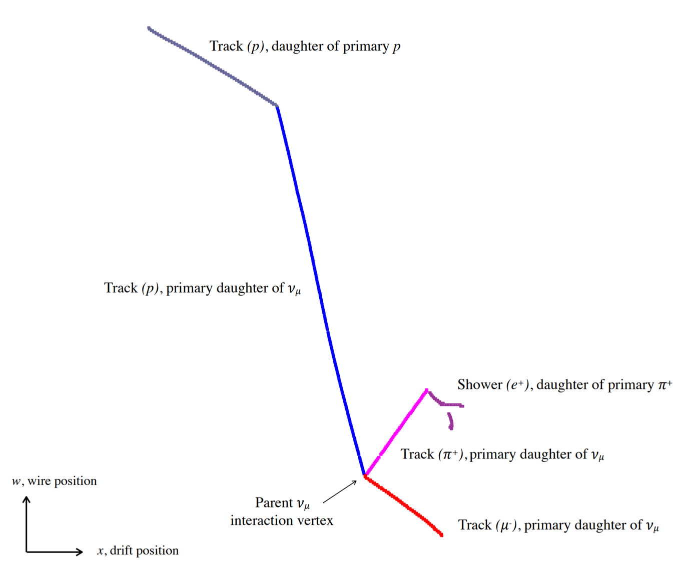
NuGraph3: Toward Full LArTPC Reconstruction using GNNs

Adam Aurisano, for the Exa.TrkX/NuGraph Collaboration

Department of Physics, University of Cincinnati – adam.aurisano@uc.edu

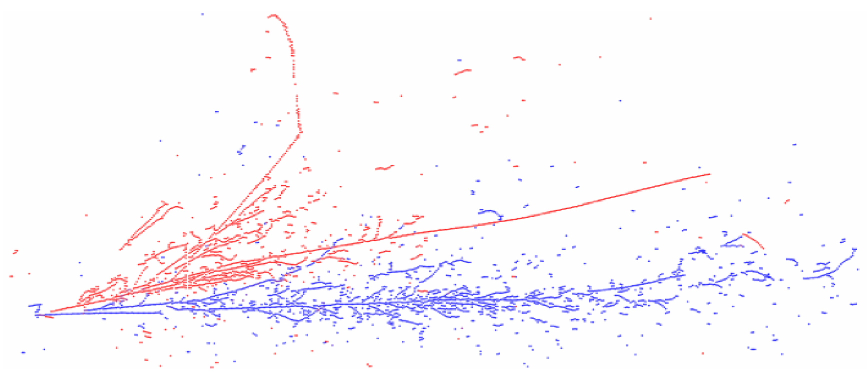
Traditional Reconstruction

- Standard reconstruction package for LArTPC experiments is Pandora
- Large number of pattern recognition algorithms applied adaptively in a series of stages
- Goal: build a full particle hierarchy
  - Low-level objects stitched together into high-level particles
  - High-level particles stitched into an event



R. Acciarri et al, arXiv:1708.031351

- Pandora is sophisticated, but with some shortcomings
  - Starts with 2D reconstruction
    - Some ambiguities cannot be resolved in later stages
  - Reconstruction is largely serial
    - Pathologies in early stages compound in later stages

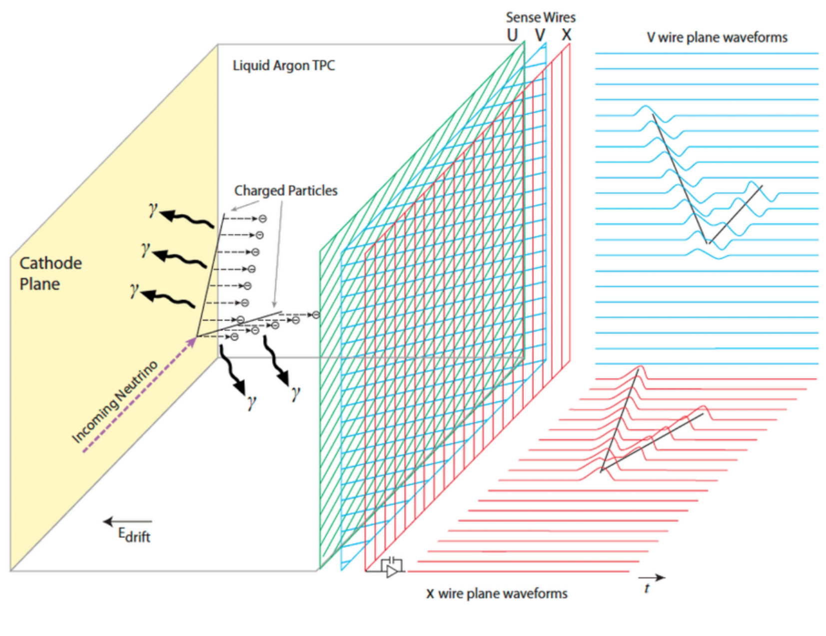


See **posters #130 and #389** in this session for more details on using GNNs for tau neutrino identification

- Tau neutrino events are important analysis target in the DUNE era
  - Frequently high multiplicity
  - Separating from other interactions requires excellent reconstruction of internal kinematics
- Success depends on avoiding reconstruction pathologies

NuGraph2

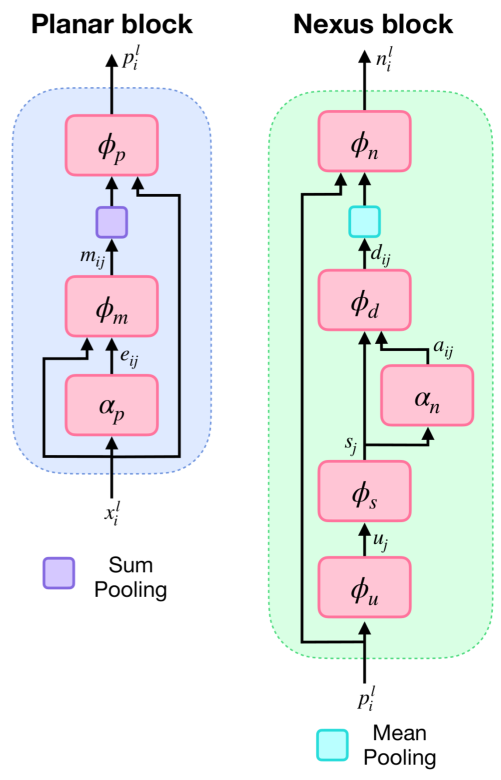
- Graphs are a mathematical structure that represents objects **(nodes)** and binary relations between them **(edges)**
- Message-passing graph neural networks iteratively learn smart embedding of graph structure
  - Graph structure provide **inductive bias** to improve learning for problem being solved
- NuGraph2 is designed to classify each detector hit according to the type of particle that created it



Use separately reconstructed 3D space-points as **nexus nodes**

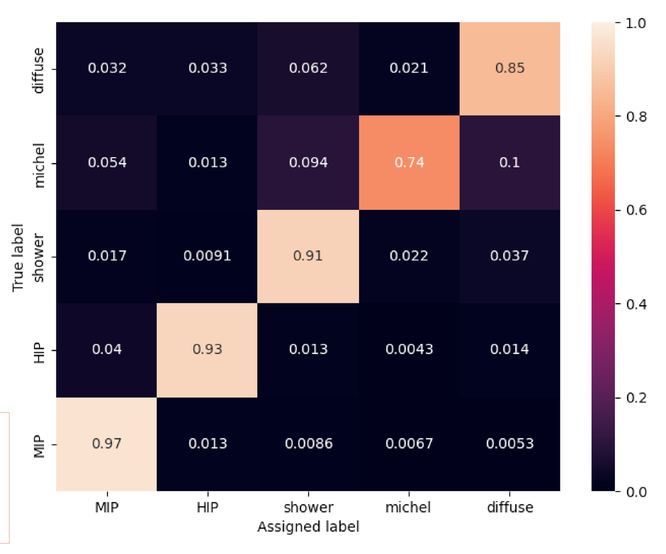
Use 2D hits from each detector plane as **planar nodes**

- TPC design provides three 2D measurements of energy deposits
- Constant drift time allows for hits to be associated for 3D hit reconstruction
- Incorporate information through message passing within three planar graphs **and** between 3D nexus nodes
  - Allows algorithm to learn consistency between planes



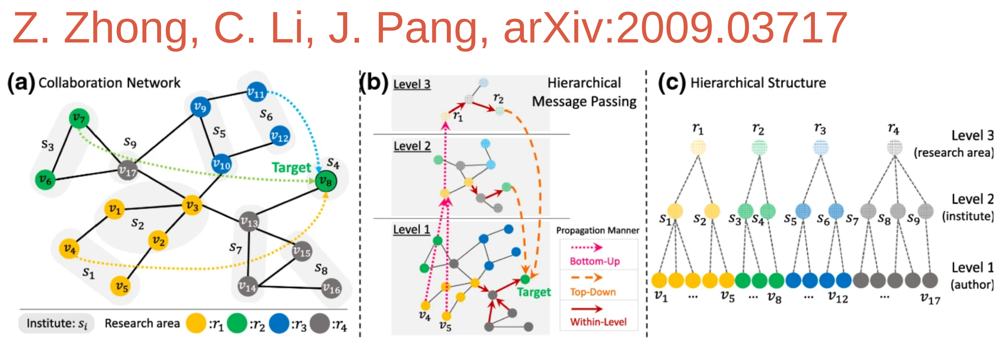
See **poster #162** in this session for more details on NuGraph2

- NuGraph2 achieves ~95% overall efficiency and purity
- ~98% consistency between planes
  - Without 3D connections, ~70% consistency



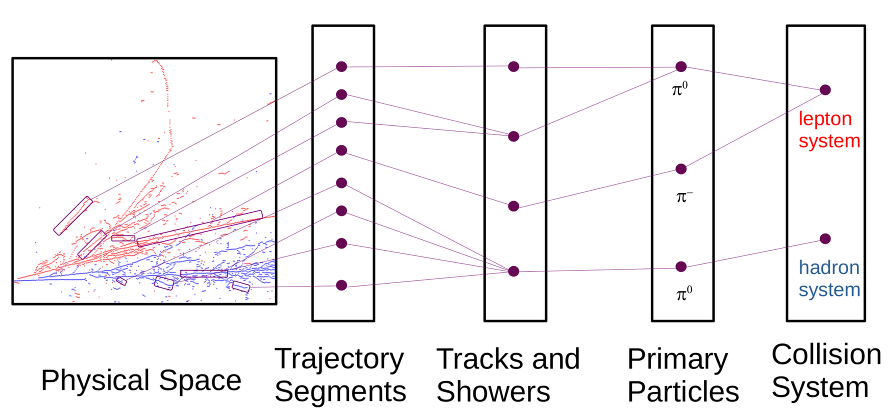
Hierarchical GNNs

Z. Zhong, C. Li, J. Pang, arXiv:2009.03717



- Flat message-passing GNNs have some weaknesses
  - Each message-passing iteration expands distance between connected nodes
  - Too many iterations degrades messages
    - **"oversquashing"**

- Hierarchical GNNs solve problem by allowing long-distance information flow through different hierarchical layers
- Hierarchical layers captures rich, multi-scale information in a natural way
  - Better reflects the inductive bias of the problem
- Message passing can occur both between and within levels

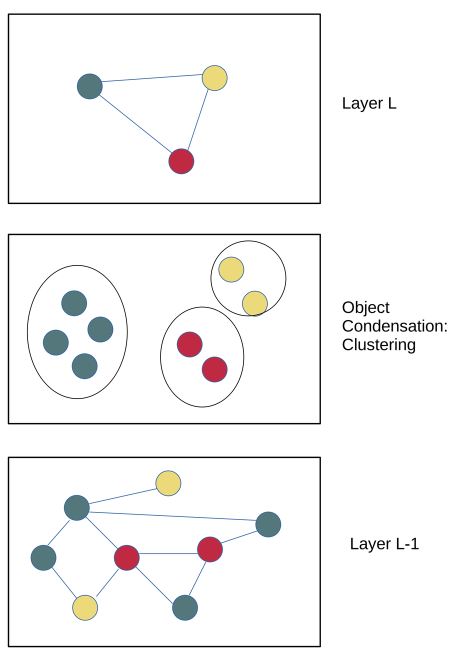


Definition hierarchy levels can be used to naturally represent different reconstruction stages and permit learning the structure of neutrino events at different resolution scales

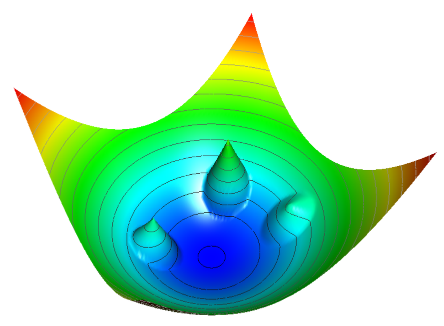
- Nodes on layer L are only connected to nodes in adjacent layers
- Hierarchical structure must be learned in-situ
- Possible layers include
  - 2D planar input graphs
  - 3D space-points and particle trajectories
  - Primary particles
  - Collision systems
  - Events

Building the Hierarchy

- In NuGraph2, graphs are constructed in advance using Delaunay triangulation
  - Graph structure is tuned to maximize information flow and is not a reconstruction product of interest
- Hierarchical graph structure directly mirrors the reconstructed particle tree
  - Is a reconstruction output of interest

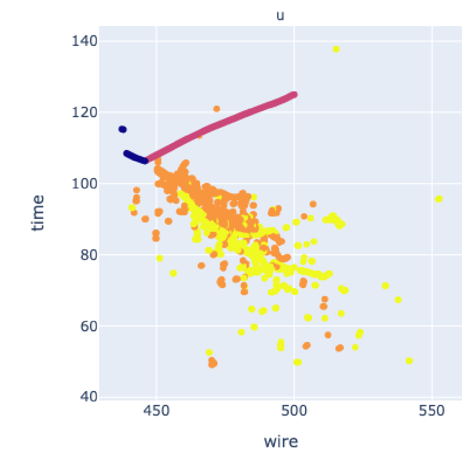


- Hierarchical graphs can be generated dynamically
- Message-passing iterations in layer L-1 are used to predict clustering coordinates
- Nodes close in clustering space are aggregated into a single node in layer L
- Ground truth definition in predicting clustering coordinates shapes the meaning of each layer



- Predict coordinates in clustering space for each node
- Electrostatic-inspired loss functions encourage nodes from same object to cluster together
- Currently implementing to cluster hits into particles

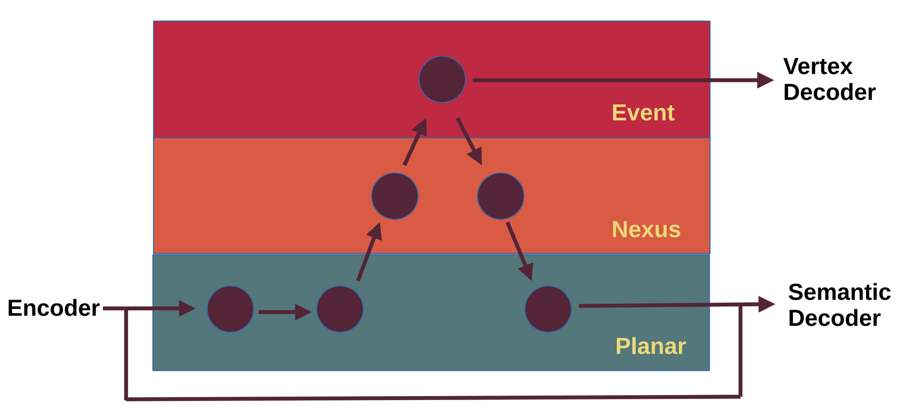
- Object condensation is a grid-free clustering approach based on an electrostatic analog
- Predict a "charge" per point to determine how strongly points should attract each other in abstract clustering space

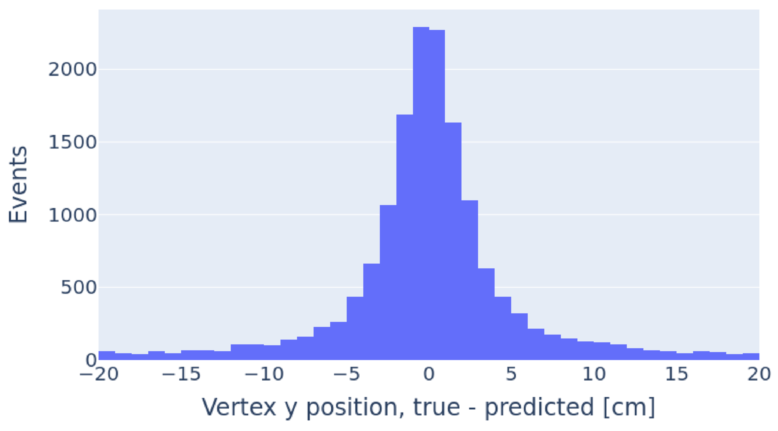


J. Kieseler, arXiv:2002.03717

NuGraph3

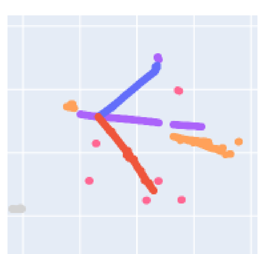
- First step in developing NuGraph3 is adding in a single event node
- Event node aggregates information from all nexus nodes through hierarchical message-passing mechanism



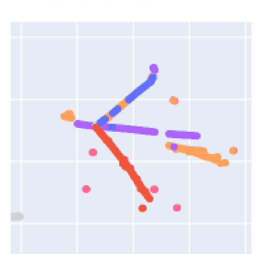


- Semantic decoder head is attached to the planar graphs in NuGraph2/3
- Event node aggregates information across full graph
  - Ideal for extracting reconstructed quantities associated with full events
- First test: regress interaction vertex position from event-level features

True Semantic Labels



Predicted Semantic Labels



Semantic performance of NuGraph3 is comparable to NuGraph2 despite breaking MIP category into muons and pions

Future:

- Replace externally reconstructed 3D space-points with in-situ reconstruction
- Integrate particle reconstruction with object condensation
- Regress relevant reconstructed quantities at each hierarchical level
- Enforce physical consistency in full reconstruction