End-to-end ML-based Reconstruction Chain for the DUNE Near Detector

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on behalf of the SLAC ML group

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U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

ML for LArTPCs

SLAC Group

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At SLAC, research supported by DoE ML grants (**K. Terao**):

- **Deep-learning-based data reconstruction chain for liquid argon time-projection chambers**
- μBOONE, pDUNE, ICARUS, ArgonCube 2x2, DUNE

Group consists of three **scientists**, three **postdocs**, three **grad students**

T. Usher
ICARUS

F. Drielsma
ICARUS

Q. Lin
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L. Domine
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P. Tsang
pDUNE

R. Itay
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D.H. Koh
ICARUS

P. Cotes de Soux

High rate LArTPCs

DUNE ND

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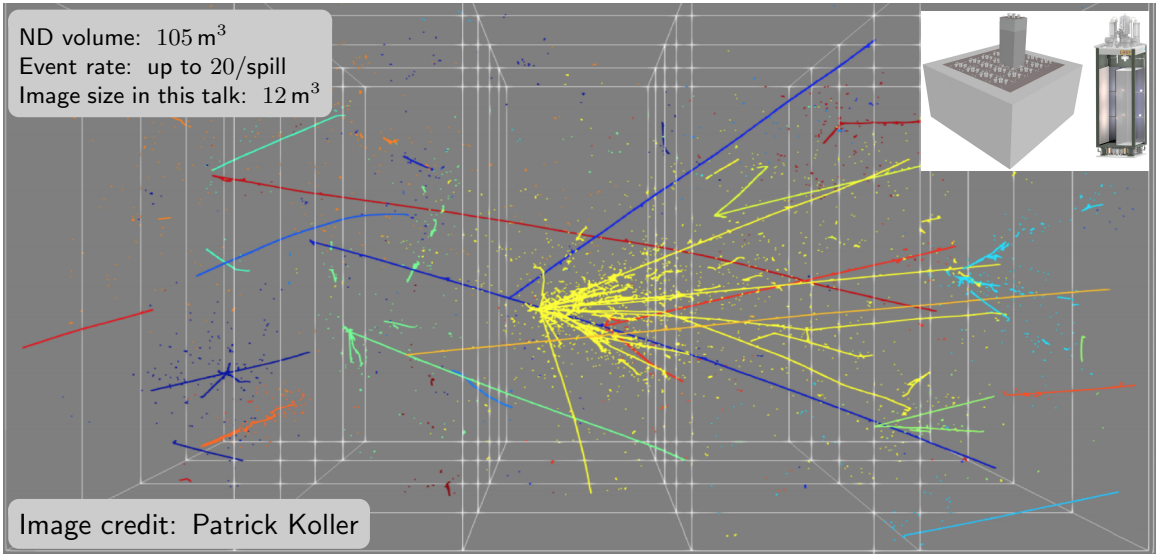

High rate LArTPCs | NuMI Example

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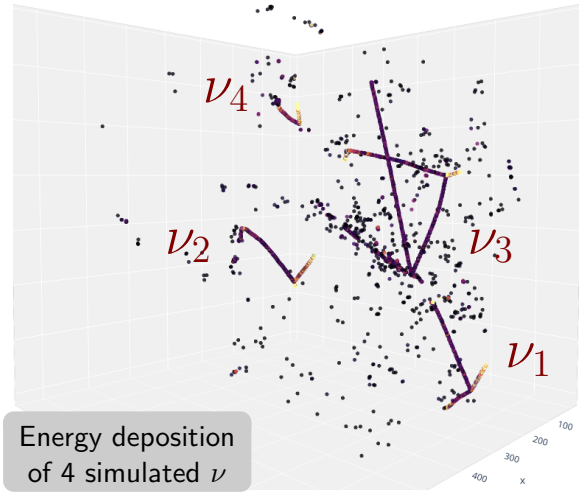

Energy deposition of 4 simulated ν

ν_1 0.70 GeV ν_μ CC interaction

- 0.17 GeV μ^-, 1.09 GeV p^+, 0.37 GeV π^+

ν_2 0.81 GeV ν_μ CC interaction

- 0.30 GeV μ^- (32 MeV e^-), 1.13 GeV p^+, 0.99 GeV p^+

ν_3 3.14 GeV ν_μ CC interaction

- Primary: 1.81 GeV μ^-, 0.88 GeV π^+, 0.22 GeV $\pi^0 \rightarrow$ (198 MeV γ + 24 MeV γ)
- Secondary: 0.31 GeV π^-, 1.03 GeV p^+
- Tertiary: 1.02 GeV p^+

ν_4 0.35 GeV ν_μ CC interaction

- 0.18 GeV μ^- (24 MeV e^-), 1.06 GeV p^+

High rate LArTPCs

NuMI Example

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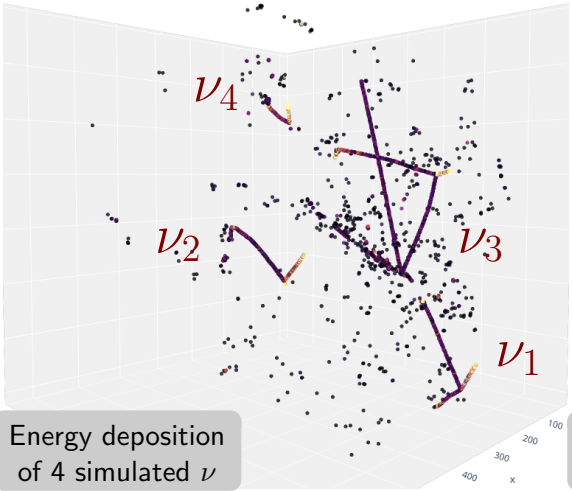
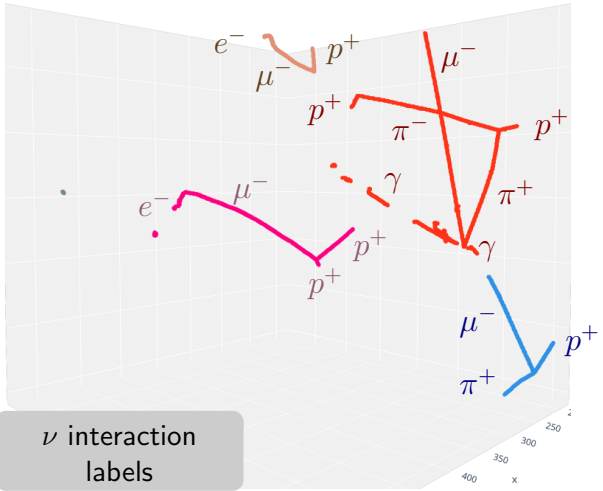


Energy deposition of 4 simulated ν



ν interaction labels

High rate LArTPCs

NuMI Example

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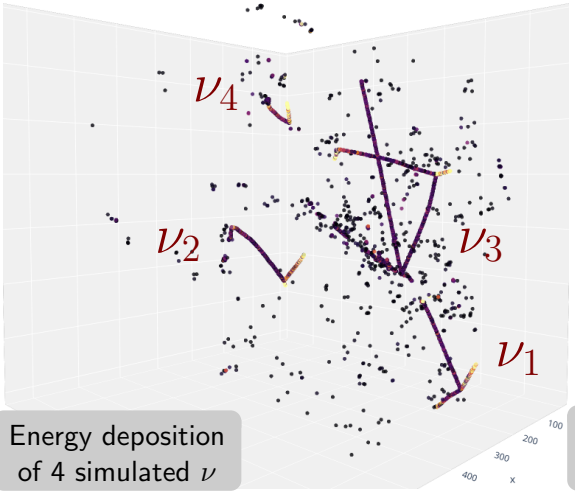
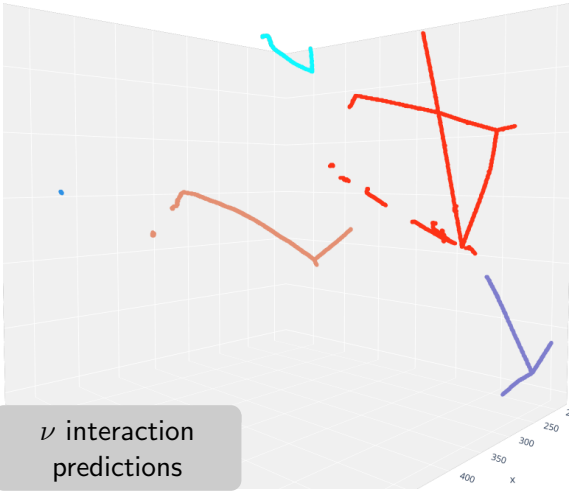


Energy deposition of 4 simulated ν



ν interaction predictions

High rate LArTPCs

NuMI Example

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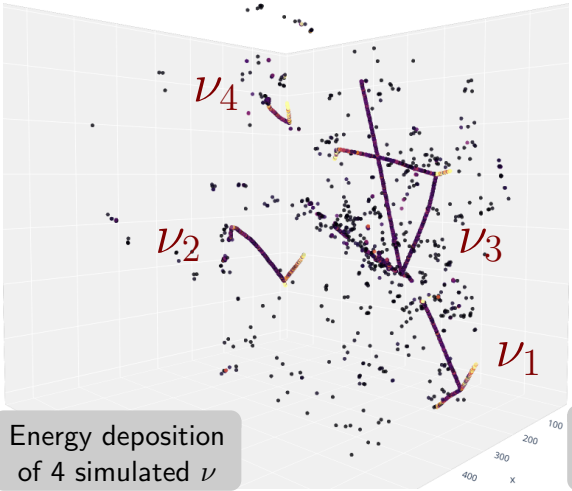
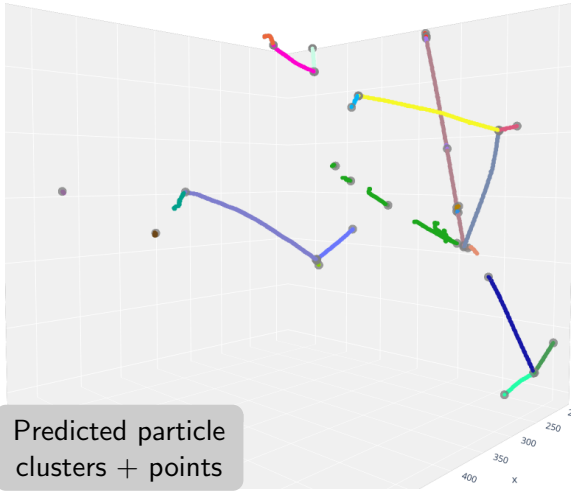
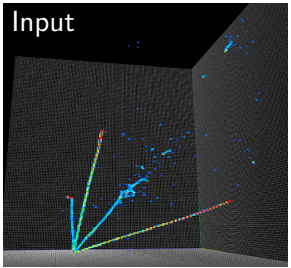


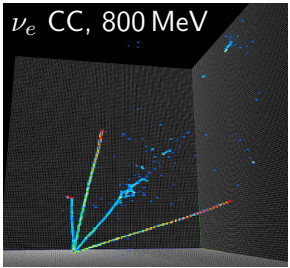
Energy deposition of 4 simulated ν

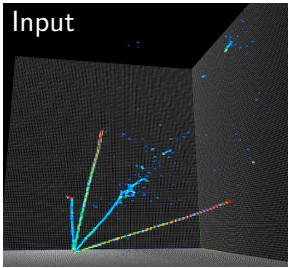


Predicted particle clusters + points

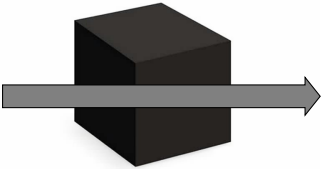
Hierarchical feature extraction | Big Picture

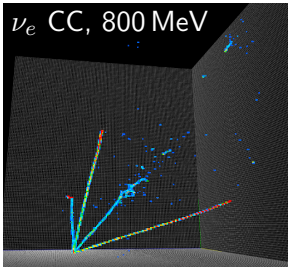






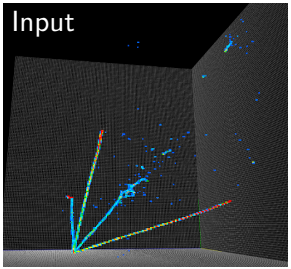
CNN ?





Hierarchical feature extraction | Big Picture

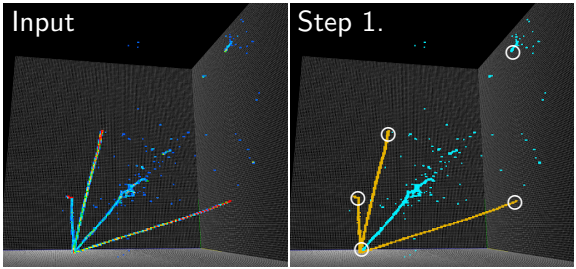
Enforce extraction of **hierarchical physics features**



Hierarchical feature extraction | Big Picture

Enforce extraction of **hierarchical physics features**

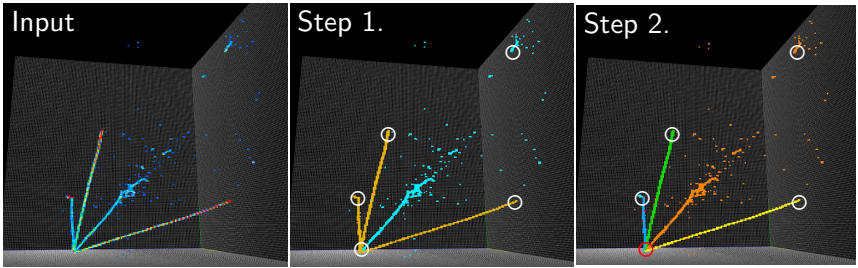
1. Pixel feature extraction + key points (particle start/end)



Hierarchical feature extraction | Big Picture

Enforce extraction of **hierarchical physics features**

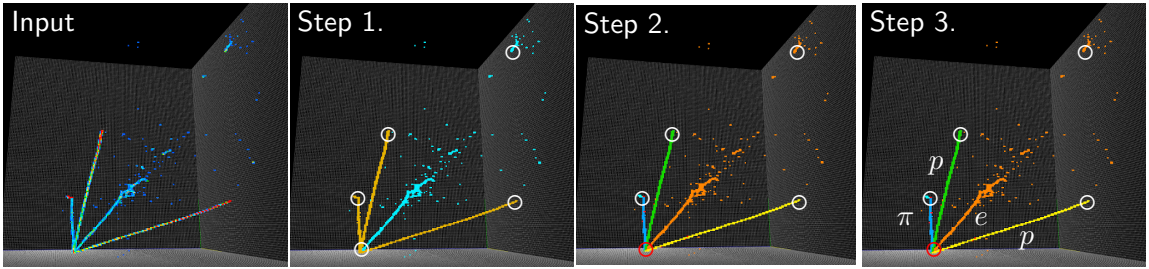
1. Pixel feature extraction + key points (particle start/end)
2. Vertex finding + particle clustering



Hierarchical feature extraction | Big Picture

Enforce extraction of **hierarchical physics features**

1. Pixel feature extraction + key points (particle start/end)
2. Vertex finding + particle clustering
3. Particle type + energy/momentum



Hierarchical feature extraction | Big Picture

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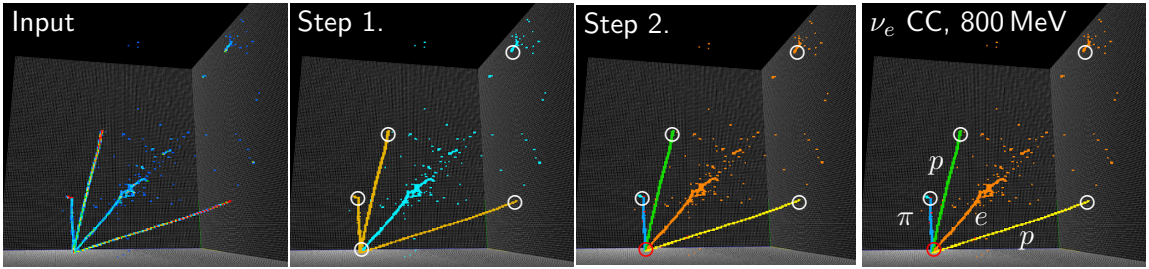
Enforce extraction of **hierarchical physics features**

1. Pixel feature extraction + key points (particle start/end)
2. Vertex finding + particle clustering
3. Particle type + energy/momentum
4. Interaction (particle flow) reconstruction



Hierarchical feature extraction | Big Picture

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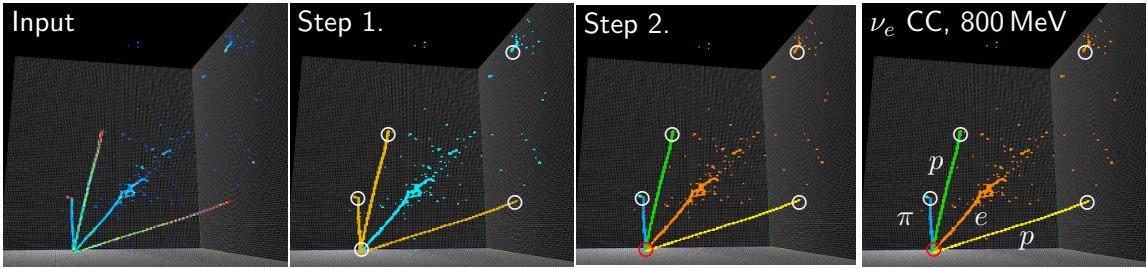
Enforce extraction of **hierarchical physics features**

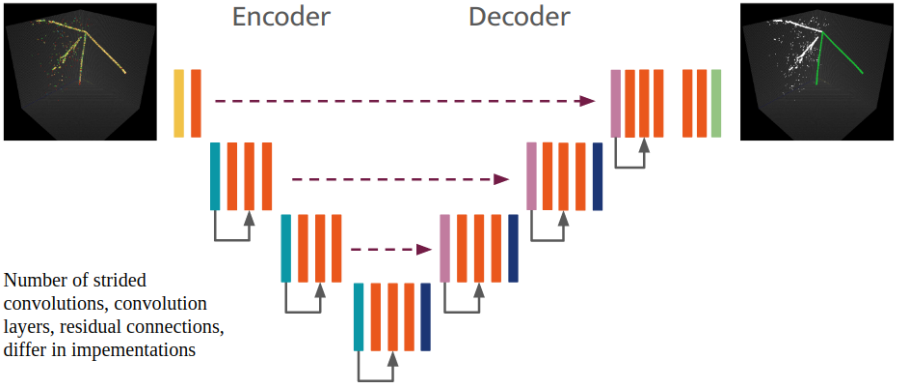
1. Pixel feature extraction + key points (particle start/end)
2. Vertex finding + particle clustering
3. Particle type + energy/momentum
4. Interaction (particle flow) reconstruction

Whole chain can be optimized together



Pixel feature extraction | Architecture

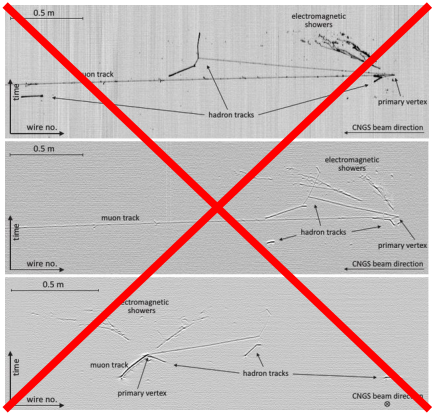
UNet + Residual connections + Sparse convolution → **Sparse UResNet**



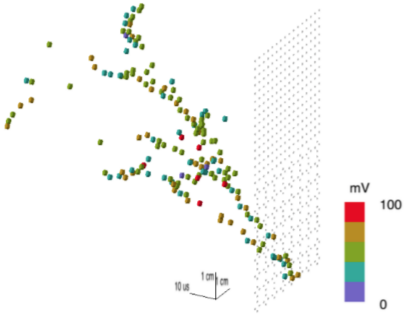
arXiv:1903.05663

L. Domine

Pixel feature extraction | Input

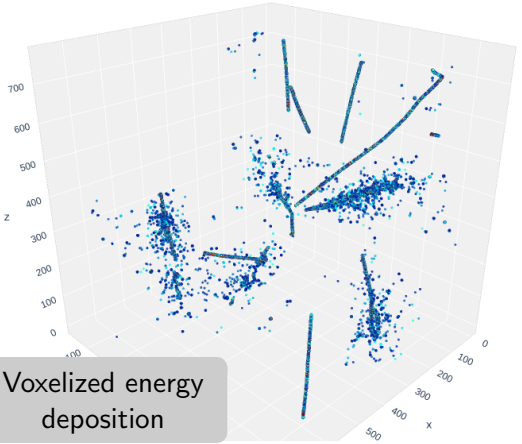


ICARUS, arXiv:1210.5089

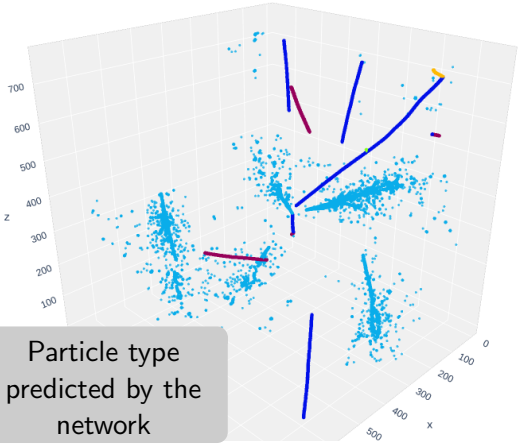


LArPix, arXiv:1808.02969

Pixel feature extraction | Particle type



Voxelized energy deposition



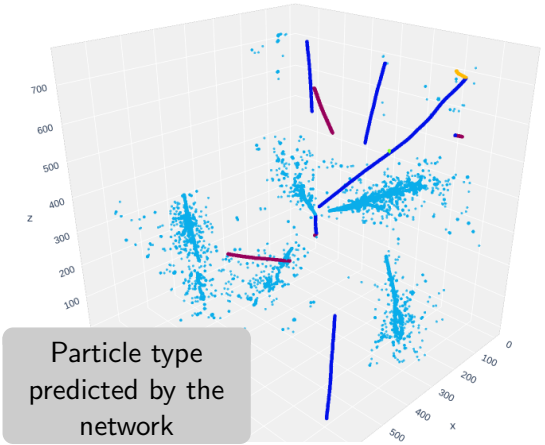
Particle type predicted by the network

Pixel feature extraction | Particle type

Particle type identification accuracy:

Particle type	Voxel fraction	Accuracy
HIP	17 %	98.2 %
MIP	34 %	99.4 %
Showers	47 %	99.2 %
Delta rays	1 %	96 %
Michel	1 %	94.7 %
Total		**99 %**

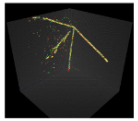
Network adapted to very sparse data,
see paper for details: arXiv:1903.05663

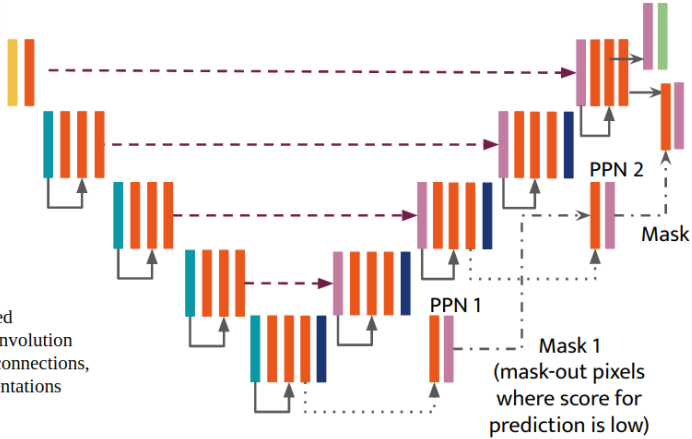


Particle type predicted by the network

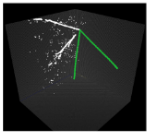
Pixel feature extraction

Point proposal





Number of strided convolutions, convolution layers, residual connections, differ in impementations

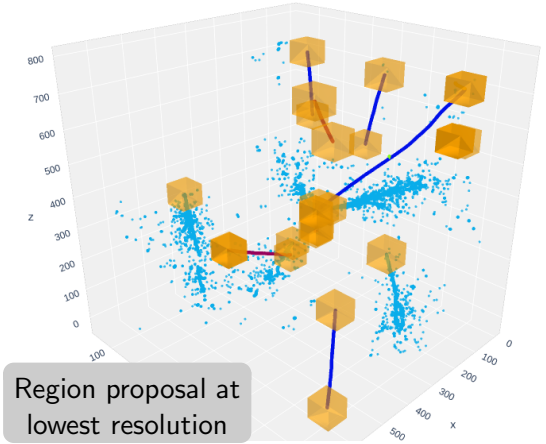


input
conv
conv-s2-finc
tconv-s2-fde
conv-fdec
softmax
Residual connections
Concatenation

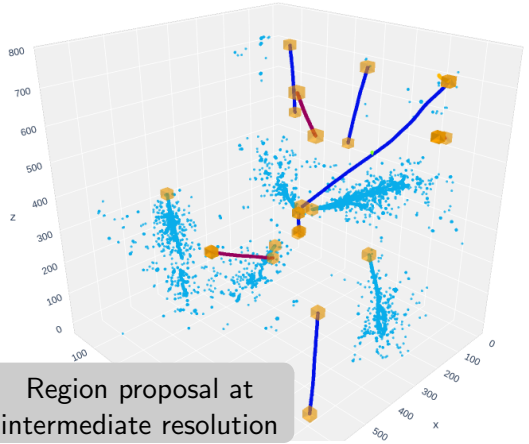
doi.org/10.5281/zenodo.1300713

L. Domine

Pixel feature extraction | Point proposal



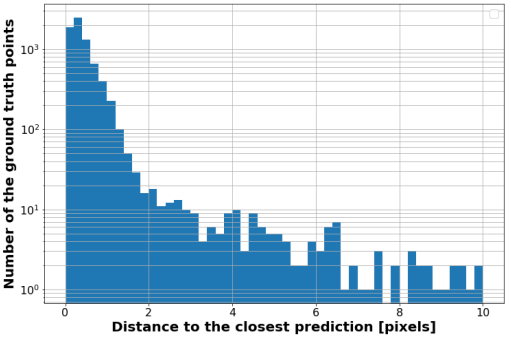
Region proposal at lowest resolution

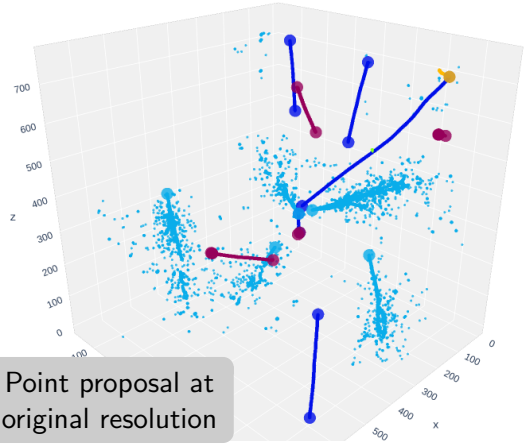


Region proposal at intermediate resolution

Pixel feature extraction | Point proposal

Point proposal efficiency (97 % $<$ 10 px):



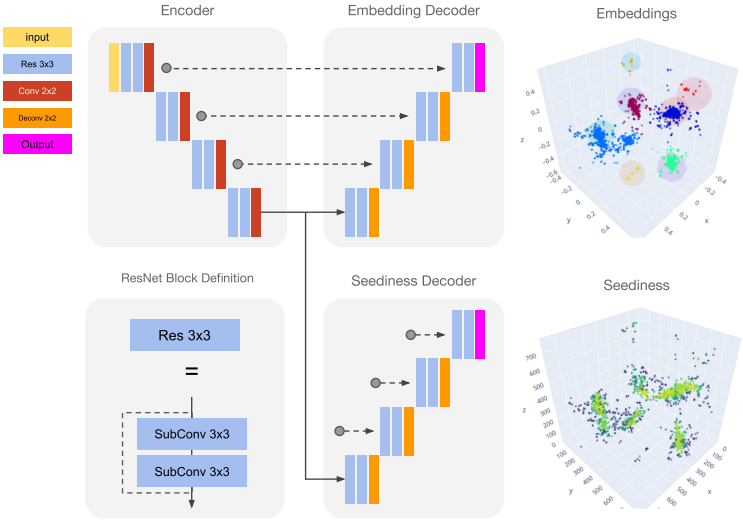


Point proposal at original resolution

doi.org/10.5281/zenodo.1300713

Pixel feature extraction

Dense clustering



Network predicts 3 things:

- **Embedding**: space in which fragments are spatially separated
- **Seediness**: likelihood that a voxel is a cluster centroid in embedding space
- **Margin**: Size of the cluster in embedding space

D. H. Koh

arXiv:1906.11109

Pixel feature extraction

Dense clustering

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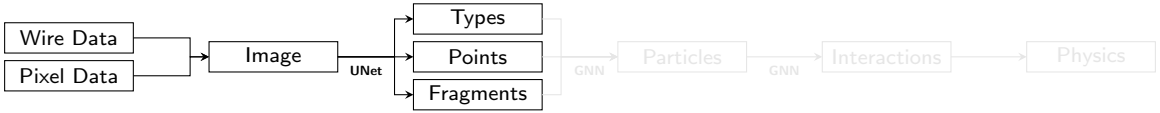
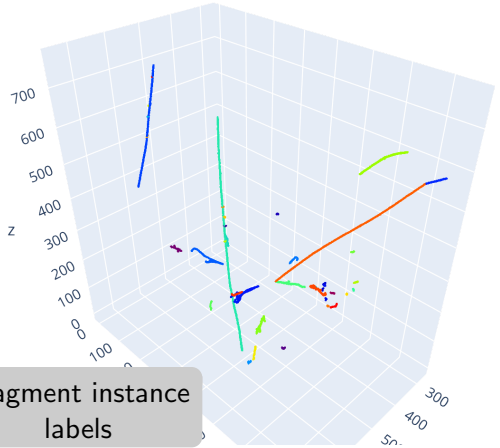
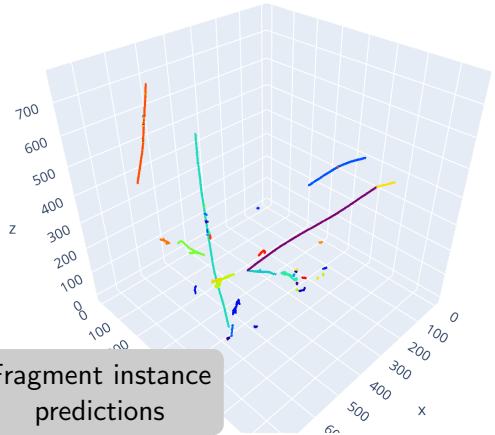


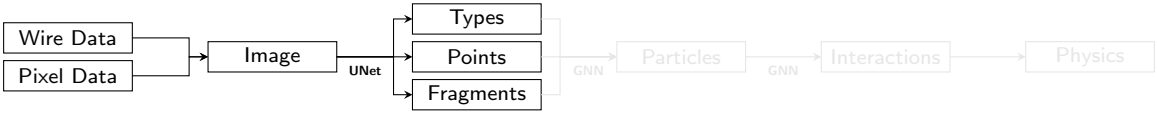


Fragment instance labels



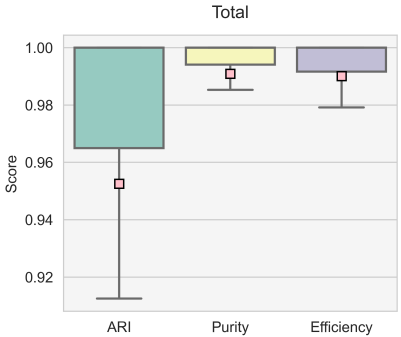
Fragment instance predictions

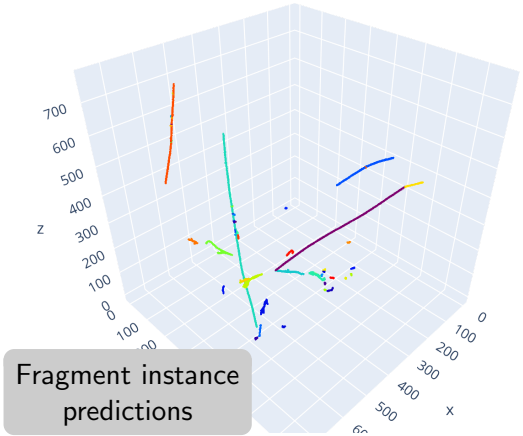
Pixel feature extraction



Dense clustering accuracy:

- Mean ARI: **95.2 %**





Fragment instance predictions

Shower clustering | Architecture

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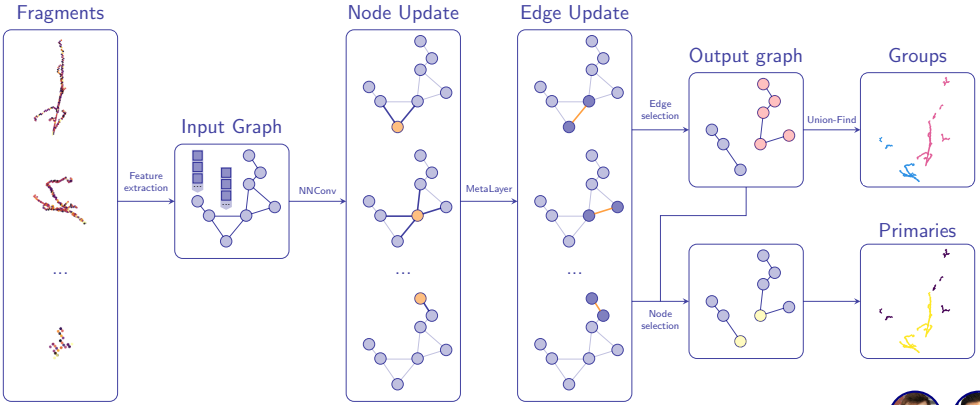
Graphical Neural Networks (GNN) are ideal to cluster spatially detached objects:

- Based on *nodes* and *edges*. Features propagate by *message passing* (MP)



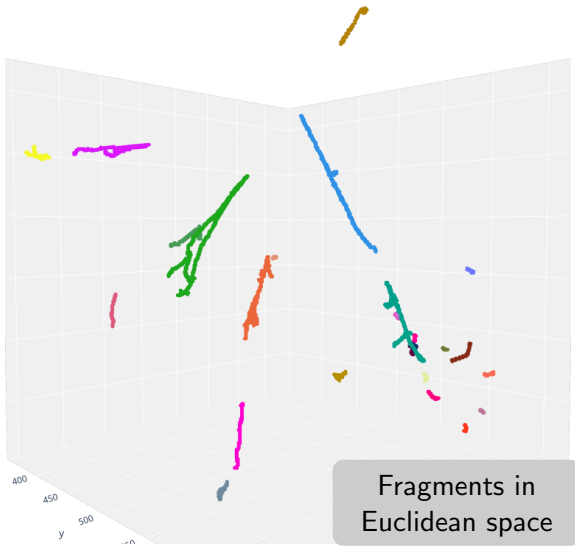
F. Drielsma, Q. Lin, P. Cotes de Soux

Shower clustering

Network input

Input:

- Fragmented EM showers



Fragments in Euclidean space

Shower clustering

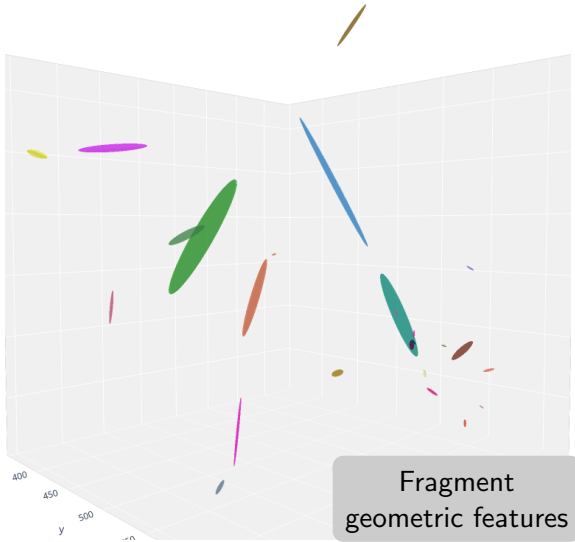
Network input

Input:

- Fragmented EM showers

Node features:

- Centroid
- Covariance matrix + PCA
- Start point + direction



Fragment geometric features

Shower clustering

Network input

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Input:

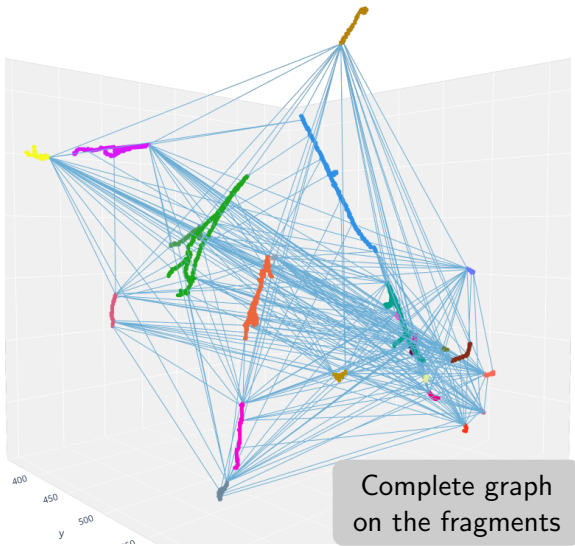
- Fragmented EM showers

Node features:

- Centroid
- Covariance matrix + PCA
- Start point + direction

Input graph:

- Connect every node with every other node (**complete graph**)



Complete graph on the fragments

Shower clustering

Network input

Input:

- Fragmented EM showers

Node features:

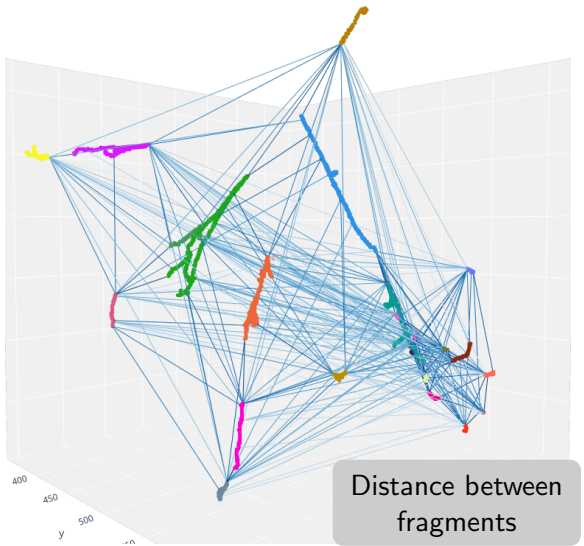
- Centroid
- Covariance matrix + PCA
- Start point + direction

Input graph:

- Connect every node with every other node (**complete graph**)

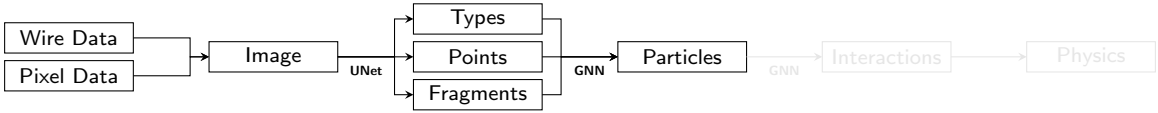
Edge features:

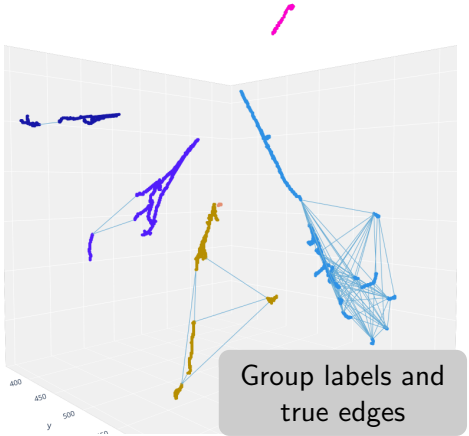
- Displacement vector (+variations)
- Closest points of approach



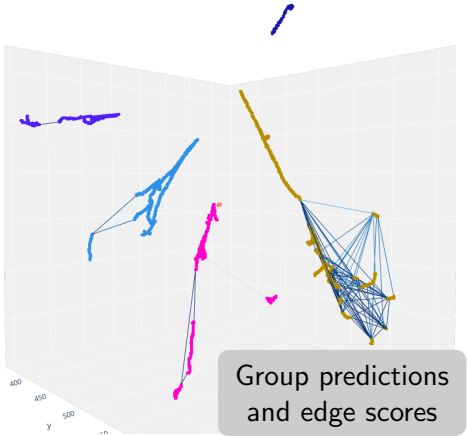
Shower clustering

Performance





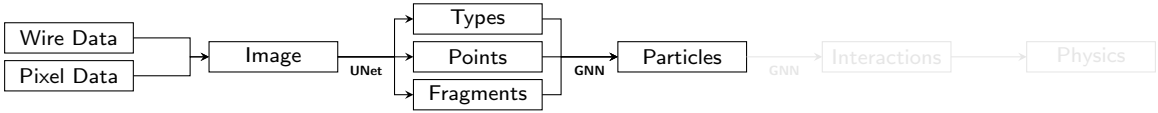
Group labels and true edges



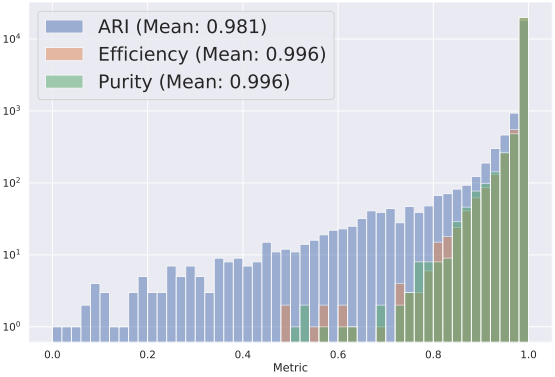
Group predictions and edge scores

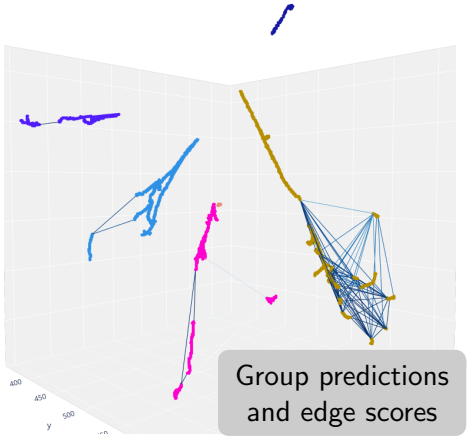
Shower clustering

Performance

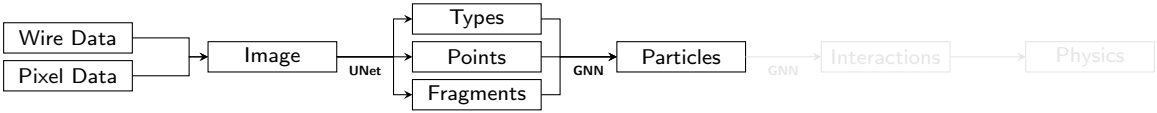


Shower clustering accuracy:





Shower Clustering | Start identification

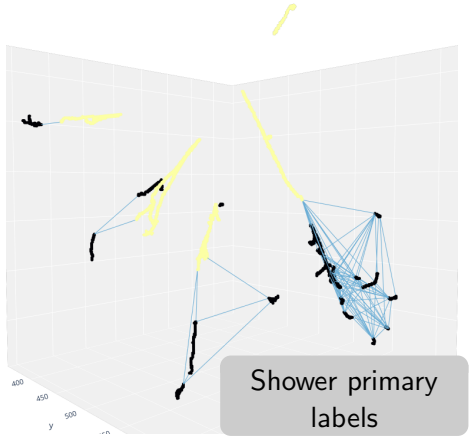


Identifying shower starts is a very useful task

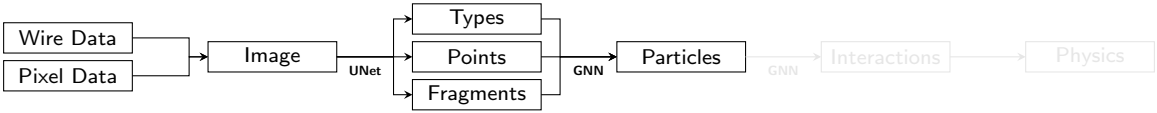
- Start point, direction
- Shower matching for π_0 reconstruction

Given the **predicted** partition of nodes:

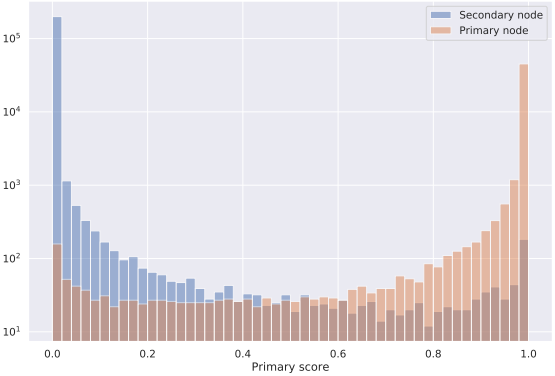
- In each group, identify the node with the highest primary score, tag as primary
- All other fragments are secondaries

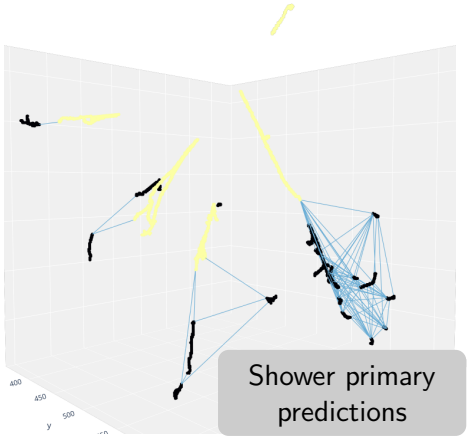


Shower Clustering | Start identification

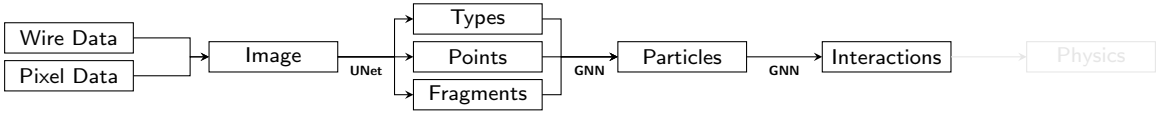


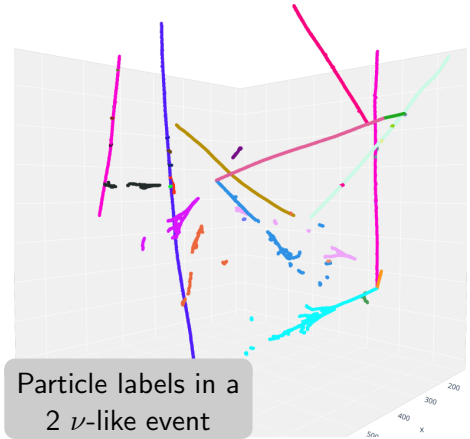
Shower primary accuracy (**99.6 %**):





Interaction Clustering | Performance





Particle labels in a 2 ν-like event

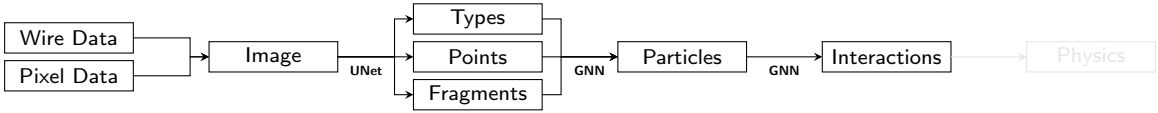
The shower clustering task can be extended to **interaction clustering**:

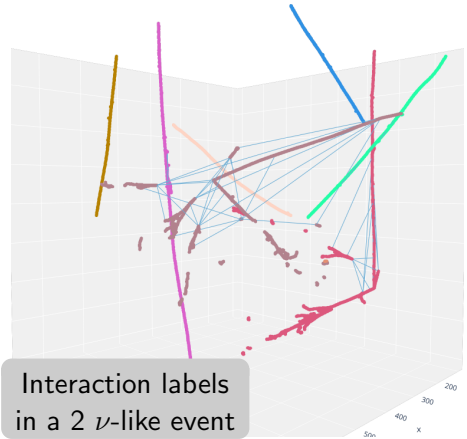
- Interaction group = particles that originate from the same vertex
- Fragment ID $\rightarrow$ Particle ID
- Particle ID $\rightarrow$ Interaction ID

Crucial to:

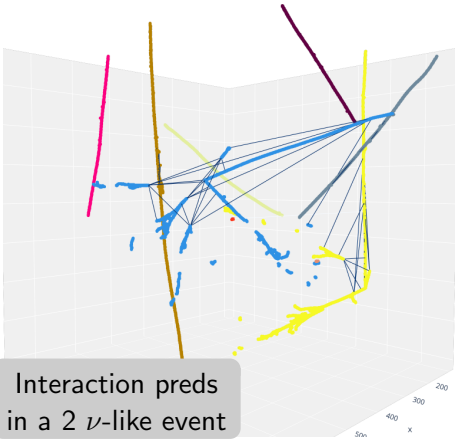
- Separate signal from background
- **Resolve pileup**

Interaction Clustering | Performance



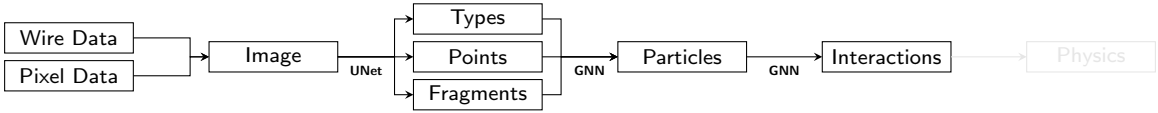


Interaction labels in a 2 ν-like event

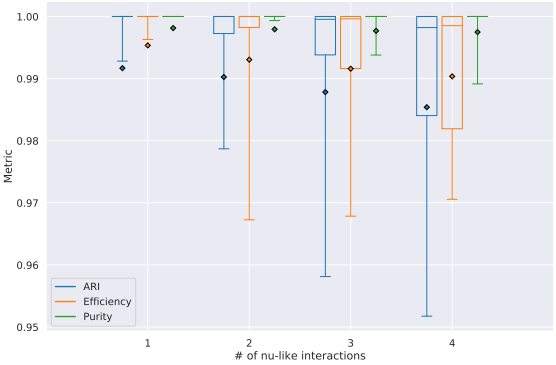


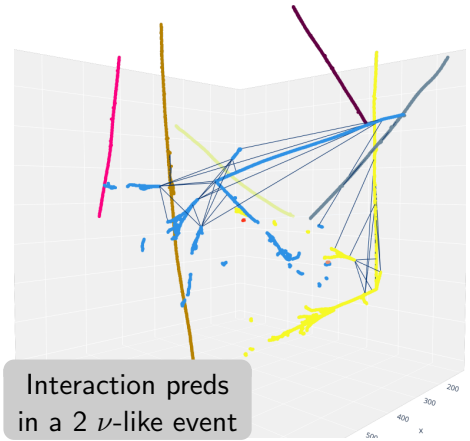
Interaction preds in a 2 ν-like event

Interaction Clustering | Performance



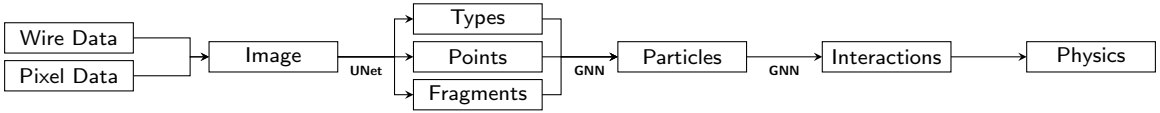
Interaction clustering performance:





Interaction preds in a 2 ν-like event

Summary



ML-based hierarchical feature extraction very successful

What is now available:

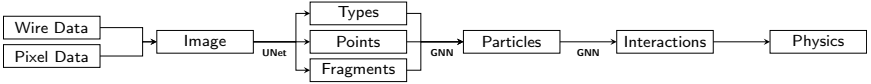
- List of interactions per event
- List of particles per interaction
- Particle class (e.g. track vs shower)
- Start and end point of particles

What we don't have:

- Momentum/energy estimation
- Particle identification
- Interaction vertex
- Particle flow

$\rightarrow$ Goals for this summer research !

Now engaging physics analysis needs in SBN/DUNE: your help is very welcome !



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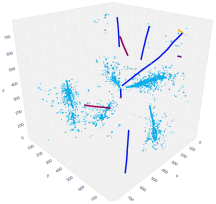
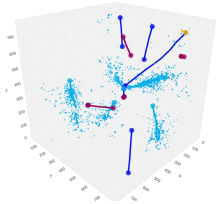
Particle types

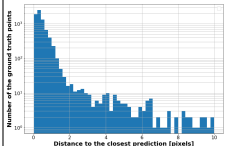


Particle type	Accuracy
HIP	98.2 %
MIP	99.4 %
Showers	99.2 %
Delta	96 %
Michel	94.7 %
Total	**99 %**

See paper for details:
arXiv:1903.05663

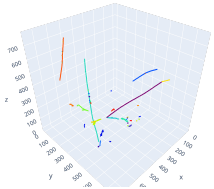
Point proposal





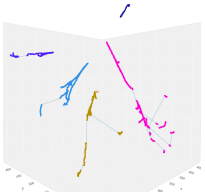
	< 10 voxels
Eff.	97.2 %
Pur.	97.6 %

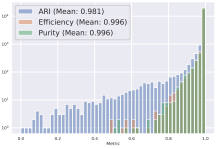
Dense clustering



	Mean
Eff.	99.0 %
Pur.	99.1 %
ARI	95.2 %
SBD	91.8 %

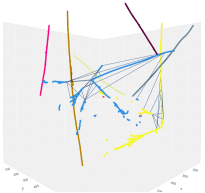
Shower clustering

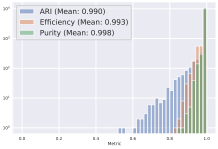




	Mean
Eff.	99.6 %
Pur.	99.6 %
ARI	98.1 %

Interaction grouping





	Mean
Eff.	99.3 %
Pur.	99.8 %
ARI	99.0 %

Here $\#\nu = 2$/image

Back-up slides

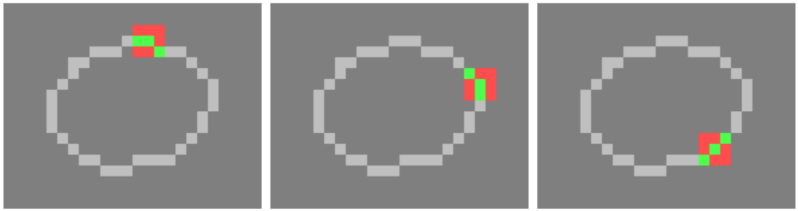
Submanifold Sparse Convolutions

1. Resources waste of dense convolutions on sparse data
2. Dilation problem
   - One nonzero site leads to 3d nonzero sites after 1 convolution
   - How to keep the same level of sparsity throughout the network?

https://arxiv.org/pdf/1711.10275.pdf

In more details, two new operations:

- Sparse convolutions (SC)
  - Discards contribution of non-active input sites
  - Output site active if at least one input site is active
- Sparse submanifold convolutions (SSC)
  - Output size = Input size
  - Output site active iff center of receptive field active
  - Only compute features for active output sites



https://arxiv.org/pdf/1711.10275.pdf

PPN outputs **voxel location**, **position within voxel** and **point class**

Three components to the point proposal loss:

- Pixel classification loss at each of three depth (pixel contains point or not)

$$\mathcal{L}_{\text{class},i} = \frac{1}{N_i} \sum_{k=1}^{N_i} y_k \log(p_k) + (1 - y_k) \log(1 - p_k)$$

- L^1 distance from true point at highest resolution **on active voxels**

$$\mathcal{L}_{\text{dist}} = \frac{1}{N_3^*} \sum_{k=1}^{N_3^*} \min_j ||\vec{p}_i - \vec{q}_j||$$

- Particle type loss at highest resolution **on active voxels**

$$\mathcal{L} = \frac{1}{N_3^*} \sum_{k=1}^{N_3^*} \sum_c y_{k,c} \log(p_{k,c})$$

Fragment clustering | Loss

Instance Segmentation:

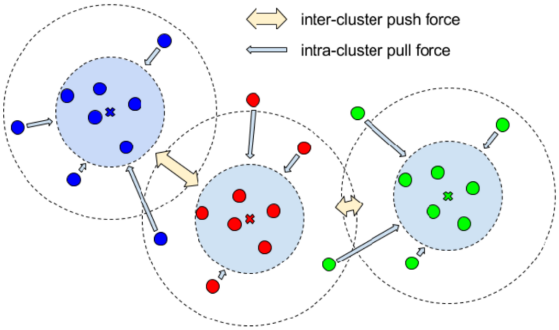
- Three component loss: pull together points that belong to the same cluster, keep distance between clusters, and regularization

$$L = \alpha L_{var} + \beta L_{dist} + \gamma L_{reg},$$

$$L_{var} = \frac{1}{C}\sum_{c=1}^{C}\frac{1}{N_c}\sum_{i=1}^{N_c}[\max(0, \|\mu_c - x_i\| - \delta_v)]^2$$

$$L_{dist} = \frac{1}{C(C-1)}\sum_{\substack{c_A,c_B=1 \\ c_A \neq c_B}}^{C}[\max(0, 2\delta_d - \|\mu_{c_A} - \mu_{c_B}\|)]^2$$

$$L_{reg} = \frac{1}{C}\sum_{c=1}^{C}\|\mu_c\|$$

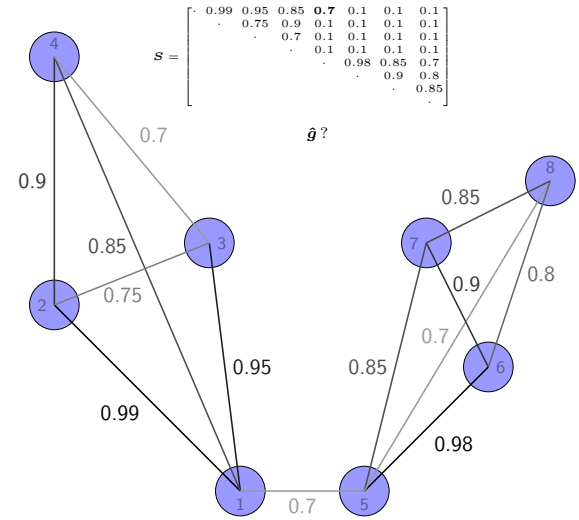


arXiv:1708.02551

Shower clustering

The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

- How to recover a set partition $\hat{\boldsymbol{g}}$?

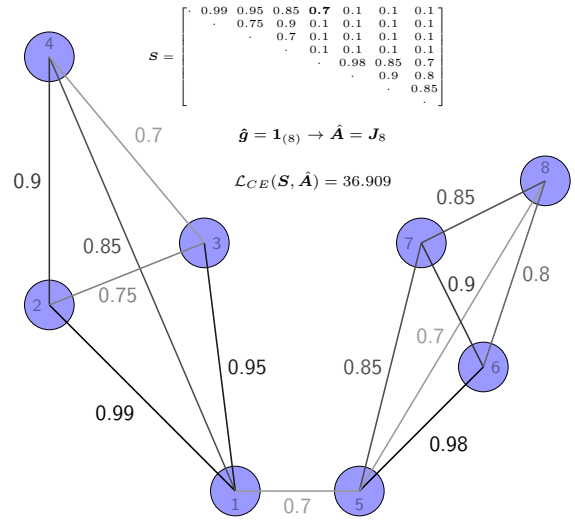


The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

- How to recover a set partition $\hat{\boldsymbol{g}}$?

We want the partition $\hat{\boldsymbol{g}}$ that minimizes the CE loss, given $\hat{A}_{ij} = \delta_{\hat{g}_i, \hat{g}_j}$, e.g.

$$\hat{\boldsymbol{g}} = \min_{\boldsymbol{g} \in G} \mathcal{L}_{CE}(\boldsymbol{S}, \hat{\boldsymbol{A}}(\boldsymbol{g}))$$



Shower clustering

Inference

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The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

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$$\hat{\boldsymbol{g}} = \min_{\boldsymbol{g} \in G} \mathcal{L}_{CE}(\boldsymbol{S}, \hat{\boldsymbol{A}}(\boldsymbol{g}))$$

G is the set of all possible partitions

- Bell number, huge ($B_{20} \simeq 5 \times 10^{13}$), cannot brute force, how to optimize?
- Start with an empty graph

$$\boldsymbol{S} = \begin{bmatrix} \cdot & 0.99 & 0.95 & 0.85 & \mathbf{0.7} & 0.1 & 0.1 & 0.1 \\ & \cdot & 0.75 & 0.9 & 0.1 & 0.1 & 0.1 & 0.1 \\ & & \cdot & 0.7 & 0.1 & 0.1 & 0.1 & 0.1 \\ & & & \cdot & 0.1 & 0.1 & 0.1 & 0.1 \\ & & & & \cdot & 0.98 & 0.85 & 0.7 \\ & & & & & \cdot & 0.9 & 0.8 \\ & & & & & & \cdot & 0.85 \\ & & & & & & & \cdot \end{bmatrix}$$

$$\hat{\boldsymbol{g}} = (1, 2, 3, 4, 5, 6, 7, 8) \rightarrow \hat{\boldsymbol{A}} = \boldsymbol{I}_8$$

$$\mathcal{L}_{CE}(\boldsymbol{S}, \hat{\boldsymbol{A}}) = 29.998$$

The network predicts a score matrix $\boldsymbol{S}$, estimate of the true adjacency matrix $\boldsymbol{A}$

- How to recover a set partition $\hat{\boldsymbol{g}}$?

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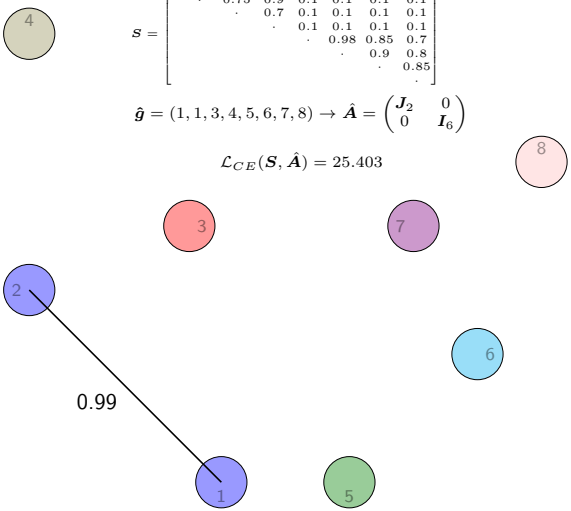
- Start with an empty graph
- Iteratively attempt to add most likely edges until edge score < 0.5

$$\boldsymbol{S} = \begin{bmatrix} \cdot & 0.99 & 0.95 & 0.85 & \mathbf{0.7} & 0.1 & 0.1 & 0.1 \\ & \cdot & 0.75 & 0.9 & 0.1 & 0.1 & 0.1 & 0.1 \\ & & \cdot & 0.7 & 0.1 & 0.1 & 0.1 & 0.1 \\ & & & \cdot & 0.1 & 0.1 & 0.1 & 0.1 \\ & & & & \cdot & 0.98 & 0.85 & 0.7 \\ & & & & & \cdot & 0.9 & 0.8 \\ & & & & & & \cdot & 0.85 \\ & & & & & & & \cdot \end{bmatrix}$$

$$\hat{\boldsymbol{g}} = (1, 1, 3, 4, 5, 6, 7, 8) \rightarrow \hat{\boldsymbol{A}} = \begin{pmatrix} \boldsymbol{J}_2 & 0 \\ 0 & \boldsymbol{I}_6 \end{pmatrix}$$

$$\mathcal{L}_{CE}(\boldsymbol{S}, \hat{\boldsymbol{A}}) = 25.403$$



Shower clustering

Inference

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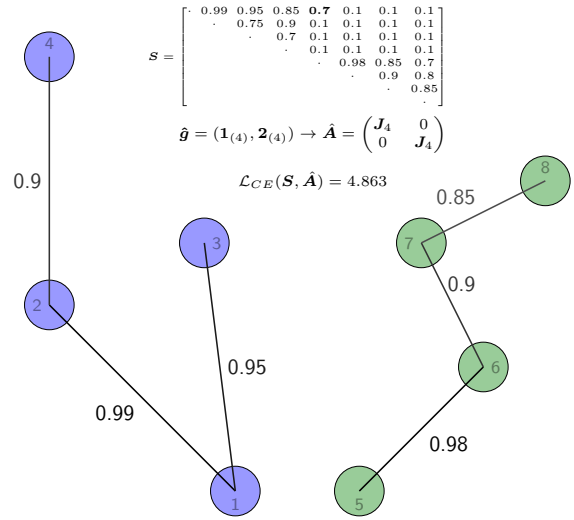


Shower clustering

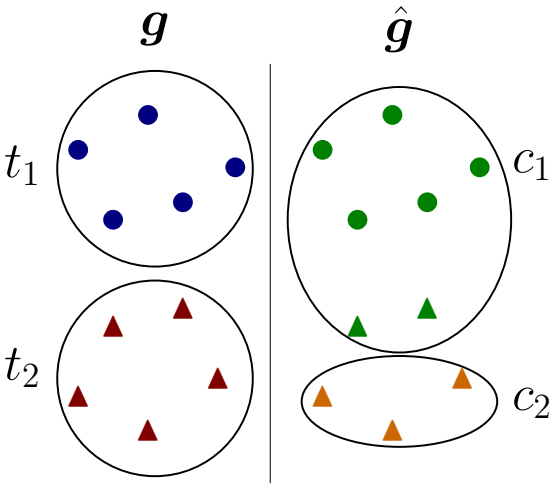
Metrics

Purity $= \frac{1}{N}\sum_{i=1}^{n_p} \max_j |c_i \cap t_j|$

- c_i predicted cluster
- t_j true cluster with highest count in c_i

Efficiency $= \frac{1}{N}\sum_{i=0}^{n_t} \max_j |c_j \cap t_i|$

- c_j pred. cluster with highest count in t_i
- t_i true cluster



Purity $= \frac{1}{N}\sum_{i=1}^{n_p} \max_j |c_i \cap t_j|$

- c_i predicted cluster
- t_j true cluster with highest count in c_i

Efficiency $= \frac{1}{N}\sum_{i=0}^{n_t} \max_j |c_j \cap t_i|$

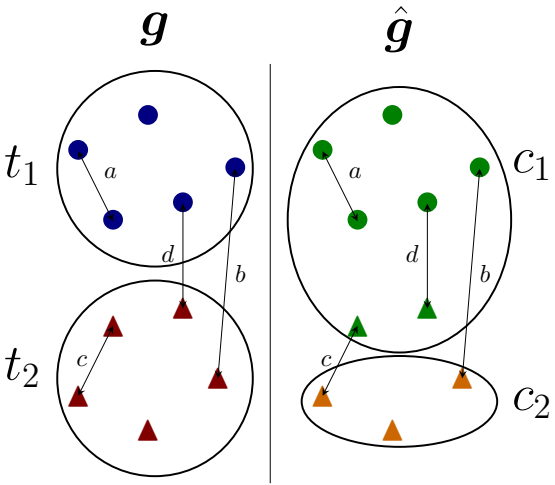
- c_j pred. cluster with highest count in t_i
- t_i true cluster

Adjusted Rand Index (ARI)

- Measure of overlap of prediction and truth, adjusted for random chance

$\text{RI} = \frac{a+b}{a+b+c+d}$

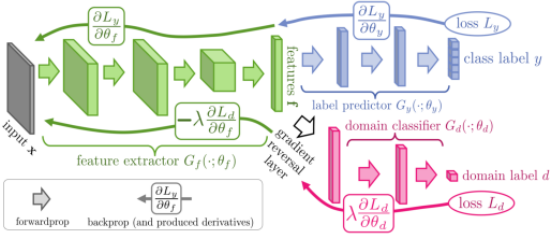
$\text{ARI} = \frac{RI - E(RI)}{1 - E(RI)}$



Domain discrepancies | GAN

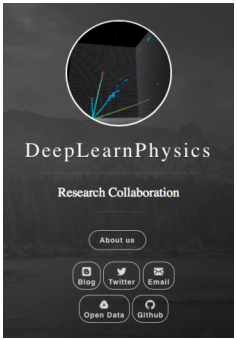
What can we do about imperfect simulation ?

- Issue: the signal distribution learned by the algorithm may be different in two domains!
- Mitigation techniques in ML domain ?
  - Can try CNN to locate where it is
  - Can try CNN to fix the discrepancy
  - Can try a training technique to minimize the effect



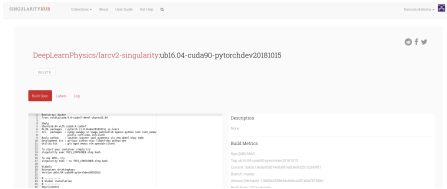
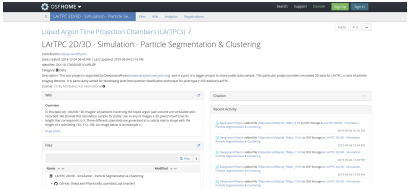
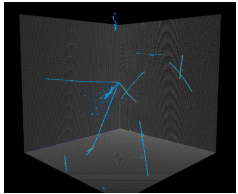
Maximize the loss to discriminate data vs. simulation, feature extractors are penalized to key on simulation specific information

Domain-Adversarial Training of Neural Networks: J. Mach. Learn. Res. 17 (2016)



DeepLearnPhysics: Collaboration for ML technique R&D

- Open simulation sample (used throughout this talk)
  - Open real data ? Soon ! (3D prototype R&D at SLAC)
- Open source container (Singularity)
- Open source code (GitHub)
  - All the code used to make this talk is available

→ **Reproducible results** !

- Readers have reproduced arXiv:1903.05663