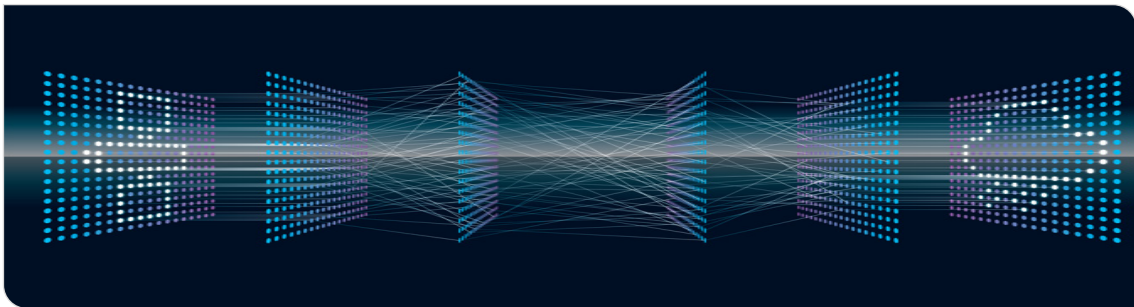


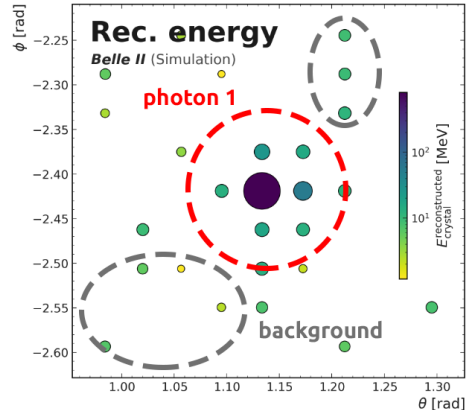
Clustering Energy Depositions in the ECL using Graph Neural Networks (GNNs)

Florian Wemmer, Torben Ferber | September 20, 2022



Setting and Objective

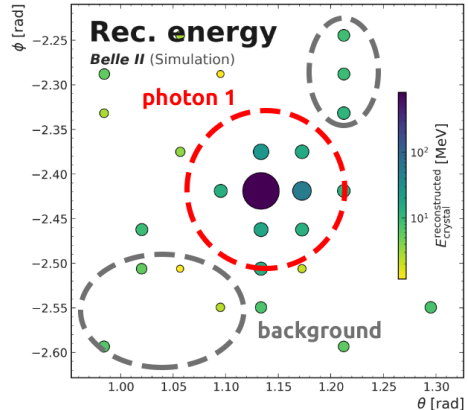
- 9×9 grid of crystals
- One photon cluster
- Nominal phase 3 beam background



Setting and Objective

- 9×9 grid of crystals
- One photon cluster
- Nominal phase 3 beam background

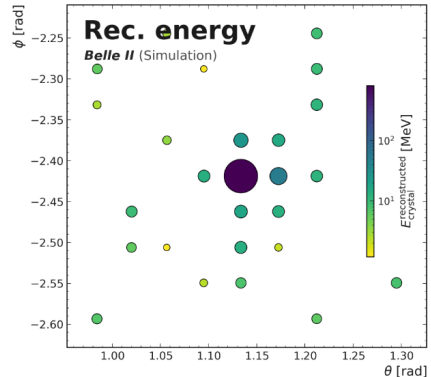
- Cluster energy depositions
- Soft clustering including background
 - ⇒ Assign weights $w_i \in [0, 1]$ with $i \in \{\text{photon, bkg}\}$
 - ⇒ $\sum_i w_i = 1$ per crystal



Why (this) Graph Neural Network?

(and not a 'regular' Convolutional Neural Network)

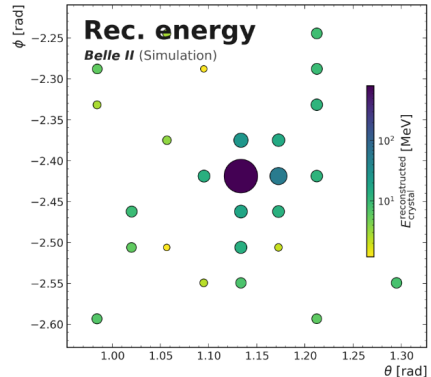
- Additional valuable input features
- Learns representation space
- Can handle irregular detector geometry (endcaps)



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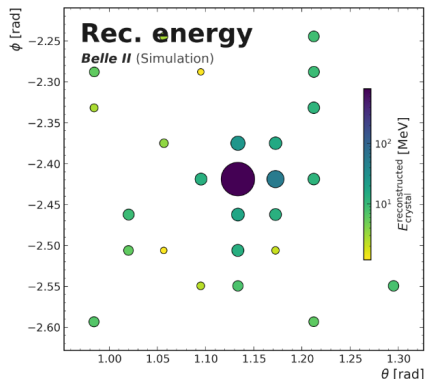
- Additional valuable input features
 - Learns representation space
 - Can handle irregular detector geometry (endcaps)
 - Resources:
 - Only ≈ 16000 parameters and few computations
 - Small input: One hit $\hat{=}$ one node
- \Rightarrow Potential real time application for L1 trigger



Approach

Conversion of an event to a graph

- Crystal hit in 9 x 9 view port becomes node
- Crystal measurements become node features
- No edges (yet)



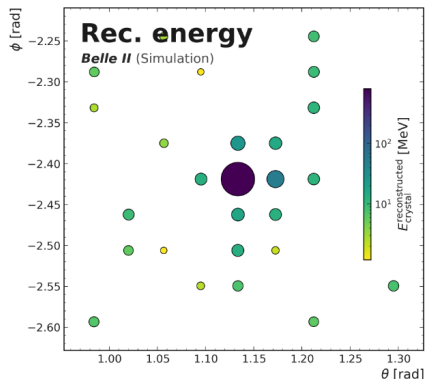
Approach

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Node features

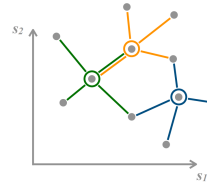
- Reconstructed Energy
- Reconstructed Time
- Pulse Shape Discrimination (PSD)
- Crystal coordinates (local and global)
- Crystal mass



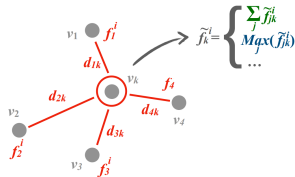
GravNet block



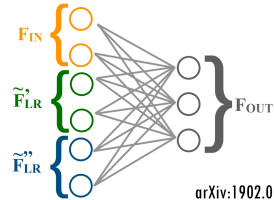
1 Learn representation and feature space



2 Connect k nearest neighbours



3 Message passing



arXiv:1902.07987

4 Concatenate messages

Model and Loss Function

Model

- Stack three GravNet blocks
- Add batch normalization
- Fully connected layers into softmax

Model and Loss Function

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- Add batch normalization
- Fully connected layers into softmax

$$L_2 = \sum_{i, k} (p_{ik} - t_{ik})^2$$

- E_i reconstructed energy in node i
- t_{ik} true fraction of cluster k in node i
- p_{ik} pred. fraction of cluster k in node i

- i : number of nodes per event (varies)
- $k \in \{0, 1\}$: number of classes

Model and Loss Function

Model

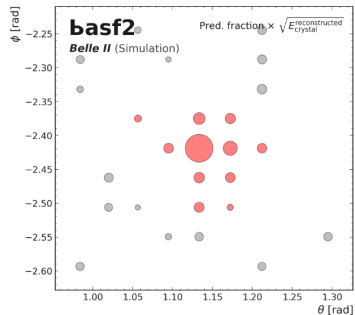
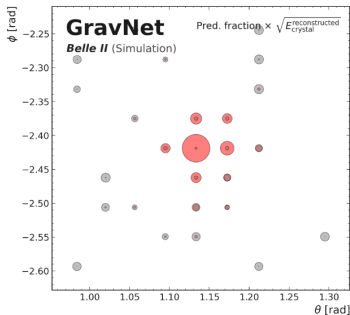
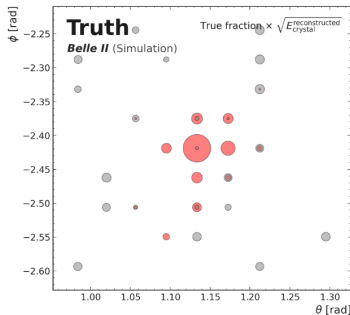
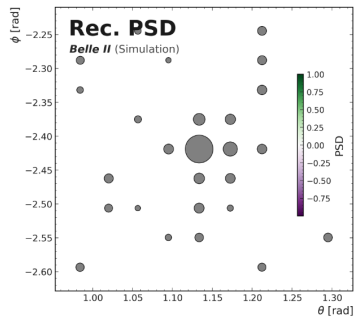
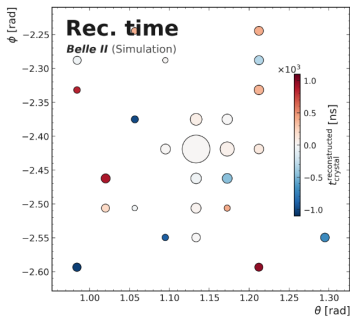
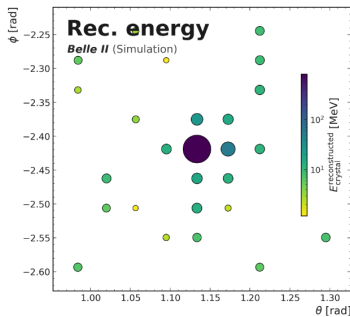
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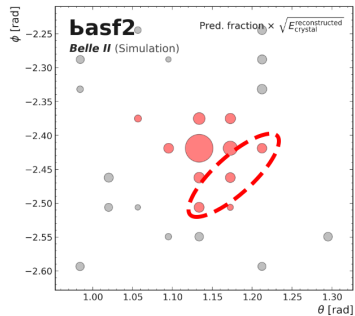
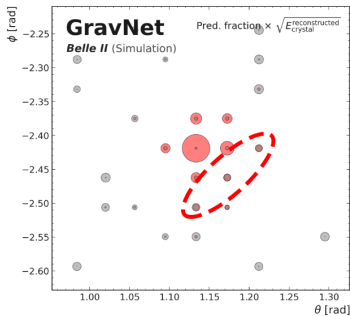
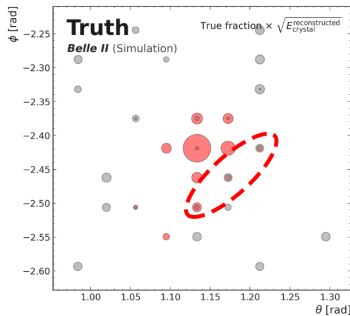
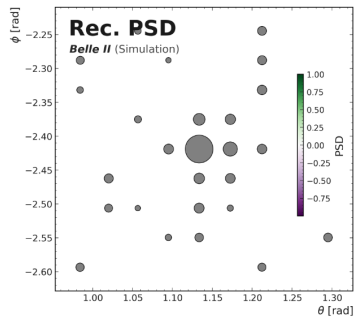
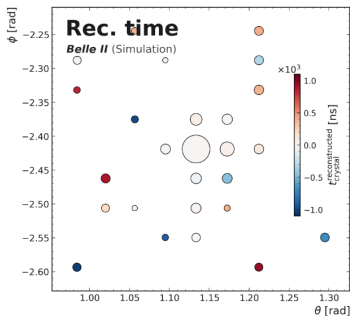
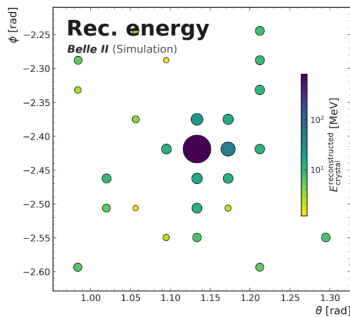
Machine Learning Settings

- Implemented in PyTorch Geometric
- 2 million MC events for training
- 200000 MC events for testing

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- t_{ik} true fraction of cluster k in node i
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- i : number of nodes per event (varies)
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Generated Photon Energy Resolution

$$\frac{E_{\text{pred}} - E_{\text{gen}}}{E_{\text{gen}}}$$

$$E_{\text{pred}} = \begin{cases} \sum_i E_i p_i & \text{GravNet} \\ \text{ClusterE} & \text{basf2} \end{cases}$$

$$E_{\text{gen}} = E_{\gamma}$$

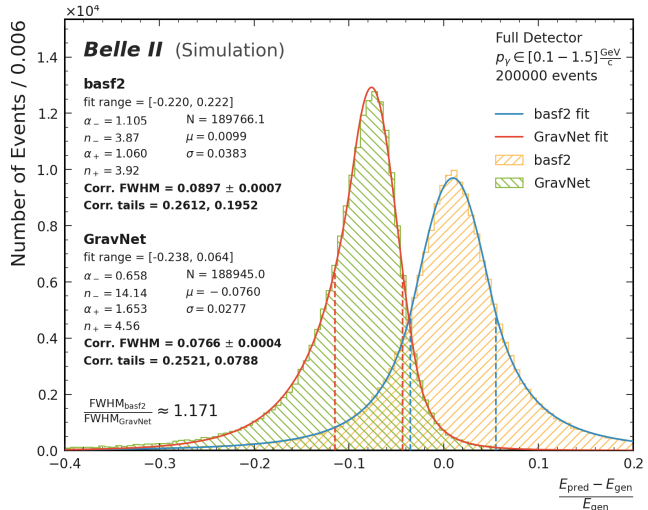
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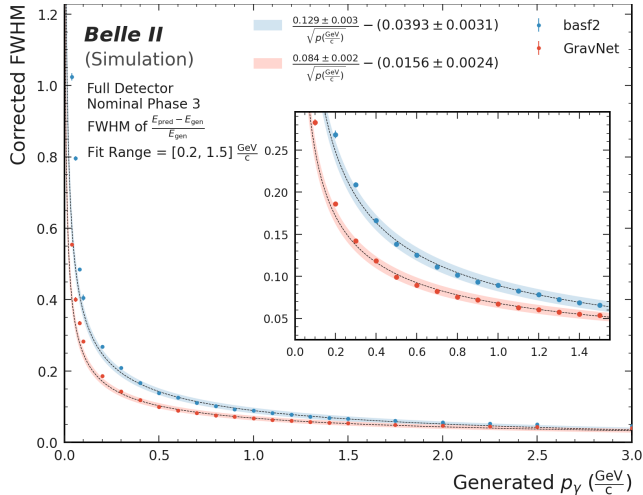
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$$E_{\text{gen}} = E_{\gamma}$$

⇒ 17.1 % improvement



Resolution Energy Dependence



π^0 Invariant Mass Resolution

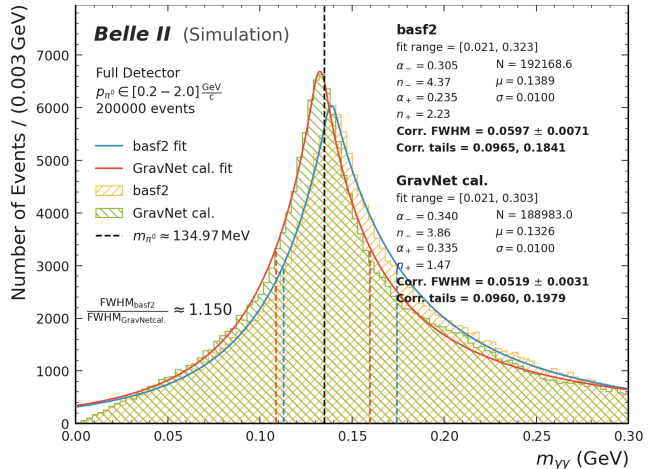
- Shot π^0 particle gun with
 $p_{\pi^0} \in [0.2 - 2.0] \frac{\text{GeV}}{c}$
- Two separate photon signatures
in detector

π^0 Invariant Mass Resolution

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- Reconstruction of π^0 mass from
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- \Rightarrow 15% improvement



Summary and Outlook

Summary

- Few parameters and computations
- Well-suited for soft clustering with nominal phase 3 background
- Significant improvements to photon and π^0 resolution

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- Few parameters and computations
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Further Work

- Early phase 3 background analysis
- Network for overlapping photons
- π^0 rec. from overlapping photons

Outlook

- Technical paper
- Evaluation on data
- Investigate feasibility for basf2

Deposited Photon Energy Resolution

$$\frac{E_{\text{pred}} - E_{\text{dep}}}{E_{\text{dep}}}$$

$$E_{\text{pred}} = \begin{cases} \sum_i E_i p_i & \text{GravNet} \\ \text{rawEnergy} & \text{basf2} \end{cases}$$

$$E_{\text{dep}} = \sum_i E_i t_i$$

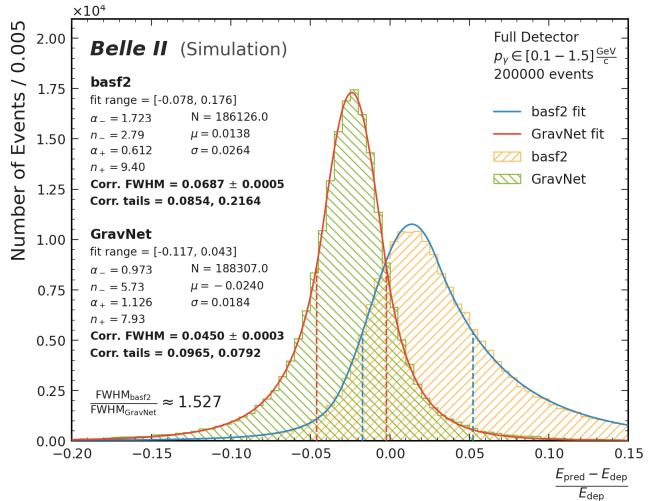
Deposited Photon Energy Resolution

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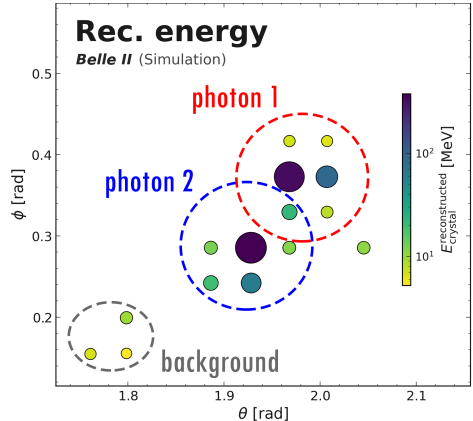
⇒ 52.7% improvement



Setting and Objective Overlap

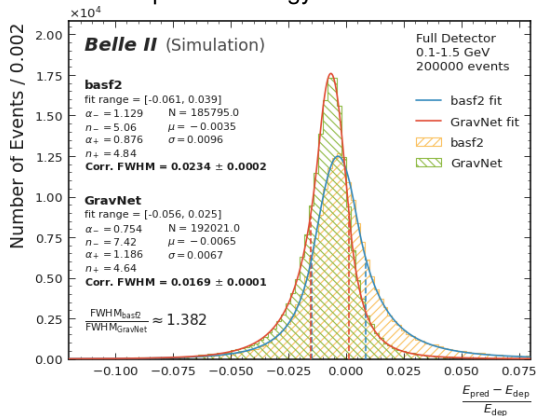
- Two clusters with overlap in 5×5 region
- 9×9 grid of crystals
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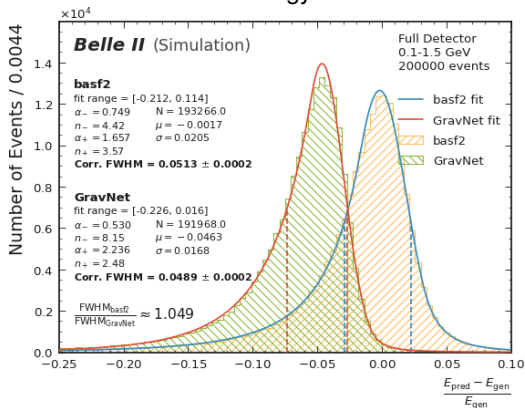
Early Phase 3

Deposited energy



⇒ 38.2% improvement

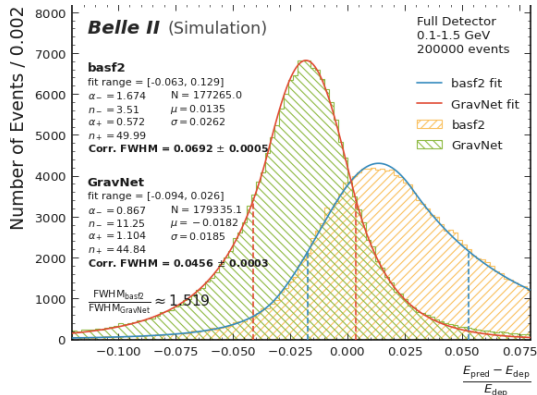
Generated energy



⇒ 4.9% improvement

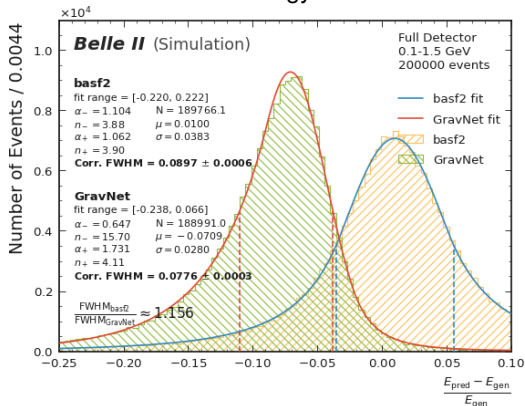
Nominal phase 3 Background

Deposited energy



\Rightarrow 51.9% improvement

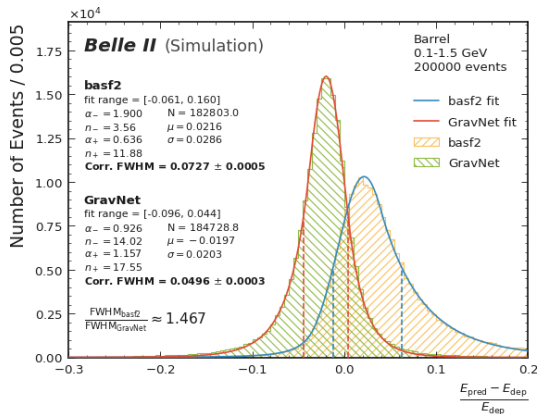
Generated energy



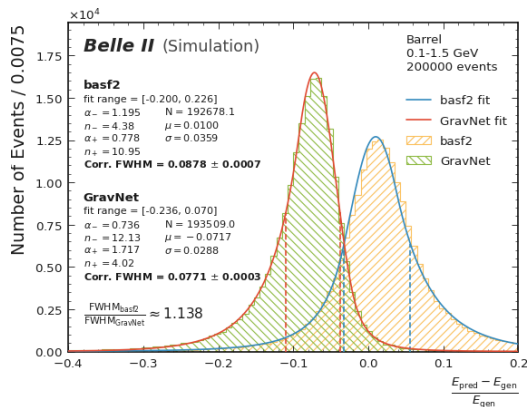
\Rightarrow 15.6% improvement

Barrel

Deposited Energy

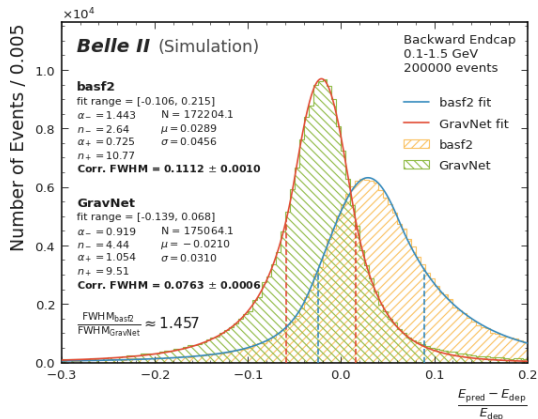


Generated Energy

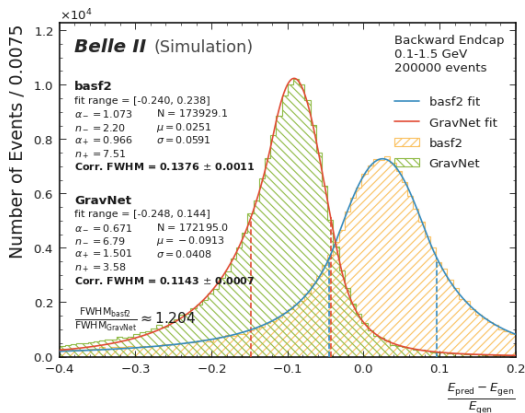


Backward Endcap

Deposited Energy

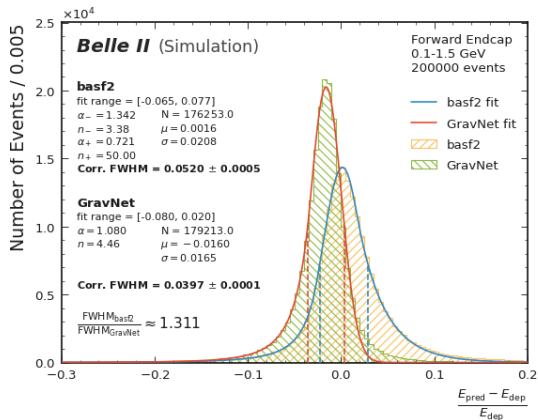


Generated Energy

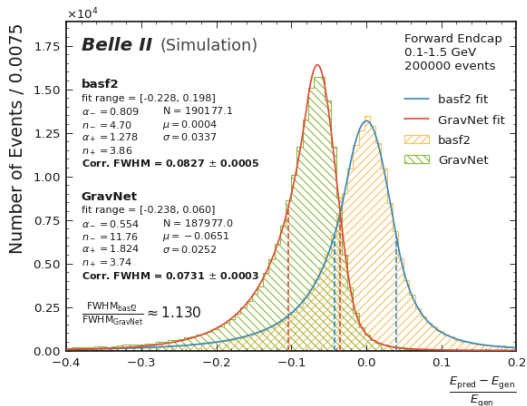


Forward Endcap

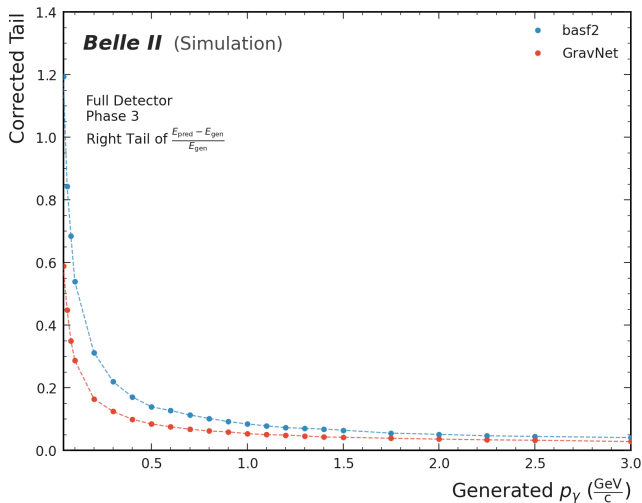
Deposited Energy

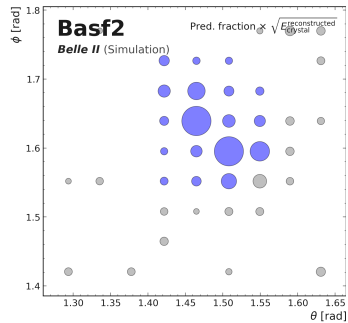
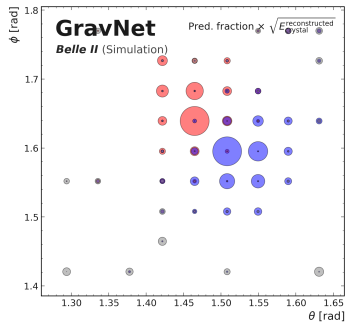
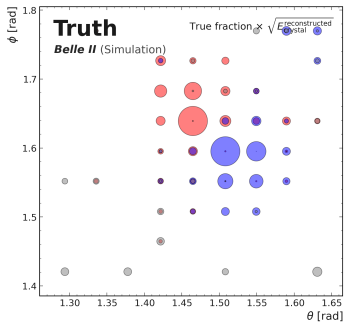


Generated Energy

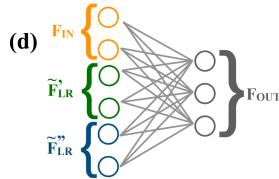
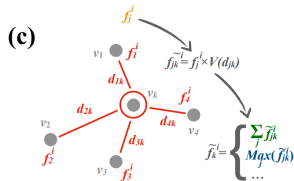
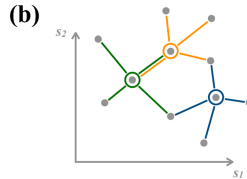
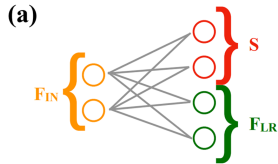


Tails Energy Dependence





Full Model



(a)

- Three fully connected layers
- Representation space dim = 3
- Learned node features = 16

(b)

- Nearest neighbours = 12

(c)

- Mean and maximum aggregation

(d)

- One fully connected layer

Input / Output Details

Features

- Rec. energy, rec. time, rec. PSD
- Crystal weight
- Global coordinates
- Local coordinates in 9 x 9 region

Softmax (sum fractions = 1)

- Fraction particle 1
- Fraction particle 2
- Fraction background

Full Machine Learning Settings

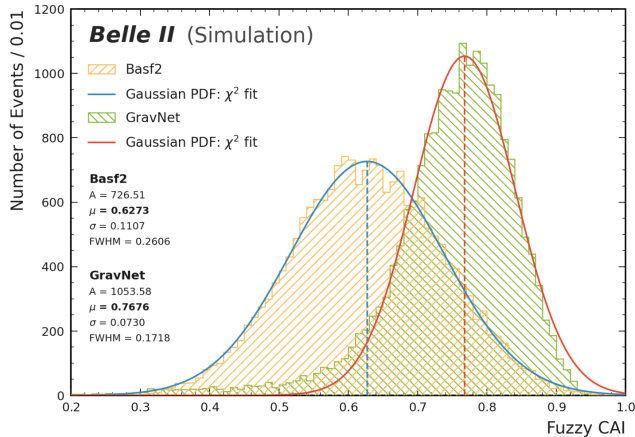
Training

- Random initialization
- Adam Optimizer
- Learning rate: 0.005
- Decaying learning rate on plateau

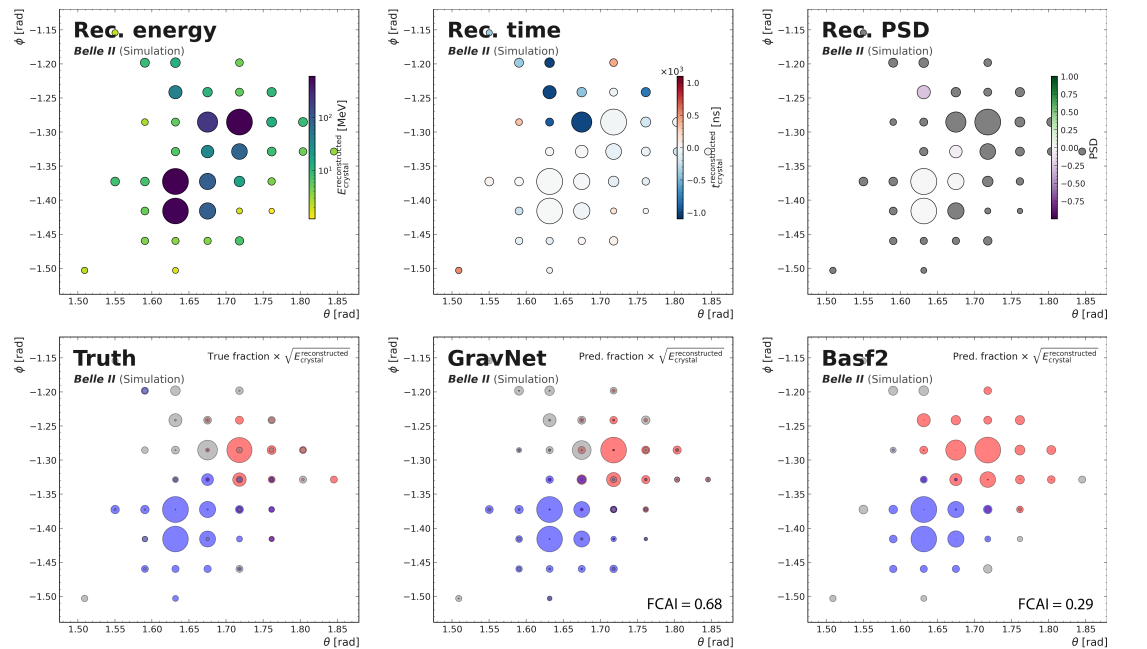
More details

- Batchsize: 512
- Number of epochs: ≈ 50 to convergence
- Batch normalization after each GravNet Layer
- (Mostly) Elu activation

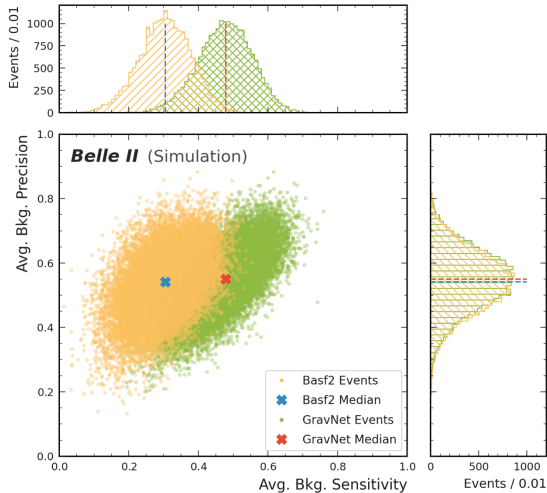
Clustering Metrics



- Evaluate quality of soft-clustering
- Use overlap between different classes at each data point as basis for pairwise comparison
- doi: 10.1609/aaai.v31i1.10905.



Clustering Metrics



- Sensitivity:

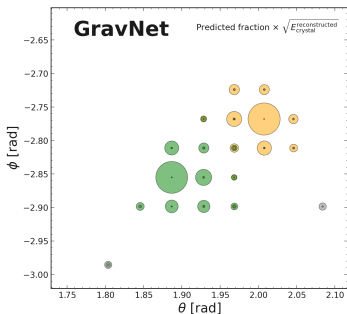
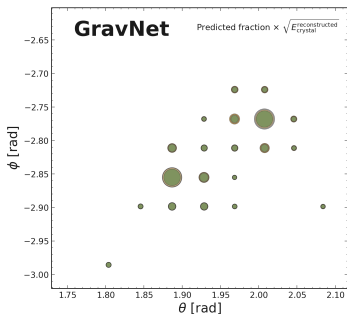
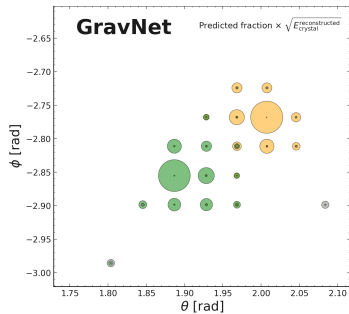
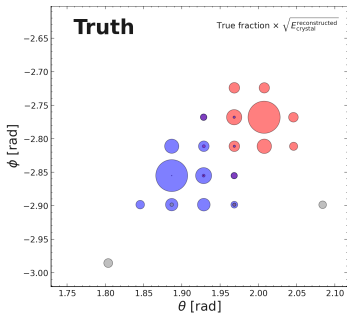
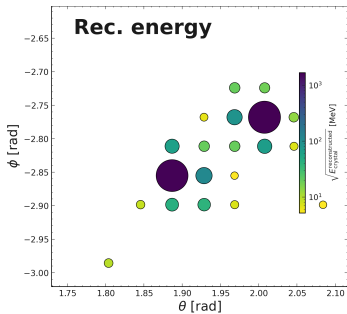
$$\frac{1}{n} \sum \frac{(\text{identified and correct background})}{(\text{total true background})}$$

- Precision:

$$\frac{1}{n} \sum \frac{(\text{identified and correct background})}{(\text{total identified background})}$$

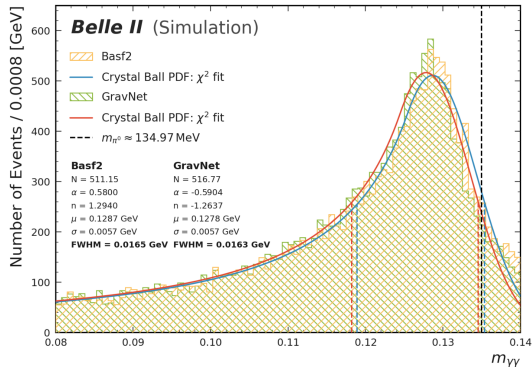
Data Selection

- Two separated local maxima
- At least 10 MeV measured energy
- At least 80% true physics deposition in local maxima
- Overlap in 5×5 area around local maxima

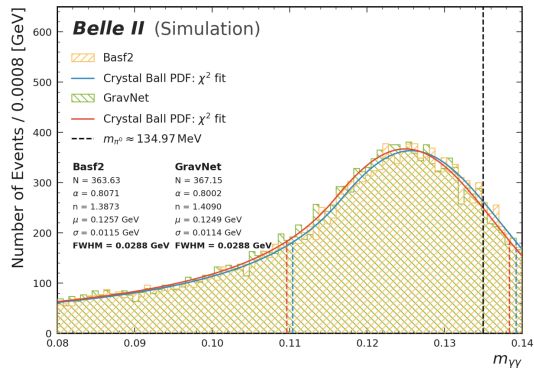


π^0 Invariant Mass Resolution

Reconstructed energy + MC position

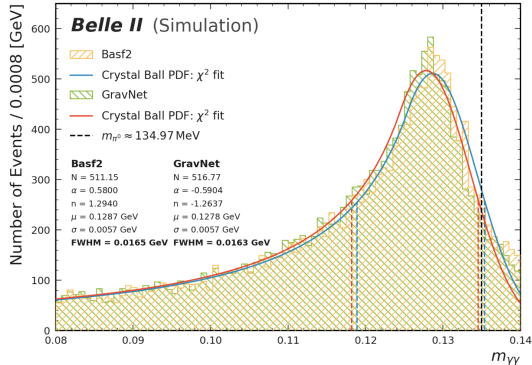


Reconstructed energy + reconstructed position

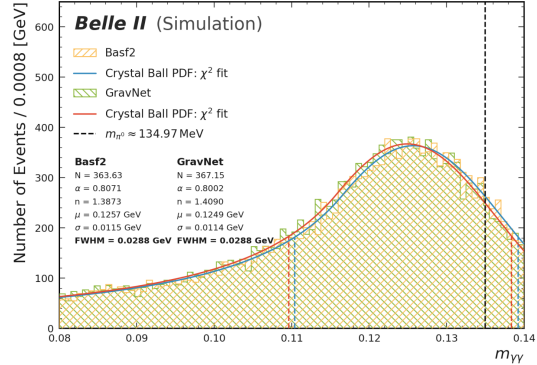


π^0 Invariant Mass Resolution

Reconstructed energy + MC position



Reconstructed energy + reconstructed position



⇒ Significant improvement in photon resolution does not transfer to invariant mass resolution:

$$\sigma_{m^2}^2 \approx m_{\pi^0}^4 \left(\frac{\sigma_{E\gamma_1}^2}{E_{\gamma_1}^2} + \frac{\sigma_{E\gamma_2}^2}{E_{\gamma_2}^2} + \frac{4\sigma_{\alpha}^2}{\alpha^2} \right)$$