Hadronic Shower Substructure Reconstruction using Graph Neural Networks

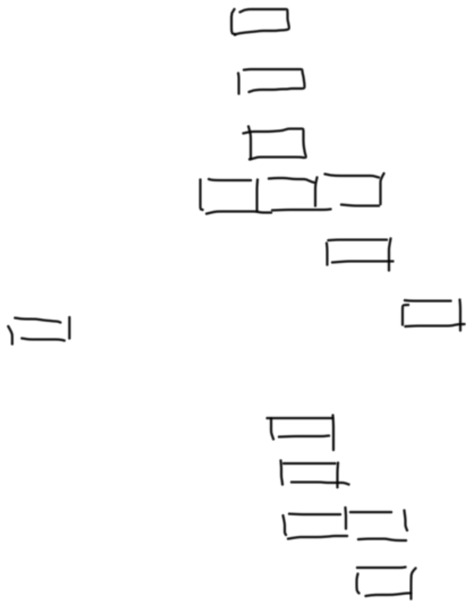
AHCAL main meeting

Vladimir Bocharnikov (DESY)
8 Dec 2021

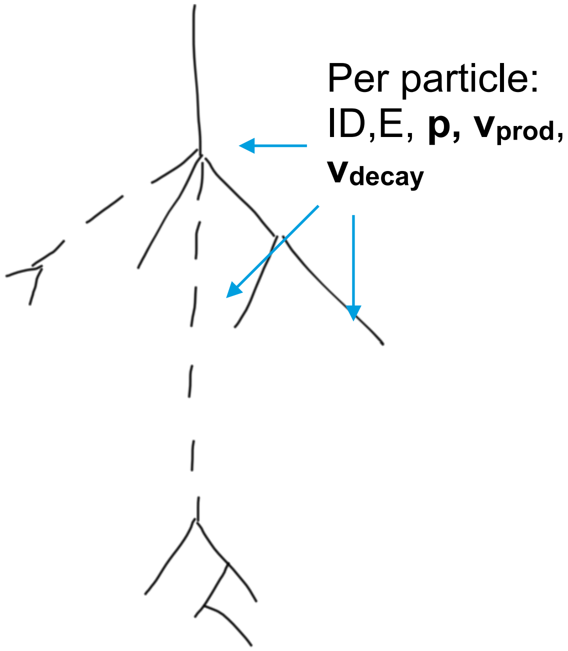
Calorimeter vision for hadronic showers

Ultimate goal and general approach

Set of hits in highly granular calorimeter



Particle interaction tree



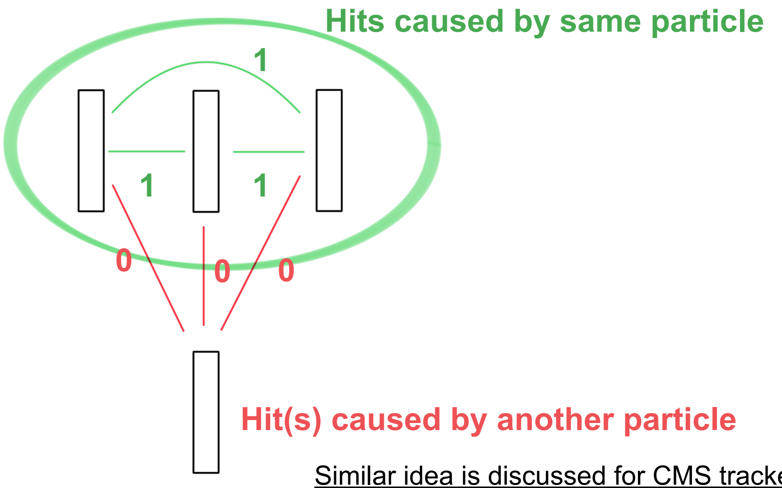
Potential applications of hit to secondary particle association:

- Hadronic energy reconstruction
- Shower separation algorithms:
  - Recombination of secondaries between overlaid showers
- Validation of simulation performance:
  - Comparison of global physical distributions
  - Shower description on single event basis is possible

    ➡ essential for adversarial networks

Graph representation of calorimeter event

First steps

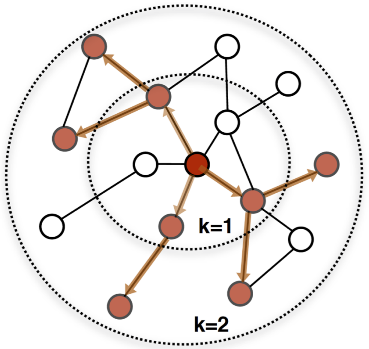


Similar idea is discussed for CMS tracker and HGCAL

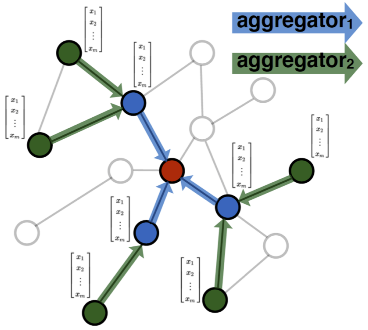
Event graph:

- Nodes - calorimeter hits
- Node features - position, energy, (time)
  - — Edges - neighbours within distance < R_{max} (Radius graph)
  - — Edge weights - 1 if pair of hits belong to same **fundamental object** (e/m sub-shower, track), otherwise 0
- ML **objective** - **predict edge weights** given the radius graph of event

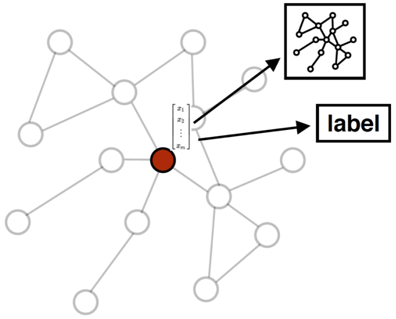
GraphSAGE (**SA**mple and aggre**G**at**E**) architecture (Graph neural network model (GNN)):



Sample neighbourhood of graph nodes

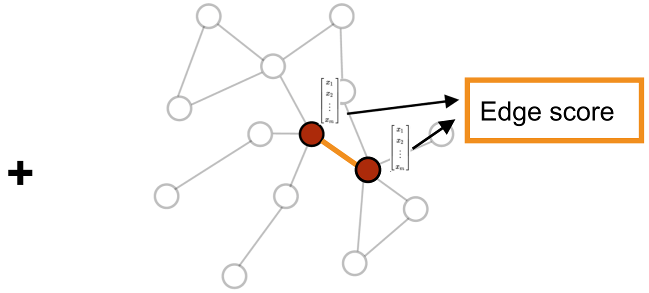


Aggregate feature information from neighbours



Get graph context embeddings for node using aggregated information

Custom output layer



Predict edge score for each pair of connected nodes using embedded features

Truth information from Monte-Carlo

Algorithm to find truth e/m objects

Simulations

Geant4 (v10.03.p02) QGSP_BERT_HP using CALICE AHCAL geometry

Pure energy deposition in cells (before digitalisation and reconstruction)

Truth electromagnetic sub-shower definition:

"**Electromagnetic**" particles: $e^{\pm}$,γ, π^0, η

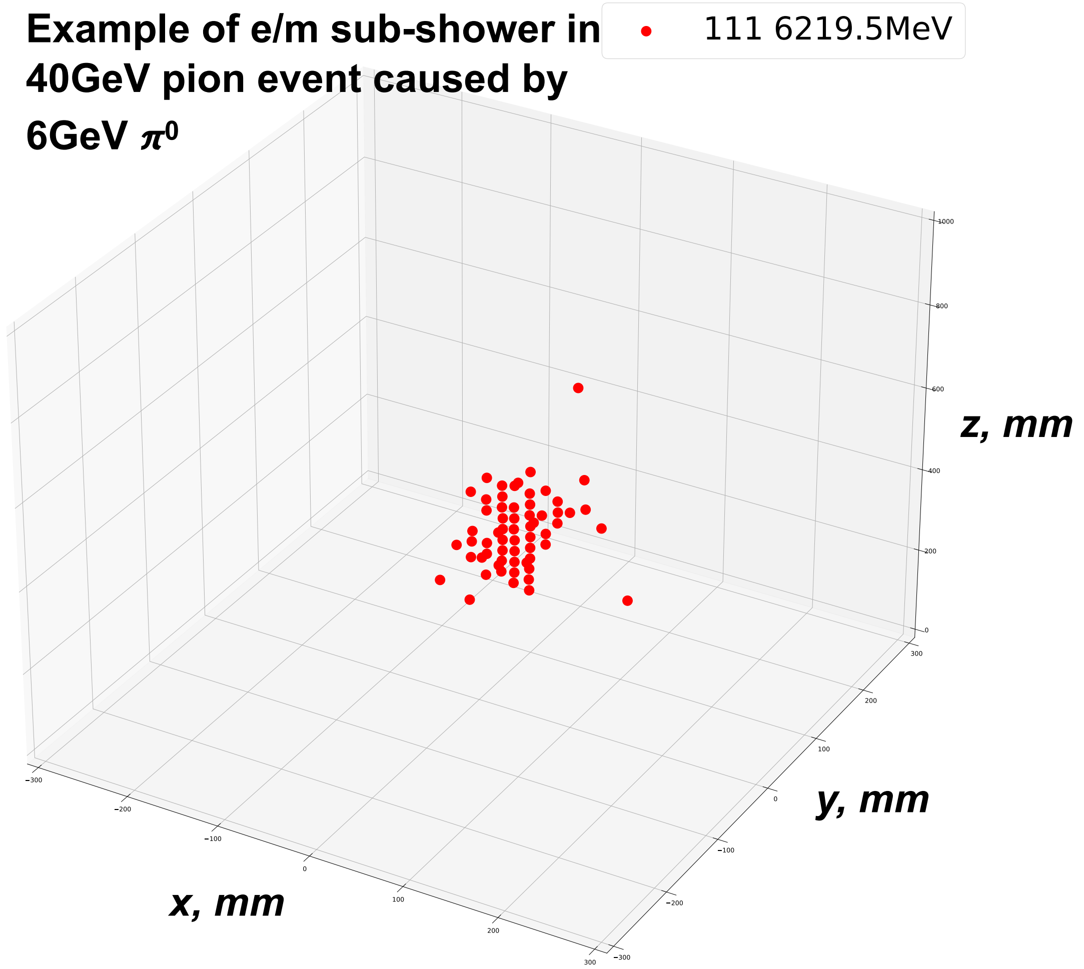
Energy threshold - *0.1GeV* (arbitrary now)

If MC particle is "electromagnetic", all it's "electromagnetic" daughters compose e/m shower are removed from further consideration

Corresponding simulated hits compose sub-shower,

0.5MIP cut: $E_{hit}>0.25MeV$

Example of e/m sub-shower in 40GeV pion event caused by 6GeV π^0



MC history for **ionising particles** is more complicated to easily define individual objects (tracks). Work in progress

Datasets and model parameters

Edge score model

Train&test dataset:

- ~6000 MC event graphs (50/50 split)
  - Pure energy deposition in calorimeter cells (before digitalisation and reconstruction)
  - **10-100 GeV pion** samples

➡ Radius graphs with calorimeter hit nodes (x,y,z,E_{hit}) R_{max} = ***59 mm***

- Electromagnetic relation between hits is encoded in edge scores (0/1)

Model:

GraphSAGE GNN

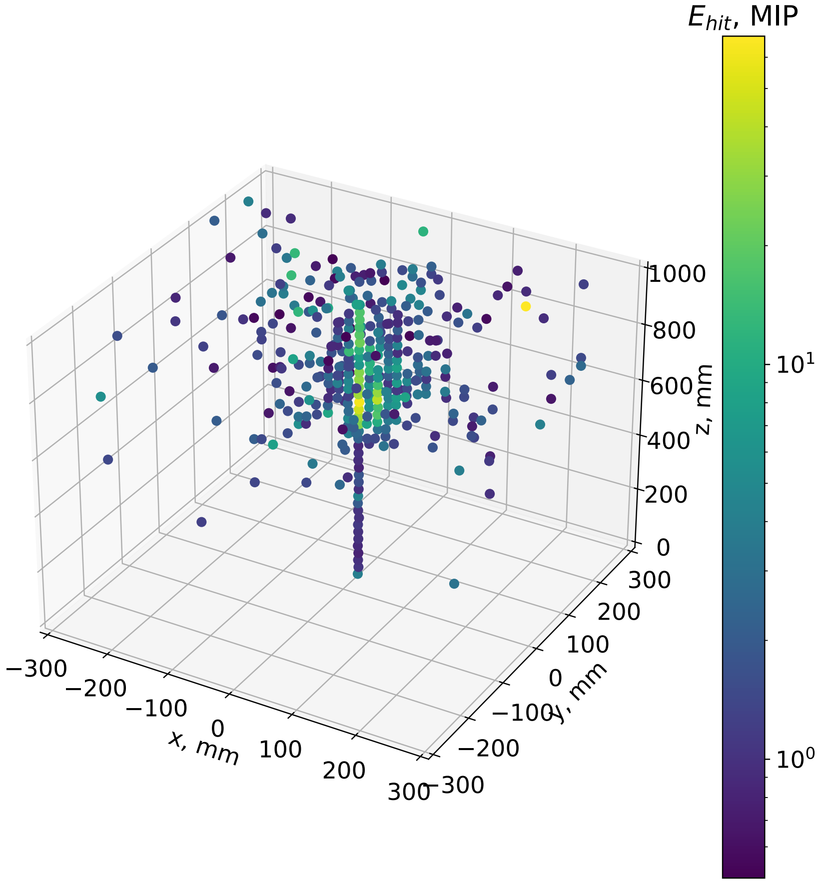
8 layers with 16 hidden channels + 1 linear output layer to convert node embeddings to edge scores

Objective: prediction of edge scores

Loss: binary cross entropy

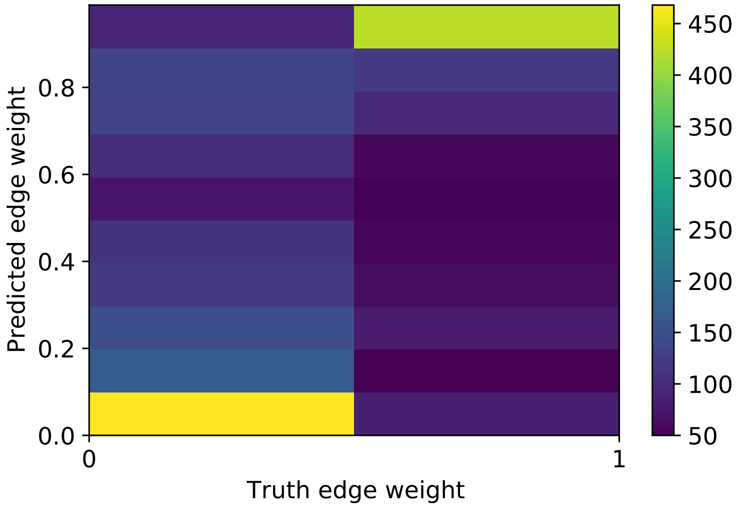
Hadronic shower reconstruction with GNN

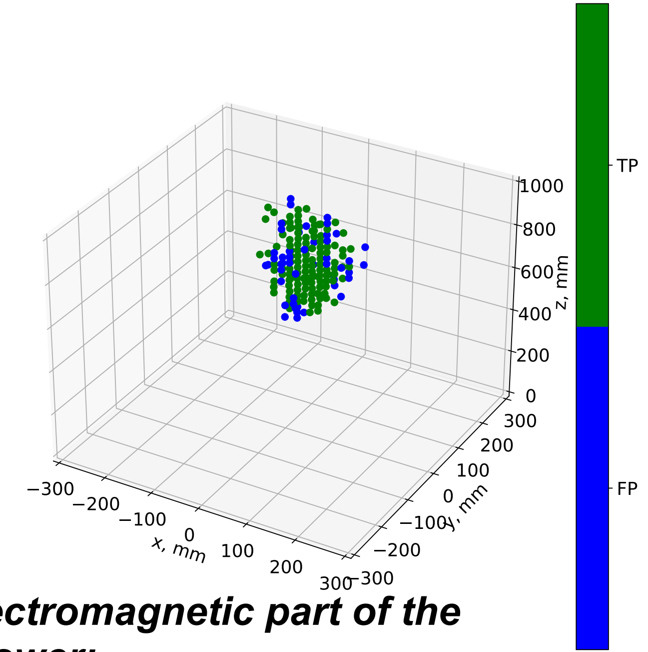
Results for single test event.



Electromagnetic relation between hits is encoded in graph edge weights:

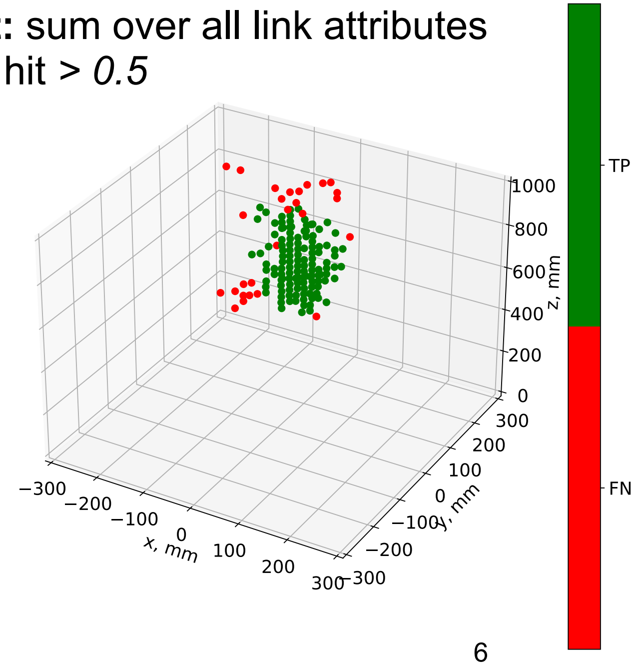
2650 graph edges





Electromagnetic part of the shower:

Cut: sum over all link attributes per hit > *0.5*

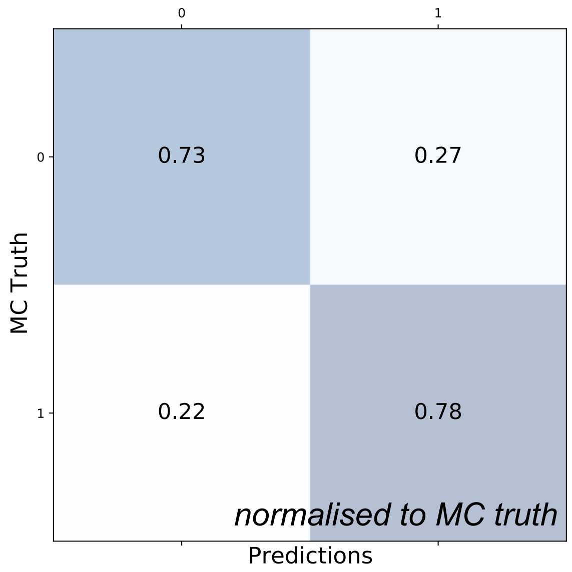


W o r k i n p r o g r e s s …

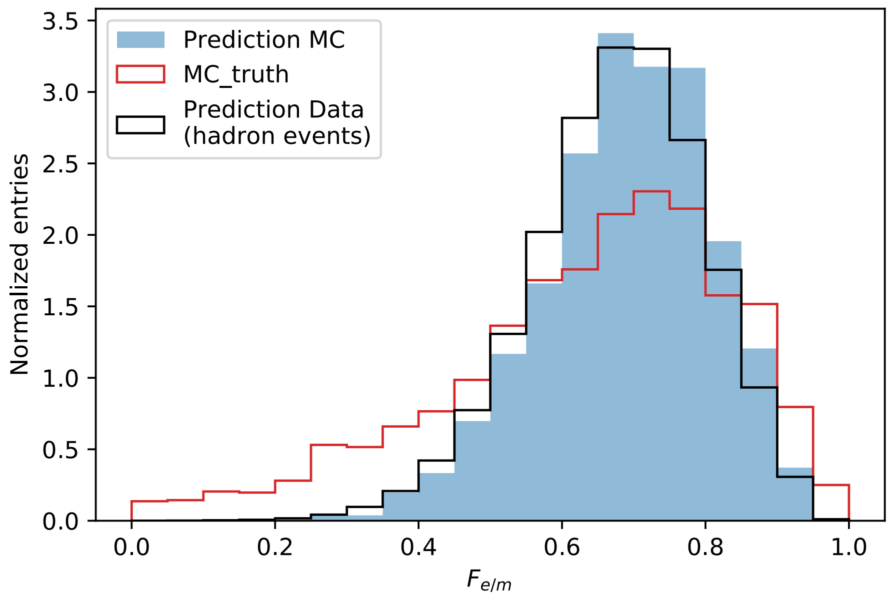
Electromagnetic fraction of hadronic showers

Results for 10,20,30,40,60,80 GeV pions

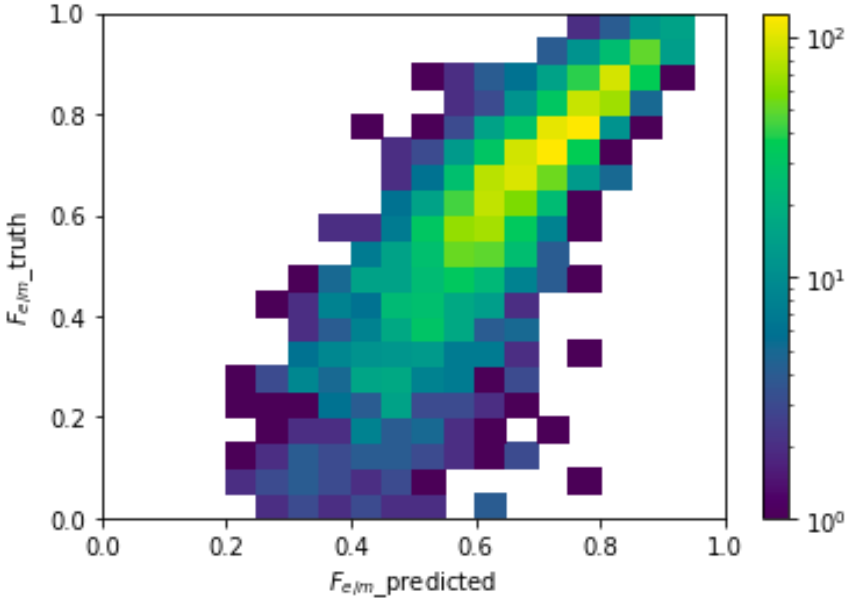
Hit classification



Electromagnetic fraction



Prediction vs truth correlation



- ~75,5% hit classification accuracy
- Higher MPV for F_{em} than expected
  - ➡ Non-e/m contributions to the hits are not taken into account
- Less pronounced tails for F_{em} prediction than for MC truth

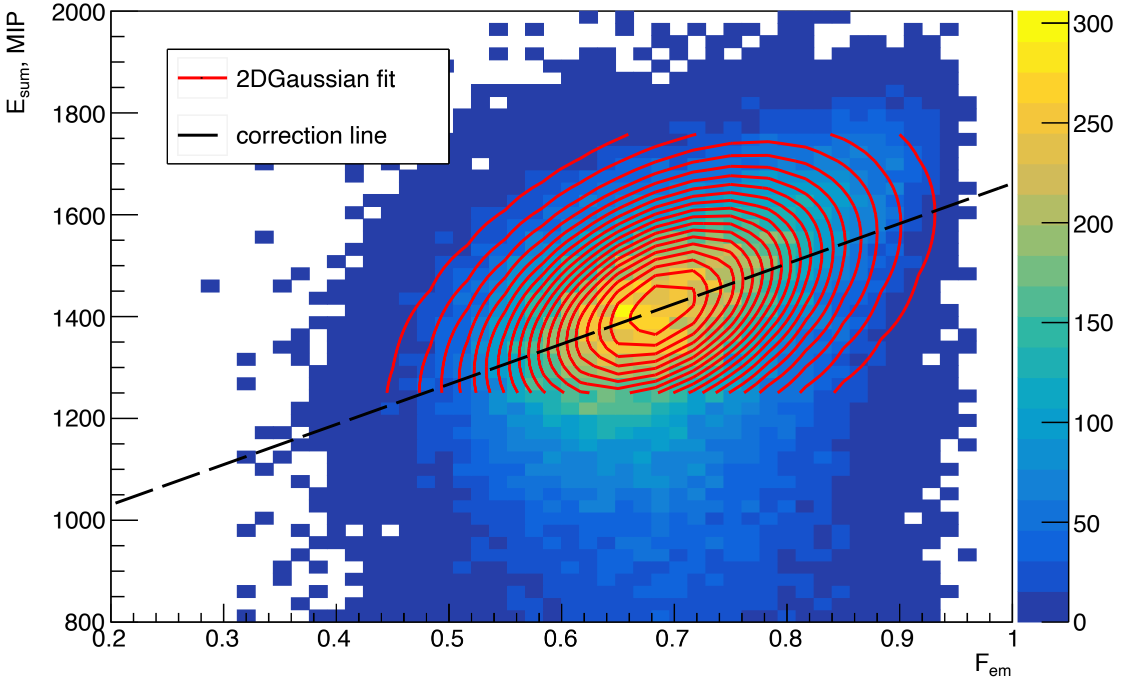
- Reasonable correlation of predicted EM fraction with truth in MPV region

Work in progress…

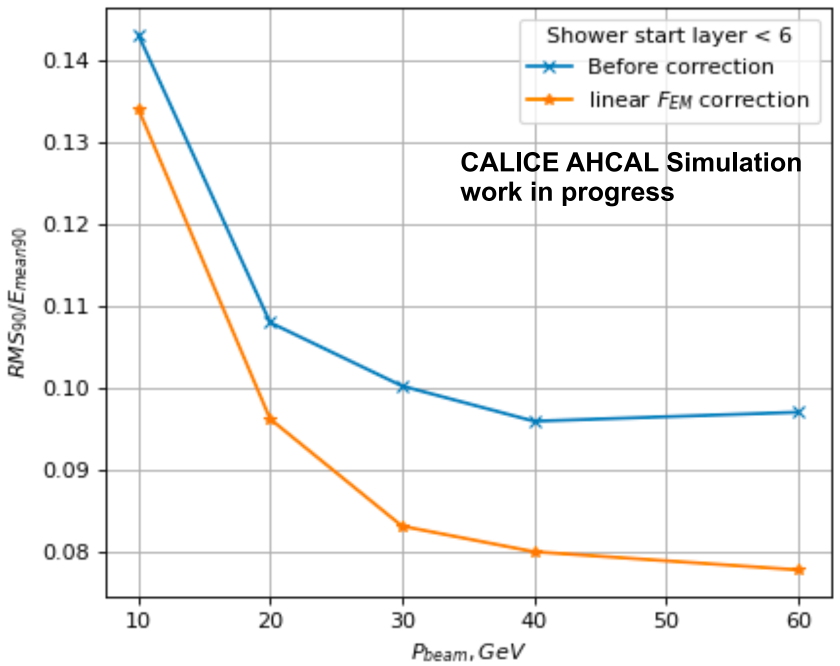
Hadronic shower reconstruction with GNN

Using reconstructed EM fraction for energy correction

Correlation example for 40 GeV pion



Energy resolution estimation



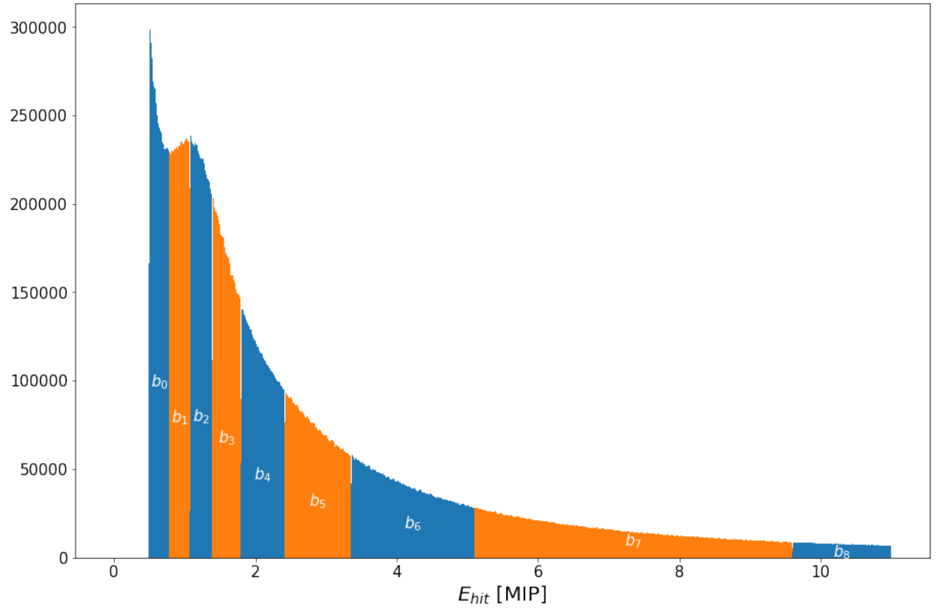
- Well pronounced correlation between E_{sum} and F_{em} observed for all energies
- For each energy point simultaneous gaussian fit is performed to extract the correction line

- Simple linear correction gives resolution improvement of ~6-20%
- Promising resolution improvement, baseline for more complex compensation algorithms using reconstructed EM information

"Standard" LSC

Code provided by Jack (used as a reference)

- E_{hit} **distribution** split into **bins** of **equal frequency probability**;
- i.e. **equal likelihood (on average!)** of **hits** falling into **each bin**.
- **Three weights defined, per bin,** using **Chebyshev Polynomial;**
- **Fraction of shower energy** falling into **each bin** is **weighted** according to the E_{sum}.



$$w_b = w_{b0} + w_{b1}\left(\frac{E_{sum}}{S}\right) + 2w_{b2}\left(\left(\frac{E_{sum}}{S}\right)^2 - 1\right) \quad (1)$$

S is a normalization constant, 150 GeV

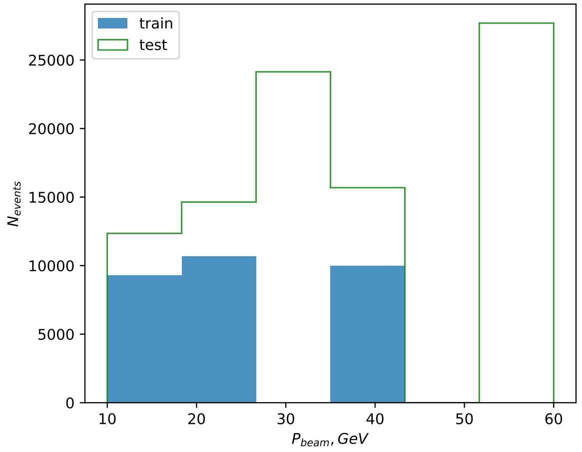
Jack Rolph | UHH | March 24, 2021 | Page 8

- Binning and weights are updated with latest available simulations
- 10-80 GeV range
  - 10K events before shower start cut:
    - 2 < st < 15
    - 28652 events in total

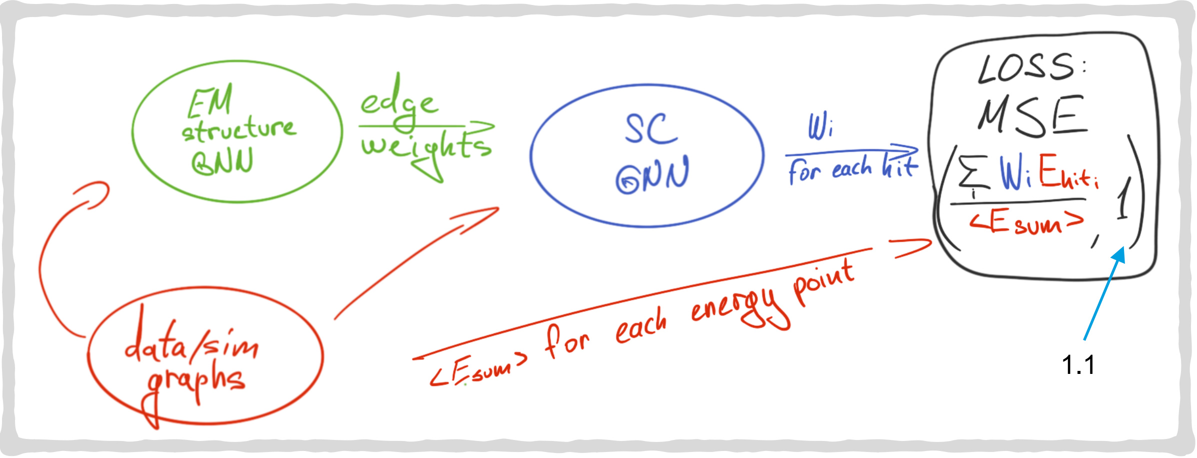
Energy reconstruction using predicted EM information

SC experiment

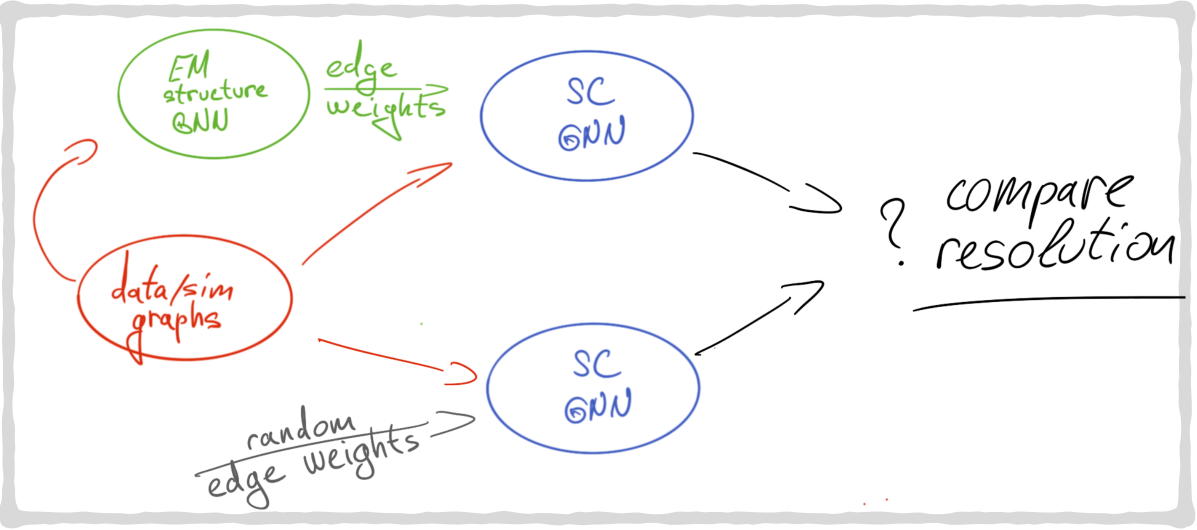
- Test if use of predicted edge weights improves the energy resolution
- Almost same GNN as for EM structure prediction:
  - 1 GraphSAGE layer replaced with ARMAConv (capable to exploit edge attributes during message passing), output has shape [N_{nodes}]
  - Train using predicted EM edge weights
    - Simulations: 10,20,40 GeV, st<6, 30 Kevents
  - Compare resolution for the test sample using predicted EM attributes or random edge weights
    - Simulations: 10,20,30,40,60 GeV, st<6



Training:

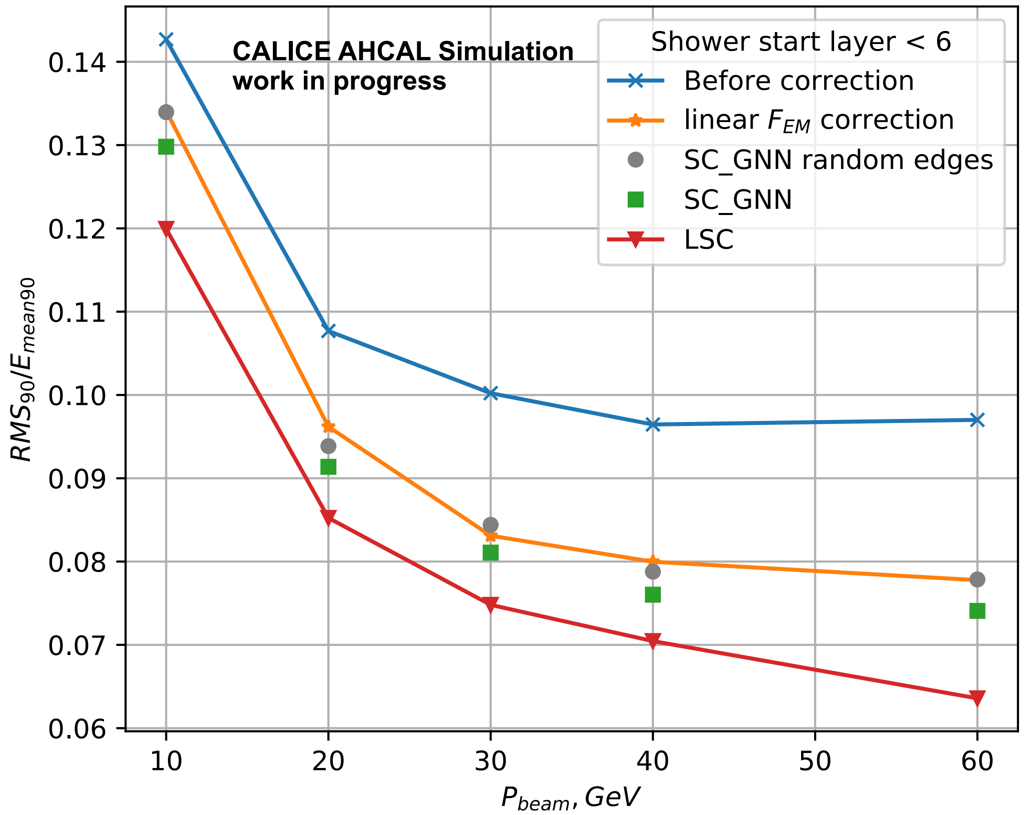


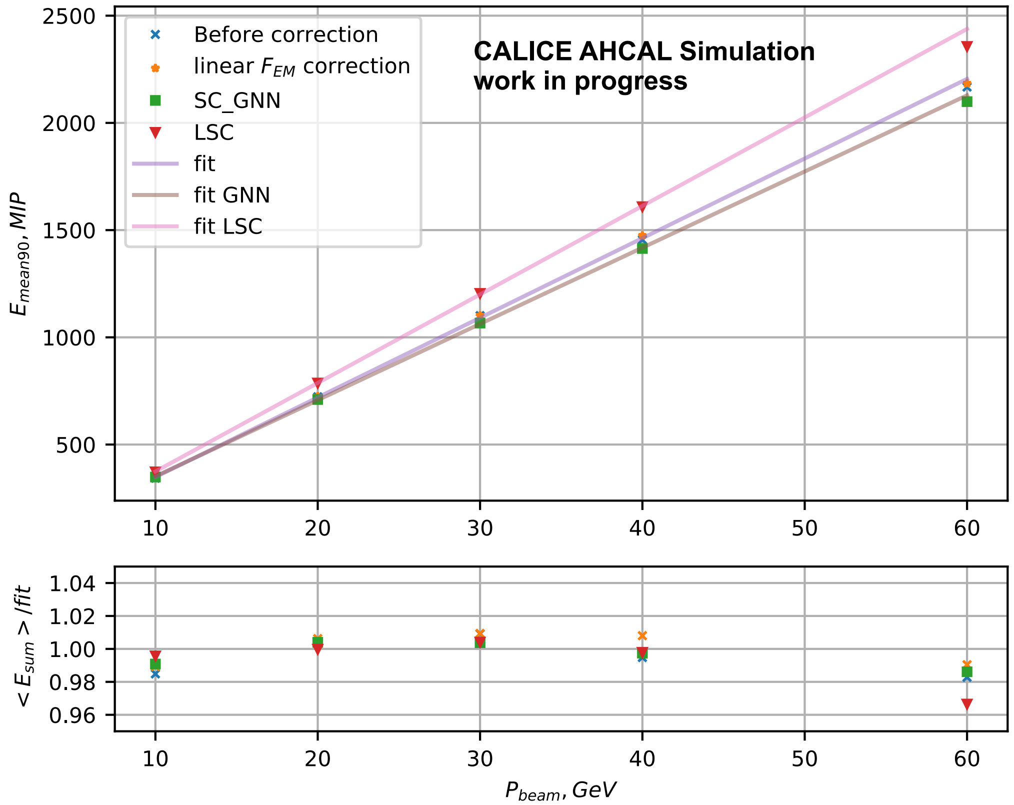
Experiment:



Resolution and linearity

10-60 GeV. Simulations only.





- SC_GNN gains some resolution performance by using reconstructed EM connections between hits
- Problems with LSC linearity are already visible at 60GeV (fit range was up to 80 GeV)

TODOs:

- Estimate leakage effect (check if methods are doing leakage correction in addition to SC) using tail catcher information
- Compare with TB data

Towards distinct secondary particle reconstruction

Outlook

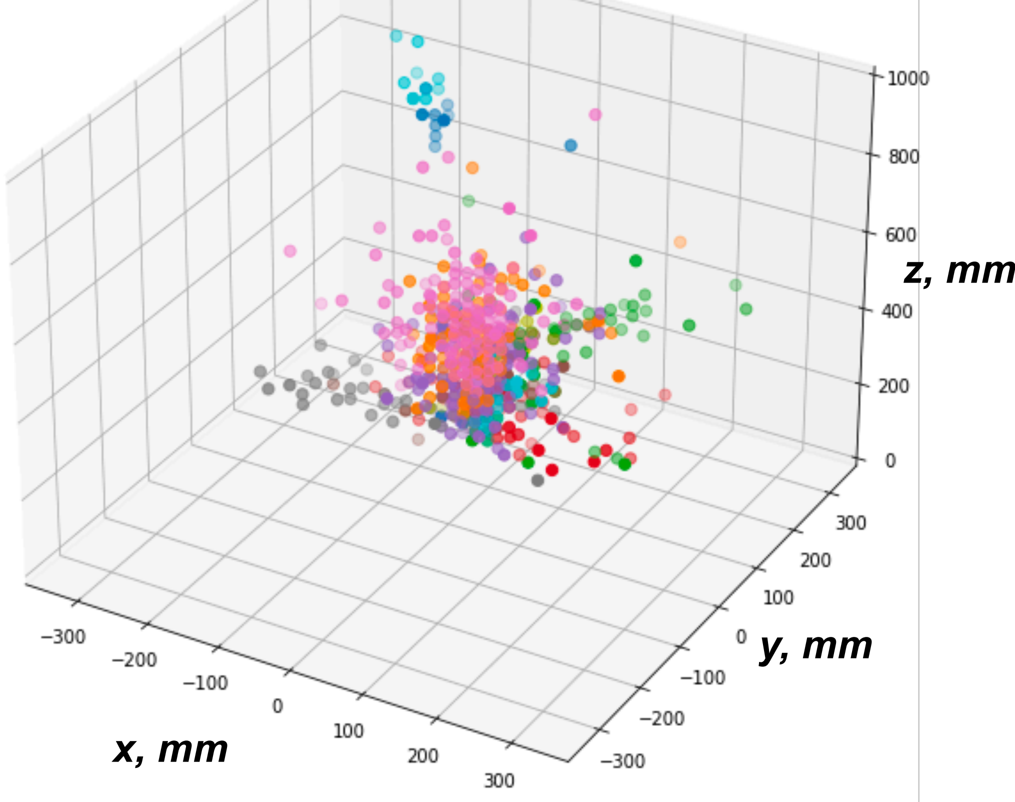
Motivation:

- In HAD showers we can have many EM subshowers at first HAD interaction (overlaid) and later in the had cascade (displaced)
- Further look into the structure of EM fraction:
  - Reconstruct distinct particle components
    - No easy rule-based algorithm to merge overlaid subshowers on MC truth level ➡ go unsupervised!
    - Test Bayesian Gaussian Mixture model with Dirichlet process on point clouds from calorimeter events
      - SKlearn implementation is tested, own flexible Pyro implementation is planned

    ➡ Tune training dataset for substructure GNN
      - e.g. energy thresholds (some EM sub showers have topology closer to ionising tracks)

Event display for MC truth EM fraction of 40 GeV π^-.

Colour code represents different EM subshowers:



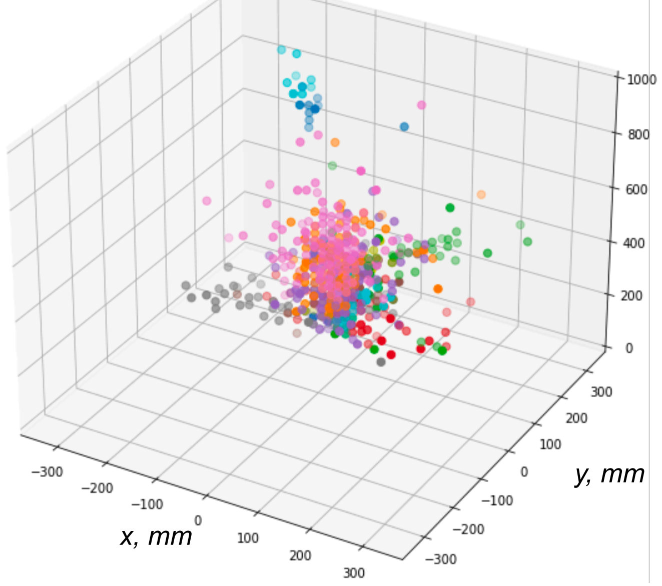
Applying Bayesian GM to EM component of had showers

Truth EM component

- SKlearn implementation can handle only scatter plots
- To keep hit energy information, artificial scatter plot is produce:
  - 10 points per MIP
  - uniformly distribute within cell volume: ±15mm,±15mm,±1mm
  - Normalise coordinates: *(-0.36m,0.36m) (-0.36m,0.36m) (0m,1m)*
- Max number of components = 10,
- Object size can be optimised by modifying covariance prior
- Clusters can be filtered by likelihood and energy density

MC truth EM fraction of 40 GeV MC π^-.

Colour code represents different EM subshowers:

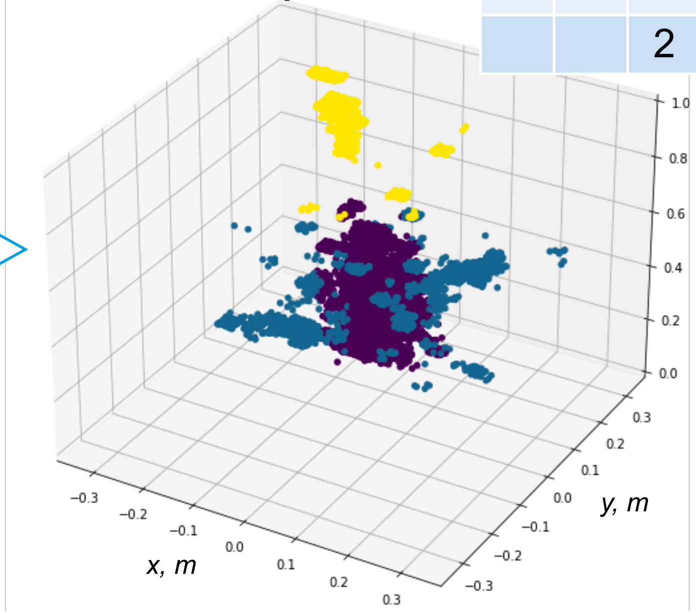


1st BGM iteration:

3 Gaussian components

Cov prior 1st iter

2		
	2	
		2

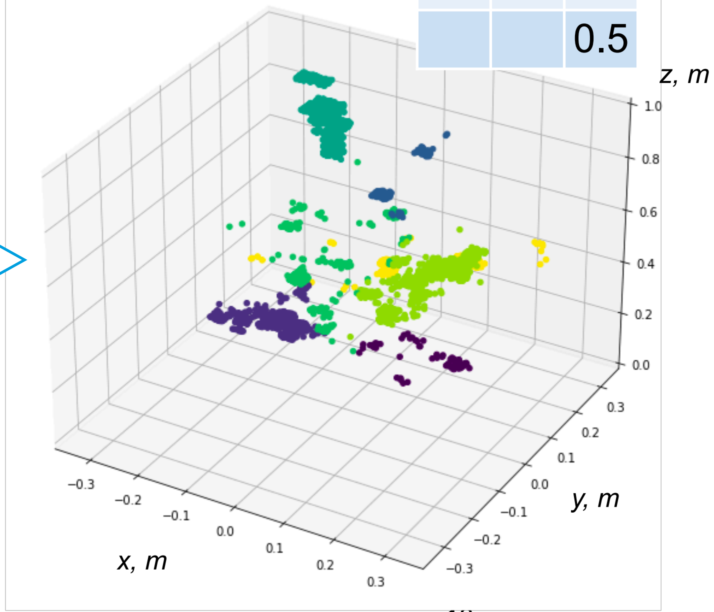


2nd BGM iteration:

7 components

Cov prior 2d iter

0.5		
	0.5	
		0.5



Applying Bayesian GM to EM component of had showers

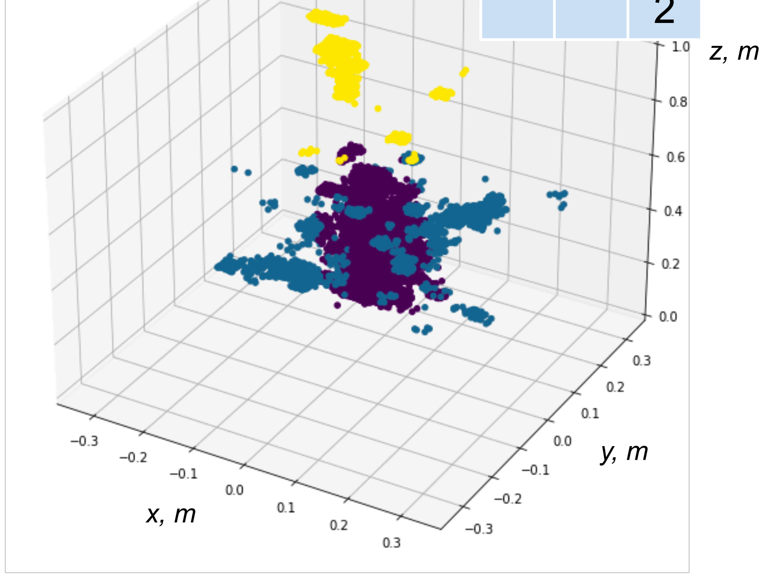
Truth vs reco EM component

1st BGM iteration (truth EM):

3 Gaussian components

Cov prior truth EM

2		
	2	
		2

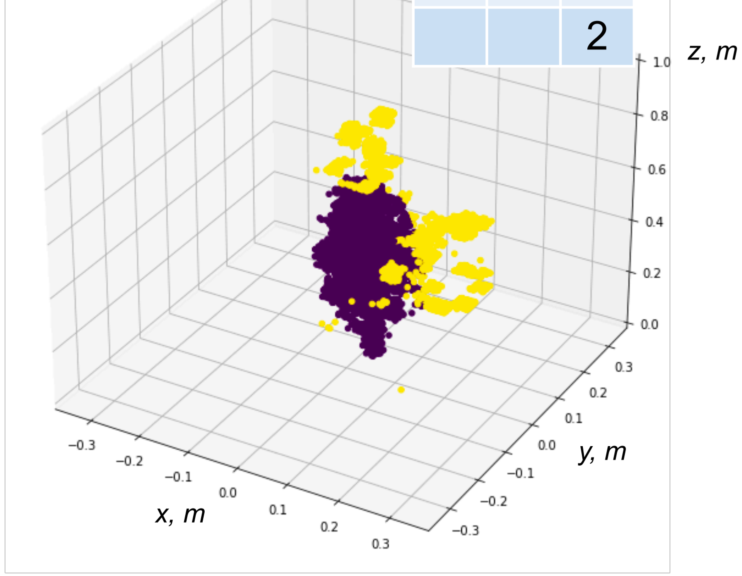


1st BGM iteration (predicted EM):

2 Gaussian components

Cov prior 1st iter

2		
	2	
		2

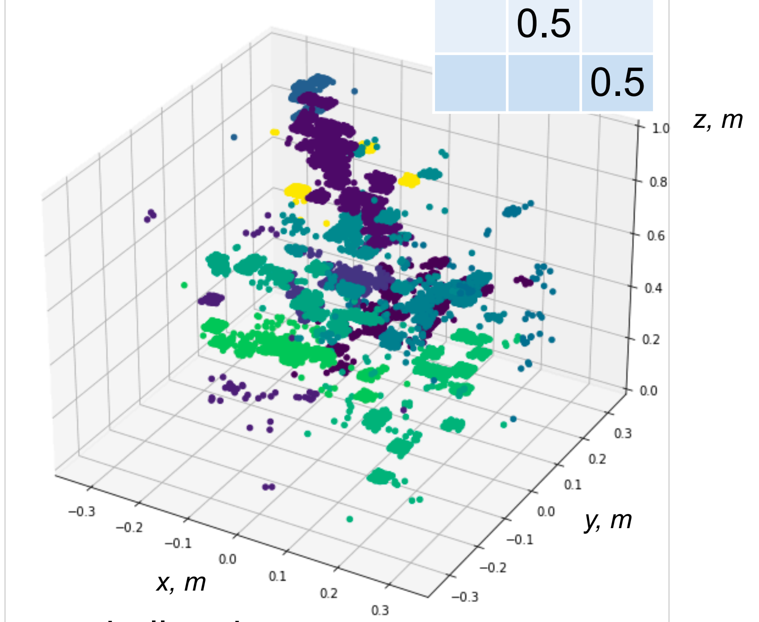


2nd BGM iteration (rest of event) :

20 components

Cov prior 2d iter

0.5		
	0.5	
		0.5



- Visual similarity for main gaussian component
  - Hints of agreement for E_{sum} and $E_{density}$ on several hundred events between truth and predicted EM fraction (see backup slides)
- Physical observables to be determined and compared with TB data
  - some examples of main GM component distributions in the backup

- Smaller clusters are more challenging

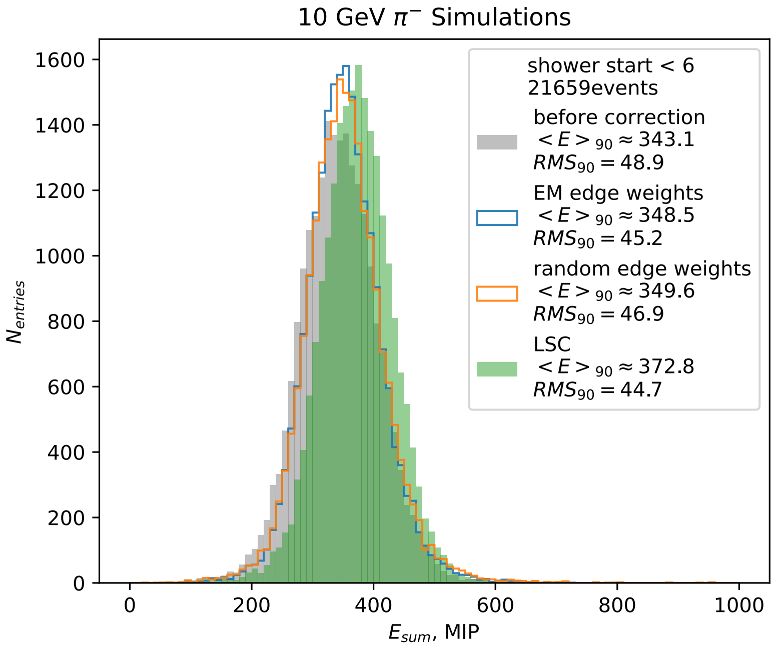
➡ Room for improvement

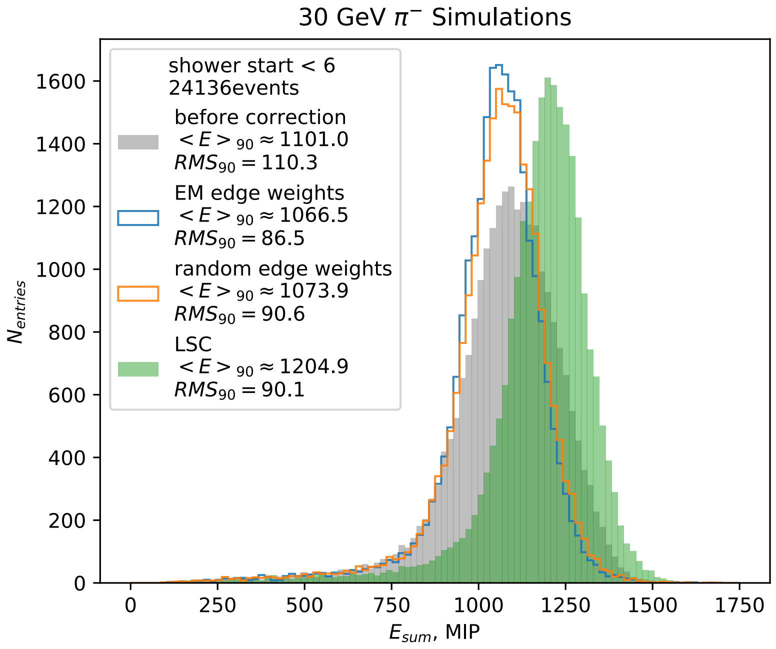
Conclusion

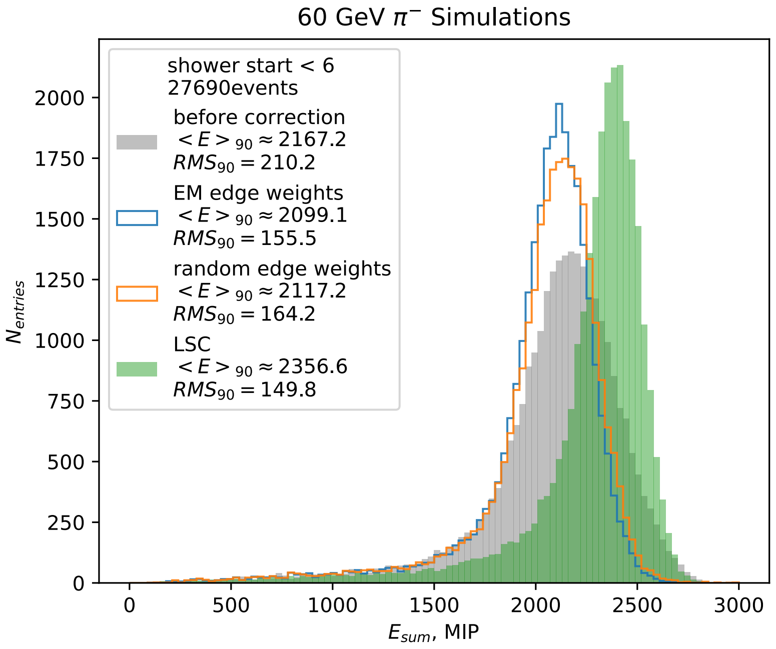
- Reconstruction method for electromagnetic substructure of hadronic showers using Graph Neural Networks is presented
- Reconstructed electromagnetic structure can be used to improve hadronic energy resolution
  - GNN software compensation model is capable to exploit EM information
    - can extrapolate and interpolate to different energies
  - Better performance for “standard” local SC to be understood
- Gaussian Mixture model is a promising tool to reconstruct distinct particle contributions within hadronic showers

Backup

Single energy examples

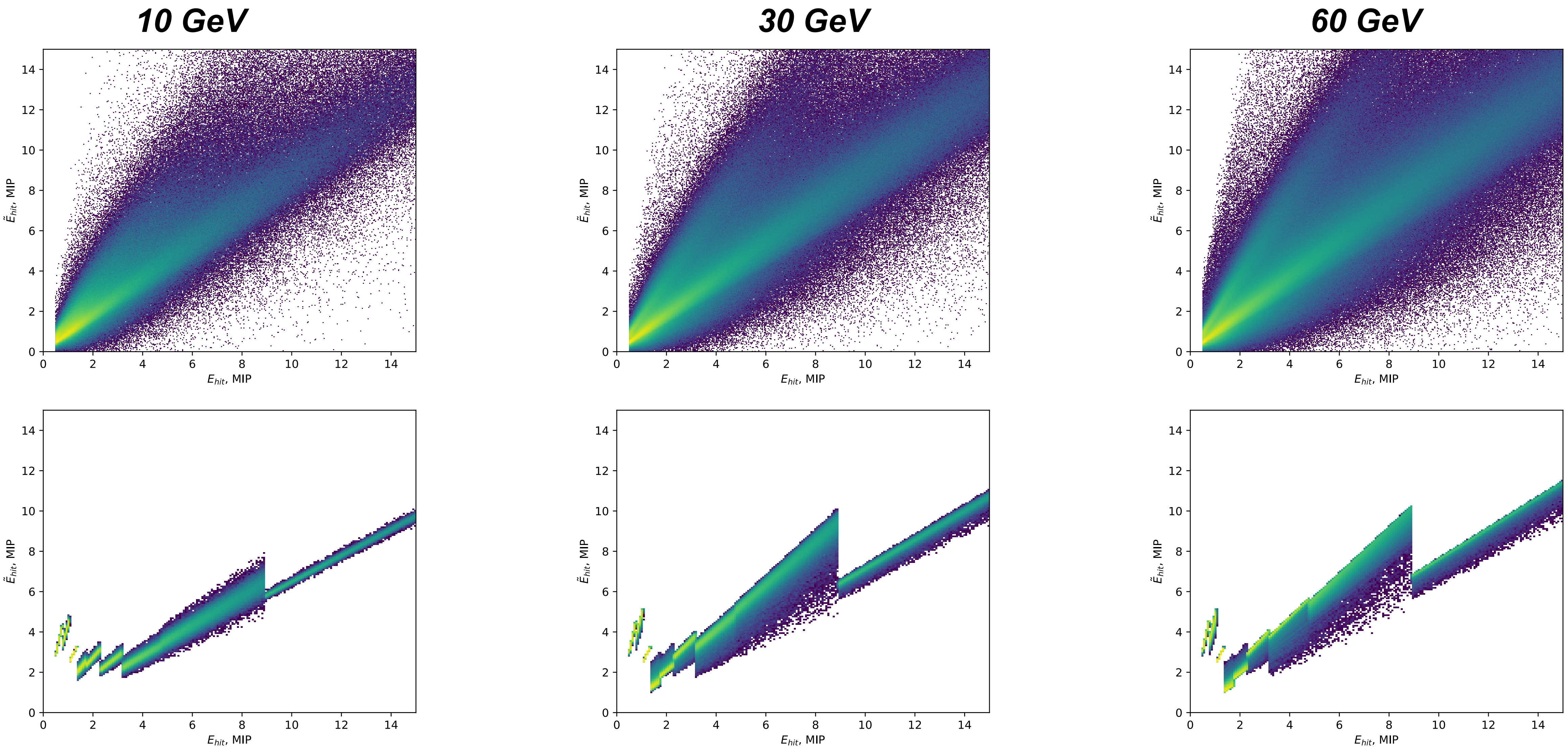






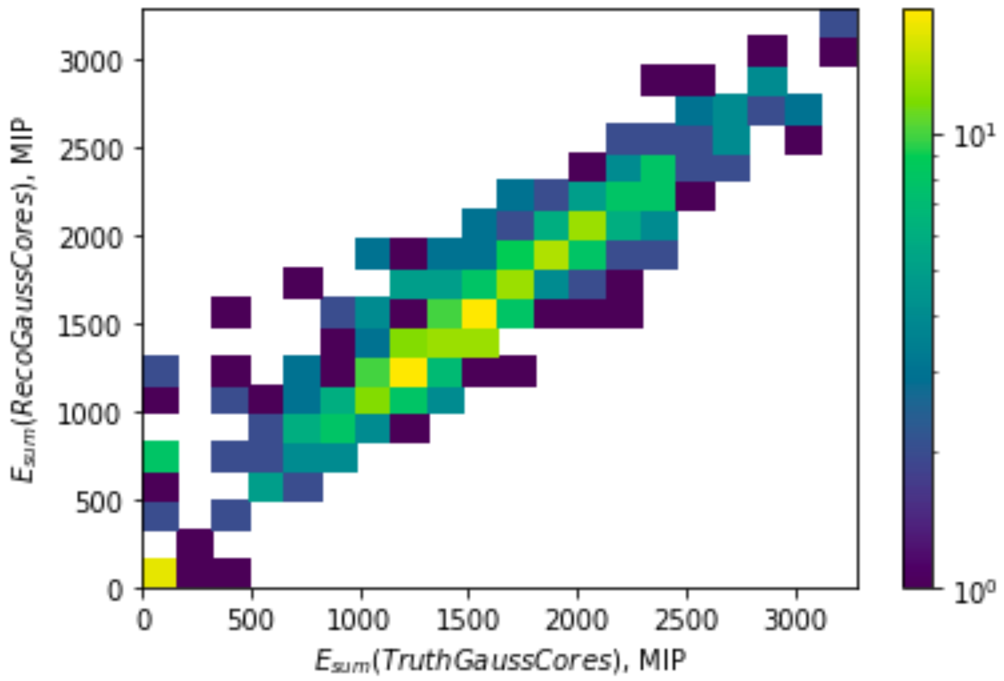
Hit energies

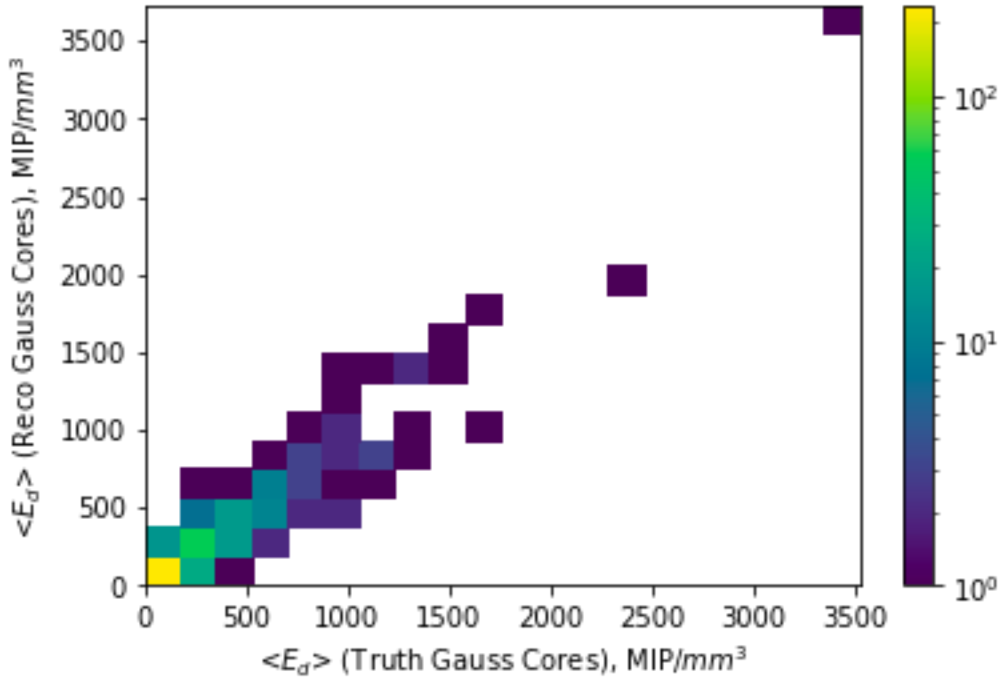
GNN vs LSC. Simulations



Truth vs reco EM

500 40GeV pion events



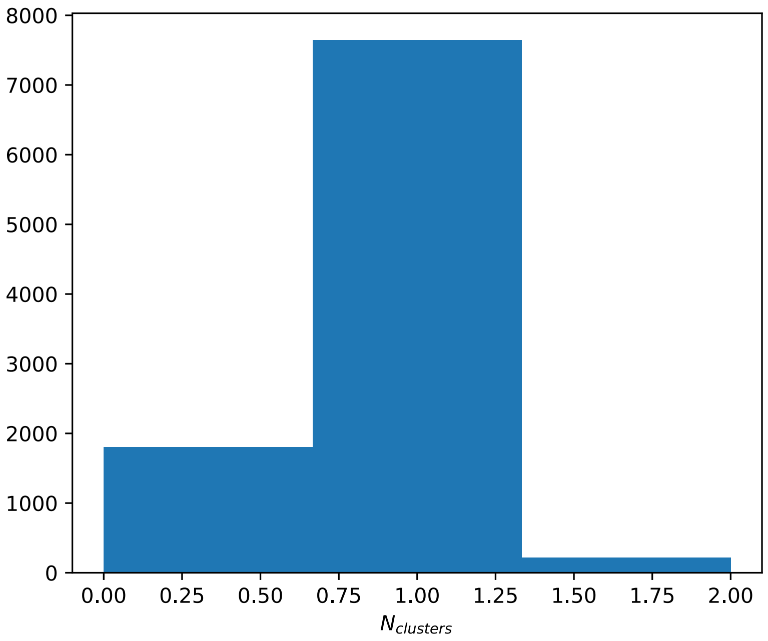


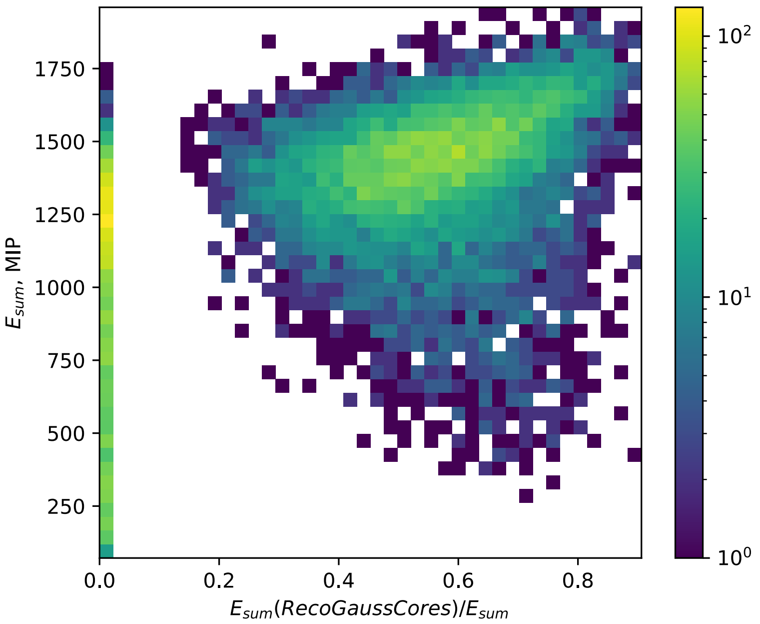
Applying GM to larger dataset

Some distributions for simulated 40 GeV pions. 10 Kevts.

- Reconstructed EM fraction.
- Shower start found

- Quality metrics (optimised on several events)
  - likelihood > 2 (first guess)
  - energy density in ellipsoid [MIP/mm^3] > 20 (first guess)





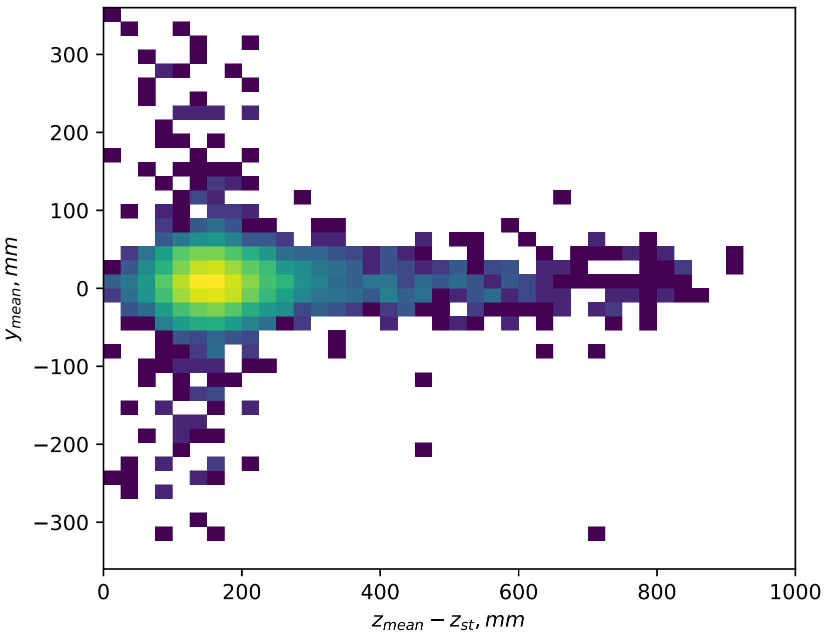
Main gaussian component (shower core)

Some distributions for simulated 40 GeV pions. 10 Kevts.

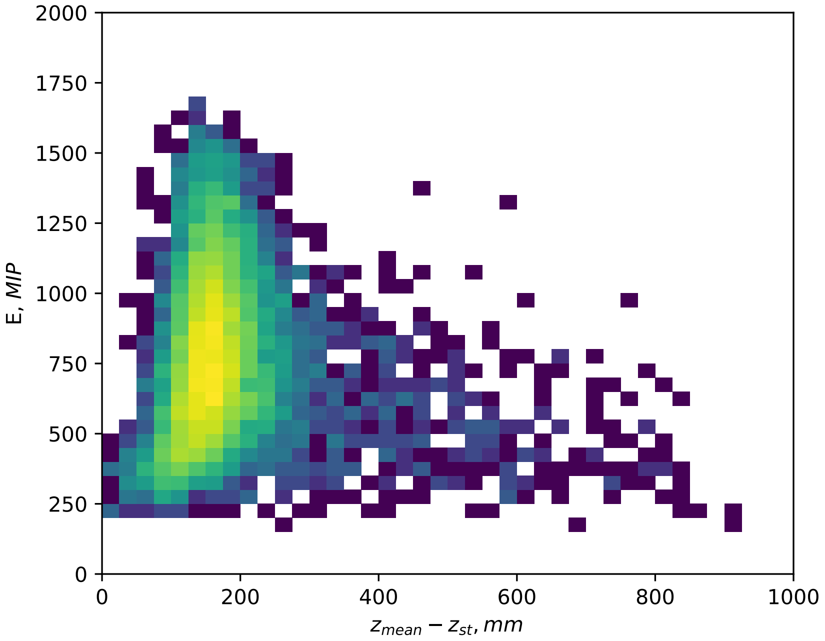
- Reconstructed EM fraction.
- Shower start found

- Quality metrics (optimised on several events)
  - likelihood > 2 (first guess)
  - energy density in ellipsoid [MIP/mm^3] > 20 (first guess)

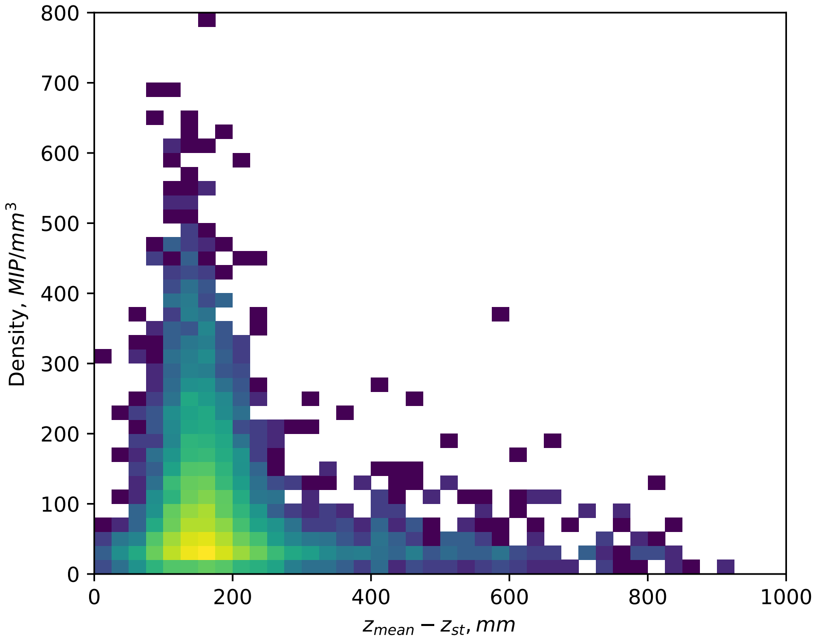
Mean position in XY plane

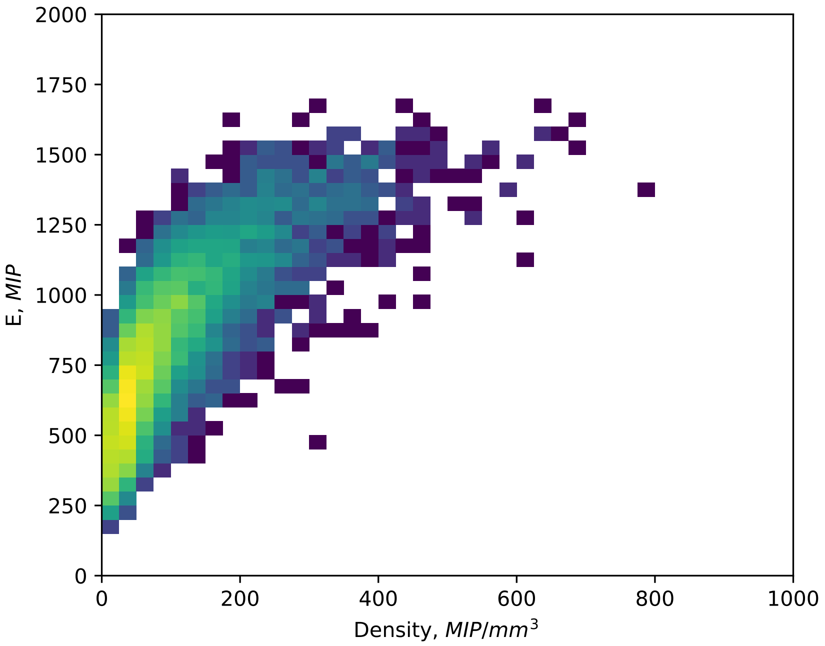


Cluster energy vs Z mean



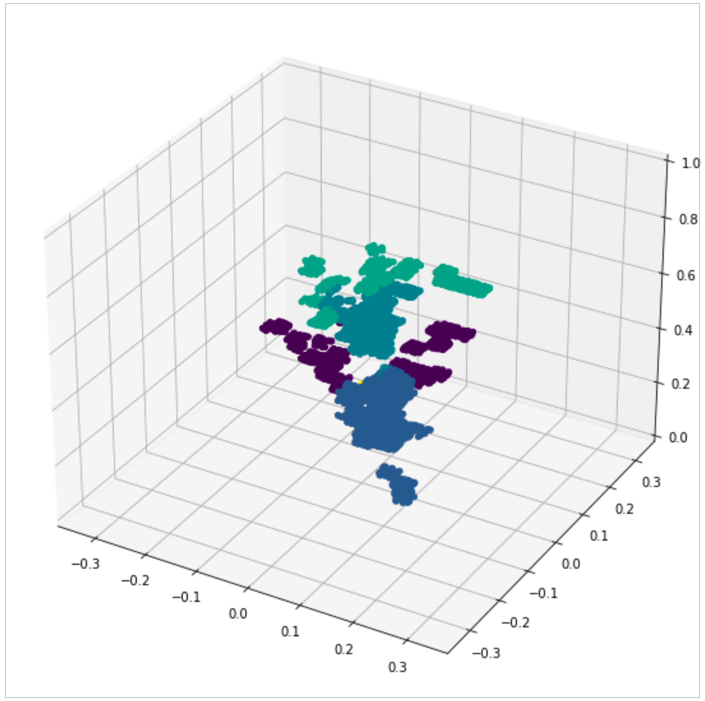
Cluster energy density vs Z mean

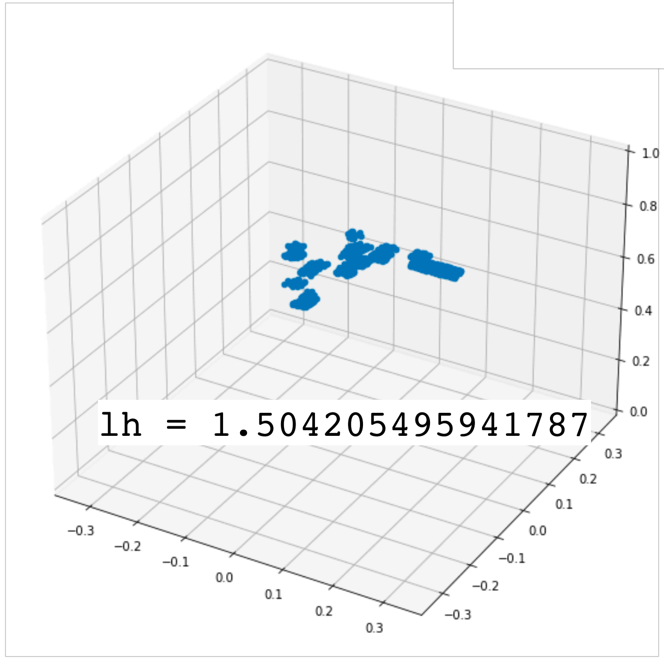


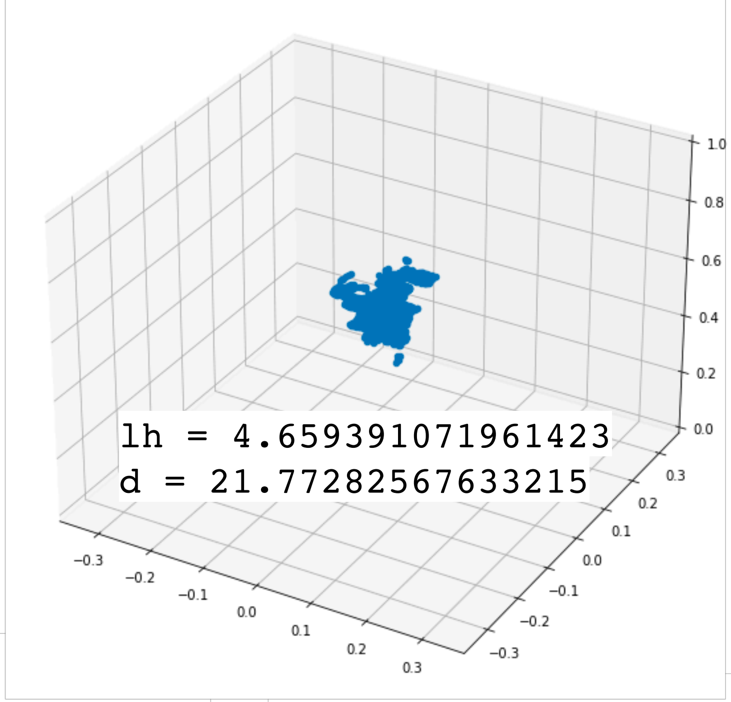

2000
1750
1500
1250
1000
750
500
250
0
E, MIP
0
200
400
600
800
1000
Density, MIP/mm^3

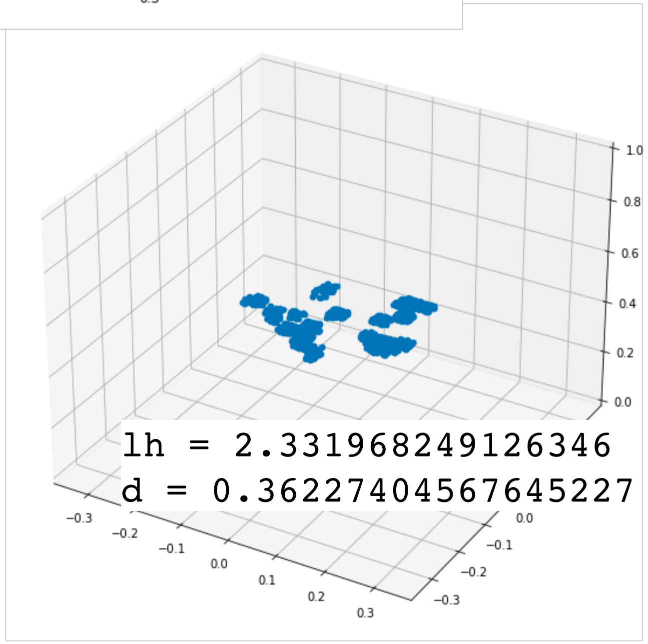
Dealing with background clusters

- Quality metrics (optimised on several events)
  - likelihood > 2 (first guess)
  - energy density in ellipsoid [MIP/mm^3] > 20 (first guess)



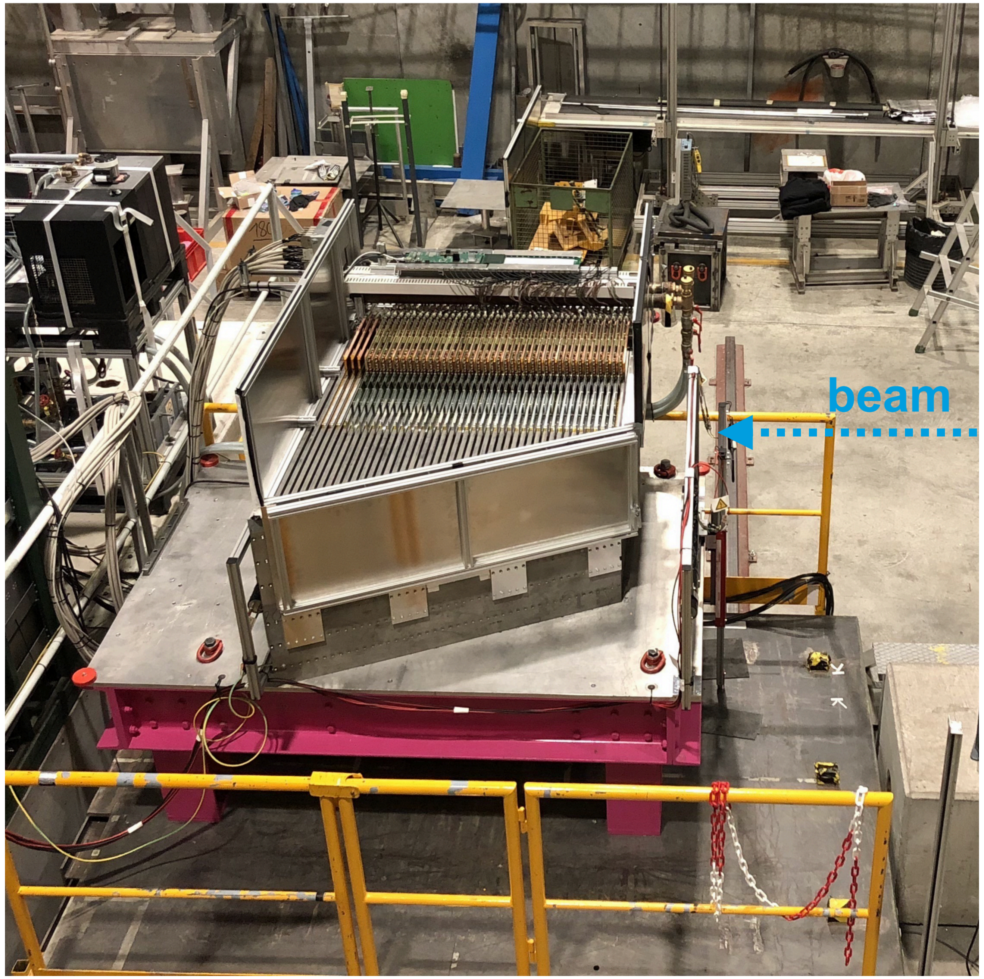






CALICE AHCAL

Test beam prototype.



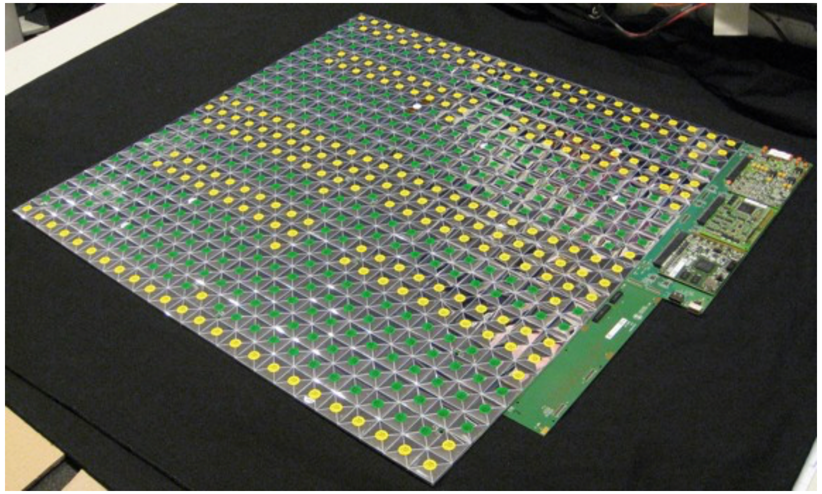
***39* active layers** of *24x24* scintillator tiles (*3x3* cm^2 each) with individual SiPM readout. Active layers alternate with ~*2 cm* steel absorber.

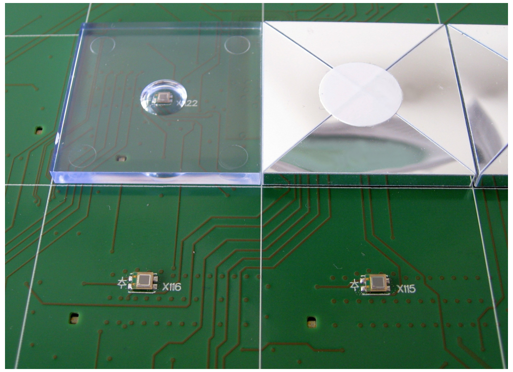
In total: ***~22000* channels** (*<1‰ dead channels*), **~*4* λ, ~*38*X_0**

Beam particles: muons, electrons, **pions**

Energy range: ***10-200 GeV*** *in 10-40 GeV steps*

O(1M) hadron events per energy point





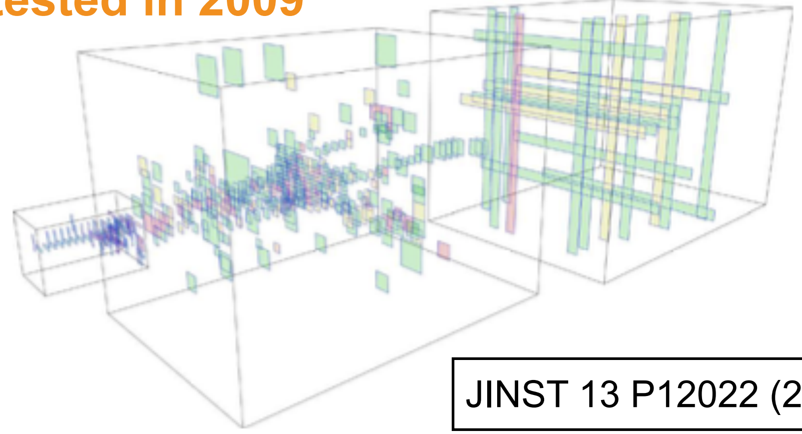
Software compensation method

Example for CALICE combined setup ECAL+AHCAL+Tailcatcher tested in 2009

- h/e response compensation by assigning energy-dependent weights to hit energies (⇒local energy density)
    - Higher weights for **low energy hits** - dominated by **HAD** component
    - Lower weights for **high energy hits** - dominated by **EM** component
- 8 bins for hit energies
    - Polynomial fit to get energy dependent weight for each bin

➡ Energy resolution improvement 10-20%

- Disadvantages: limited to fit energy range, polynomial dependence has no physics motivation, additional topological information of hit context is not used



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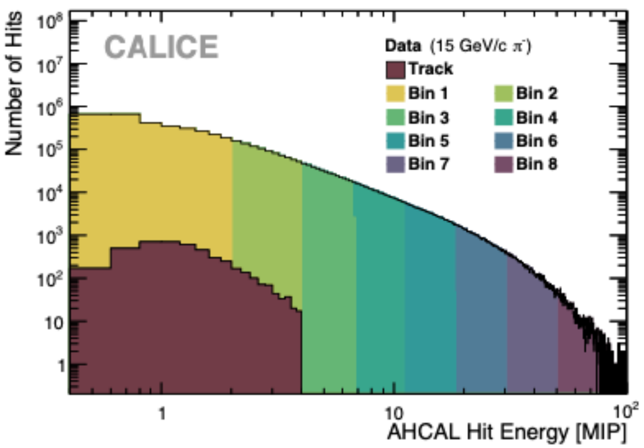
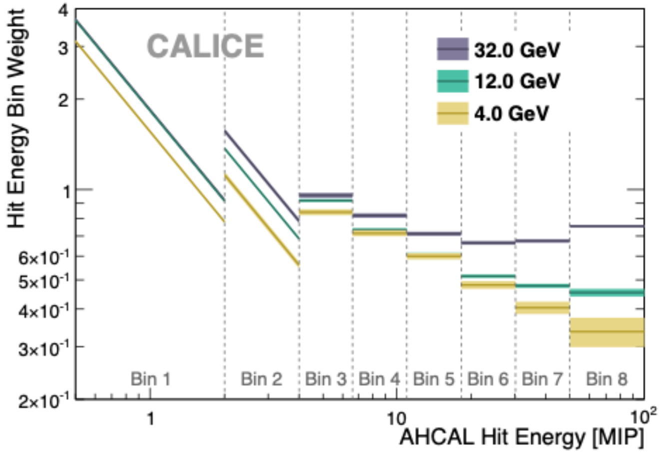
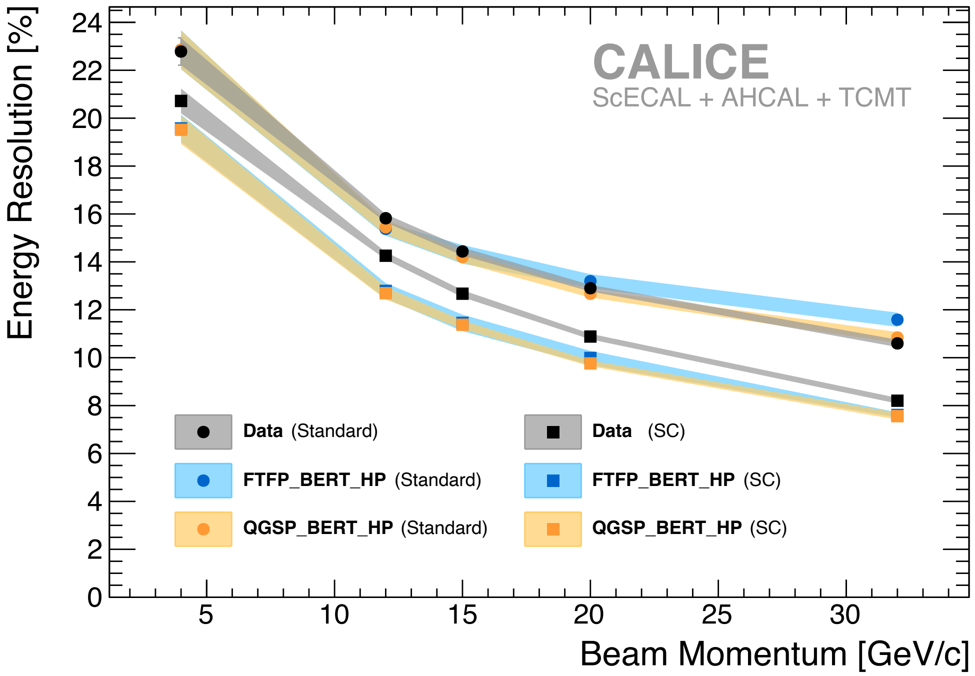


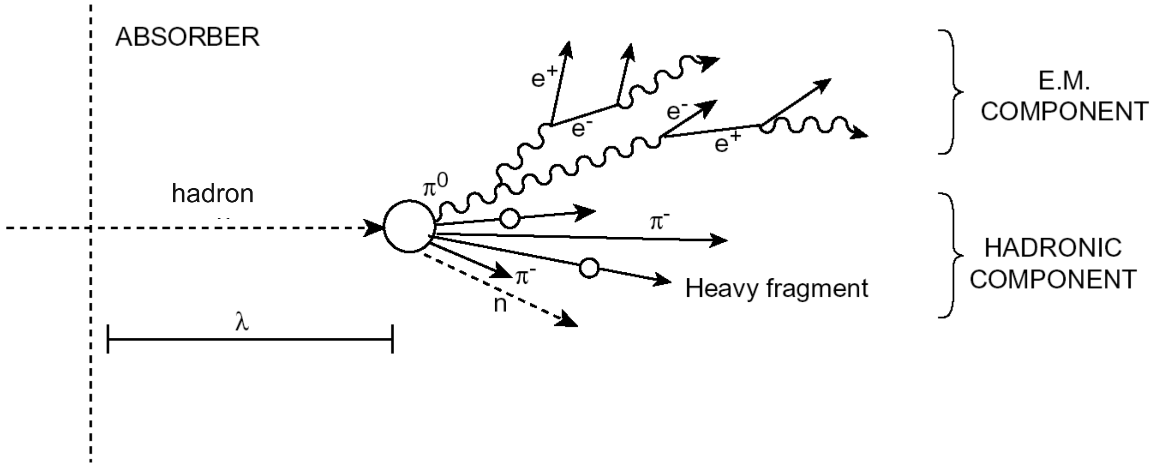


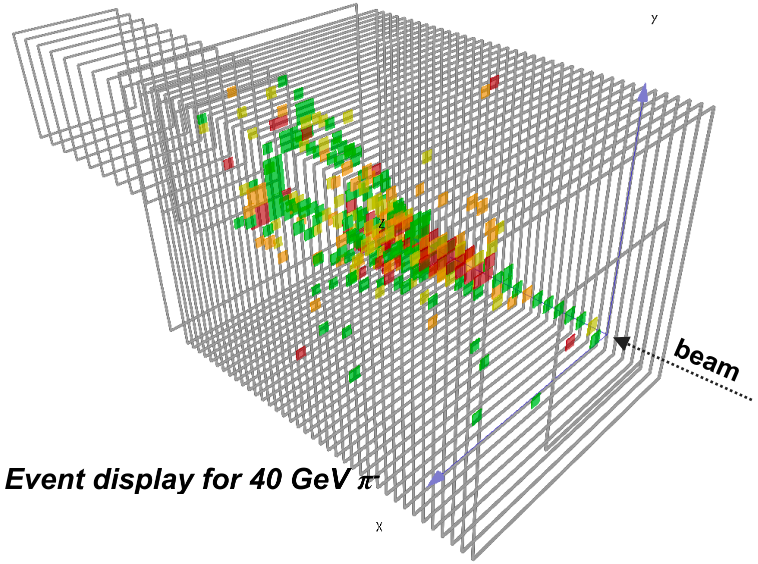


Hadronic showers

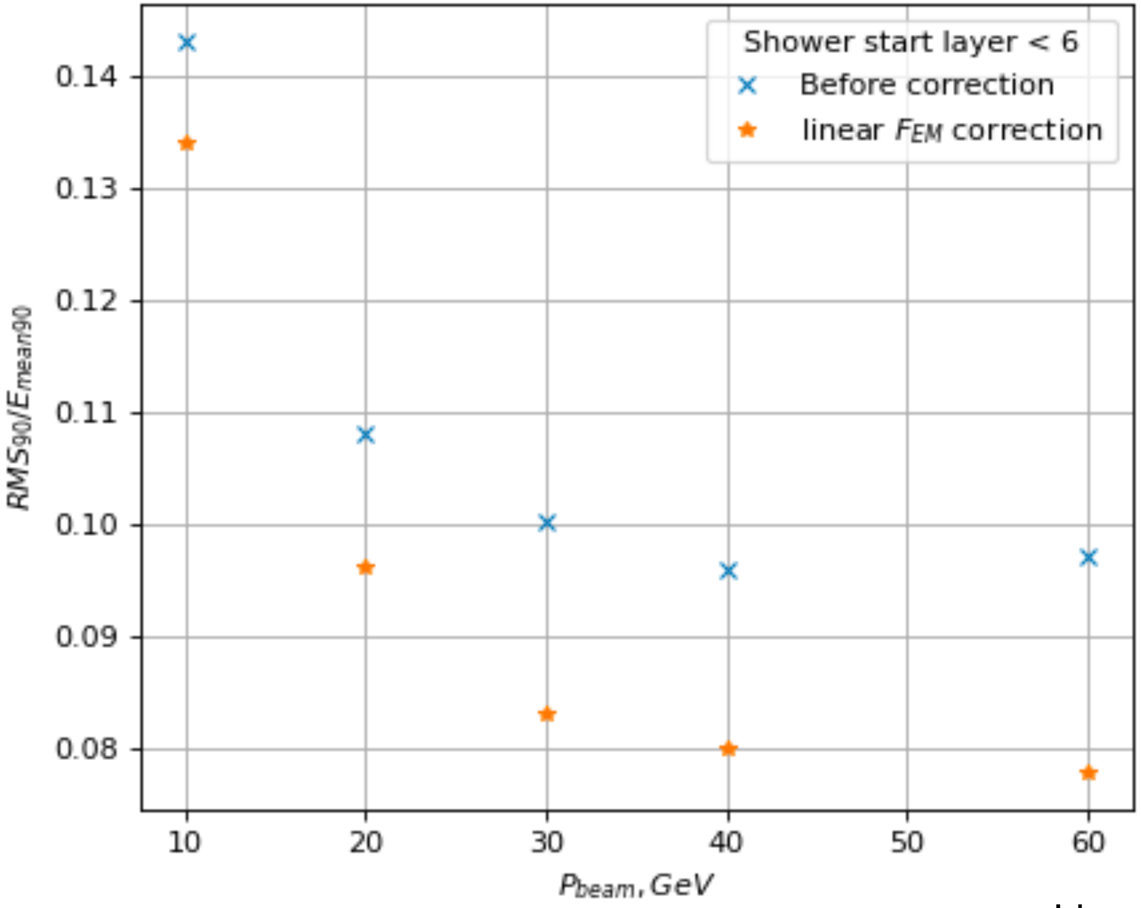
General properties

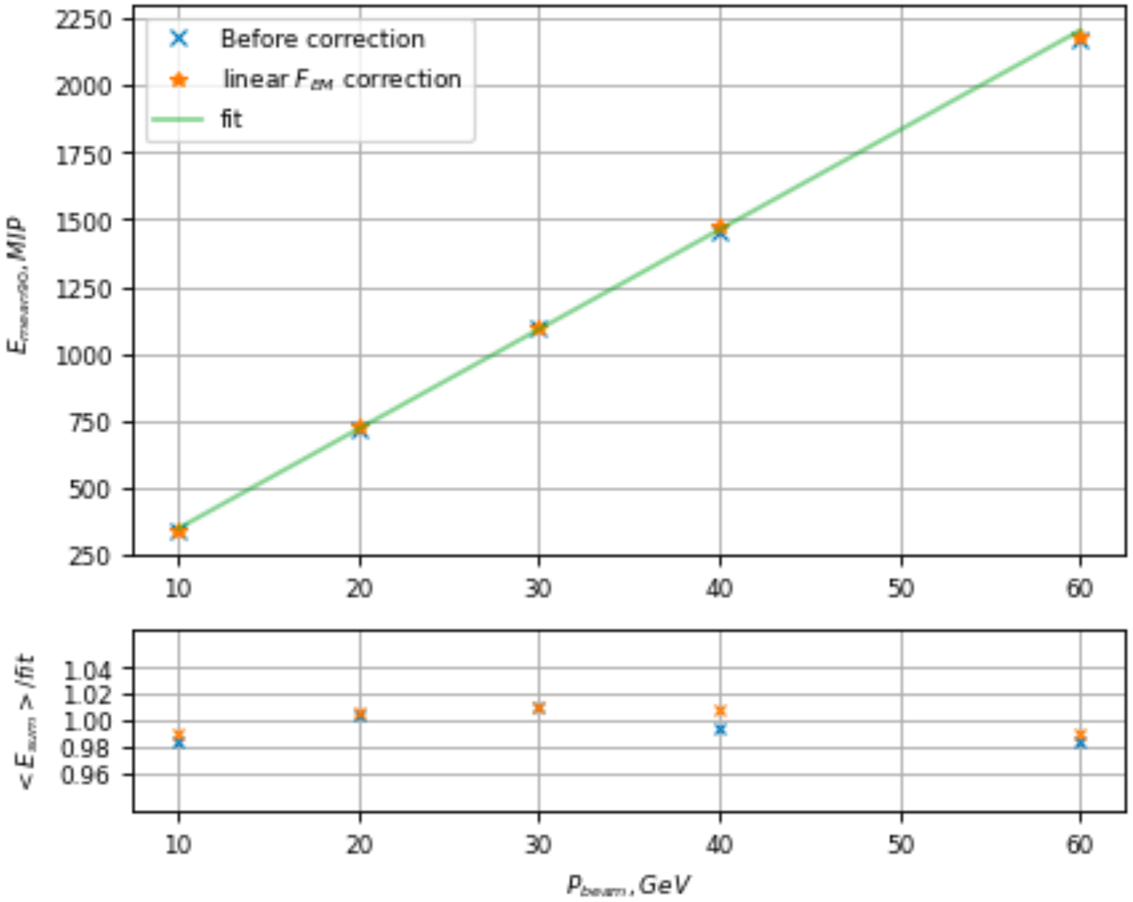
- Hadronic shower development is rather complex:
  - Narrow EM core component from π^0/η
  - Surrounding halo dominated by charged hadrons
  - Large event-by-event fluctuation of EM/HAD ratio
  - Response to EM and HAD components is different in non-compensating calorimeters
  - Invisible energy as binding energy, nuclear recoil, neutrinos + late component
  - ➡ Limited hadronic energy resolution
  - ➡ Detailed simulation is challenging
- Highly granular calorimeter prototypes
  - Imaging capabilities provide detailed calorimetric images
  - Real test beam data for crosschecks and development of data-driven algorithms





Event display for 40 GeV π^-





- Linear $E_{sum}(F_{em})$ correction:

  $E_{cor} = C*E_{sum}$

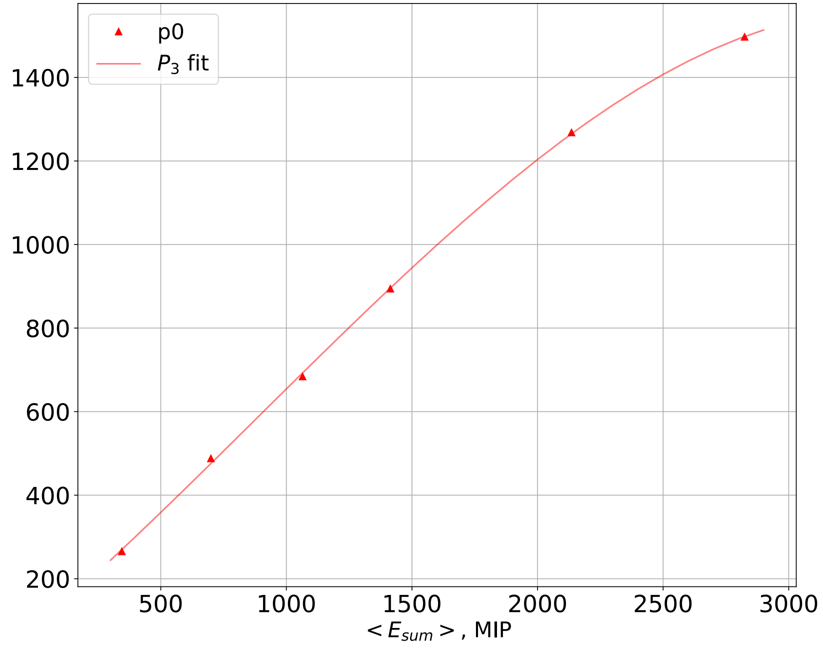
  $C = <F_{em}>/(p_1 . F_{em} + p_0)$

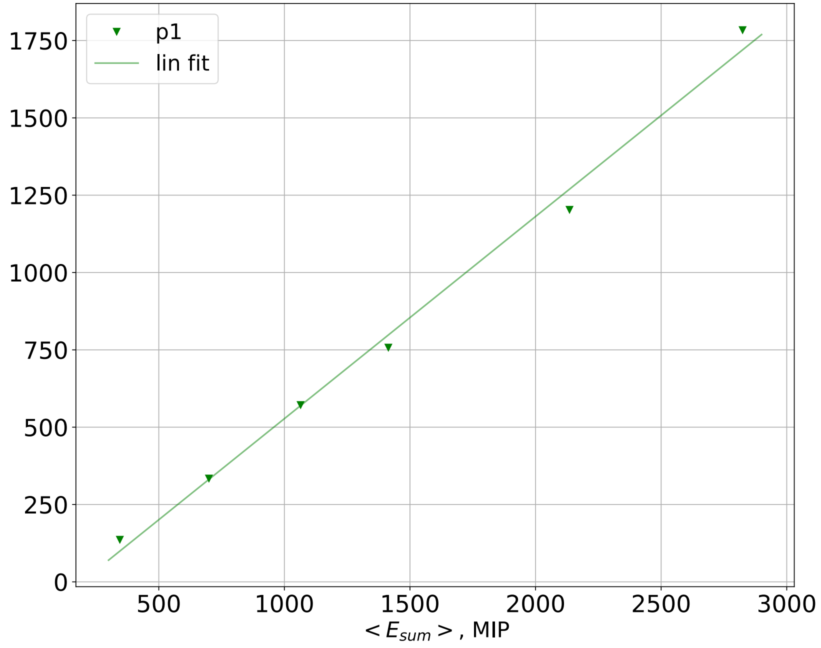
Unified correction

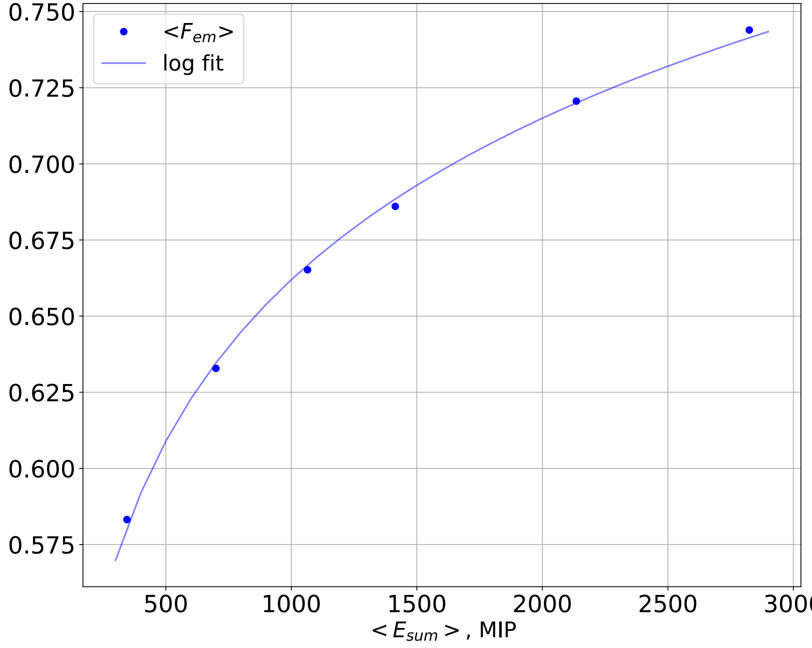
Getting P_{beam}-independent correction

Work in progress…

Correction parameters as a function of $\langle E_{sum} \rangle$:







- p_0,p_1 and $\langle F_{em} \rangle$ are calculated for each event from the observed energy using resulting fits
  - More energy points need to be included to check the overfitting
  - Parameter uncertainties are not taken into account
  - Performance decrease for resolution ~3%