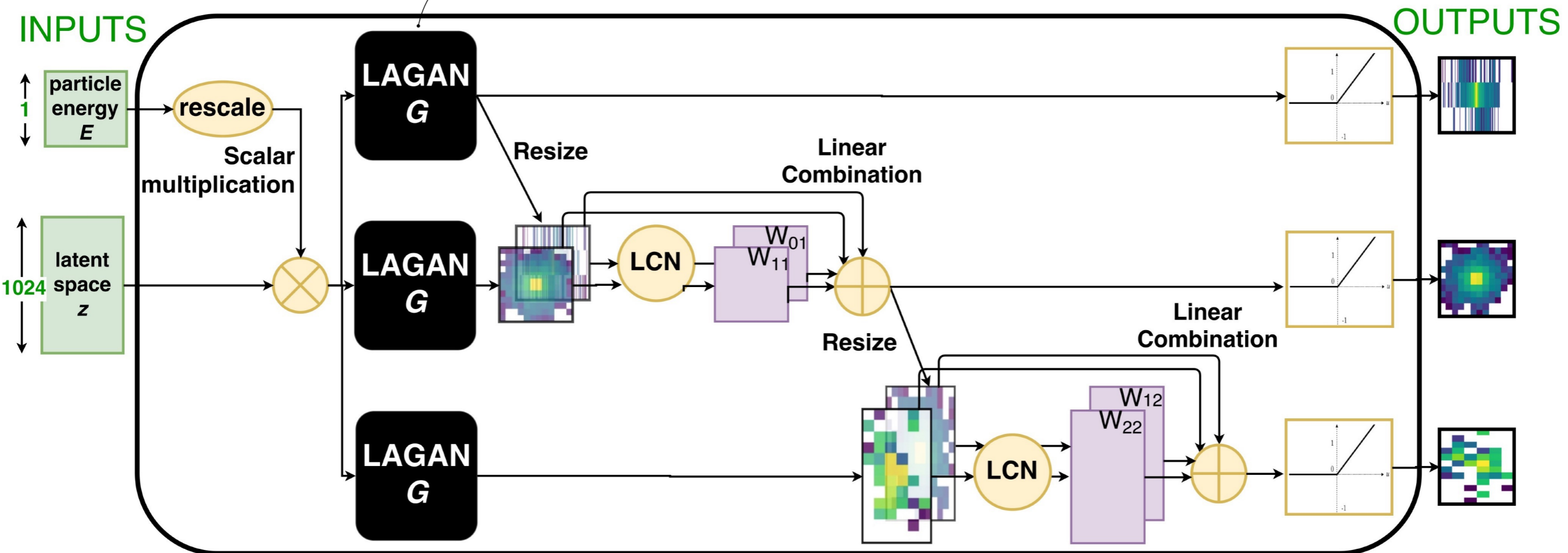




# CaloGAN Generator

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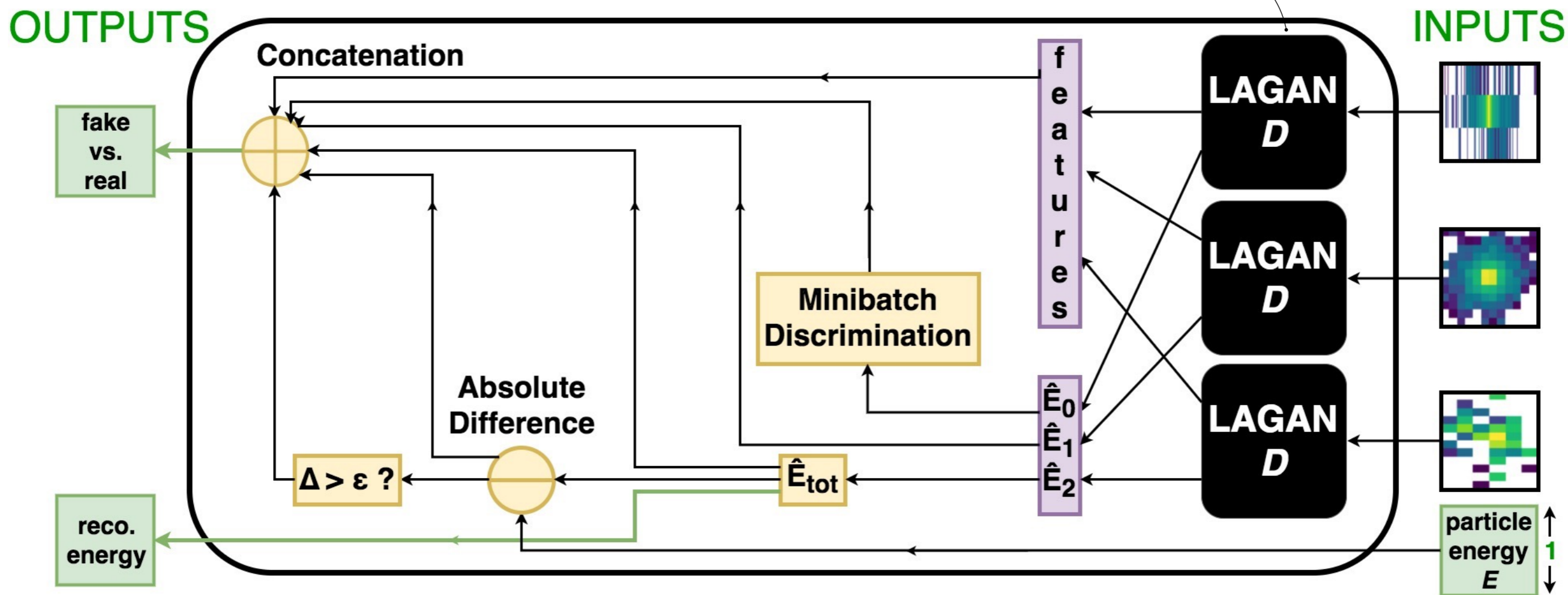
arXiv:1701.05927



# CaloGAN Discriminator

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arXiv:1701.05927



# Shower Shape Variables

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| Shower Shape Variable                           | Formula  | Notes  |
|---|--|--|
| $E_i$   | $E_i = \sum_{\text{pixels}} \mathcal{I}_i$   | Energy deposited in the $i^{\text{th}}$ layer of calorimeter   |
| $E_{\text{tot}}$                                | $E_{\text{tot}} = \sum_{i=0}^2 E_i$  | Total energy deposited in the electromagnetic calorimeter  |
| $f_i$   | $f_i = E_i/E_{\text{tot}}$   | Fraction of measured energy deposited in the $i^{\text{th}}$ layer of calorimeter  |
| $E_{\text{ratio},i}$                            | $\frac{\mathcal{I}_{i,(1)} - \mathcal{I}_{i,(2)}}{\mathcal{I}_{i,(1)} + \mathcal{I}_{i,(2)}}$  | Difference in energy between the highest and second highest energy deposit in the cells of the $i^{\text{th}}$ layer, divided by the sum |
| $d$   | $d = \max\{i : \max(\mathcal{I}_i) > 0\}$  | Deepest calorimeter layer that registers non-zero energy   |
| Depth-weighted total energy, $l_d$              | $l_d = \sum_{i=0}^2 i \cdot \mathcal{I}_i$   | The sum of the energy per layer, weighted by layer number.   |
| Shower Depth, $s_d$                             | $s_d = l_d/E_{\text{tot}}$   | The energy-weighted depth in units of layer number.  |
| Shower Depth Width, $\sigma_{s_d}$              | $\sigma_{s_d} = \sqrt{\frac{\sum_{i=0}^2 i^2 \cdot \mathcal{I}_i}{E_{\text{tot}}} - \left(\frac{\sum_{i=0}^2 i \cdot \mathcal{I}_i}{E_{\text{tot}}}\right)^2}$ | The standard deviation of $s_d$ in units of layer number.  |
| $i^{\text{th}}$ Layer Lateral Width, $\sigma_i$ | $\sigma_i = \sqrt{\frac{\mathcal{I}_i \odot H^2}{E_i} - \left(\frac{\mathcal{I}_i \odot H}{E_i}\right)^2}$   | The standard deviation of the transverse energy profile per layer, in units of cell numbers.   |

# Recent HEP-ML Conferences and Workshops

Yale

- NIPS Workshop 2014, 2015
- DS@HEP 2015, 2016, 2017
- Connecting the Dots 2016, 2017
- IML Workshop
- CERN OpenLab workshop on ML and Data Analytics