Contrastive Reinforcement Learning for Classifying MeV Scale Physics in LArTPCs

Nuclear Science & Security Consortium

APS April Meeting (04/03/2024)

Presented by *Nicholas Carrara* on behalf of the ***BLIP ML Group*** at **UC Davis**

DEEP UNDERGROUND NEUTRINO EXPERIMENT

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Why are neutrons important?

To turn neutrino physics into a precision science, we need to understand complex neutrino-nucleus interactions (specifically on Ar):

- Neutrons carry away a ***large fraction***[1] of energy.
- Neutron final states are ***model dependent***.
- Neutrons are ***difficult to detect*** in LAr.

Neutrons are also important for low-energy physics in LAr:

- e.g., modeling **supernova** and **solar** (and now **galactic**[2]) neutrino physics.

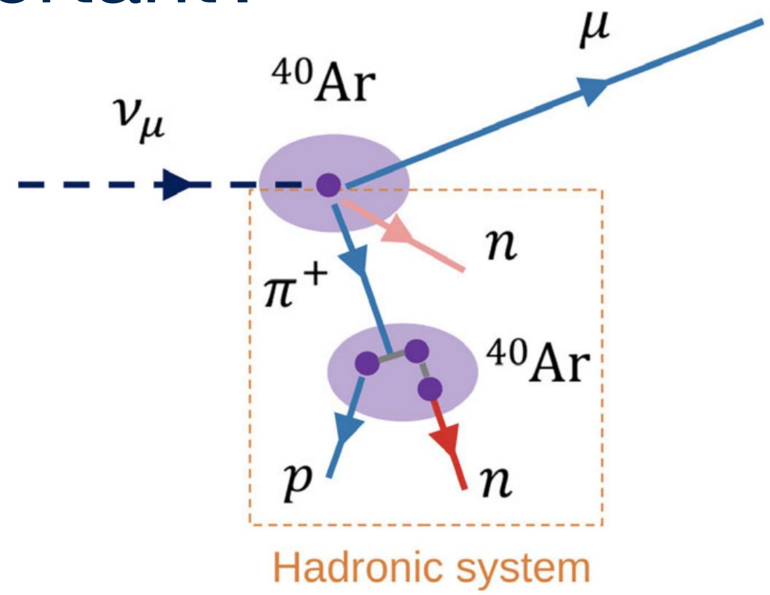

Figure from A. Friedland and W. Li (2019).

1 A. Friedland and W. Li, *Understanding the energy resolution of liquid argon neutrino detectors*, Physical Review D, **99**, 2019 (https://arxiv.org/abs/1811.06159)
2 ICECUBE Collaboration, *Observation of high-energy neutrinos from the Galactic plane*, Science, **380**, 2023 (https://www.science.org/doi/10.1126/science.adc9818)

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Difficult to detect?

It is necessary to be able to account for the neutron "missing energy" in order to make precision oscillation measurements (production and transport).

- Neutrons show up as small ***blips*** in LAr detectors.

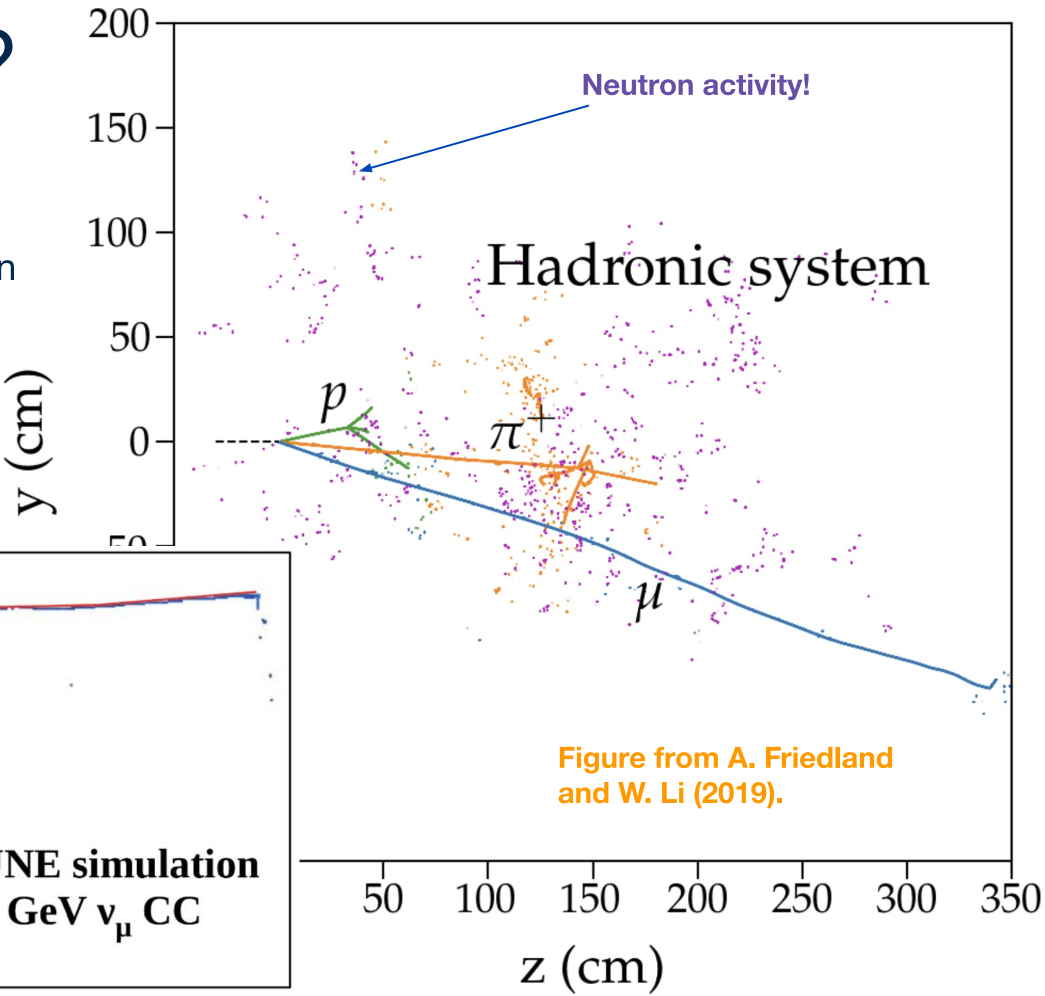
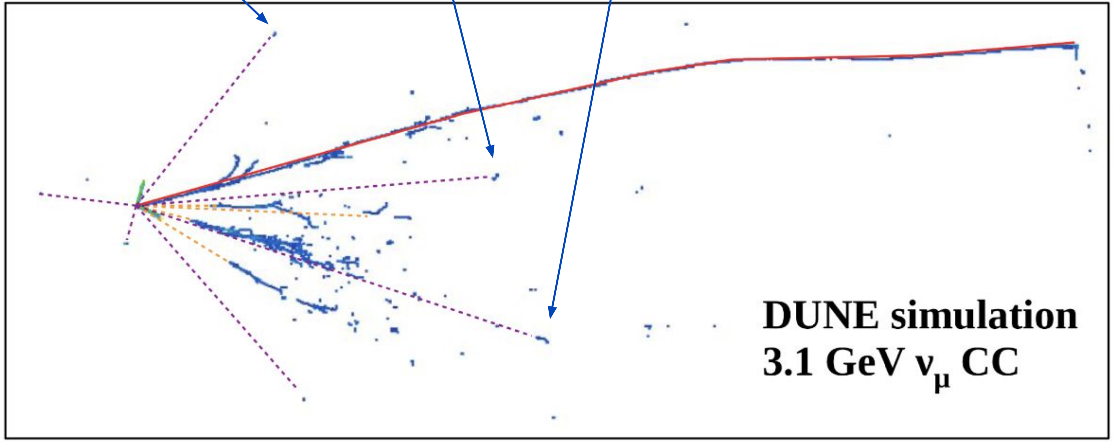


Figure from A. Friedland and W. Li (2019).



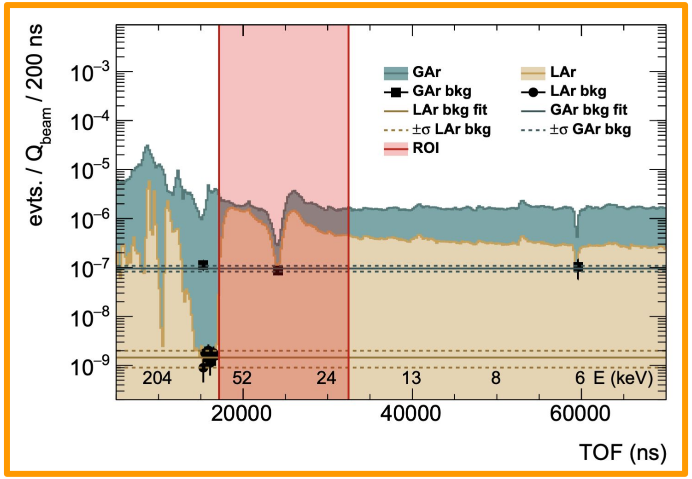
Neutron Calibration (PNS)

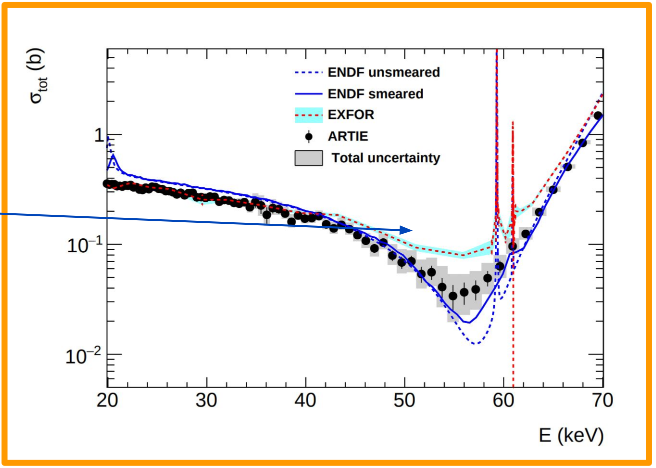
Benefits of low-energy neutrons for calibration:

- ***Standard Candle*** - Neutron captures on Ar-40 emit a 6.1 MeV gamma cascade.

$$\mathrm{n} + {}^{40}\mathrm{Ar} = {}^{41}\mathrm{Ar} + \{\gamma_j\}$$
$$\sum_j E(\gamma_j) \approx 6.1\mathrm{MeV}$$

- ***Scattering Length*** - Some percentage of neutrons above 57 keV will fall into the resonance well.
    - Average *fractional energy loss* is ~4.8%.
    - The *effective scattering length* is ~30 m.
    - The resonance well has been measured by the ARTIE[1] experiment at LANL, with a ***follow-up*** planned for this year (**ARTIE-II**).





3 *Measurement of the total neutron cross section on argon in the 20 to 70 keV energy range,* The ARTIE Collaboration, Phys. Rev. C, 2023, (https://arxiv.org/abs/2212.05448).

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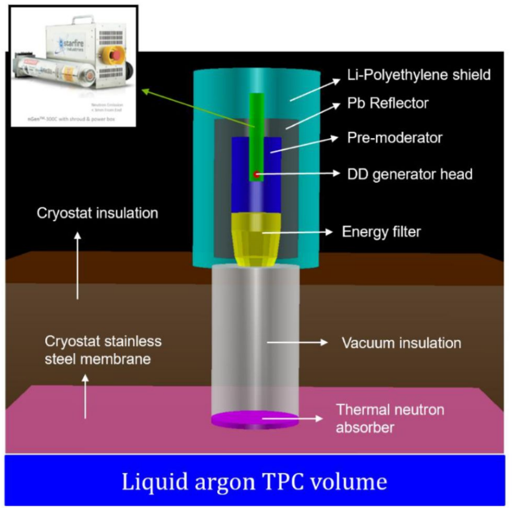
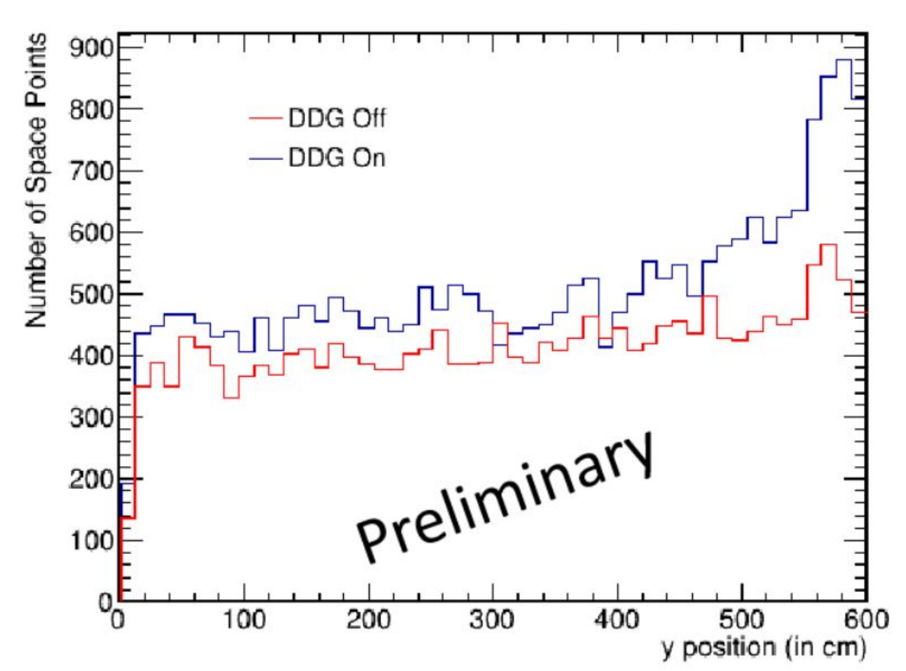
How Can We Isolate Captures?

A **pulsed neutron source**, such as a deuterium-deuterium generator (DDG), can create a *mono-energetic* spray of low-energy neutrons.

- A DDG was used in ProtoDUNE-I, from which the neutrons could be seen in the detector reconstruction.
- So far, we have not had the ability to isolate ***individual neutron captures***.





Work done by Y. Bezawada and J. Huang

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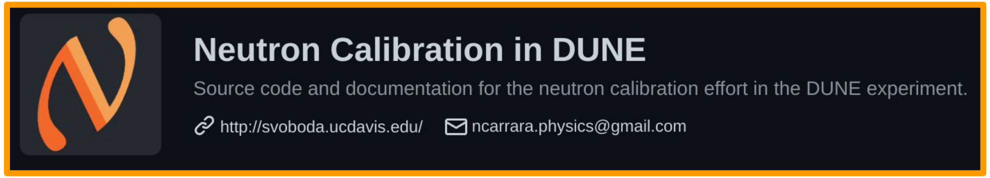
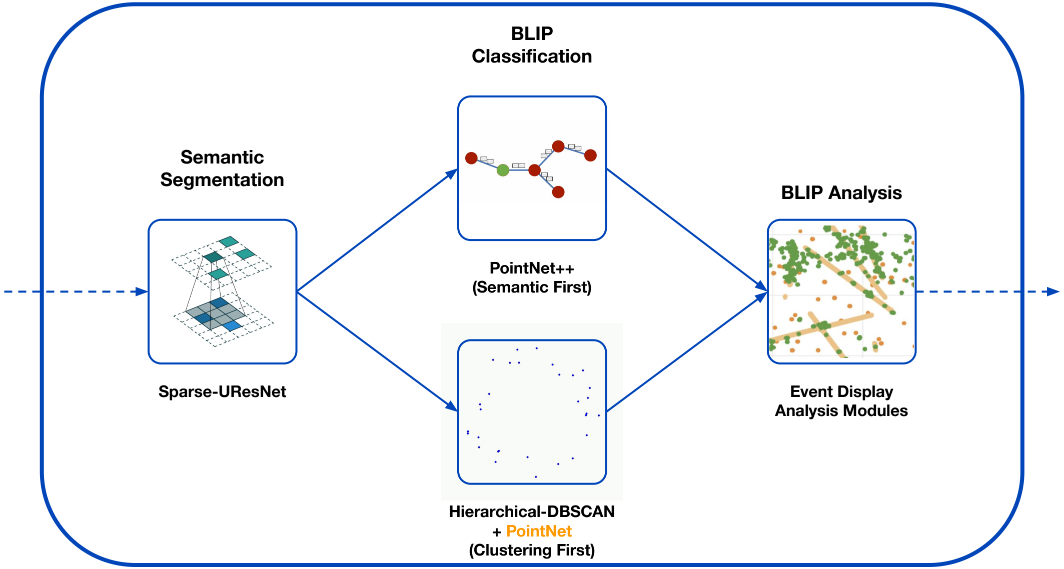
BLIP

We introduce ***BLIP***[2], a collection of ML algorithms for classifying low energy interactions in LArTPCs.

- **Semantic Segmentation**:
  - Pixel/point-cloud level classification for detector readout and/or reconstructed space points.
  - Identification of tracks/showers in order to **isolate** Blips.
- **Heirarchical Clustering**:
  - Merge-trees and Heirarchical-DBSCAN for clustering BLIPs.
- **Point-cloud Classification**:
  - BlipNet models for classifying BLIP point clouds.
- **Topological Data Analysis (TDA)**:
  - State-of-the-art algorithms for characterizing the topology of point sets (e.g. persistent homology).

2 *BLIP, BLIP ML* Group (UC Davis), 2023, (https://github.com/Neutron-Calibration-in-DUNE/Blip).





BLIP

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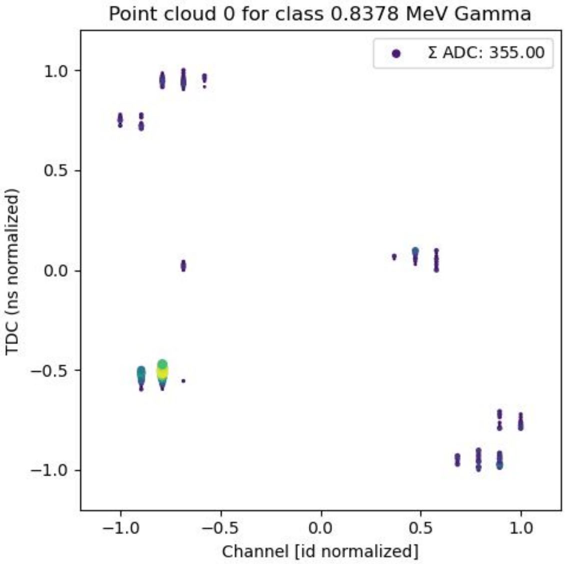
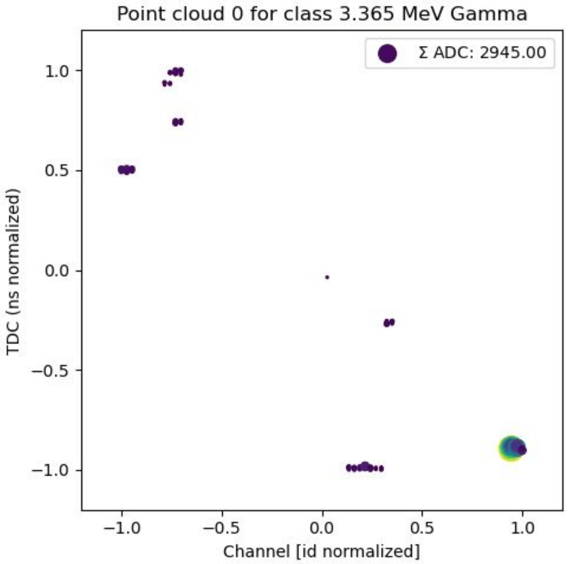
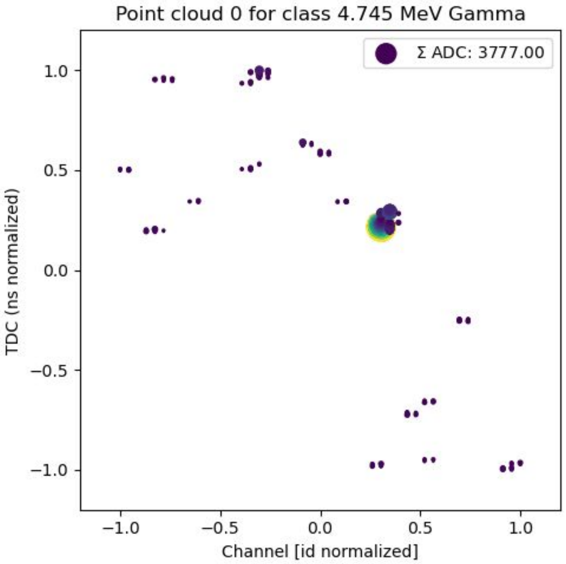
Blip Examples

Below are examples of different neutron capture gammas simulated in LArSoft.

- Each cluster is normalized so that it is centered at zero and extends from [-1,1] in each variable.
- ADC is normalized over all events.







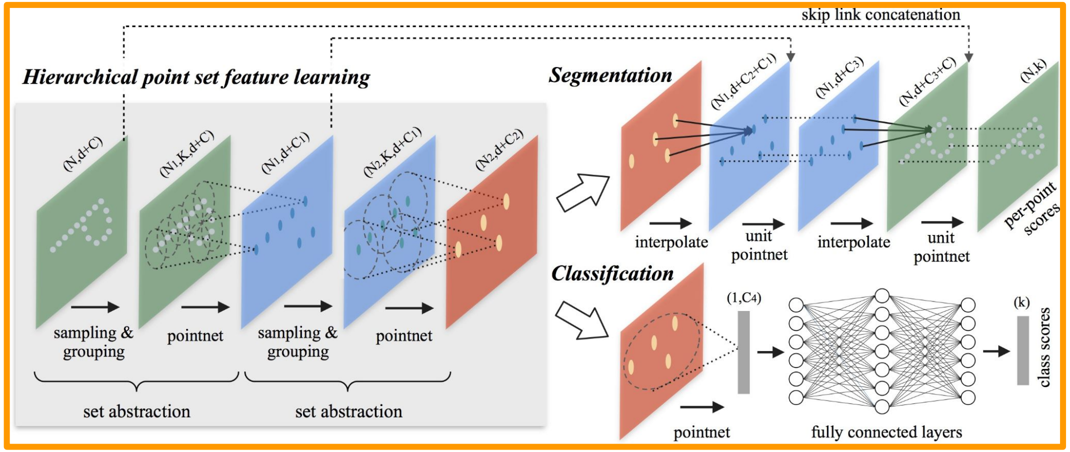
BLIP Classification

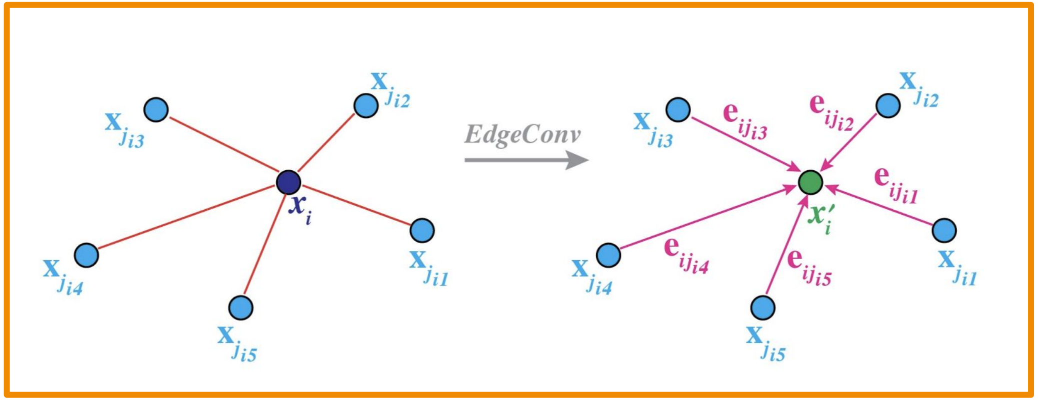
BLIP Classification will consist of at least the following model:

- **BlipGraph** - The network will learn to classify clusters at different scales (e.g. PointNet[4], DynamicEdgeConv[6]).

Point cloud neural networks take advantage of three main properties of the datasets:

1. **Unordered** - are unordered and can have a variable number of points!
2. **Distance Metric** - point clouds have a geometry and local information.
3. **Symmetries** - Due to physics/geometry, the point clouds are invariant under certain transformations.





4 *PointNet: Deep Learning on Point Sets for 3D Classification and Segmentation*, C. Qi et. al., CVPR 2017, (https://arxiv.org/abs/1612.00593).
5 *PointNet++: Deep Hierarchical Feature Learning on Point Sets in a Metric Space*, C. Qi et. al., (https://arxiv.org/abs/1706.02413)
6 *Dynamic Graph CNN for Learning on Point Clouds,* Y. Wang et. al., 2018, (https://arxiv.org/abs/1801.07829)

Contrastive Learning

We can utilize symmetries in our dataset to conduct a semi-supervised learning in which point clouds are grouped together by symmetries in their representation.

Using the *Normalized Temperature-scaled Cross Entropy Loss* (***NTXent***):

$$\ell_{i,j} = -\log \frac{\exp(\mathrm{sim}(\boldsymbol{z}_i, \boldsymbol{z}_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\mathrm{sim}(\boldsymbol{z}_i, \boldsymbol{z}_k)/\tau)}, \qquad (1)$$

we push “like” clusters closer together in the embedding space and push all others away.

? K. Sohn, *Improved Deep Metric Learning With Multi-class N-pair Loss Objective*, NIPS (2016), (https://proceedings.neurips.cc/paper_files/paper/2016/file/6b180037abbebea991d8b1232f8a8ca9-Paper.pdf)

Contrastive learning scheme
(https://ai.googleblog.com/2020/04/advancing-self-supervised-and-semi.html)

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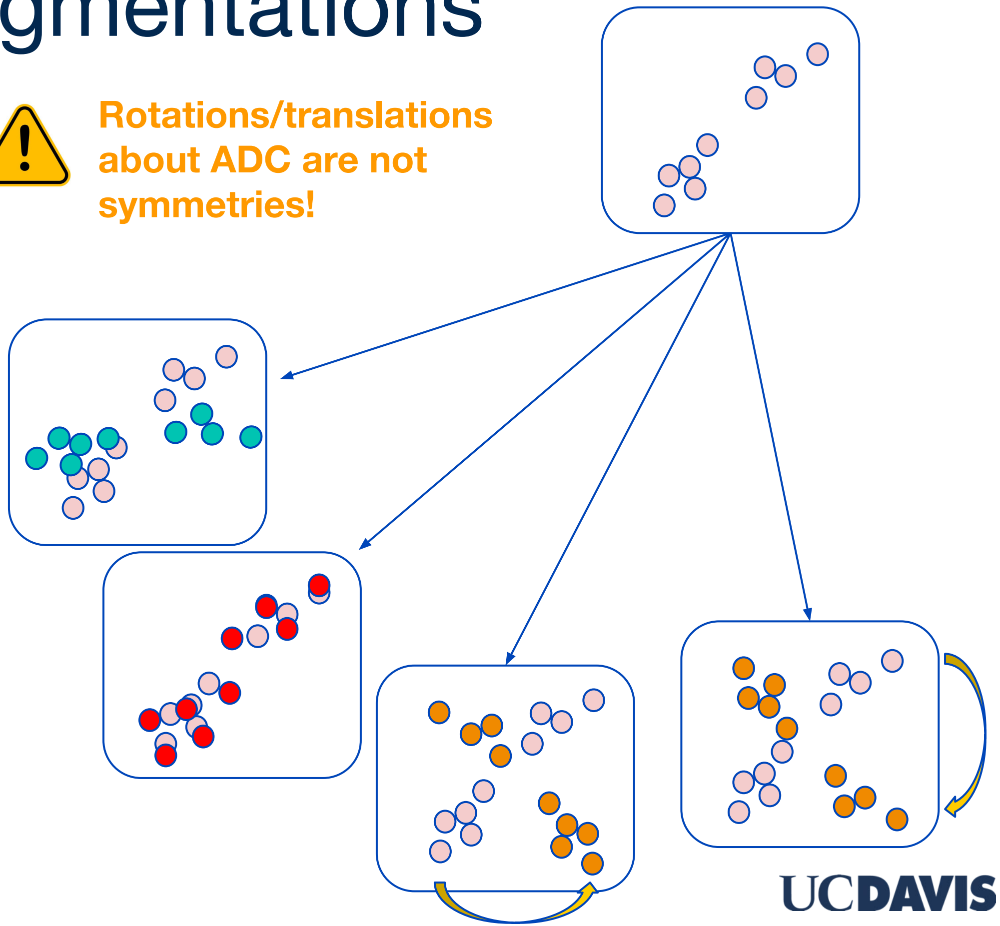
Symmetries -> Augmentations

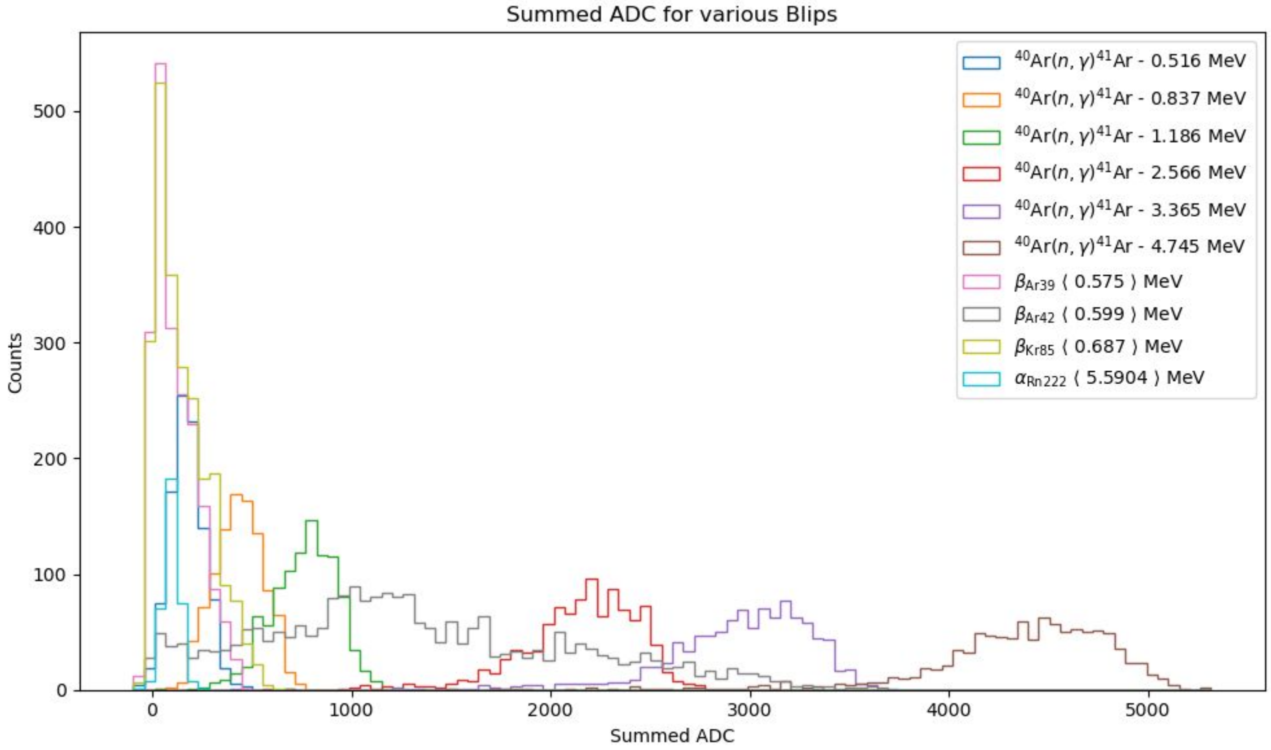
There are several symmetries in our dataset due to physics:

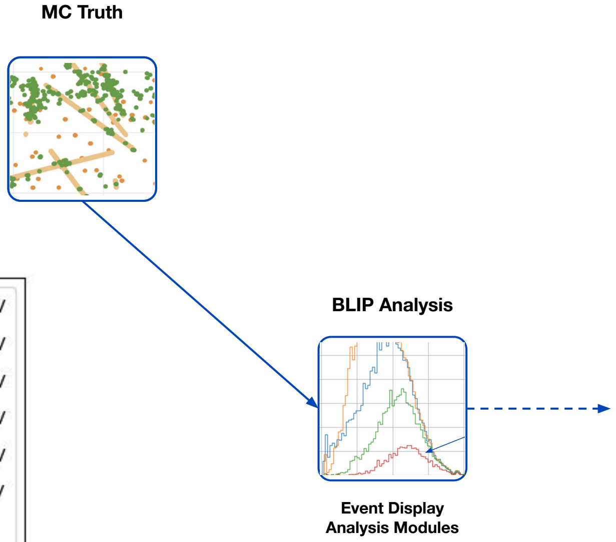
1. **Translation** - Translations in (channel,tdc) are handled by normalizing each point cloud to the origin.
2. **Rotation** - Rotations about (channel,tdc) are implemented as part of the augmentations.
3. **Fluctuations** - Fluctuations can occur from many sources including the electron drift.
4. **Parity** - Flipping of the momentum of the particle along the (channel, tdc) directions.

Rotations/translations about ADC are not symmetries!



Far Detector (channel, tdc, adc)





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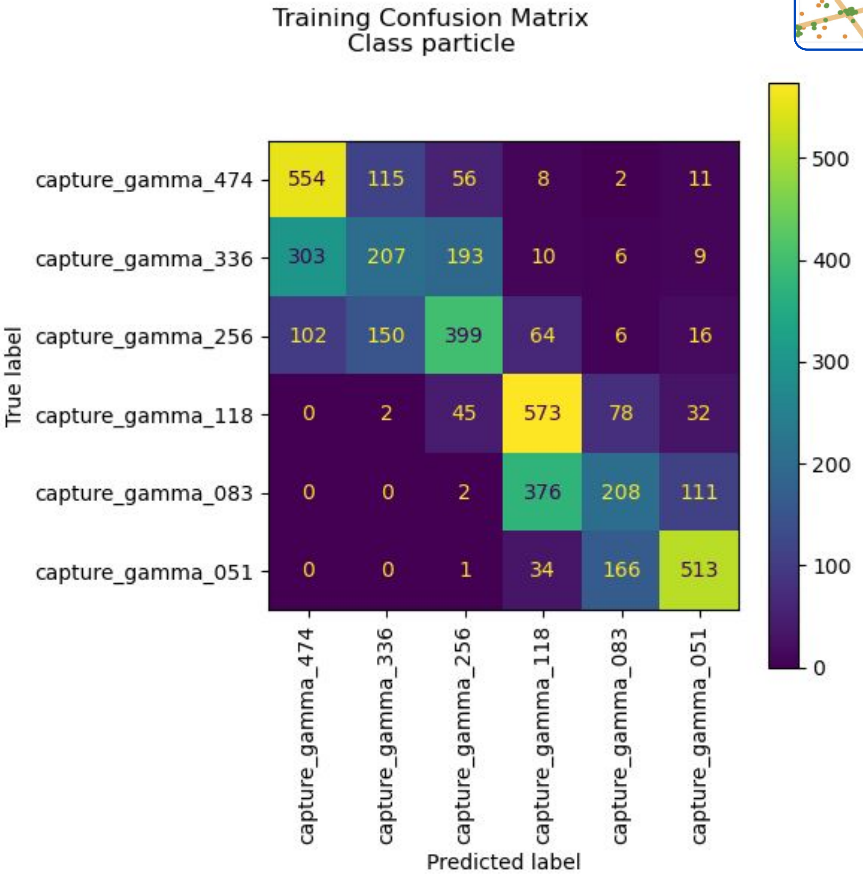
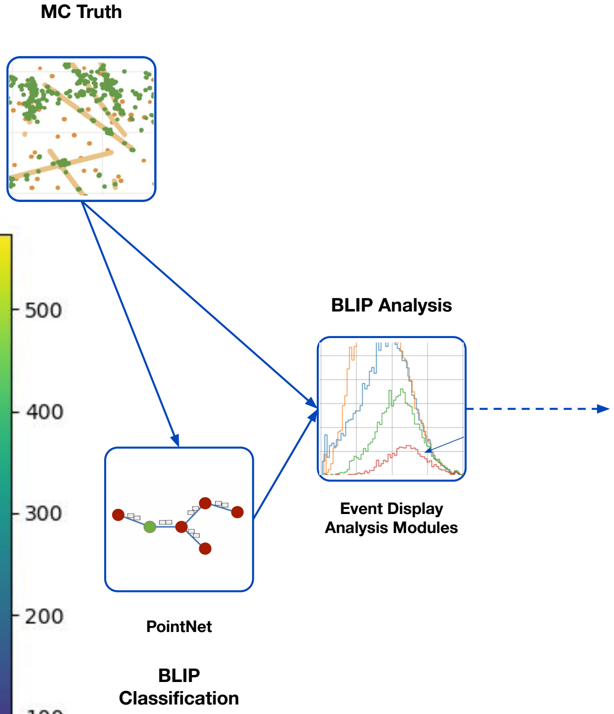
MCTruth + BlipGraph

The model needs some tuning, but the current version seems to be learning something about the shapes of the point clouds.





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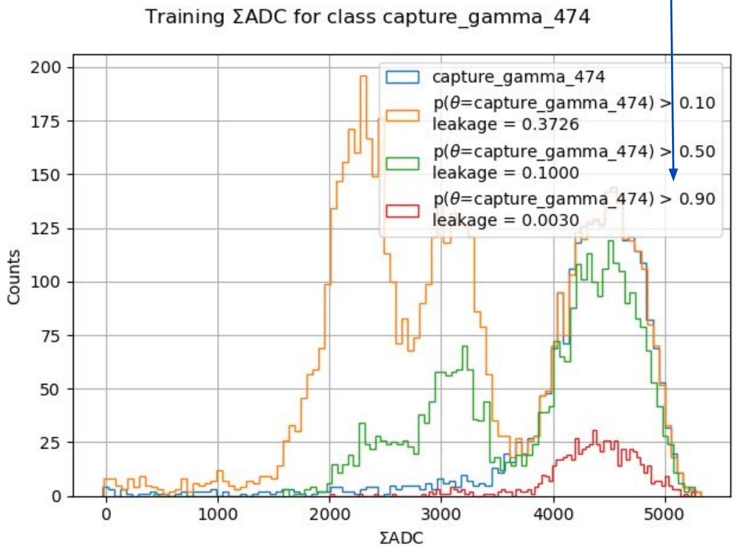
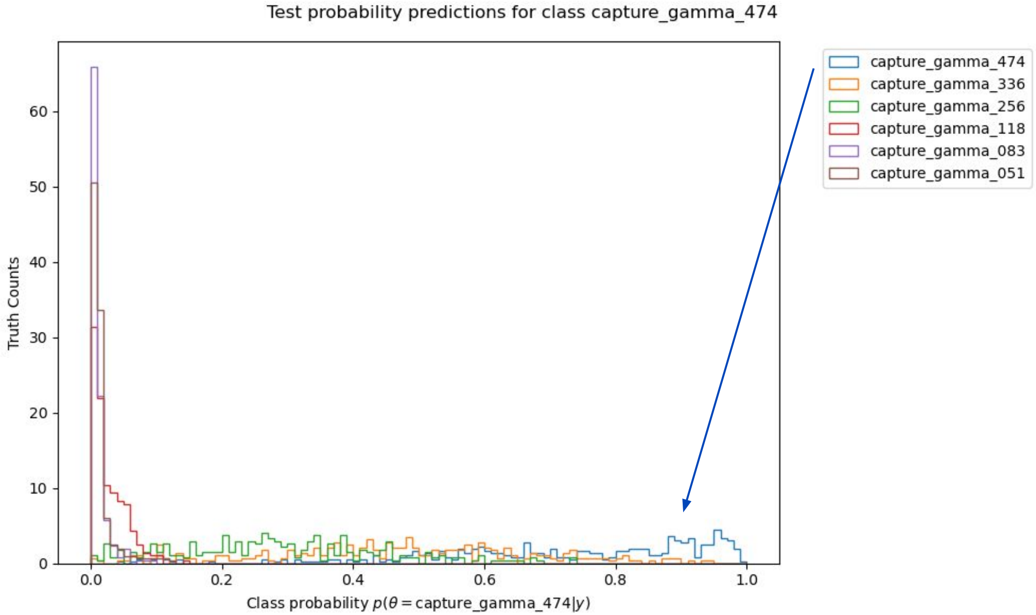
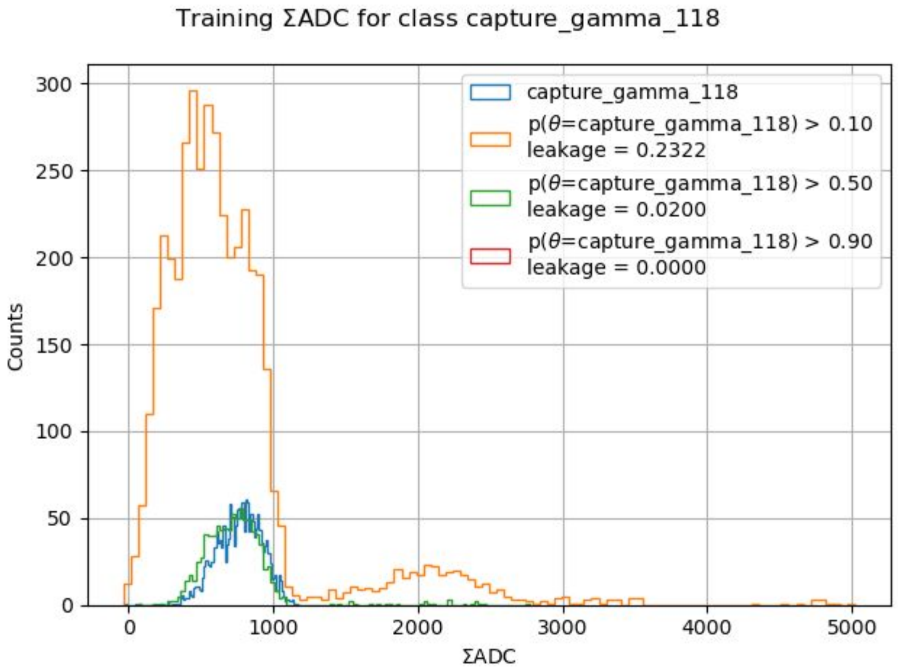
MCTruth + BlipGraph

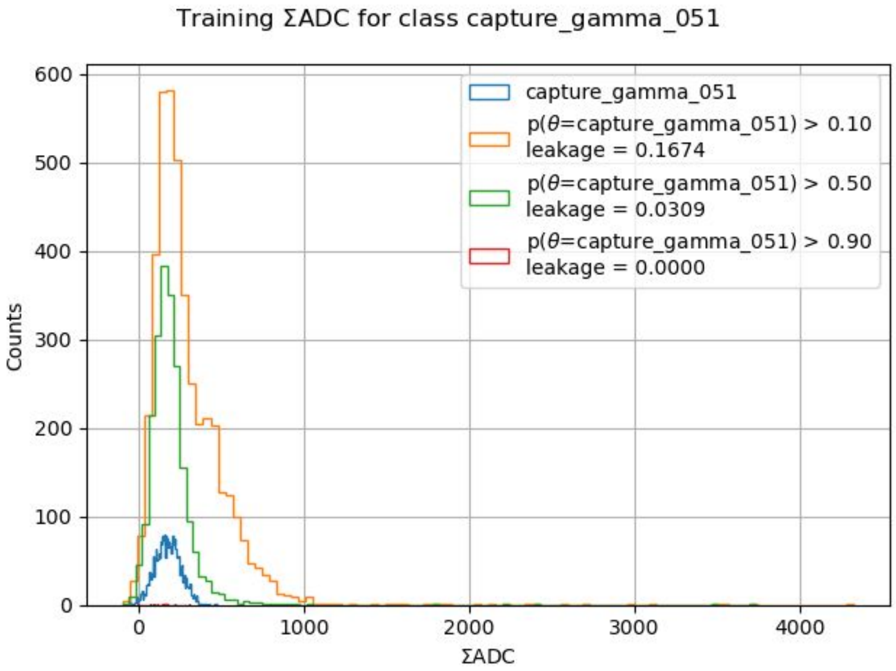
This early model rejects 99.7 % of all other blip types when imposing a 90% cut on the probability to being a 4.745 MeV gamma.





MCTruth + BlipGraph

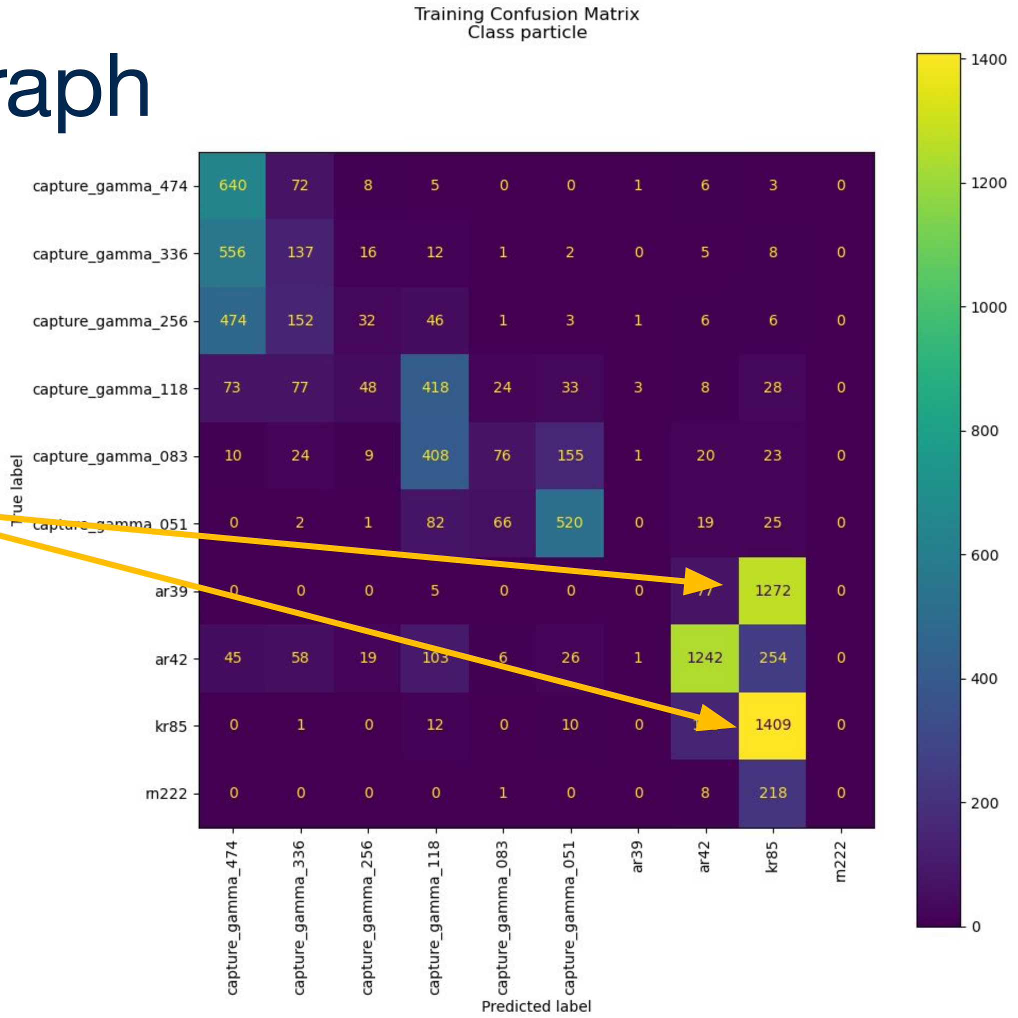




MCTruth + BlipGraph

Some preliminary results on all current blip types.

Perhaps unsurprising that Ar39 and Kr85 are difficult to distinguish given their similar physics.



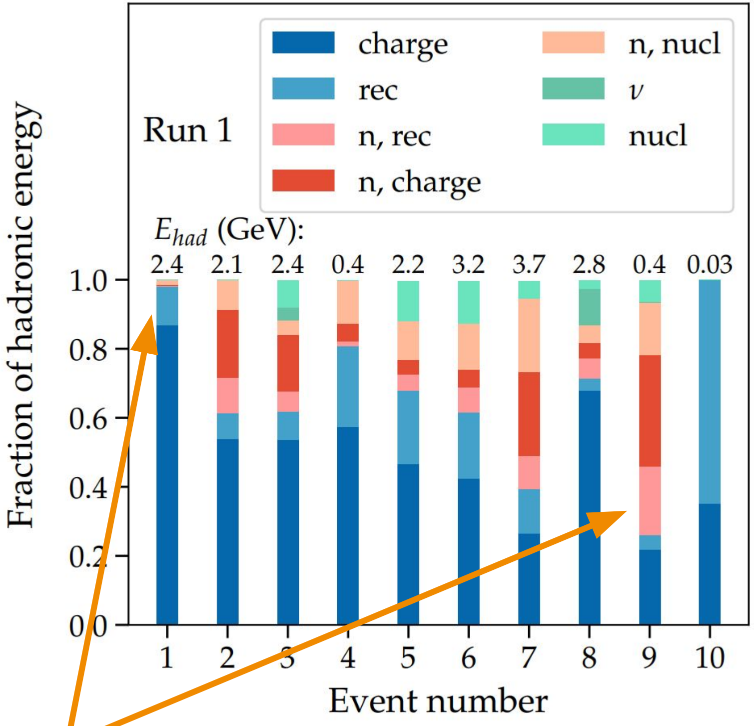
Backup

Energy resolution?

It is necessary to be able to account for the neutron "***missing energy***" in order to make precision oscillation measurements (production and transport).

A. Friedland and W. Li (2019) characterized the sources of missing energy in LArTPCs as,

1. Electronic shower sprays (**charge**)
2. Recombination effects (**rec**)
3. Nuclear breakup (**nucl**)
4. Outgoing neutrinos (***ν***)
5. Subthreshold particles
6. **Primary and secondary neutrons**



Contributions from neutrons vary widely from event to event!

Figure from A. Friedland and W. Li (2019).

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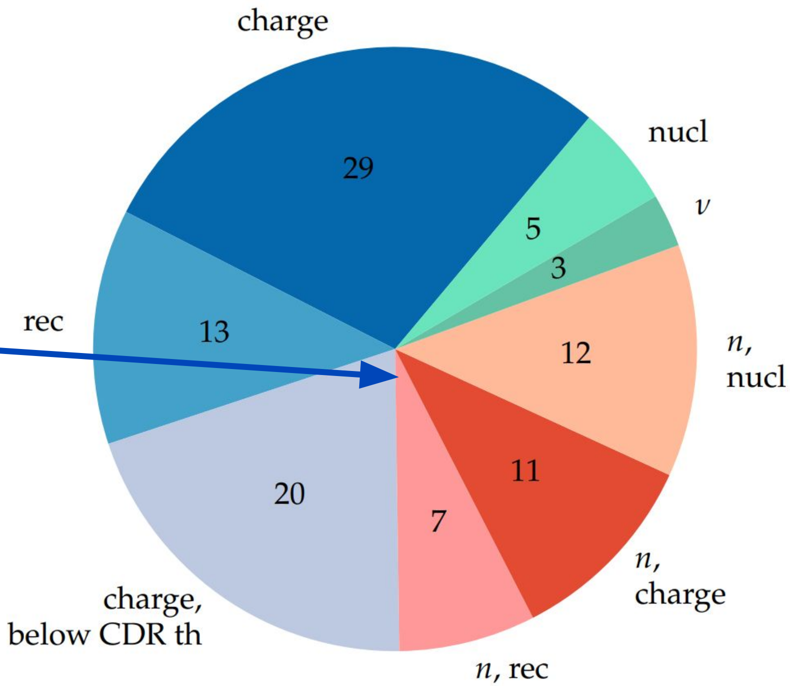
Energy resolution?

This pie chart from the same paper (2019) shows the average amount of missing energy over many events (~10K).

- Neutrons contribute nearly **~30%** of the missing energy on average!



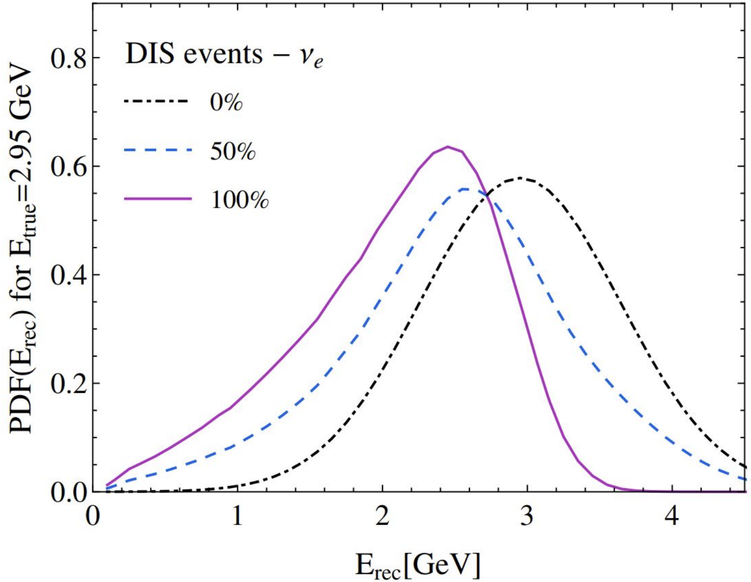


Figure from A. Ankowski et al. (2015).

Figure from A. Friedland and W. Li (2019).

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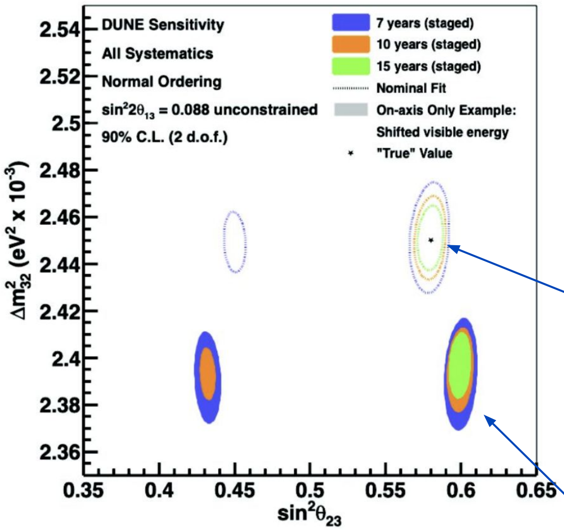
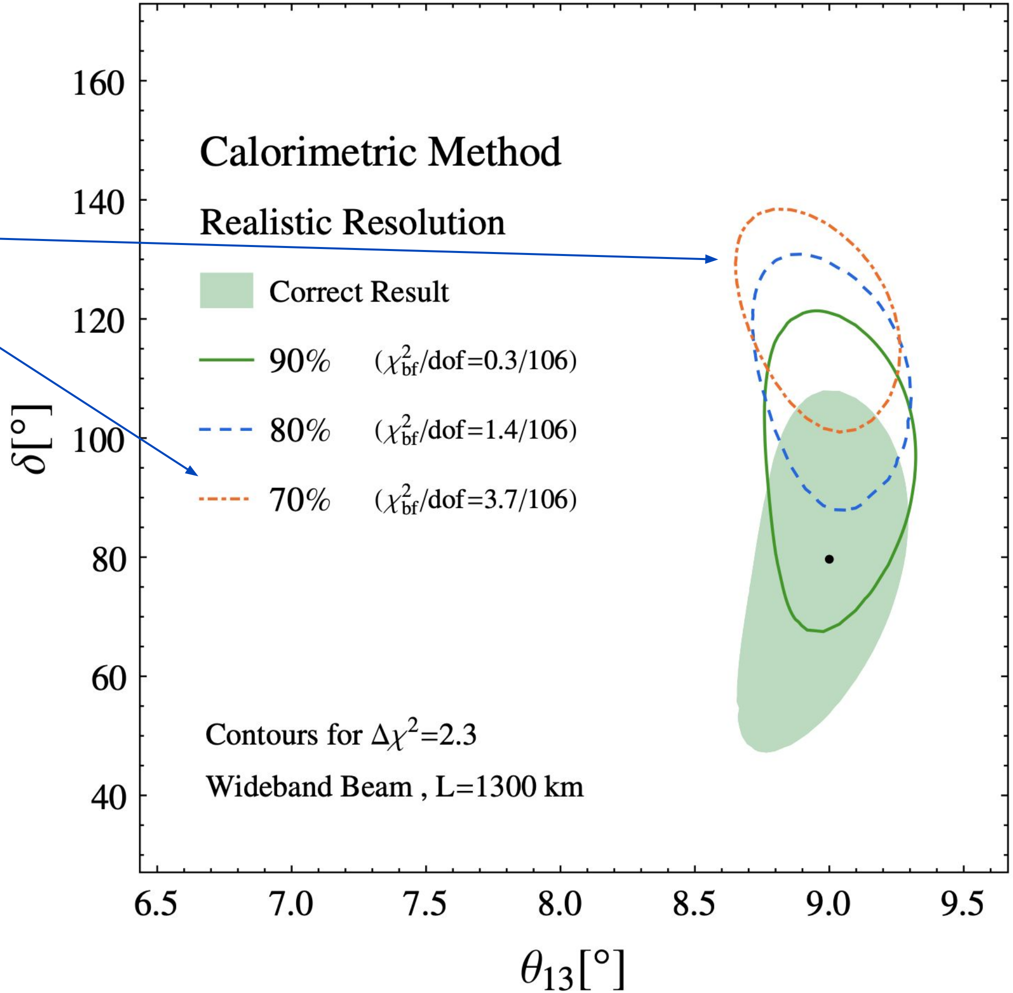
Energy resolution?

- Measurements of the CP phase[3] are shifted by a large amount if neutrons are ignored!



fit with 20% neutron energy missing

actual

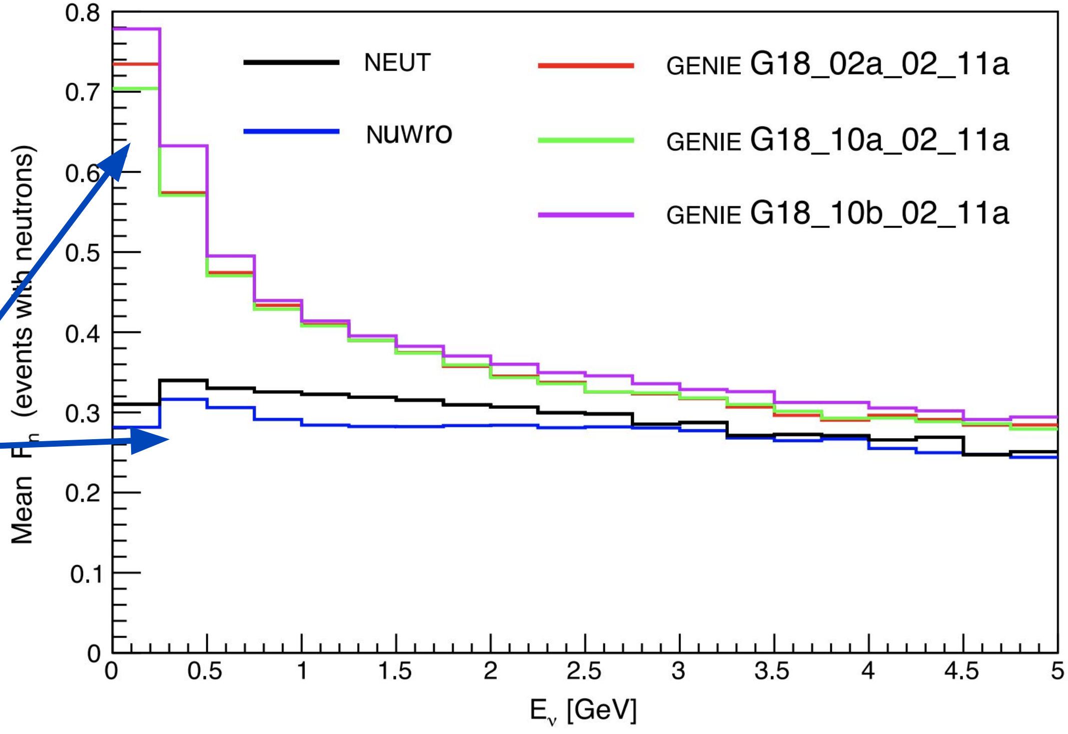


3 A. M. Ankowski et al., *Missing energy and the measurement of the cp-violating phase in neutrino oscillations*, Phys. Rev. D, **92** 2015 (https://arxiv.org/abs/1507.08561)

Model dependent final-states?

M. Buizza Avanzini et al. examined the differences in neutron final-states from the generators **NEUT**, **NuWro**, and **GENIE**.

- The fraction of total energy given to hadrons (when at least one hadron is a neutron) is shown as a function of incident neutrino energy in a CC-interaction.
- GENIE varies in the lower energy regime by a factor of 2!



4 M. Buizza Avanzini, *Comparisons and challenges of modern neutrino-scattering experiments*, Phys. Rev D, **105** 2022 (https://journals.aps.org/prd/pdf/10.1103/PhysRevD.105.092004)

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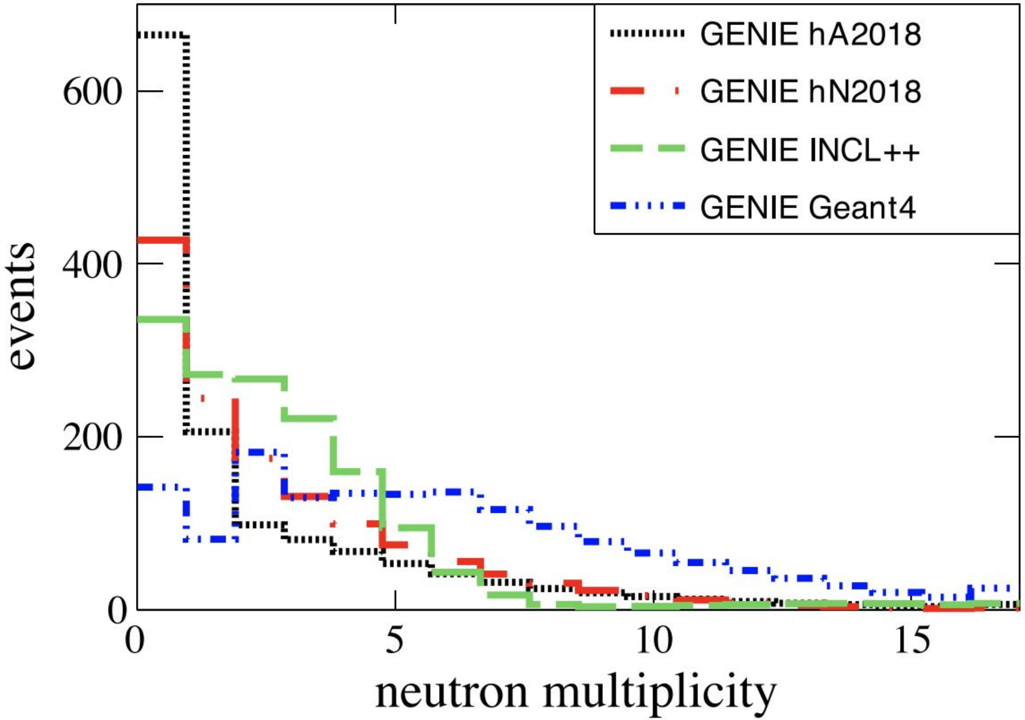
Model dependent final-states?

The various models within GENIE[5] also show a discrepancy in the predictions of neutron multiplicity.

- Neutron distributions from a simulated 2GeV muon neutrino interaction on Ar40.

Our group is working on a potential experiment to be deployed in ANNIE to measure neutron multiplicity on Ar!



5 The GENIE Collaboration, *Recent highlights from GENIE v3*, Eur. Phys. J. Spec. Top. (2021) (https://link.springer.com/article/10.1140/epjs/s11734-021-00295-7)

Arrakis LArSoft Module

The ***Arrakis***[3] LArSoft module is responsible for collecting MC truth/detector output information and generating point clouds for training.

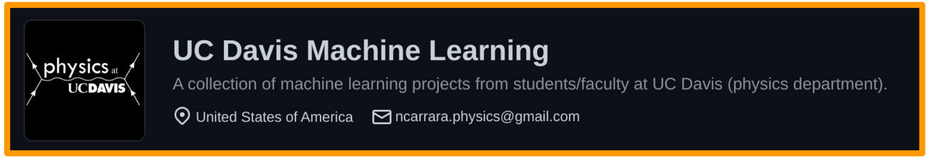
Current Labeling Schemes:

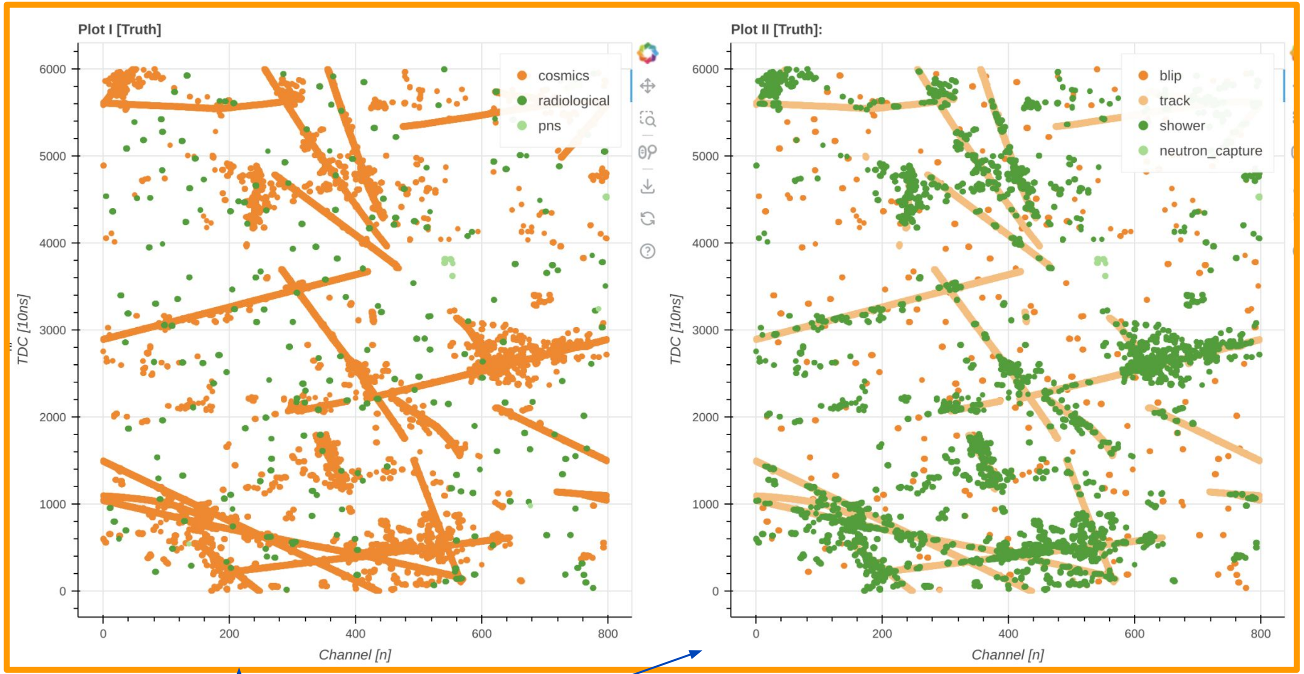
[Segmenation]

- **Source -** specifies the generator.
- **Shape -** generic topological descriptor (track, shower, blip, …)
- **Particle -** particle type responsible for the energy deposition (mu+-, neutron, proton, michel, delta, …)

[Clustering]

- **UniqueShape -** individual instance of a particular shape.
- **UniqueParticle -** individual instance of a particular particle.





‘source’ and ‘shape’ labels for a simulated ProtoDUNE event

3 *Arrakis (LArSoft module),* DUNE PNS Group (UC Davis), 2023, (https://github.com/UC-Davis-Machine-Learning/Arrakis).

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Arrakis LArSoft Module

To use Arrakis,

[Current setup]

- Can use the LArSoftArrakis repository to set up a local LArSoft install on an FNAL server.
- Download Arrakis into larana and compile.
- Add "arrakis" as an analyzer module and specify parameters.

```
#include "Arrakis.fcl"

physics:
{
    analyzers: {ana: @local::Arrakis}
    analysis:  [ana]
    trigger_paths:   [simulate]
    end_paths:       [analysis]

}
```

[Future setup]

- Eventually, Arrakis will be integrated into LArSoft and will be available as an analyzer module.
- Allow the user to register custom *logic* for generating training datasets.

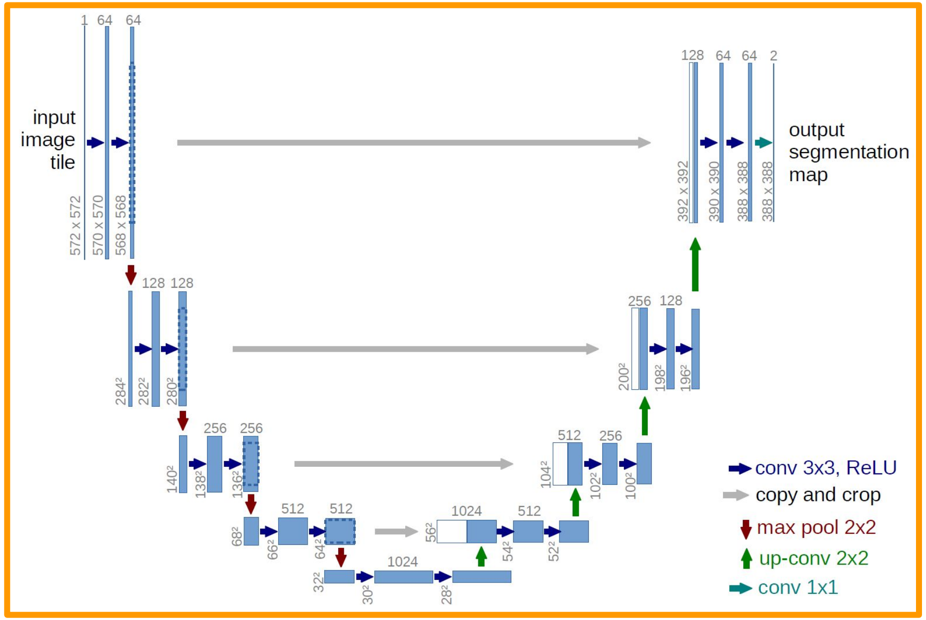
```
module_type:     "Arrakis"

# which products for the wrangler to handle
ProcessType:                 "data"  # simulation, data
ProcessMCTruth:              true
ProcessMCParticles:          true
ProcessSimEnergyDeposits:    true
ProcessSimChannels:          true
ProcessRawDigits:            true

# module labels
LArGeantProducerLabel:       "largeant"
SimEnergyDepositProducerLabel:    "IonAndScint"
SimEnergyDepositInstanceLabel:    "priorSCE"
SimChannelProducerLabel:     "tpcrawdecoder"
SimChannelInstanceLabel:     "simpleSC"
RawDigitProducerLabel:       "tpcrawdecoder"
RawDigitInstanceLabel:       "daq"

GeneratorLabels:
{
    Ar39Label:          "Ar39"
    Ar42Label:          "Ar42"
    Kr85Label:          "Kr85"
    Rn222Label:         "Rn222"
    BeamLabel:          "Beam"
    CosmicsLabel:       "Cosmics"
    HEPevtLabel:        "HEPevt"
    PNSLabel:           "PNS"
}

# which products to save
SaveMeta:        true
SaveGeometry:    true
SaveSimulationWrangler:         false    # save SimulationWrangler maps
SaveWirePlanePointCloud:        true     # save wire plane point cloud data
SaveEnergyDepositPointCloud:    true     # save energy deposit point cloud data

# whether to collect detector simulation by edep or
# by particle track id.
FilterDetectorSimulation:    "TrackID"    # ["TrackID", "EdepID"]

# labeling scheme for neutron captures,
# simple labels all gammas as "other", while medium labels
# 4.75 and 1.81 MeV gammas separately from others, and full
# labels all energies as different types.
NeutronCaptureGammaDetail:  "Simple"    # ["Simple", "Medium", "Full"]

ADCThreshold:                   20      # ADC threshold for saving points
InducedChannelInfluence:        10      # number of wires which are influenced by signals
InducedTDCInfluence:            200     # number of tdc ticks which are influenced by signals
```

FHiCL parameters

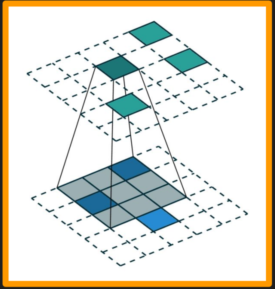
Config file training/evaluation

BLIP models can be constructed at run time with tunable parameters.

- The long term goal is to make a completely modular setup so that different models can be chained together.
- Model parameters/weights are saved in a config dictionary for reproducability.




```yaml
model:
  # uncomment the line below and specify the model to load from a checkpoint.
  # load_model:   ".checkpoints/checkpoint_200.ckpt"

  # multiple options for model_type:
  # [ "single", "composite", ... ]
  model_type: "single"
  PointNet:
    input_dimension:        3
    classifications:        ["particle"]
    augmentations:
      jitter: 0.03
      flip:
        positions:      [0, 1]
        probabilities: [0.5, 0.5]
      shear:  0.2
      rotate:
        degrees:   [15]
        axis:      [2]
    number_of_augmentations:  5
    embedding_type:         "dynamic_edge_conv"
    number_of_embeddings: 4
    number_of_neighbors:  [5, 10, 15, 20]
    aggregation:            ["max", "add", "mean", "max"]
    embedding_mlp_layers: [
      [64, 128, 64],
      [64, 128, 64],
      [64, 128, 64],
      [64, 128, 64]
    ]
    embedding_activations: ['leru', 'leru', 'leru', 'leru']
    linear_output:          512
    mlp_output_layers:      [512, 256, 128, 64, 32]
    out_channels:           [10]
```



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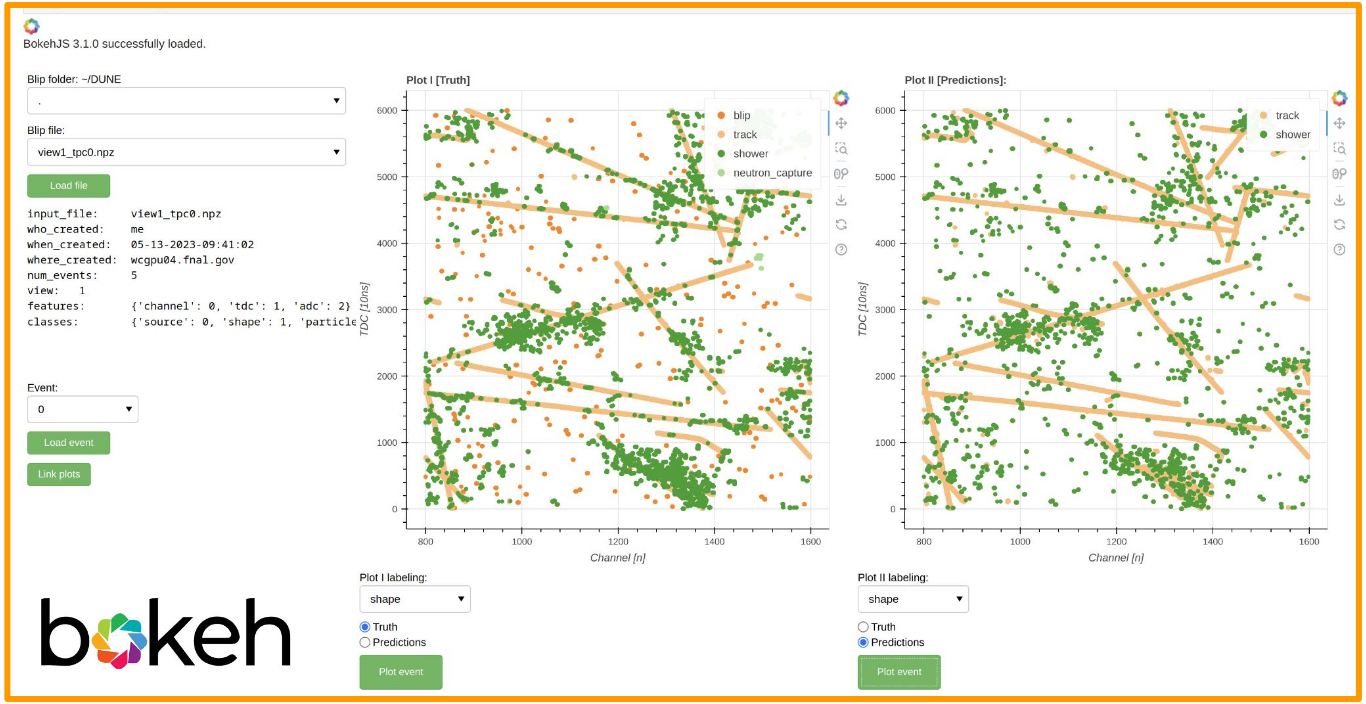
Event display

We are also working on an event display for BLIP which has the following features:

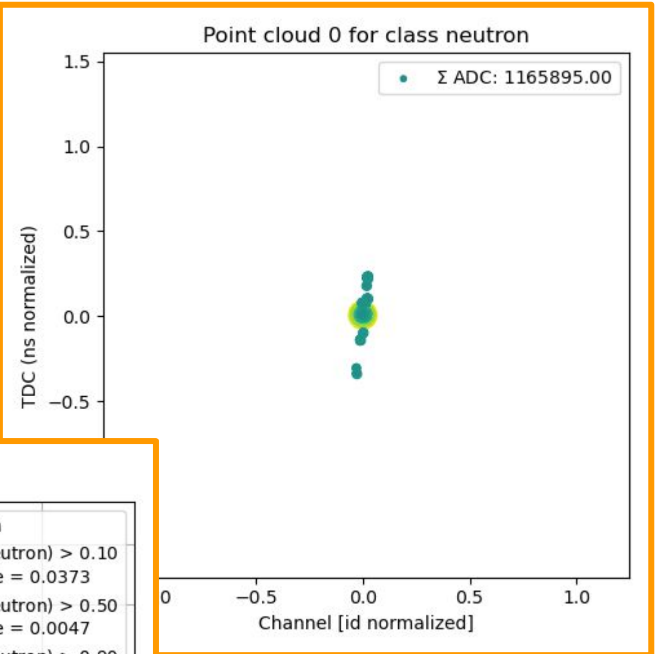
- Uses *bokeh* to create an interactive GUI.
- GUI can be run in a Jupyter notebook, or as a stand-alone html page.
- Obtain **point by point information** to quickly diagnose/access Arrakis and BLIP performance.
- Interface for analysis on network output.
- The BLIP-display could be made accessible through a **Wilson Cluster** jupyter interface.

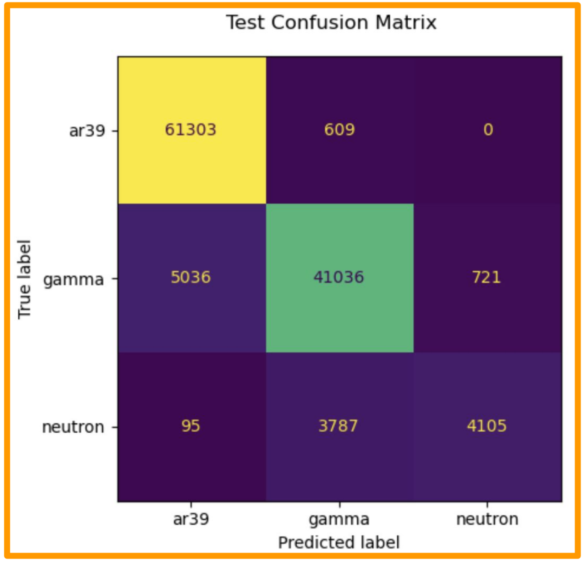


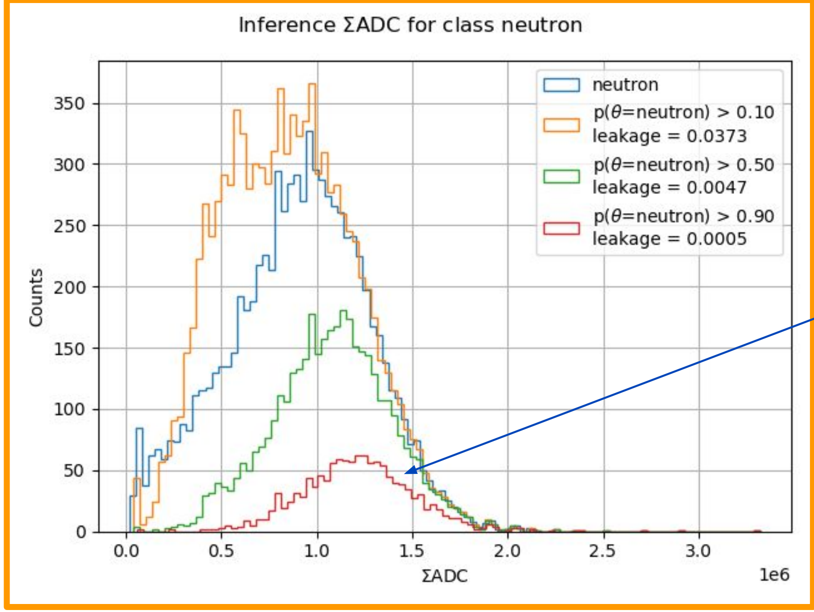
Preliminary PointNet Results

We trained a BLIP model on 116K point clouds with a 70/30 train/test split and the following classes:

- Argon-39: 61,912 events (~53%)
- Capture Gammas: 46,793 events (~40%)
- Neutron Captures: 7,987 events (~7%)







Can calibrate against this distribution!

UC DAVIS