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Graph neural networks for space experiments

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Spoke 3 II Technical Workshop, Bologna Dec 17 -19, 2024

Where we were at the meeting in Elba

We developed a GNN-driven tracking algorithm applied to a space experiment toy model.

The GNN shown promising performances on tracking purposes over the analytical/traditional approach.

All the software development has been saved on

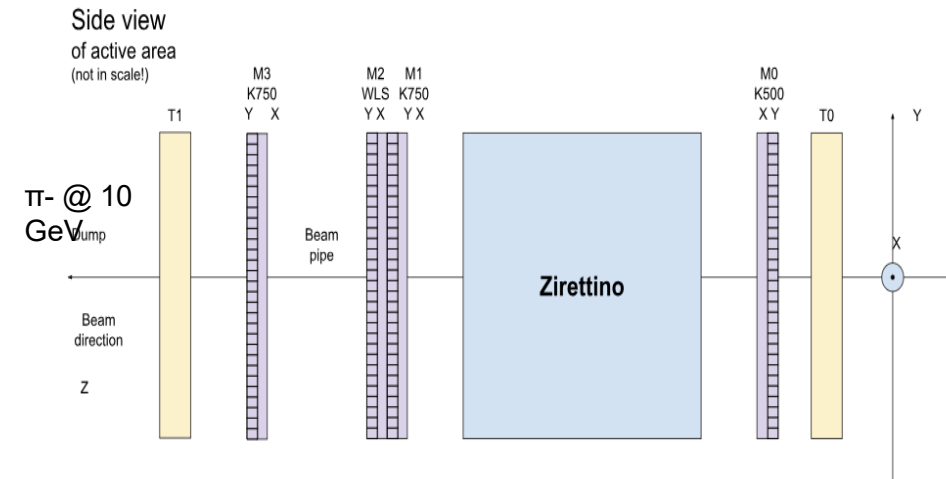
https://github.com/federicacuna/TB_Sept_2023_ml,

https://github.com/federicacuna/TestBeam_T10_2023,

https://github.com/federicacuna/nuses_M1

Next steps:

- Optimization of the GNN algorithm ✓
- Preliminary analysis and GNN development on **more complex tracking data** (ongoing)
- Development of a preliminary unified AI architecture for tracker and calorimeter (see M.Bossa talk) in space experiment (ongoing)



Results presented at
ML4Astro Catania
07/2024!!!

Scientific Rationale: AI tracking algorithm

To test our algorithm on **more complex data**, we decided to analyze HERD simulated data.

The **HERD** (High Energy cosmic-Radiation Detection) experiment is a space mission designed to directly detect cosmic rays, and it is set to be installed on the **Chinese Space Station (CSS)** in 2027.

The main goals of the mission:

- enhance our understanding of high-energy cosmic rays,
- search for indirect signals of dark matter,
- probe sources of high-energy particles such as protons, electrons, and photons.

Fiber Tracker (FIT):

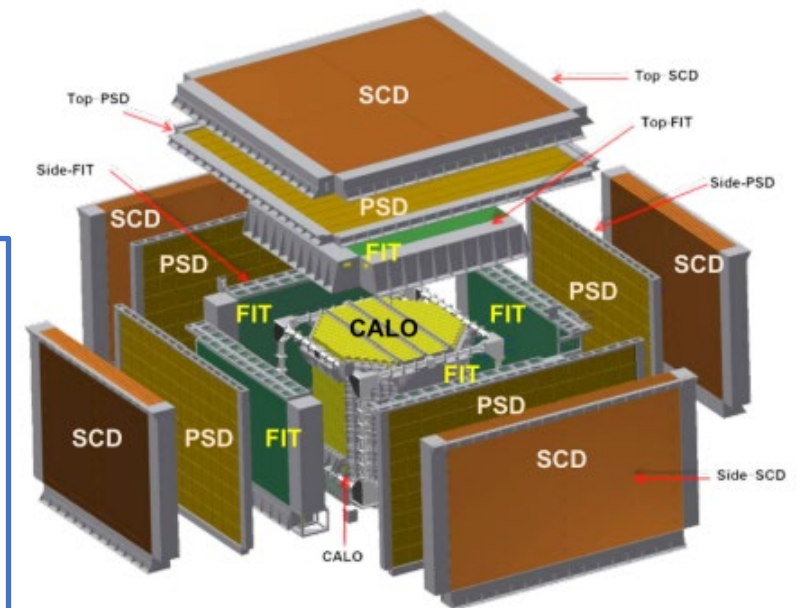
- Surrounds CALO on top and sides.
- Particle tracking and charge measurements
- 5 sectors, each with 7 X-Y scintillating fiber layers.
- Provides 7 precise position measurements.

The HERD simulation dataset

The full dataset, generated using the custom HerdSoftware simulation framework, consists of 4,300,000 events, equally divided into 2,150,000 electron events and 2,150,000 proton events.

Both event sets are simulated within a power-law energy spectrum E^{-1} , spanning an energy range from 100 GeV to 1 TeV, and are distributed within a spherical region surrounding the HERD detector.

Electrons set was used for the tracking algorithm

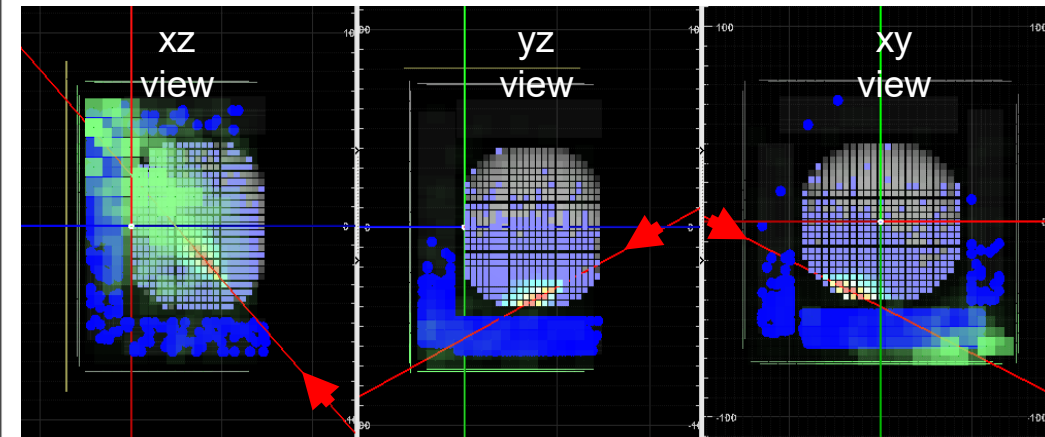
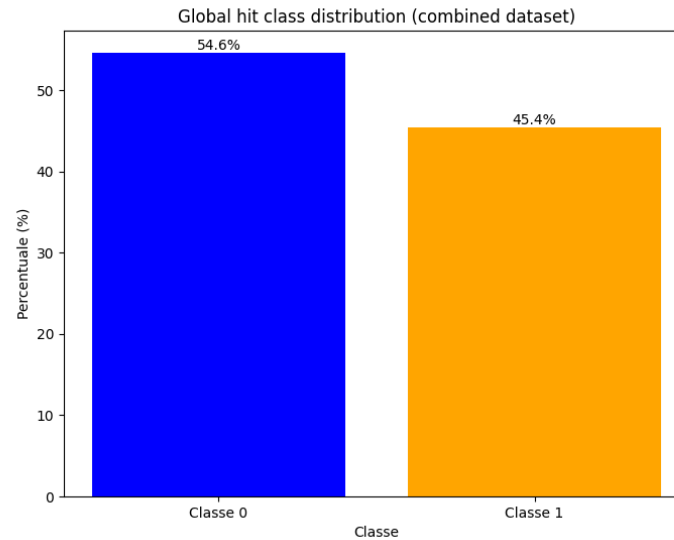
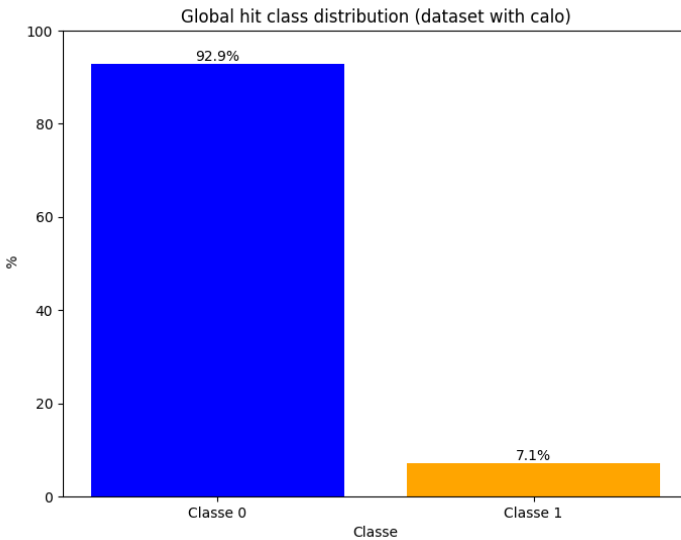
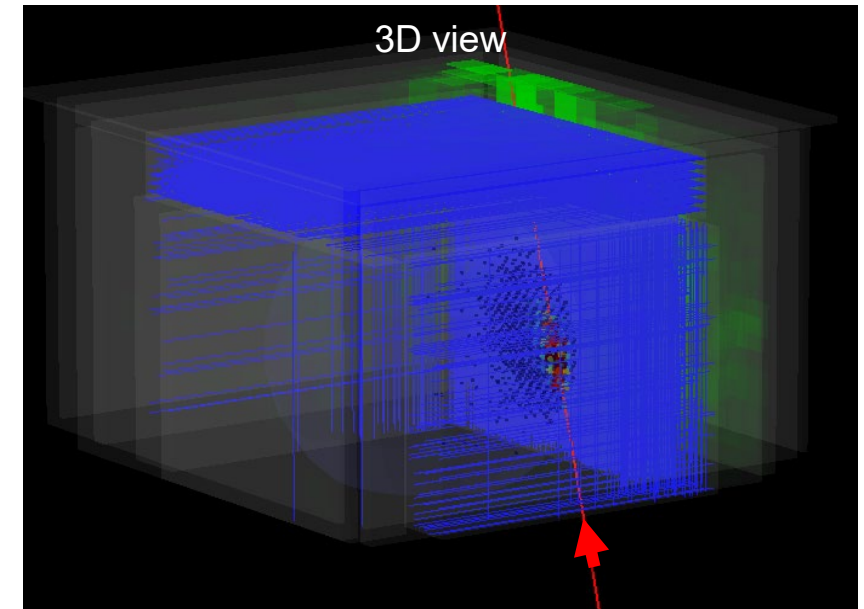


Preprocessing phase

Data are highly imbalanced, since there are many backscattering tracks originating from the calorimeter, which interfere with the correct identification of the primary particle's trajectory

To mitigate the imbalance:

1. Clustering algorithm
2. Cut of noise clusters "far away" from the primary track
3. Adding simulated events without calorimeter



The GNN algorithm

- SageConv architecture
- 18 layers
- Mean aggregation function
- 128 hidden size
- Adam optimizer
- Binary cross entropy loss function

4,5 million simulated track data
75% train-15% validation-10% test

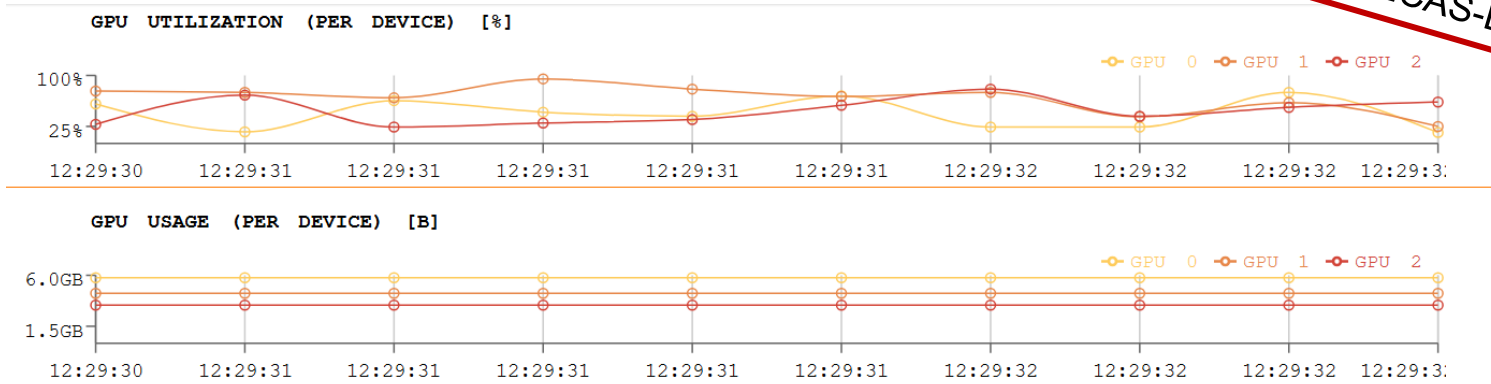
Distributed training

To enhance the time consuming we performed the distributing training by using:

- the JupyterLab instance with 3 A100 NVIDIA GPUs
- the Leonardo Hub instance with 4 A100 NVIDIA GPUs (see M.Pasqui talk!)

Leonardo-HUB

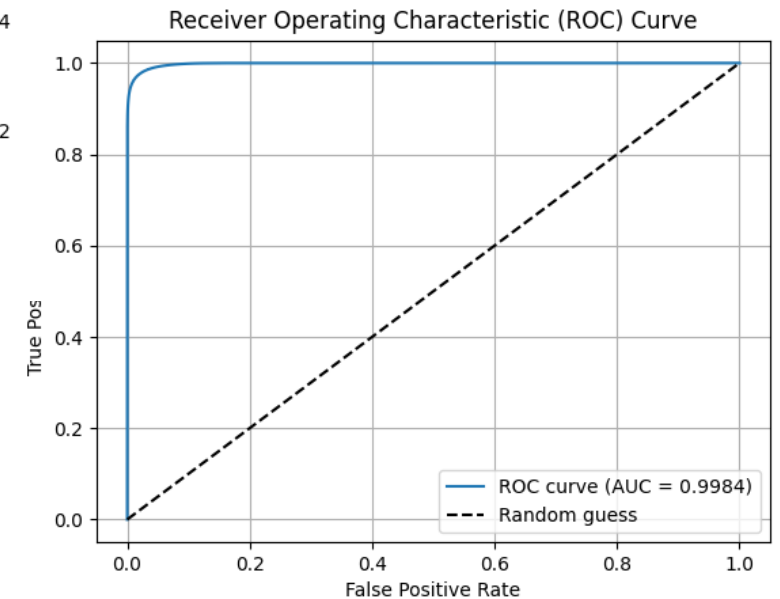
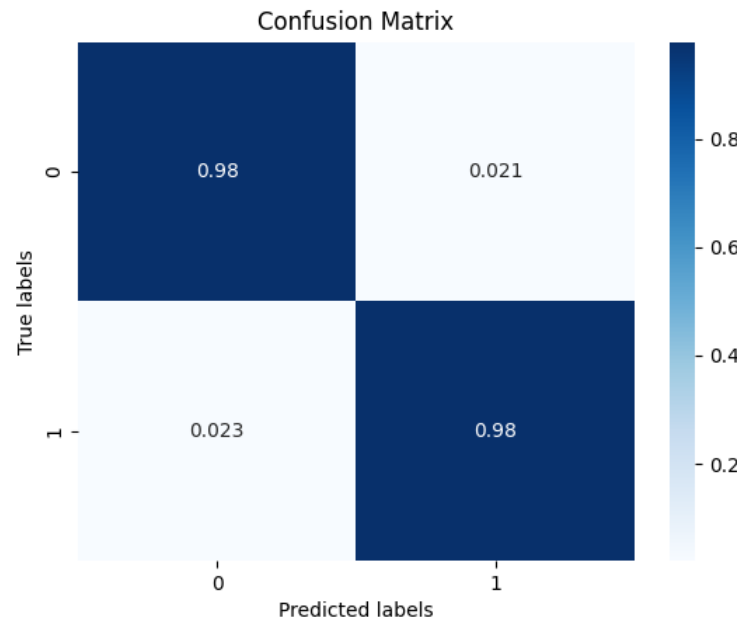
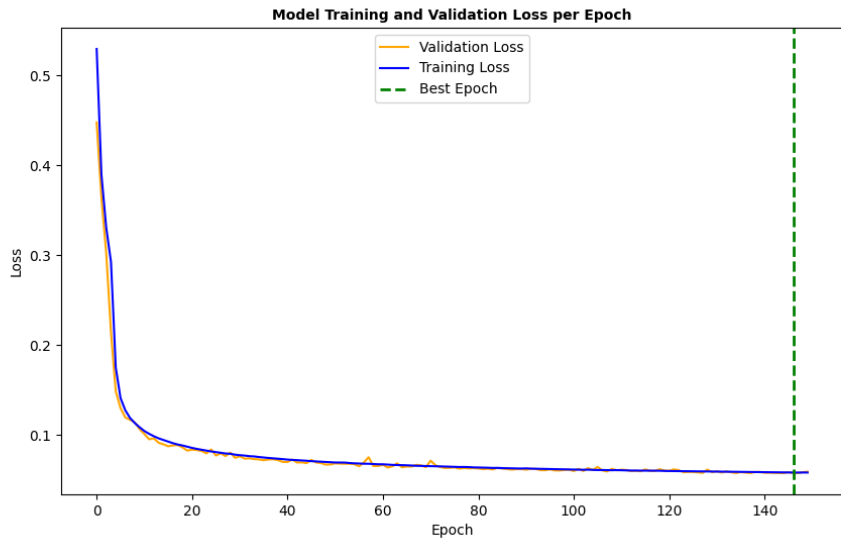
RECAS-Bari



GPU	Name	Persistence-M	Bus-Id	Disp.A	Volatile Uncorr. ECC
0	NVIDIA A100-SXM-64GB	On	00000000:1D:00.0	Off	0
1	NVIDIA A100-SXM-64GB	On	00000000:56:00.0	Off	0
2	NVIDIA A100-SXM-64GB	On	00000000:8F:00.0	Off	0
3	NVIDIA A100-SXM-64GB	On	00000000:C8:00.0	Off	0

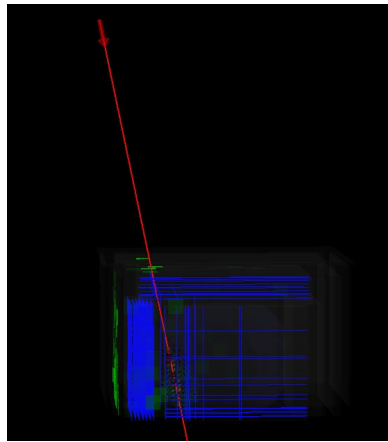
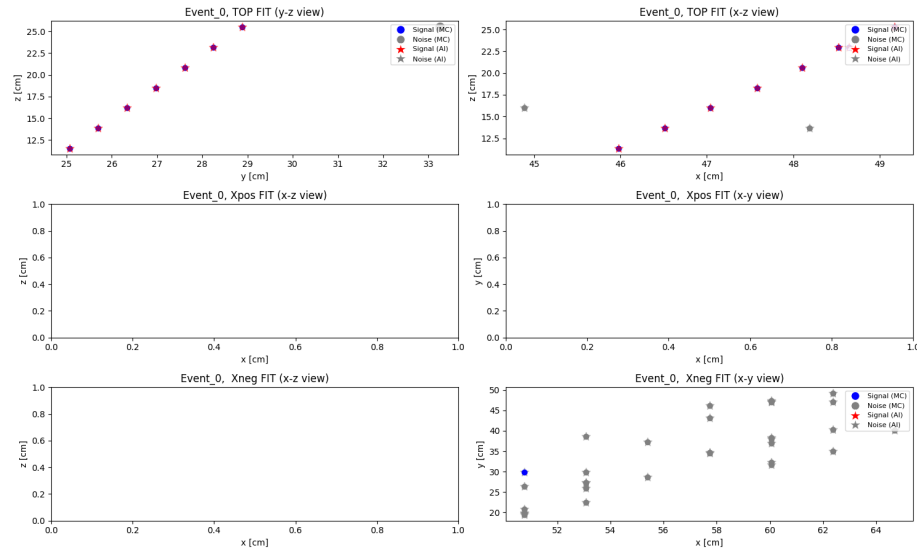
GPU	GI	CI	PID	Type	Process name	GPU Memory Usage
N/A	44C	P0				
N/A	45C	P0				
N/A	45C	P0				
N/A	44C	P0				

Main Results: gnn algorithm evaluation

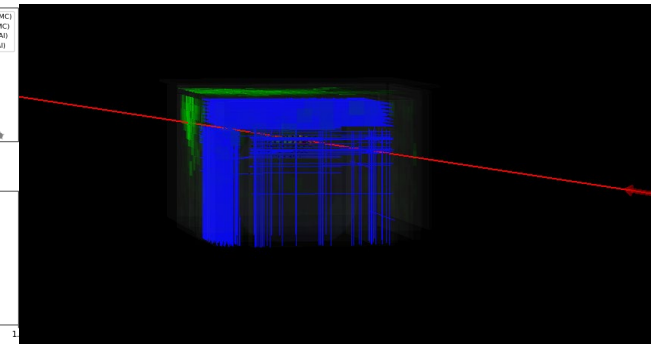
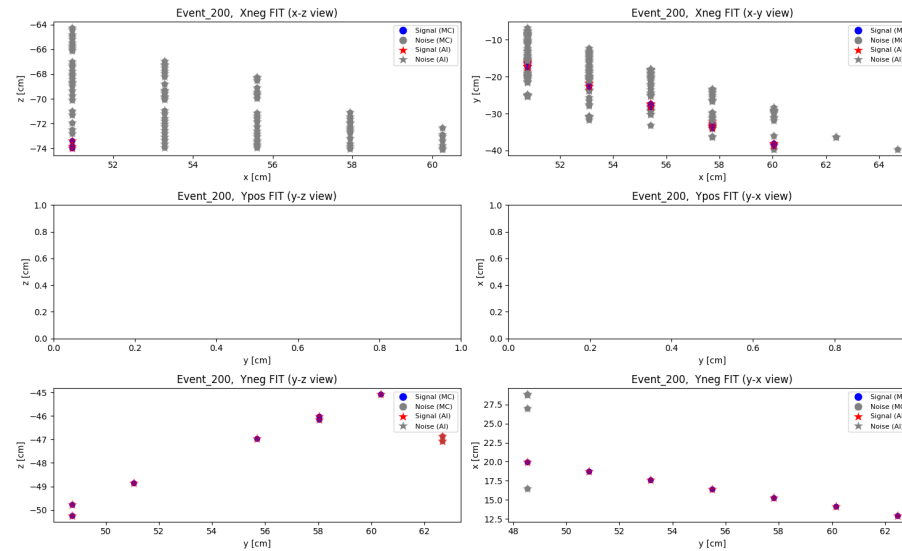


Metrics	Values
Accuracy	97.80%
Recall	97.65%
Precision	97.81%
F1-score	97.73%
ROC AUC	99.84%

Main Results: events display



Paper submitted at PDP Conference!!!



Final Steps

The results obtained by applying the GNN-tracking algorithm are quite promising, proving that the AI algorithm can handle real experiment data.

Analysis on calorimeter have been conducted by using Transformers-based algorithm for showers classification, in order to create a unified AI pipeline for HERD experiment (see Maria's talk.)

Next steps

- Improving the preprocessing phase
- Test other GNN algorithms

Cascade Funding: SPARTAN with NI

We initiated our collaboration with an in-person meeting during the last week of November.

During this meeting, we enhanced the data preprocessing to be fast enough for the FPGA utilization

Next steps:

- Test of the GNN trained algorithm on the FPGA
- Implementation of new algorithms to detect multiple tracks
- Implementation of a CNN to be tested on FPGA



Thank you
and
Happy Holidays!

Key Features of HERD:

1. Geometric Factor & Sensitivity:

1. HERD's design incorporates a **homogeneous, isotropic, and deeply segmented 3D calorimeter**, which allows for a large geometric acceptance.
2. The high energy resolution allows the experiment to measure the **proton flux** up to **1 PeV** and the **electron/positron flux** up to several tens of TeV.
3. Additionally, HERD will be able to detect **high-energy photons** and search for potential sources of cosmic rays, contributing to studies on **dark matter**

2. The other sub-detectors:

1. CALO (Calorimeter):

1. It measures the **energy** of incoming particles and helps differentiate between different types of particles (e.g., electrons vs protons and nuclei).
2. **7,500 LYSO cubic scintillating crystals** (3 cm side)
3. **charge measurement**, the FIT surrounds the CALO on all sides.

2. PSD (Plastic Scintillator Detector):

1. The PSD consists of **plastic scintillator bars** that help measure the **charge** of particles and serve as a trigger for detecting low-energy gamma rays.

3. SCD (Silicon Charge Detector):

1. A **micro-strip silicon detector** used for precise particle tracking and charge measurement.

4. TRD (Transition Radiation Detector):

1. The TRD is used primarily for **TeV nuclei calibration** and is positioned on one side of the detector.
2. It consists of **THick Gaseous Electron Multipliers (THGEM)**, which are used to detect transition radiation, a powerful tool for identifying high-energy nuclei.

Technical Objectives, Methodologies and Solutions: Graph neural networks

A graph represents the relations (edges or links) between a collection of entities (nodes).

Graph Neural Networks (GNNs) are a class of deep learning models that are designed to operate on graph-structured data.

They have shown remarkable success in tasks such as node classification, link prediction, and graph classification.

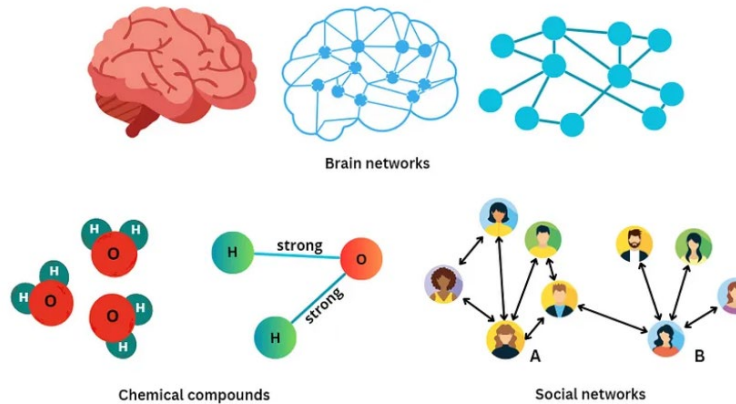
The key idea behind GNNs is to learn representations for nodes and edges in a graph by aggregating information from their local neighborhood.

A GNN consists of a number of layers, each of which updates the representation of each node based on its local neighborhood.

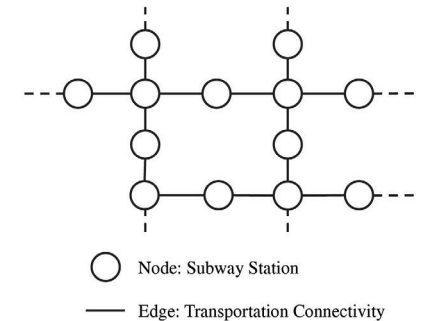
The representation of each node is typically a low-dimensional vector that encodes the node's properties and its relationships with other nodes.

The layers of a GNN are designed to capture increasingly complex features of the graph by aggregating information from the neighborhood of each node.

The key component of a GNN layer is the aggregation function, which takes as input the representations of a node's neighbors and produces a new representation for the node.



- *A Gentle Introduction to Graph Neural Networks*, <https://distill.pub/2021/gnn-intro/>
- *Hands-On Graph Neural Networks Using Python*, M.Labonne, Packt Publishing Ltd.



(a)

(b)

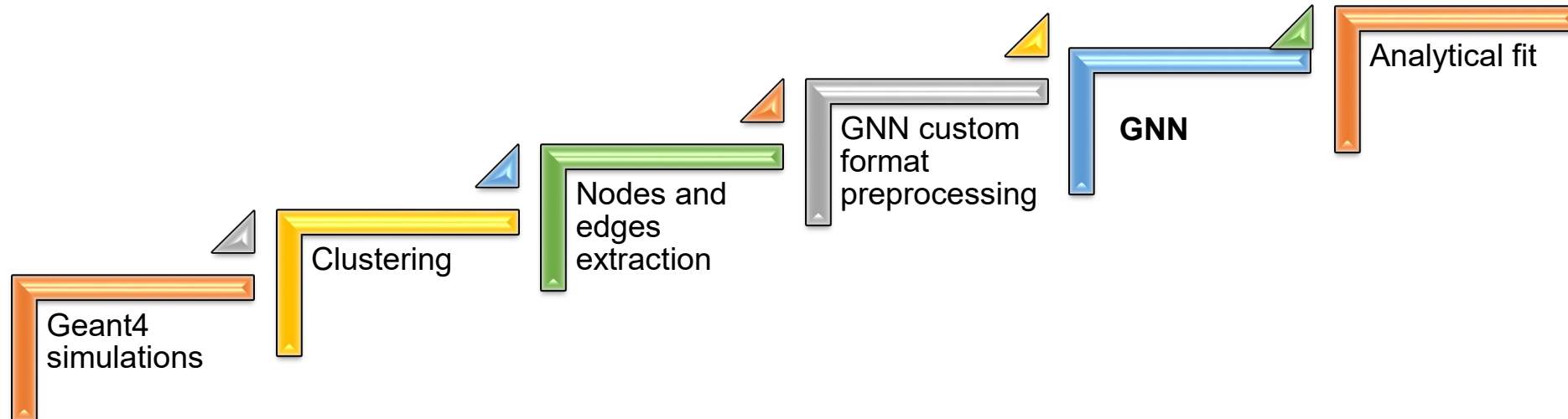
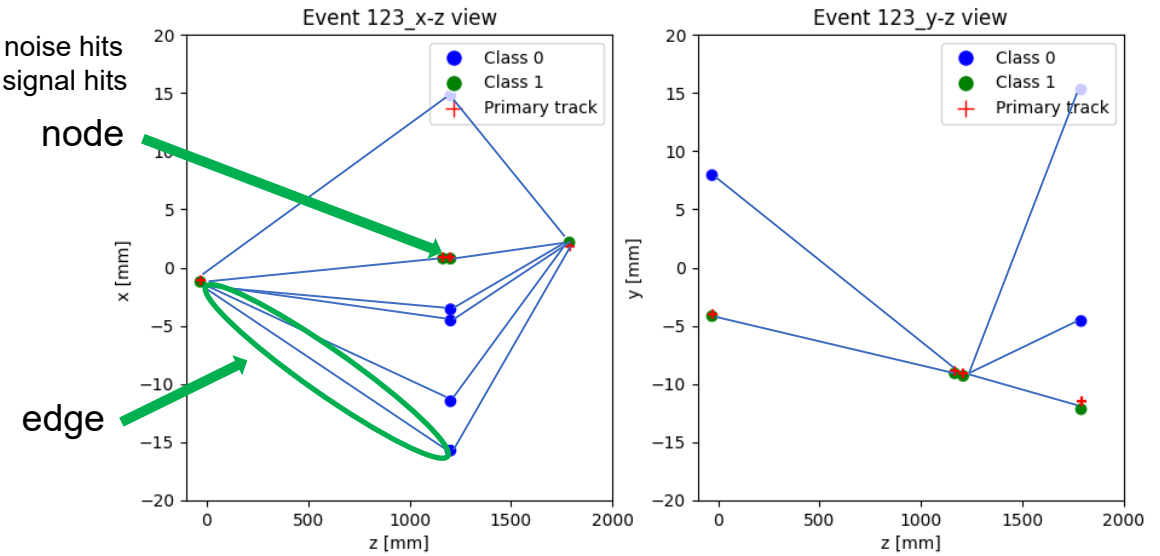
Accomplished Work, Results

Graphs are a natural way to represent tracks!

We developed graph neural networks algorithms for node classification, by using PyTorch geometric library.

Nodes are the hits inside the tracking detector and edges are the inter-layer hit connection.

Class 0: noise hits
Class 1: signal hits





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