# CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks

# Introduction

"Our judge is not God or governments, but Nature."

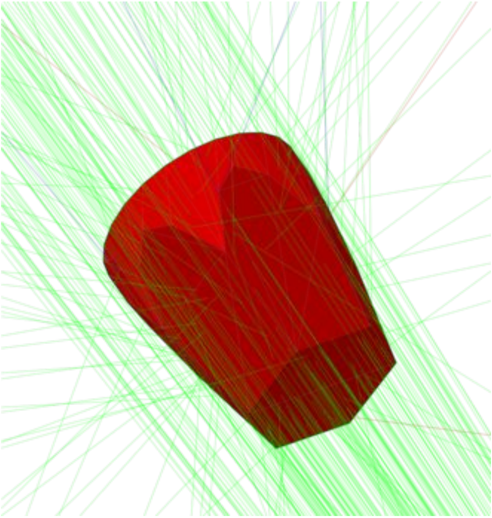
Tejinder Virdee, a spokesman for the Compact Muon Solenoid contained within the Large Hadron Collider

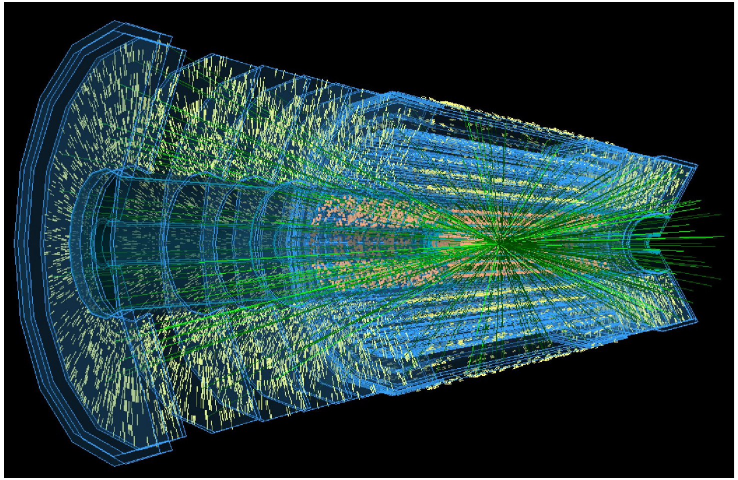
# What do they do at LHC?

Scientists use the LHC to test theoretical predictions in particle physics by colliding particles and looking at what the collisions produce.

The physics programs of all experiments based at the LHC rely heavily on detailed simulation for all aspects of event reconstruction and data analysis.

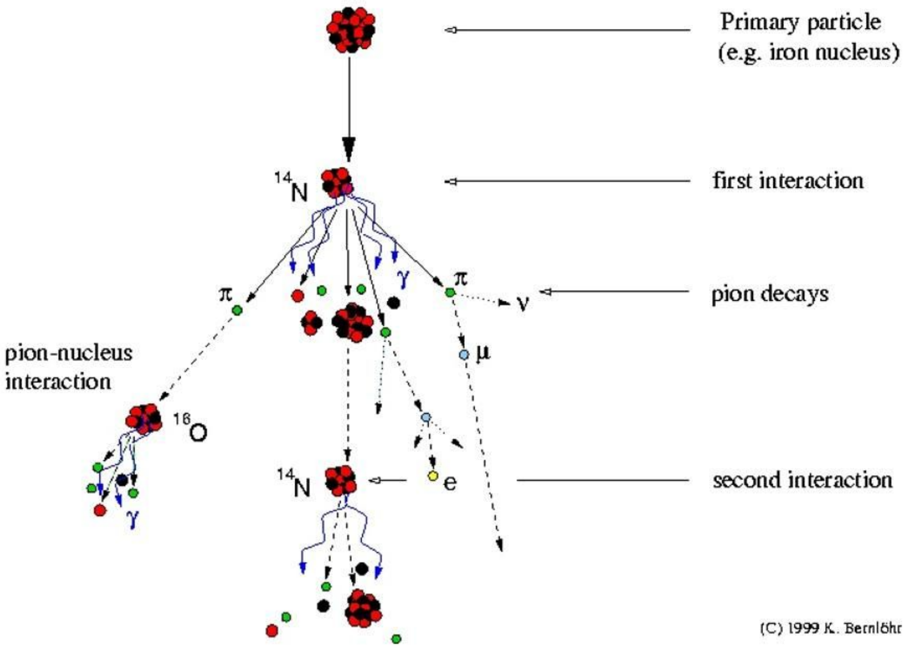
Tools like Geant4 are used to simulate the passage of particles through matter, approximating how a real detector would respond to particle showers





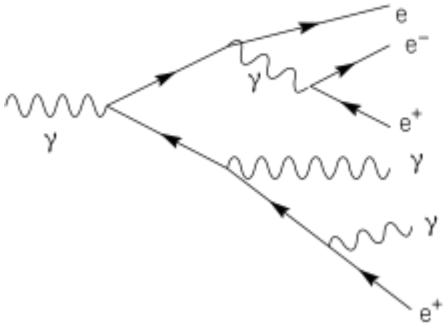
# Particle showers

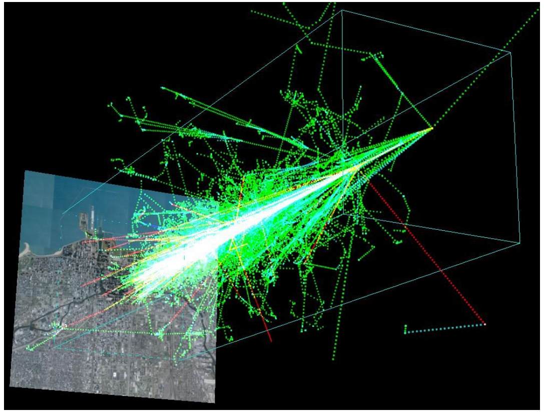
In particle physics shower is a cascade of secondary particles produced as the result of a high-energy particle interacting with dense matter. The incoming particle interacts, producing multiple new particles with lesser energy; each of these then interacts, in the same way, a process that continues until many thousands, millions, or even billions of low-energy particles are produced. These are then stopped in the matter and absorbed.



# Electromagnetic showers

An electromagnetic shower begins when a high-energy electron, positron or photon enters a material. At high energies (above a few MeV) photons interact with matter primarily via pair production — that is, they convert into an electron-positron pair, interacting with an atomic nucleus or electron in order to conserve momentum.

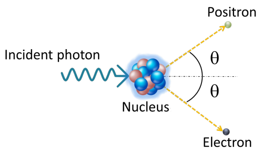


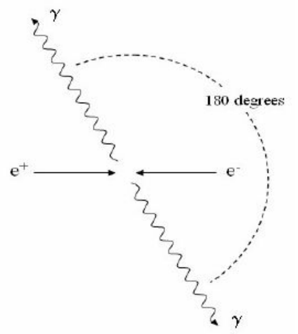
# Types of particles

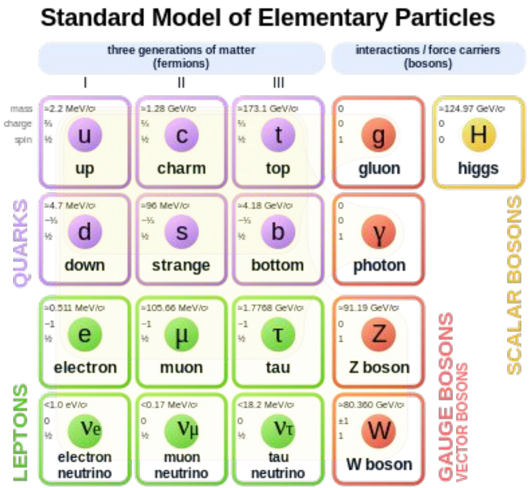
## Positrons

The positron or antielectron is the particle with an electric charge of +1e and the same mass as an electron. It is the antiparticle of the electron. When a positron collides with an electron, annihilation occurs. If this collision occurs at low energies, it results in the production of two or more photons.




$$E = \hbar\omega = h\nu = \frac{hc}{\lambda}$$



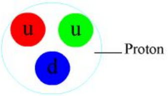




## Photon

A photon is an elementary particle that is a quantum of the electromagnetic field, including electromagnetic radiation such as light and radio waves, and the force carrier for the electromagnetic force. Photons are massless, so they always move at the speed of light in vacuum.

## Charged Pions

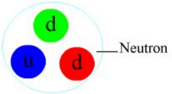
The pion can be positively, negatively or neutrally charged. The Charged pions(negatively or positively) decay into muons and neutrinos. The positively charged pion consists of a u quark and an anti-d quark and the negatively charged pion consists of a d quark and an anti-u quark.




Decay 1

$$\pi^+ \rightarrow \mu^+ + \nu_\mu$$

$$\pi^- \rightarrow \mu^- + \bar{\nu}_\mu$$




Decay 2

$$\pi^+ \rightarrow e^+ + \nu_e$$

$$\pi^- \rightarrow e^- + \bar{\nu}_e$$

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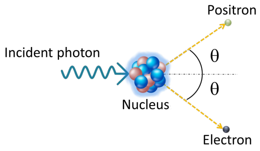


## Charged Pions

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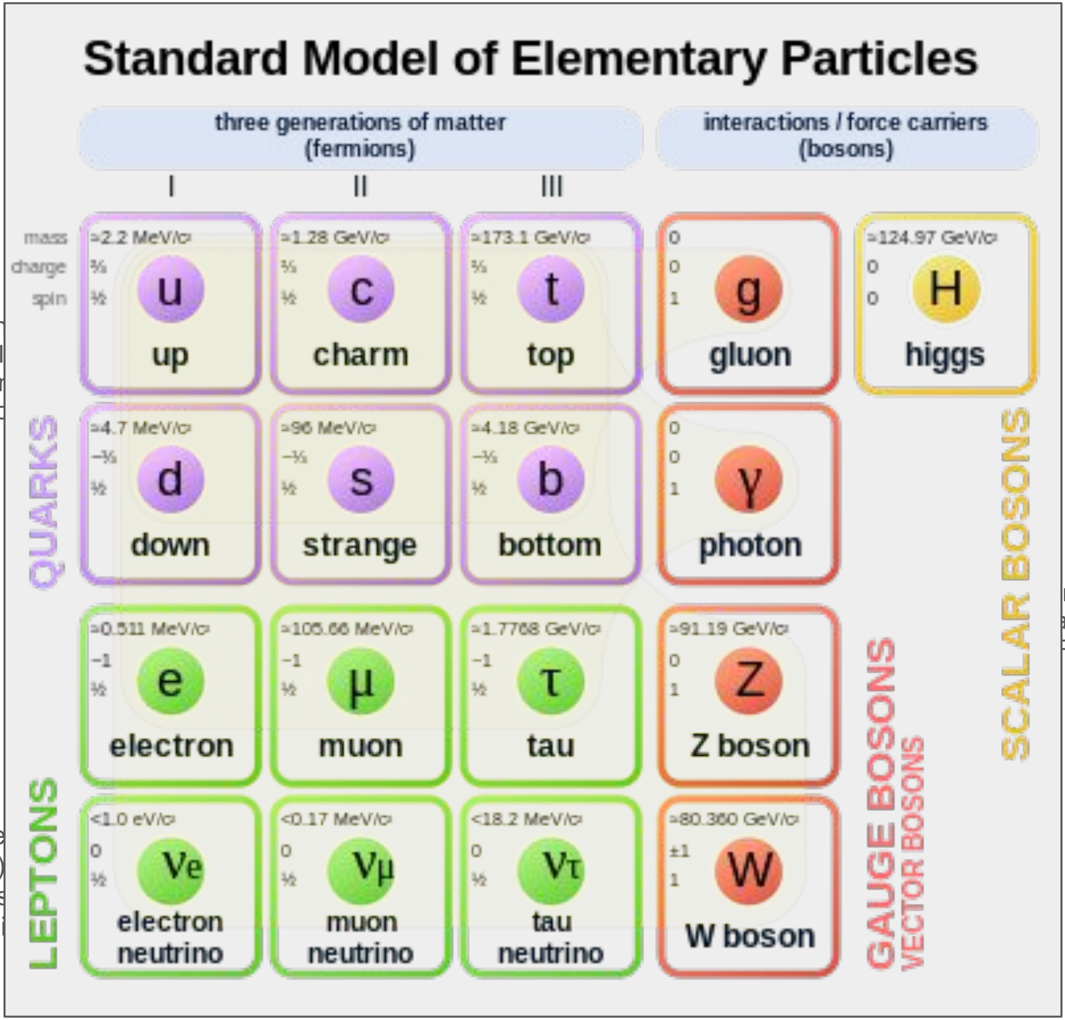


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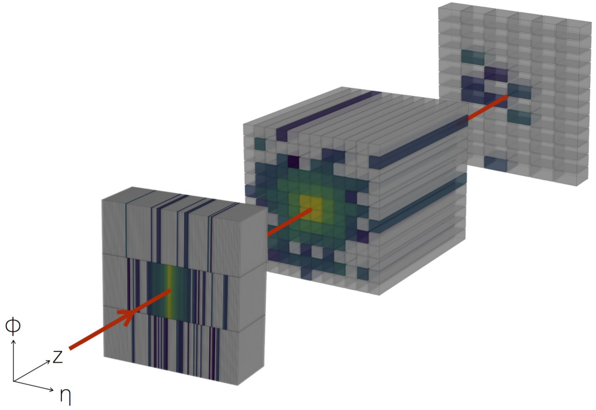
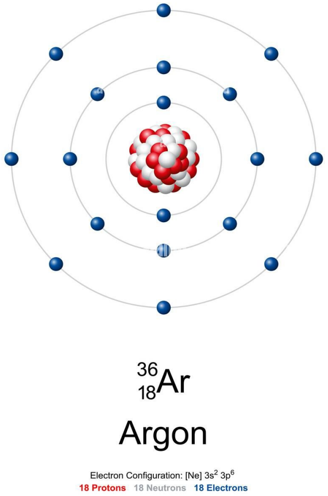
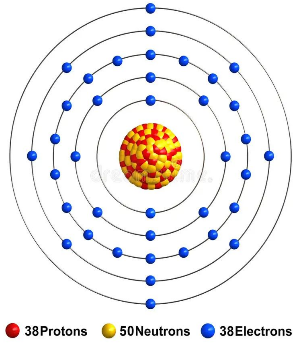
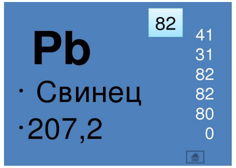
# Calorimeter

An electromagnetic calorimeter (ECAL) is one specifically designed to measure the energy of particles that interact primarily via the electromagnetic interaction such as electrons, positrons and photons.



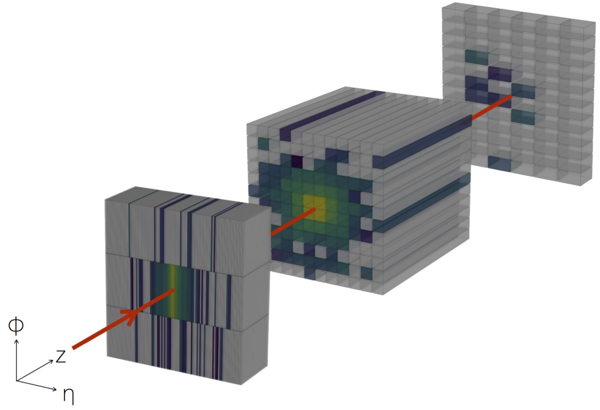

| Layer | $z$ length [mm] | $\eta$ length [mm] | $\phi$ length [mm] |
|---|---|---|---|
| 0 | 90 | 5 | 160 |
| 1 | 347 | 40 | 40 |
| 2 | 43 | 80 | 40 |

TABLE I: Dimension of a calorimeter cell. The $z$ direction is the direction of particle propagation (radial direction in a full experiment), the $\eta$ direction would be along the $pp$ beam axis in a full experiment, and $\phi$ is perpendicular to $z$ and $\eta$.

# How to make sense of all that?

In order to condense the vast amounts of raw data from each experiment there has to be software able to create images. This is what CaloGAN is supposed to do.

| | |
|---|---|
| `energy | Dataset {100000, 1}` |
| `layer_0 | Dataset {100000, 3, 96}` |
| `layer_1 | Dataset {100000, 12, 12}` |
| `layer_2 | Dataset {100000, 12, 6}` |
| `overflow | Dataset {100000, 3}` |



# Problem statement

Given:

- Type of a particle
- Its energy
- Vector from latent space

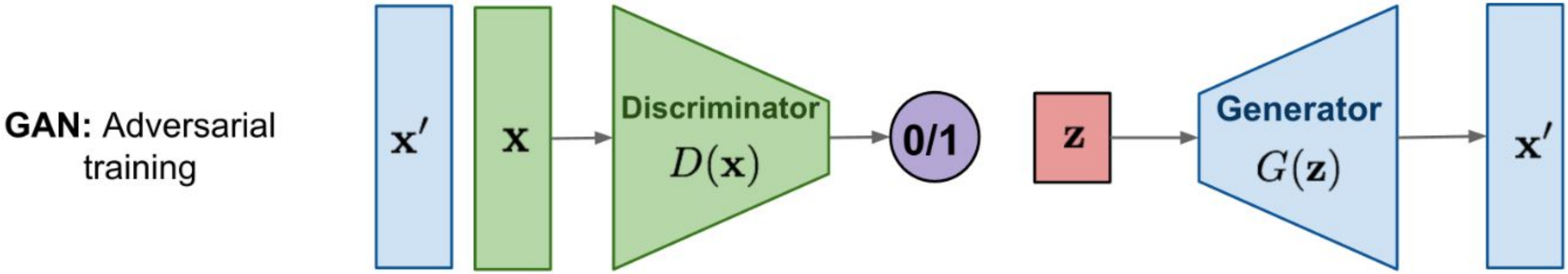
Task:

- Generate three images, which represent particle showers

Mathematically:

- $I = G(T, E, z)$, where $I$ - vector of images, $G$ - images generating function, $T$ - particle type, $E$ - particle's energy, $z$ - vector from latent space

# III. Generative Adversarial Network



# III. Generative Adversarial Network

Generator:

$z \sim p_z(z)$ → Space of generated samples

(usually chosen to be $N(0, 1)$)

Discriminator:

Space of generated samples → [0;1] - prob-ty of a sample of being real

# IV. CaloGAN

The main goal:
Speed up full simulation of particle showers in EM calorimeter.

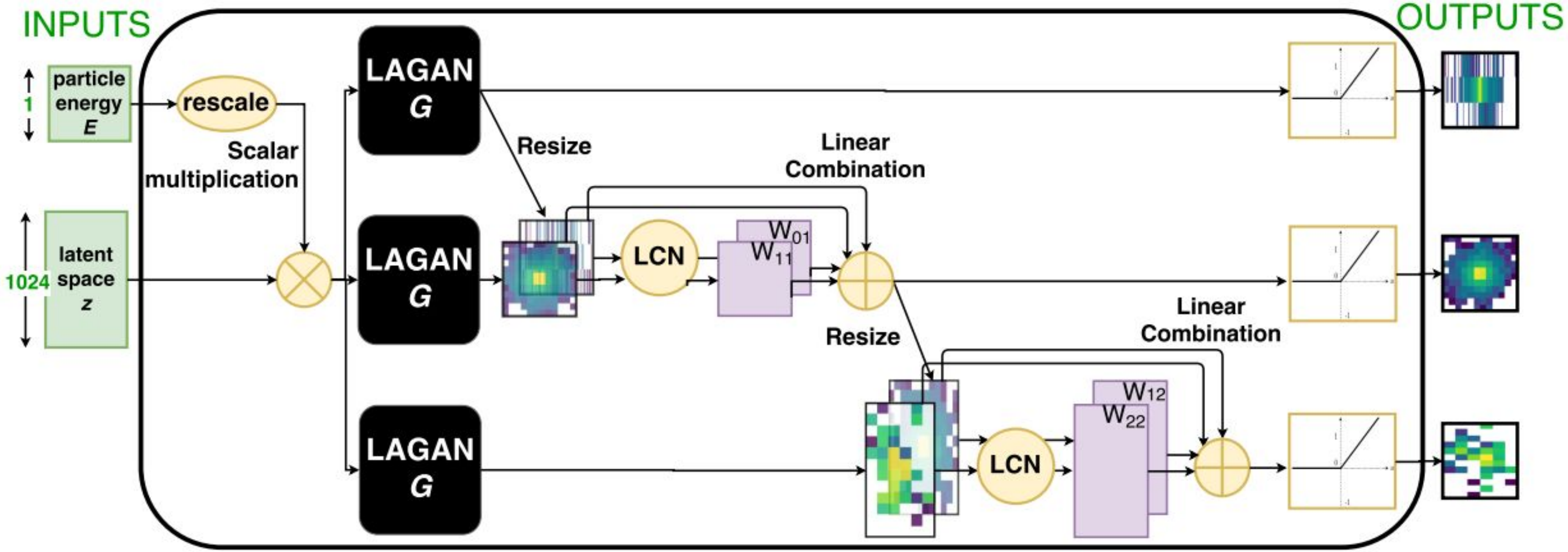
Auxiliary task: energy reconstruction

One model for each particle type: positron, pion, gamma

Model Pipeline:

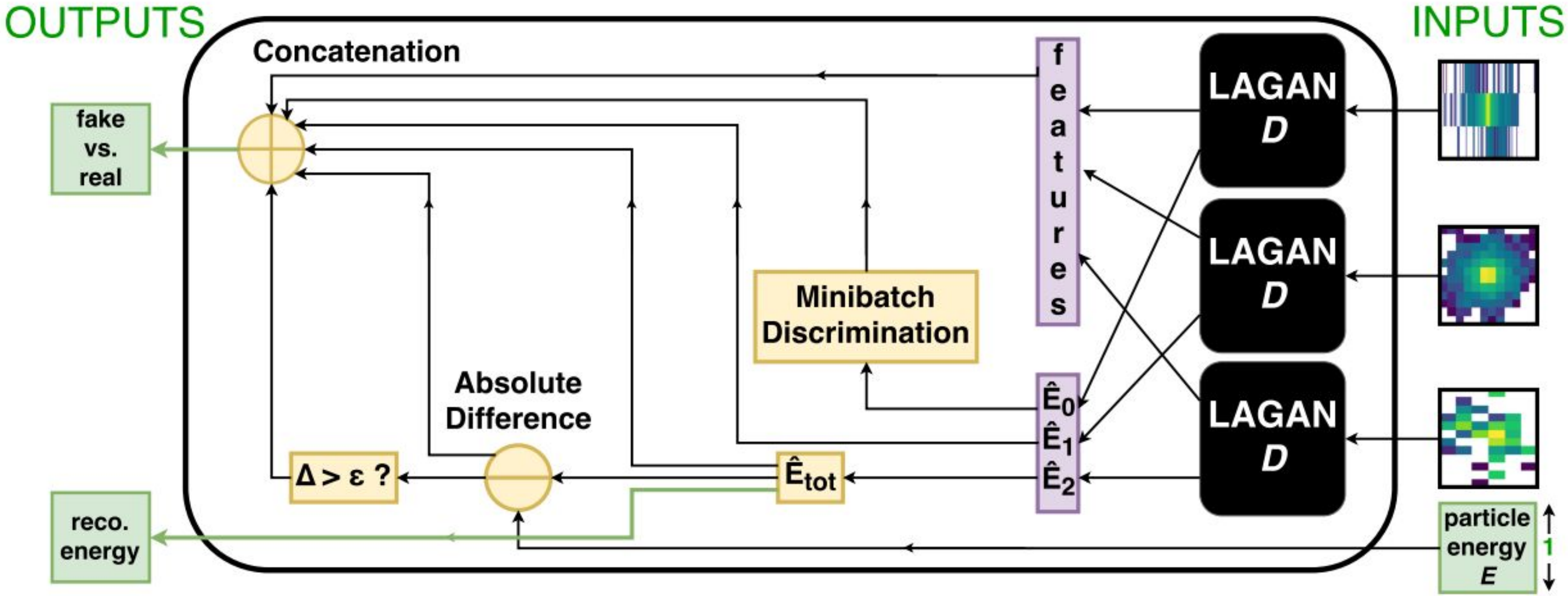
Energy scaled by 100 -> multiplied by vector from latent space $z \in \mathbb{R}^{1024}$ → Three gray-scale images → Prediction whether the shower is real or fake + Comparison of energy

# IV. CaloGAN. Generator




The LAGAN submodules are composed of a 2D convolutional unit followed by two locally-connected units with batch-normalization layers in between

# IV. CaloGAN. Discriminator




The LAGAN submodules are composed of a 2D convolutional unit followed by two locally-connected units with batch-normalization layers in between

# IV. CaloGAN. Loss Formulation

$$\mathcal{L}_{\mathsf{adv}} = \underbrace{\mathbb{E}_{z\sim p_z(z)}[\log(\mathbb{P}(D(G(z))=0))]}_{\substack{\text{term associated with the discriminator}\\ \text{perceiving a generated sample as fake}}} + \underbrace{\mathbb{E}_{I\sim f}[\log(\mathbb{P}(D(I)=1))]}_{\substack{\text{term associated with the discriminator}\\ \text{perceiving a real sample as real}}}$$

$$\mathcal{L}_E = \mathbb{E}_{z\sim p_z(z)}[\delta(E, \hat{E}(G(z)))] + \mathbb{E}_{I\sim f}[\delta(E, \hat{E}(I))]$$

$$\delta(e, e') = |e - e'|$$

$$\mathcal{L}_{\mathsf{generator}} = \lambda_E \mathcal{L}_E - \mathcal{L}_{\mathsf{adv}}$$

$$\mathcal{L}_{\mathsf{discriminator}} = \lambda_E \mathcal{L}_E + \mathcal{L}_{\mathsf{adv}}$$

# V Performance assessment and results replication

## Technical resources of authors:

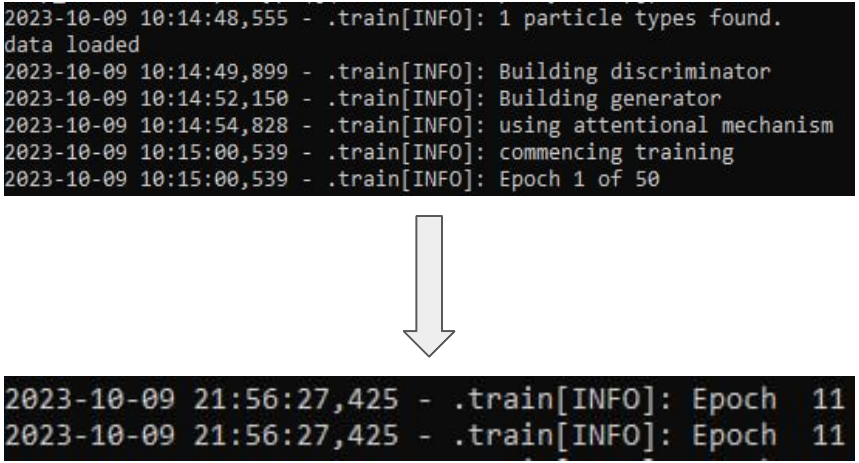
- 16 units of Nvidia K80 GPU’s
- 2 units of Nvidia Titan X GPU’s
- Technical and equipment support from Office of High Energy Physics of the U.S. Department of Energy

## Technical resources of our team:

- ~~1 unit of Nvidia RTX 3070 GPU~~ 1 unit of Intel core i5-11400f, since the older version of TensorFlow was not working properly with modern GPU’s
- A repo of non-supportable python 3.5 code which was majorly rewritten for reproducibility of results
- Technical and equipment support from working full-time

# As a result...

- Repo maintenance took us the majority of time
- A model for single-particle generation was trained due to lack of computational power
- A fifth of the suggested training computations ( 10 epochs ) were done in ~16 hours
- We would be happy to upload our trained models for other particles  as soon as they are properly trained,



# Performance assessment

## Potential problems with CaloGAN:

- Overtraining and mode collapse
- Unrealistic shower shapes compared to Geant4
- Training data energy ranges leading to inferior results when generating out-of-range energy showers
- Poor computational performance

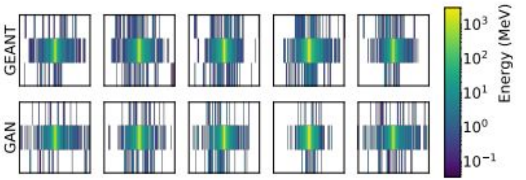
## Metrics used for assessment:

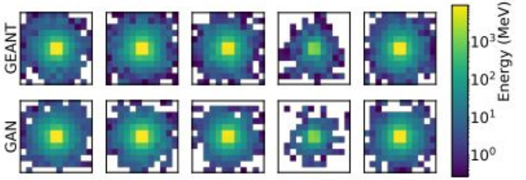
| Shower Shape Variable | Formula | *Notes* |
|---|---|---|
| $E_i$ | $E_i = \sum_{\text{pixels}} \mathcal{I}_i$ | Energy deposited in the $i^{th}$ layer of calorimeter |
| $E_{\text{tot}}$ | $E_{\text{tot}} = \sum_{i=0}^{2} E_i$ | Total energy deposited in the electromagnetic calorimeter |
| $f_i$ | $f_i = E_i / E_{\text{tot}}$ | Fraction of measured energy deposited in the $i^{th}$ 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 $i^{th}$ 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, $l_d$ | $l_d = \sum_{i=0}^{2} i \cdot E_i$ | 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 |

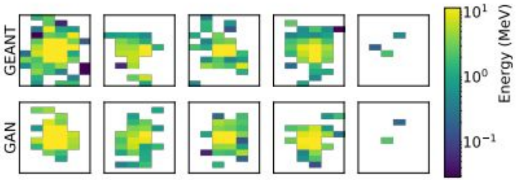
# Performance assessment: overtraining and mode collapse

- The problem was assessed by considering the nearest neighbors among the training and generated datasets

- As can be seen, the model succeeds in creating a variety of different showers and mode collapse does not seem to be a major issue



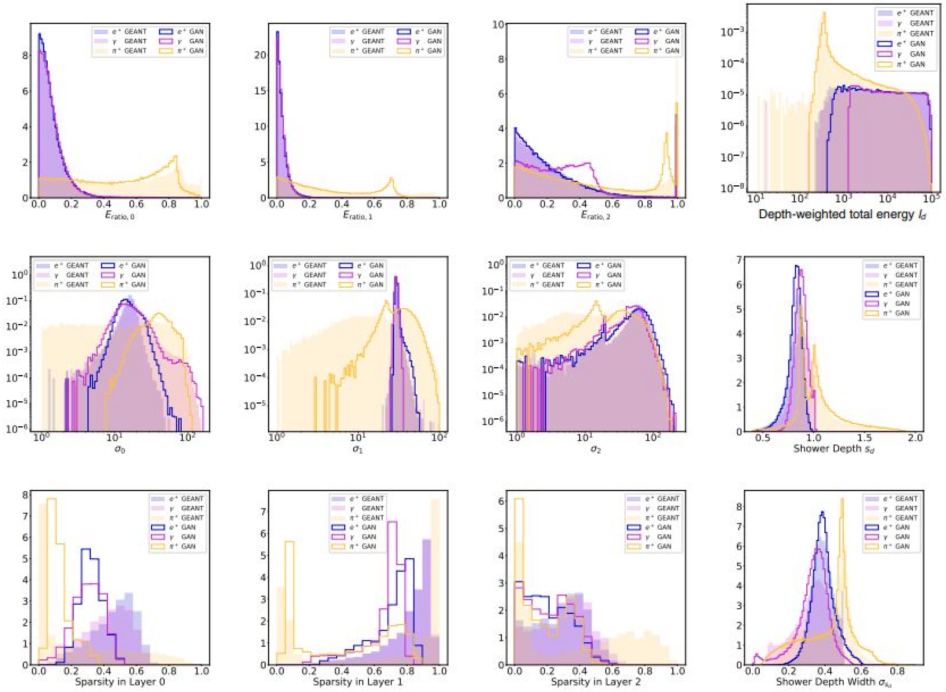



# Performance assessment: unrealistic shower shapes

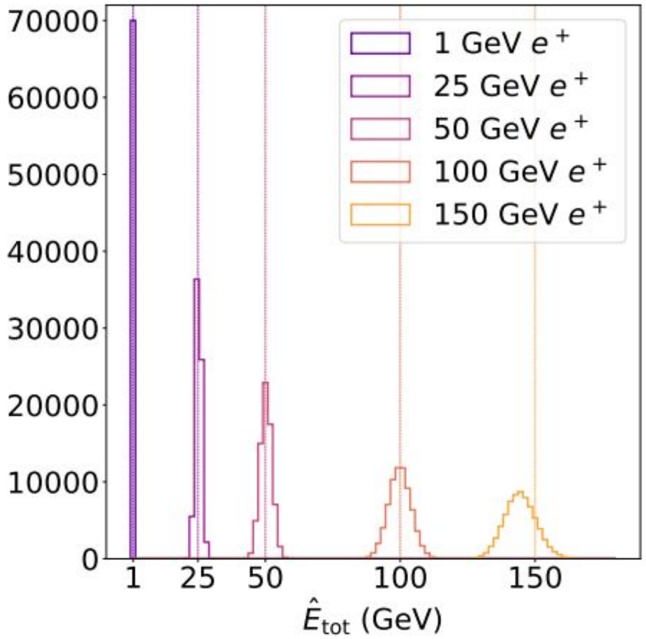
- The problem was assessed by plotting the distribution of a variety of metrics and comparing it with the ones produced by Geant4

- As can be seen, the model poorly reproduces sparsity levels per layer which are only partially matched with Geant4. However, in terms of other metrics, the 2 generation algorithms yield similar results



# Performance assessment:  out-of-range energy particles generation

The model is capable of producing post energy-conditioned empirical energy response distribution with relatively symmetrical ends for both in-range and out-of-range energies



# Performance assessment:  runtime analysis

Despite being poorly-maintained, the model seems to outperform state-of-the-art Geant4 in terms of runtime needed for generation of showers by several orders of magnitude
( 4 on average )

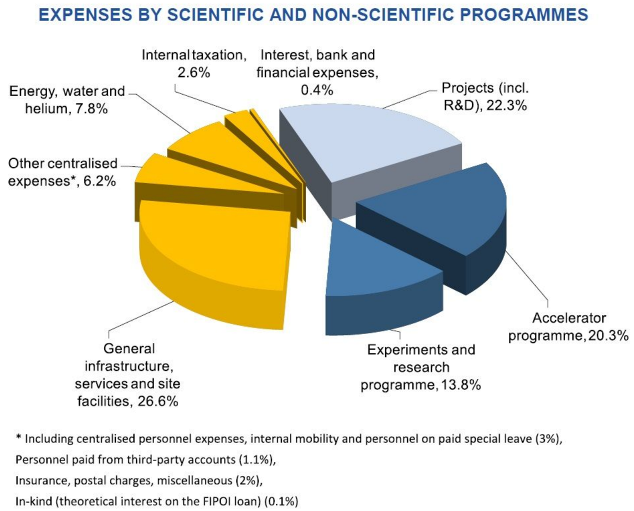
| Simulator | Hardware | Batch Size | ms/shower |
|---|---|---|---|
| GEANT4 | CPU | N/A | 1772 |
| CALOGAN | CPU | 1 | 13.1 |
| | | 10 | 5.11 |
| | | 128 | 2.19 |
| | | 1024 | 2.03 |
| | GPU | 1 | 14.5 |
| | | 4 | 3.68 |
| | | 128 | 0.021 |
| | | 512 | 0.014 |
| | | 1024 | 0.012 |

# Why is this important?

Currently,inhuman amounts of resources are used to model the experiments at LHC.

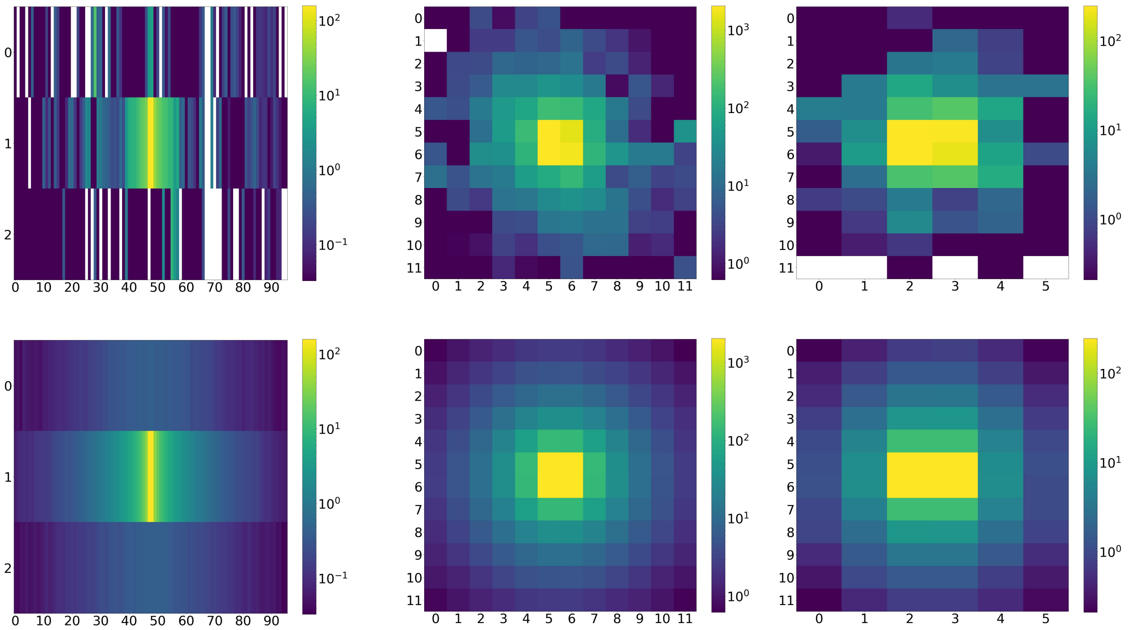
Using modern generative deep neural network techniques, generating three-dimensional electromagnetic showers in a multi-layer sampling LAr calorimeter with uneven spatial segmentation, while attempting to preserve spatio-temporal relation among layers is possible to be done with an up to five orders of magnitude decrease in computing time.These advancements may save CERN valuable resources

Future work is expected to be focused on improving performance by drawing from the recent Machine Learning developments in GAN training procedures, as well as testing the direct inclusion of important shower shape variables as constraints at training time



# Our Results

# Piplus: Generated vs Real

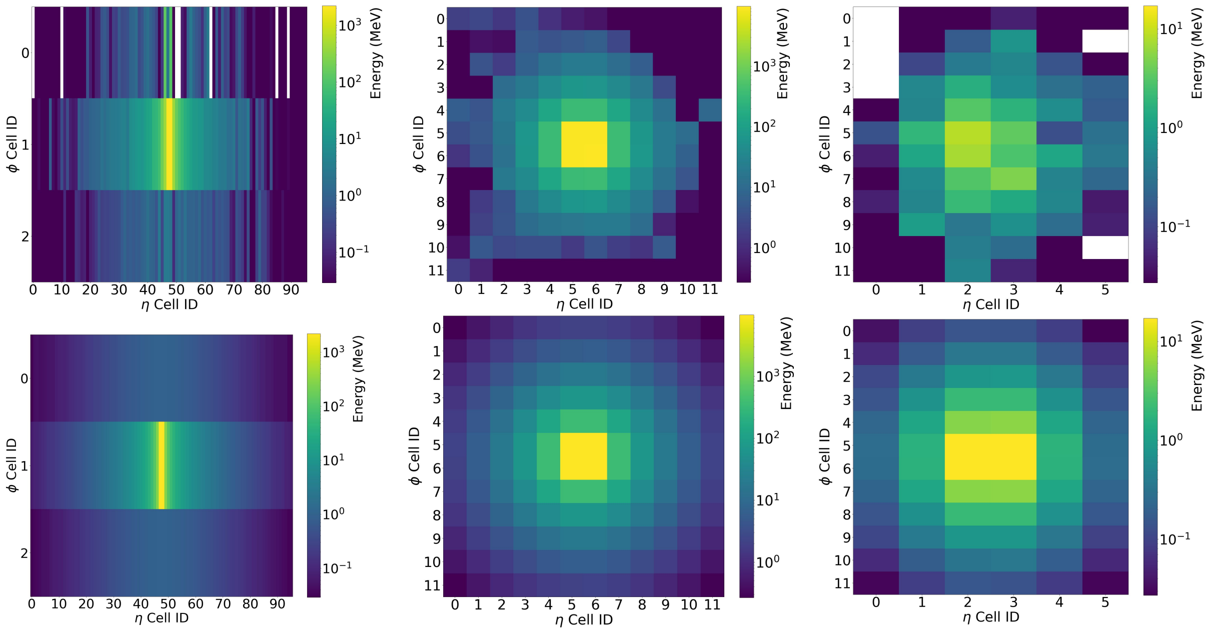



**Generated samples**

**Real samples**

## Our Results

# Eplus: Generated vs Real

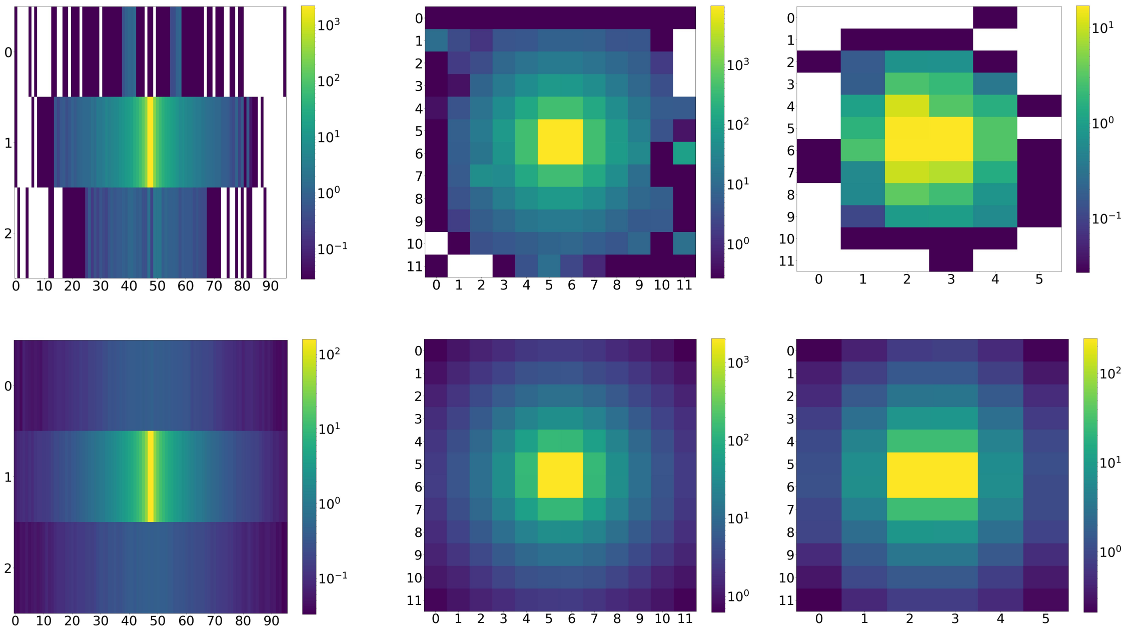



**Generated samples**

**Real samples**

# Our Results

# Gamma: Generated vs Real

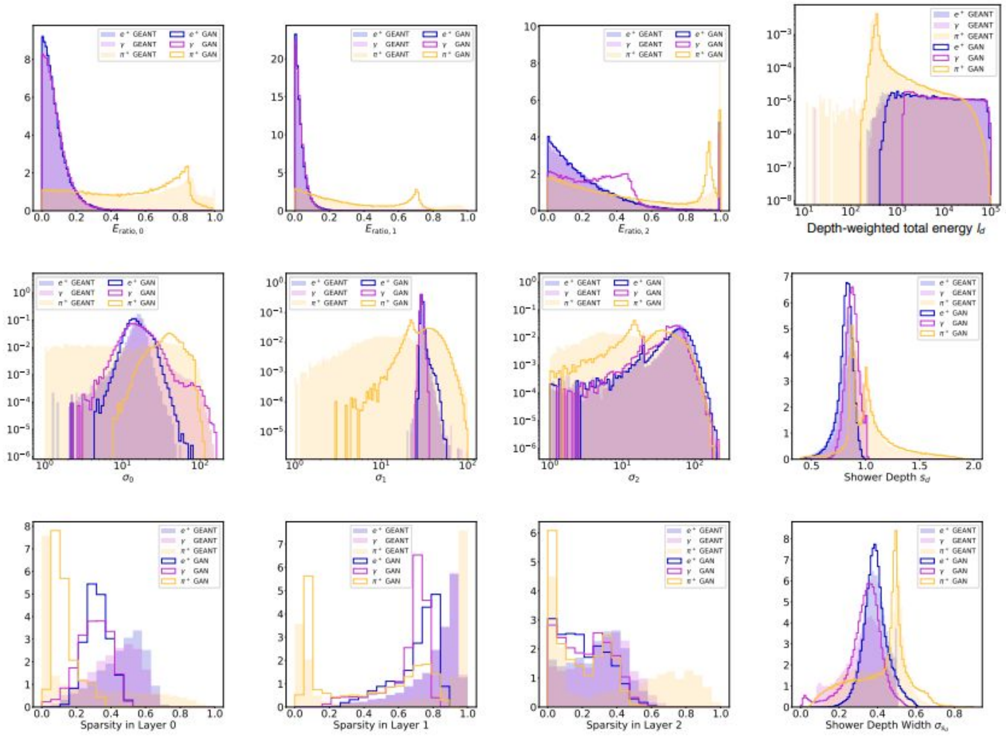



**Generated samples**

**Real samples**

Our Results

# Authors model's distributions



# Our Results

# Our model’s distributions