Scalable Particle Imaging with Neural Embeddings

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NPML 2024, ETH Zurich

SLAC NATIONAL ACCELERATOR LABORATORY

Stanford University | U.S. DEPARTMENT OF ENERGY

SPINE

Neutrino Oscillations

Neutrinos **produced as different types**

- Neutrino types are a **superposition** of **mass states**

Neutrino types

$$\boxed{\begin{pmatrix}\nu_e \\ \nu_\mu\end{pmatrix}} = \underbrace{\boxed{\begin{pmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{pmatrix}}}_{\text{Mixing matrix}} \boxed{\begin{pmatrix}\nu_1 \\ \nu_2\end{pmatrix}}$$

Mass states

Neutrino Oscillations

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- Mass wavefunctions oscillate at different rate→ **mixture changes**

Neutrino types — Mixing matrix — Mass states

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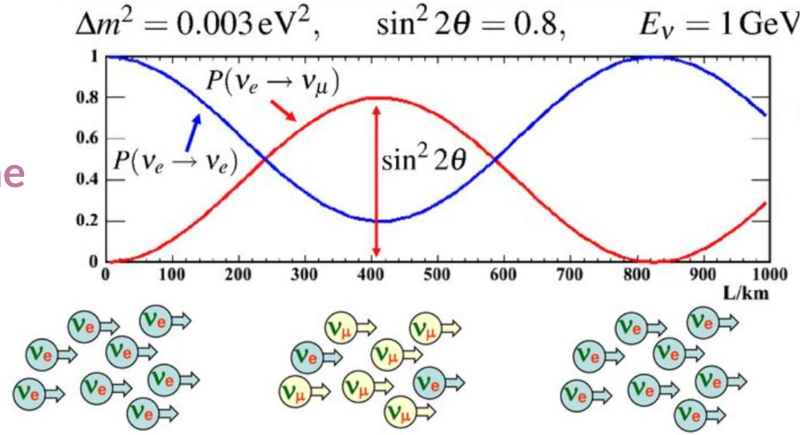
Amplitude — Frequency — Baseline

$$\boxed{P(\nu_e \to \nu_\mu)} = \boxed{\sin^2 2\theta} \sin^2\left(\frac{\boxed{\Delta m^2_{21}}\,\boxed{L}}{4\boxed{E}}\right)$$

Appearance probability — Neutrino energy



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Neutrino types | Mixing matrix | Mass states

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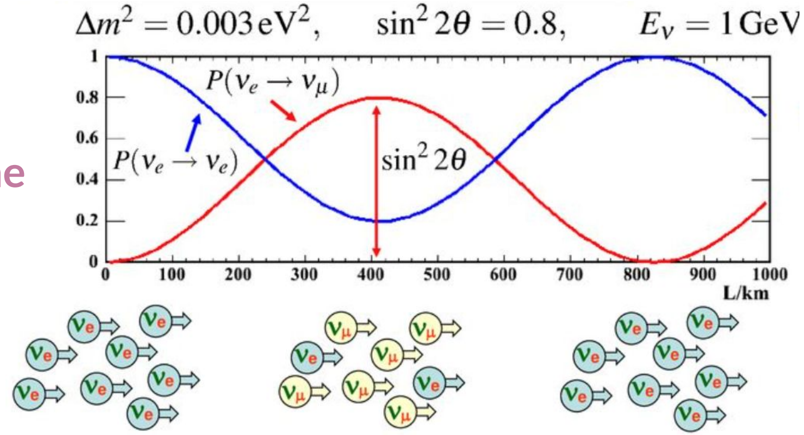
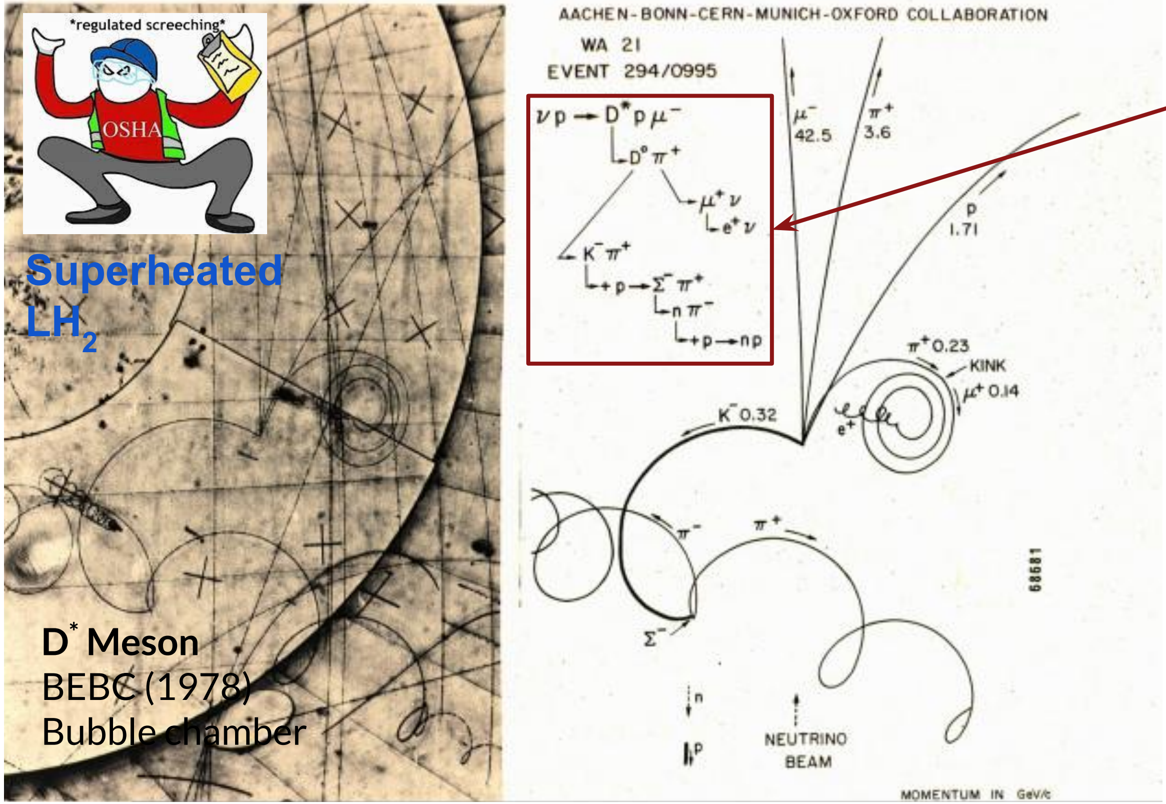
Neutrino energy



Need to measure Type + **Energy**

Particle Imaging Detectors Reconstruction



Full "particle flow"

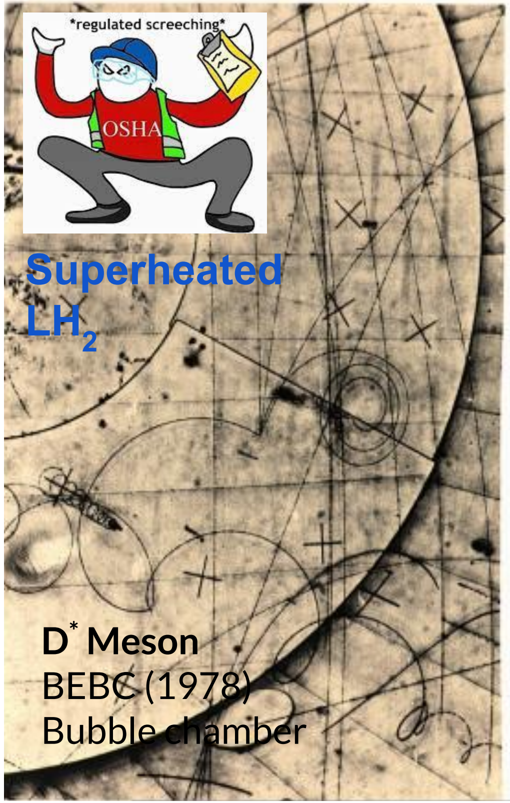
Neutrino **typing:**

- **e** vs **μ** produced (CC interaction)

Neutrino **energy:**

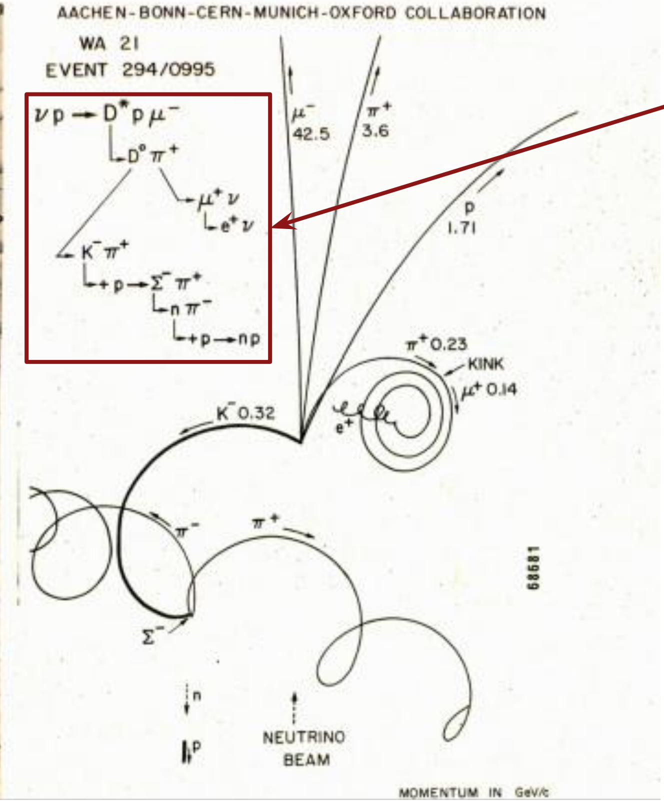
- **Particle mass (type) + range**
- **Calorimetry**

Particle Imaging Detectors Reconstruction



Superheated LH_2

D^* Meson
BEBC (1978)
Bubble chamber



Full "particle flow"

Neutrino **typing:**

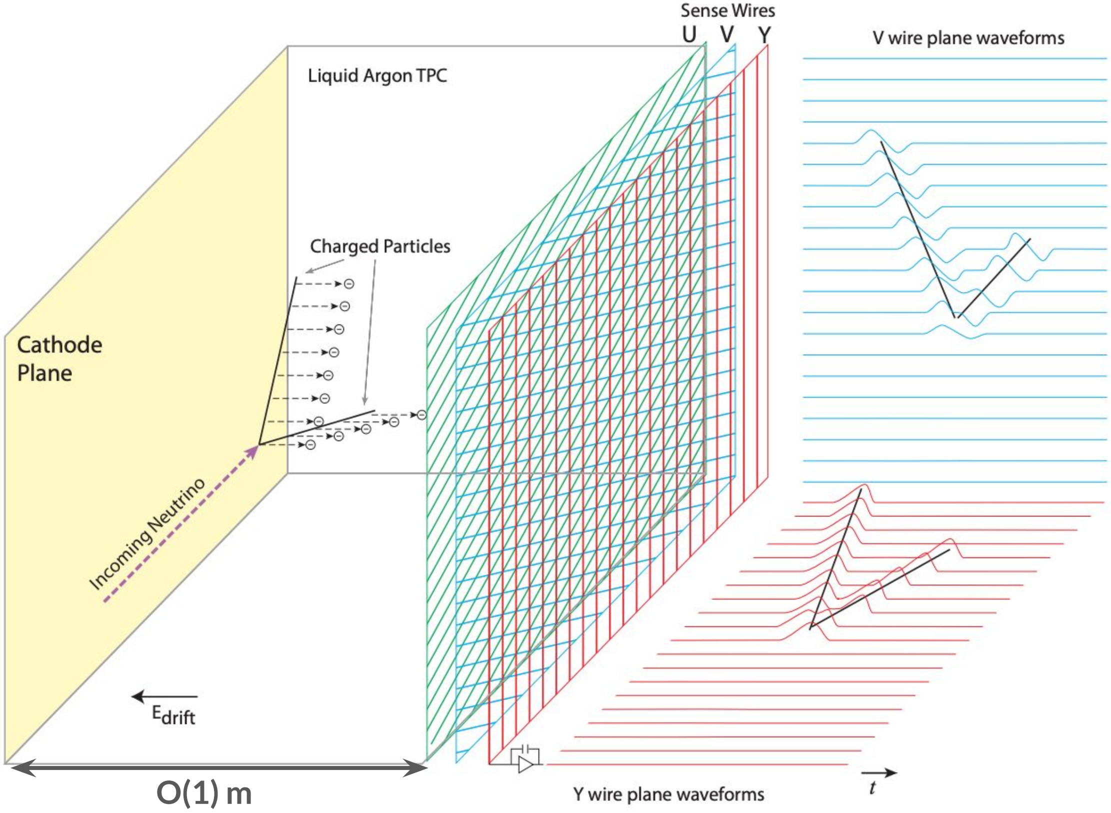
- **e** vs **μ** produced (CC interaction)

Neutrino **energy:**

- **Particle mass (type) + range**
- **Calorimetry**

→ Must be **scalable**

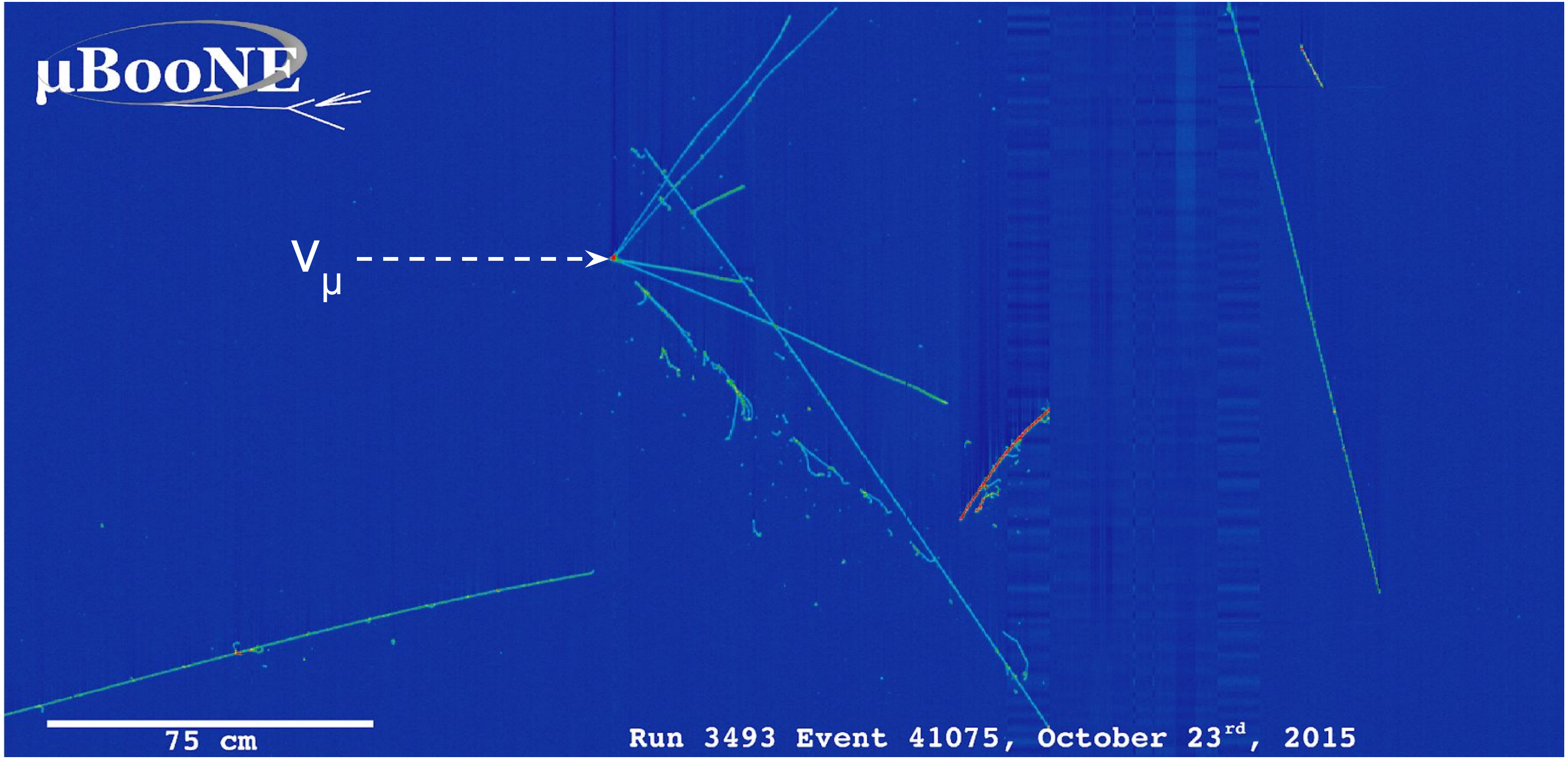
Liquid Argon Time Projection Chamber



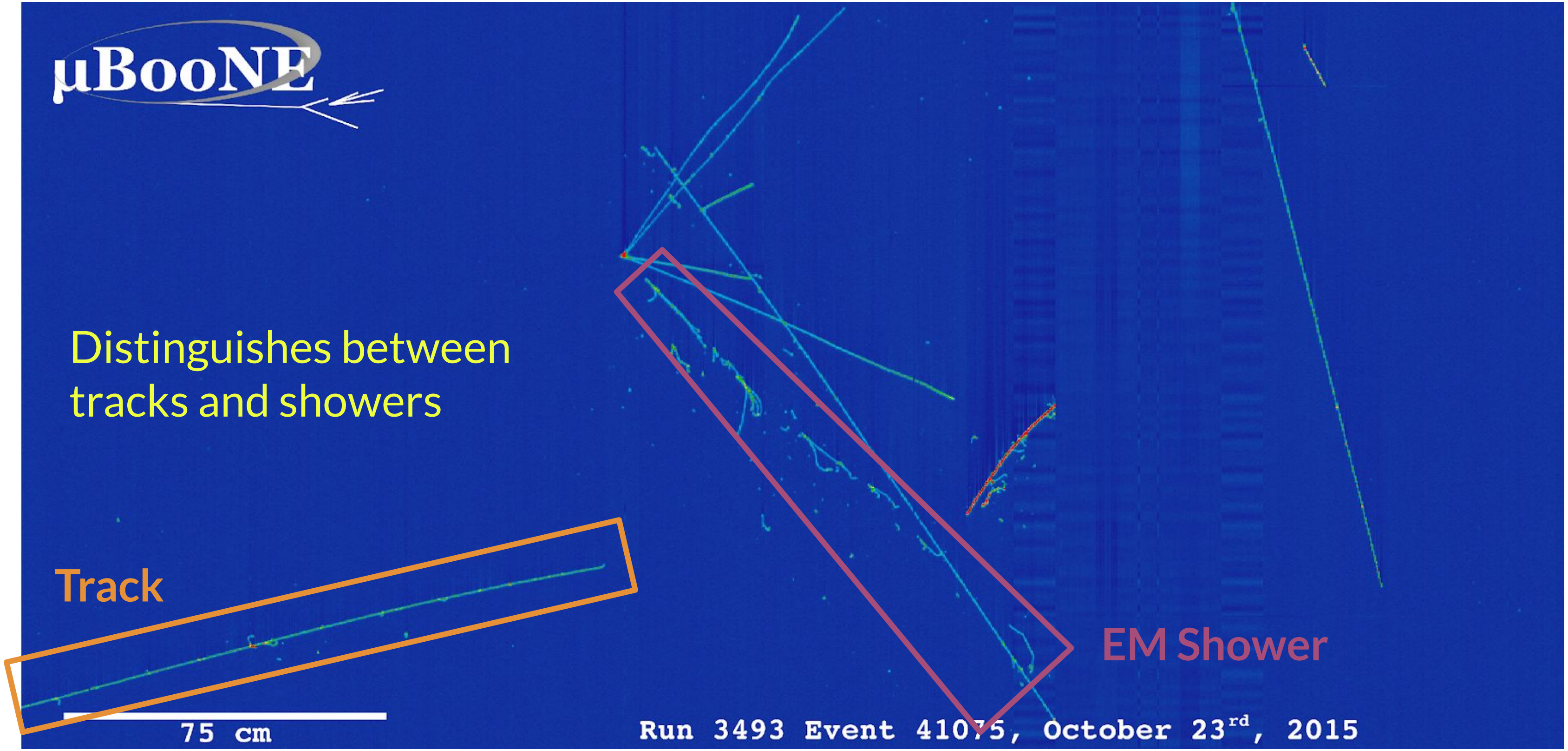
LArTPC = main detector technology in use with **high-intensity neutrino beams** in the US:

- Precise tracking
- Detailed calorimetry
- Dense (1.4 g/cm^3)
- Cheap (O(1) \$/kg)
- **Scalable**

LArTPC Image



LArTPC Image



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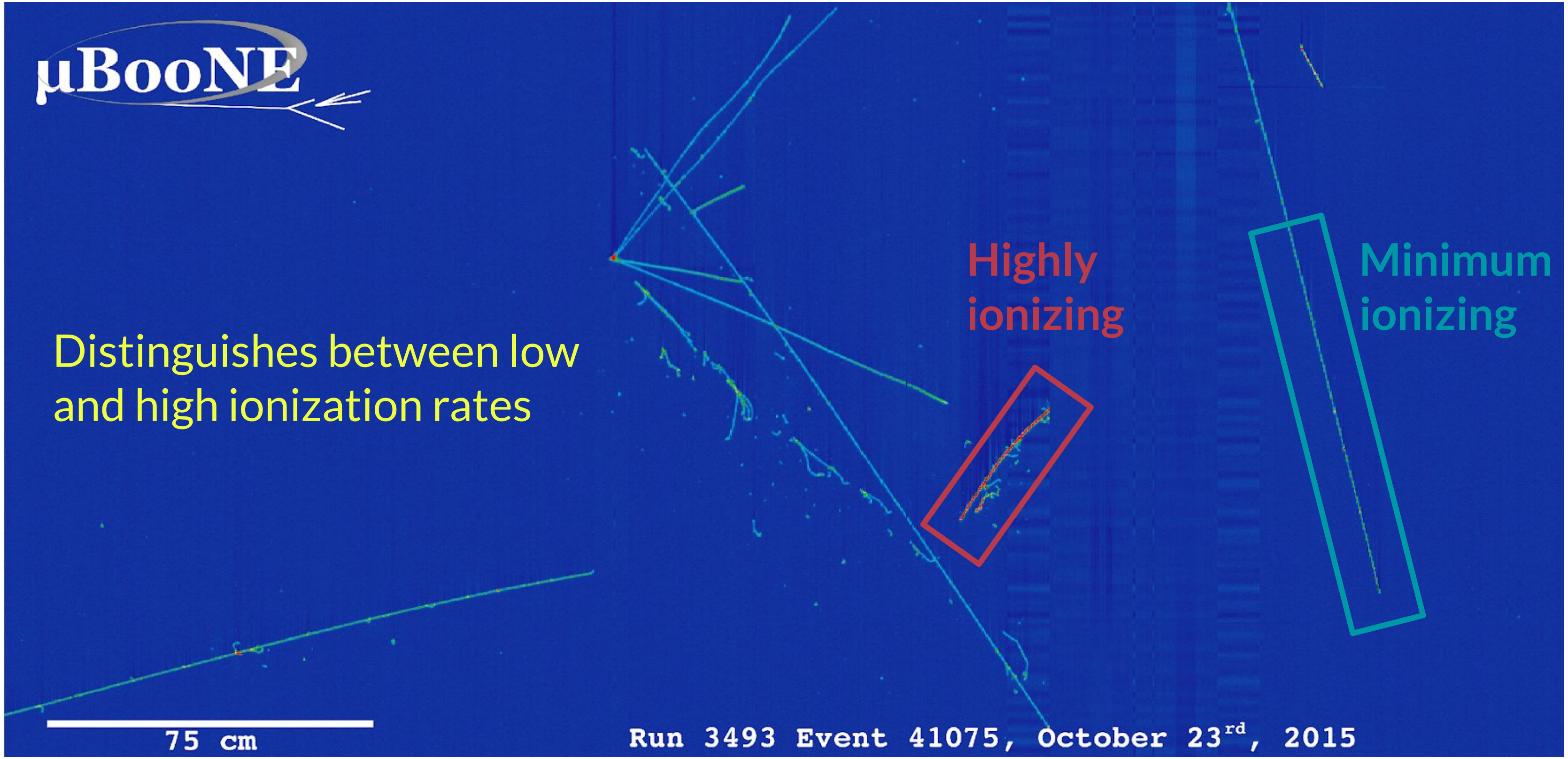

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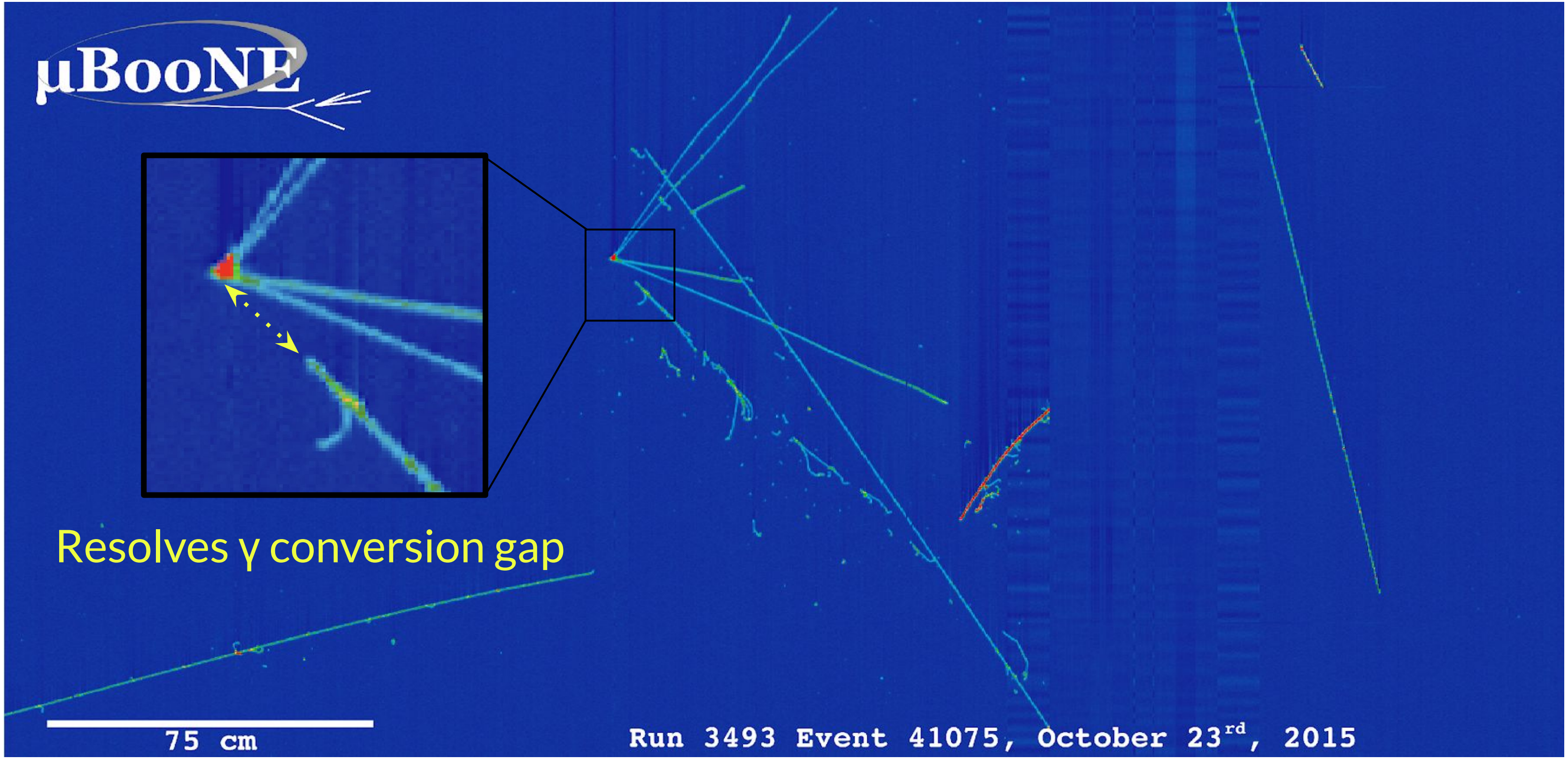
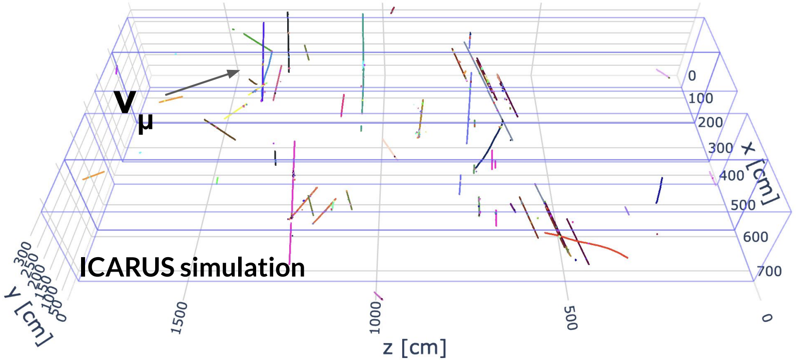


Challenges in LArTPCs

Dense medium → Slow

Electron drift velocity O(1) mm/μs

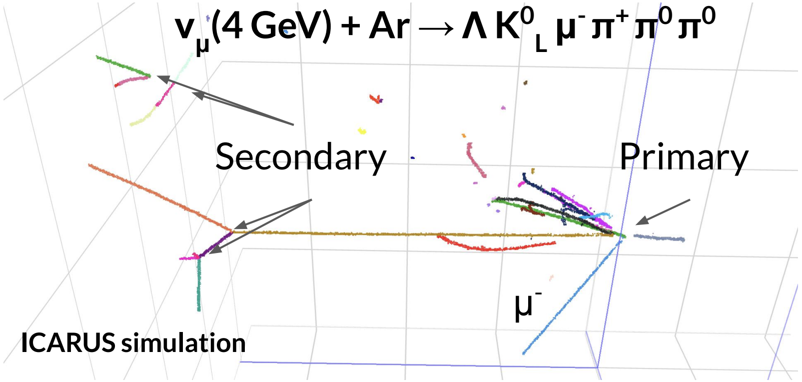
- **Long** (O(1) ms) readout **window**
- Need **light association** for timing



High Z material → Messy

Argon has a large nucleus (Z=18)

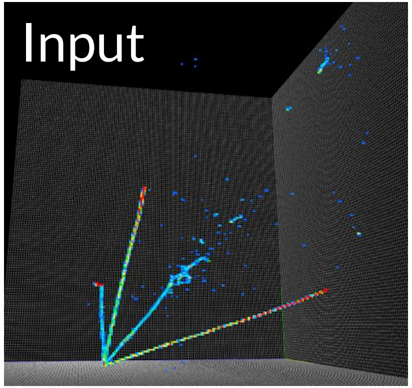
- **Complicated** nuclear physics
- **Secondary** interactions



The story so far:
In the beginning the LArTPC was created.
This has made a lot of people very angry
and been widely regarded as a bad move.

Physics-Informed ML Reconstruction

What is relevant to pattern recognition in a detailed interaction image?



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What is relevant to pattern recognition in a detailed interaction image?

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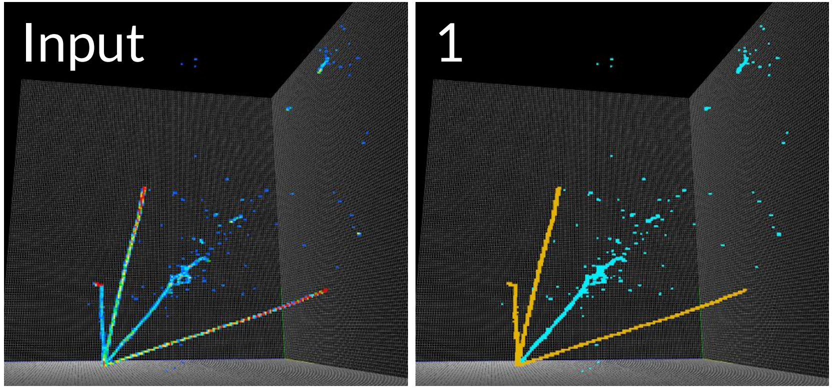
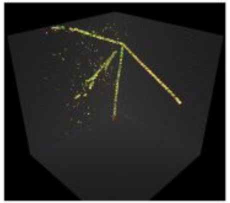


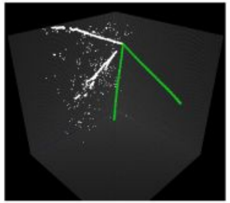
Pixel-Level Feature Extraction

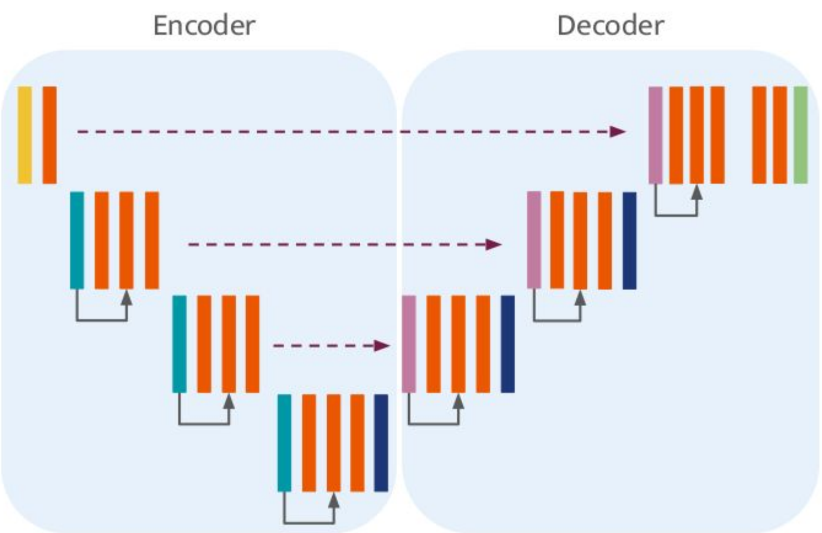
UResNet (UNet + ResNet + Sparse Conv.) as the **backbone feature extractor**

Input



Features





Paper: PhysRevD.102.012005

L. Dominé et al.

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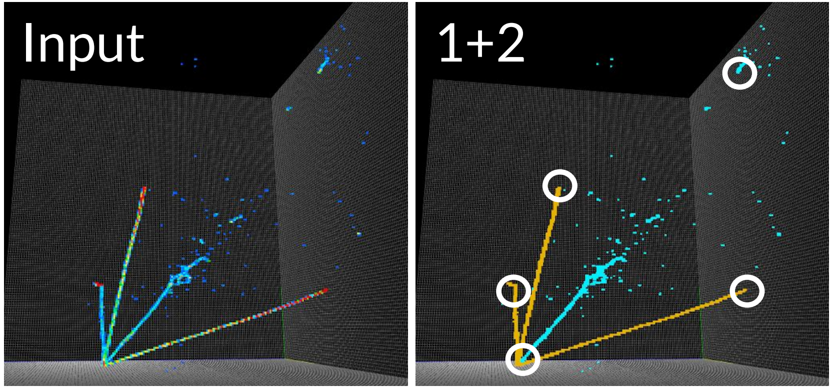
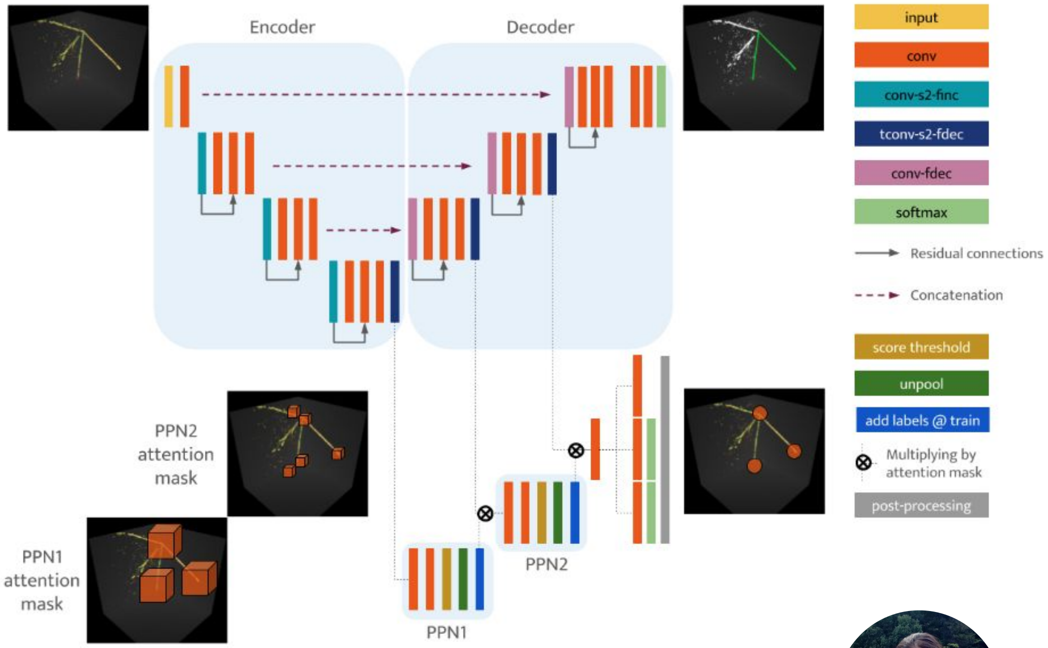


Points of Interest

The Point Proposal Network (PPN) uses decoder features

- Three CCN layers to narrow ROI
- Last layer reconstructs:
  - Relative position to pixel center of active pixel
  - Point type
- Post-processing aggregates nearby points



Paper: PhysRevD.104.032004 L. Dominé et al.

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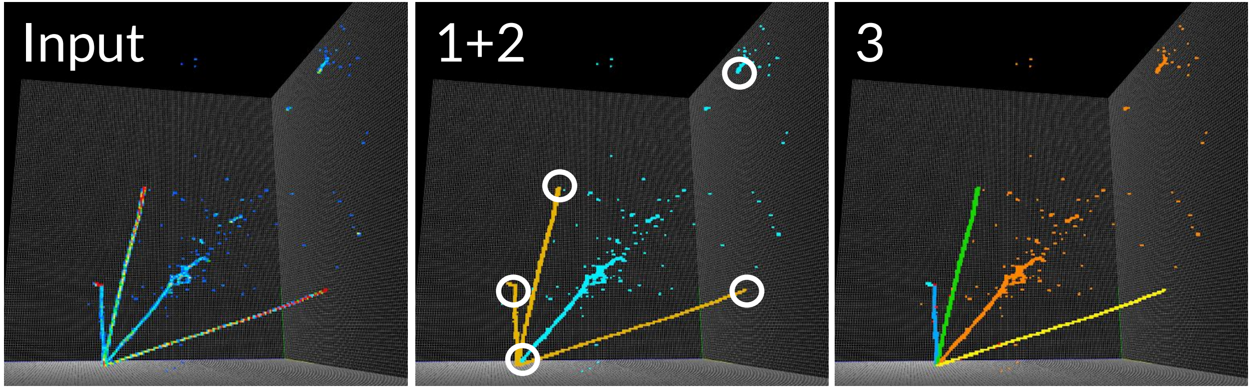
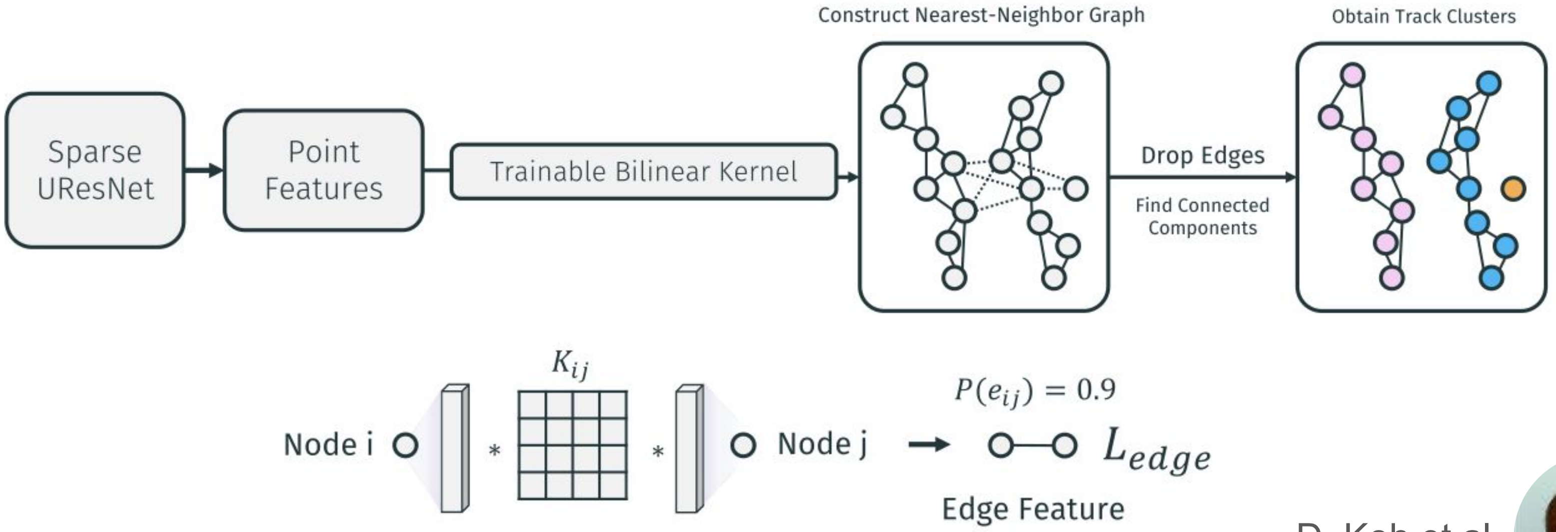
3. Cluster individual **particles** (tracks and full showers)



Supervised Connected Component Clustering

Learn a **smart** version of **DBSCAN** (connected components)



D. Koh et al.

Supervised Connected Component Clustering

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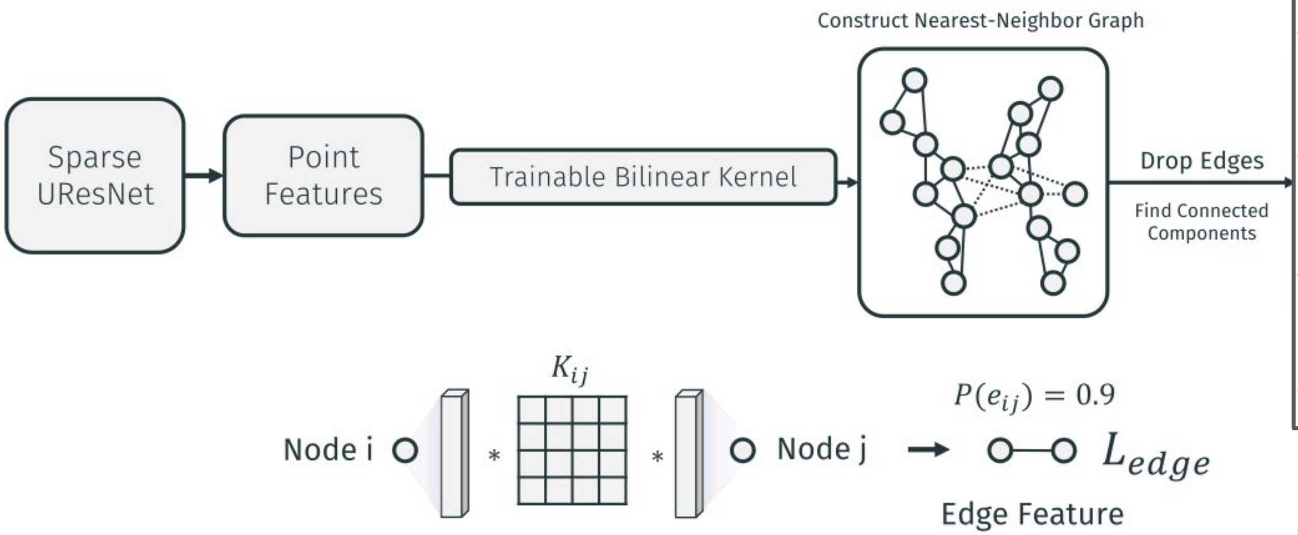
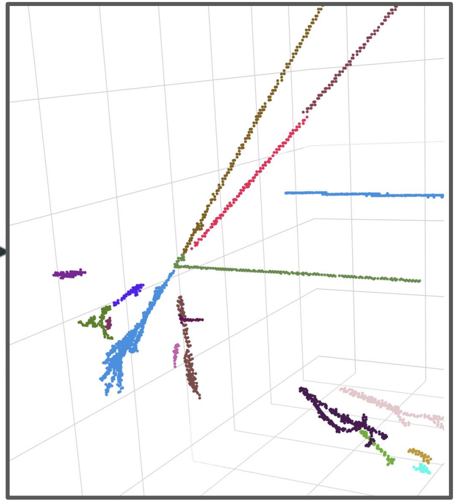


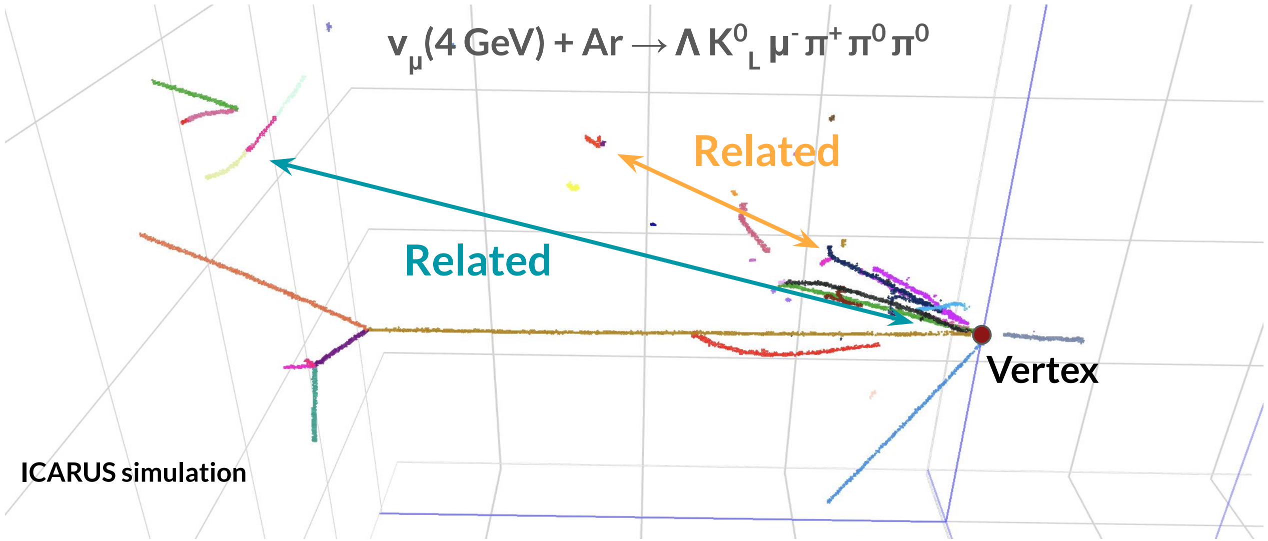


D. Koh et al.

Cluster-level feature extraction

CNN: mostly sensitive to **local neighborhood** of pixel, but…

- **EM showers**: photon mean free path in LAr = 18 cm (**60 pixels in ICARUS**)
- **Interactions**: π^0, K^0, Λ, neutrons



Cluster-level feature extraction

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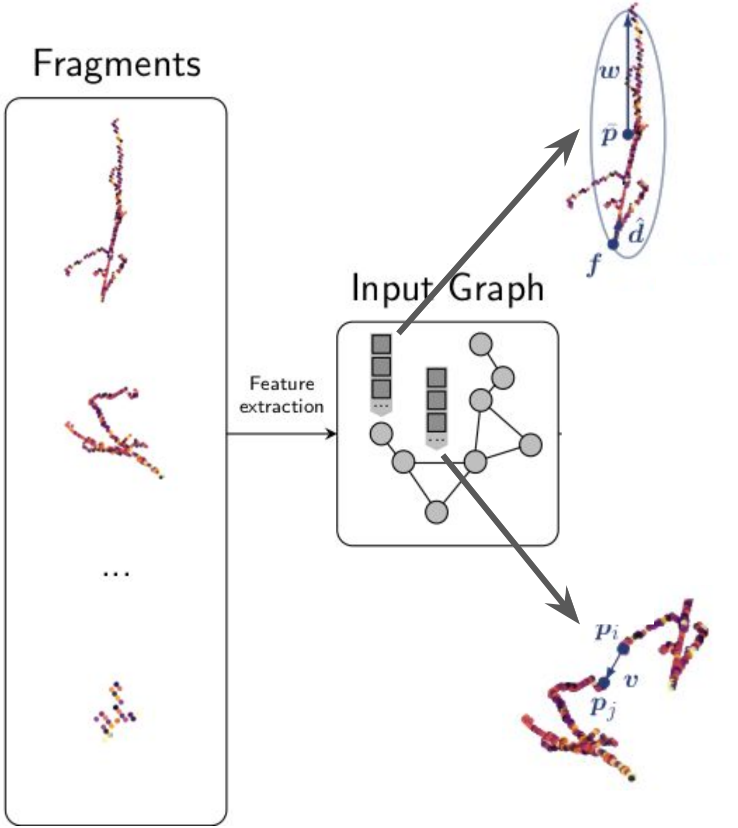
We now represent the set of fragments as a **set of nodes in a graph** where **edges represent correlations**

Node features:

- Centroid
- Covariance matrix
- Start point/direction
- . . .

Edge features:

- Displacement vector
- . . .



Cluster-level feature extraction

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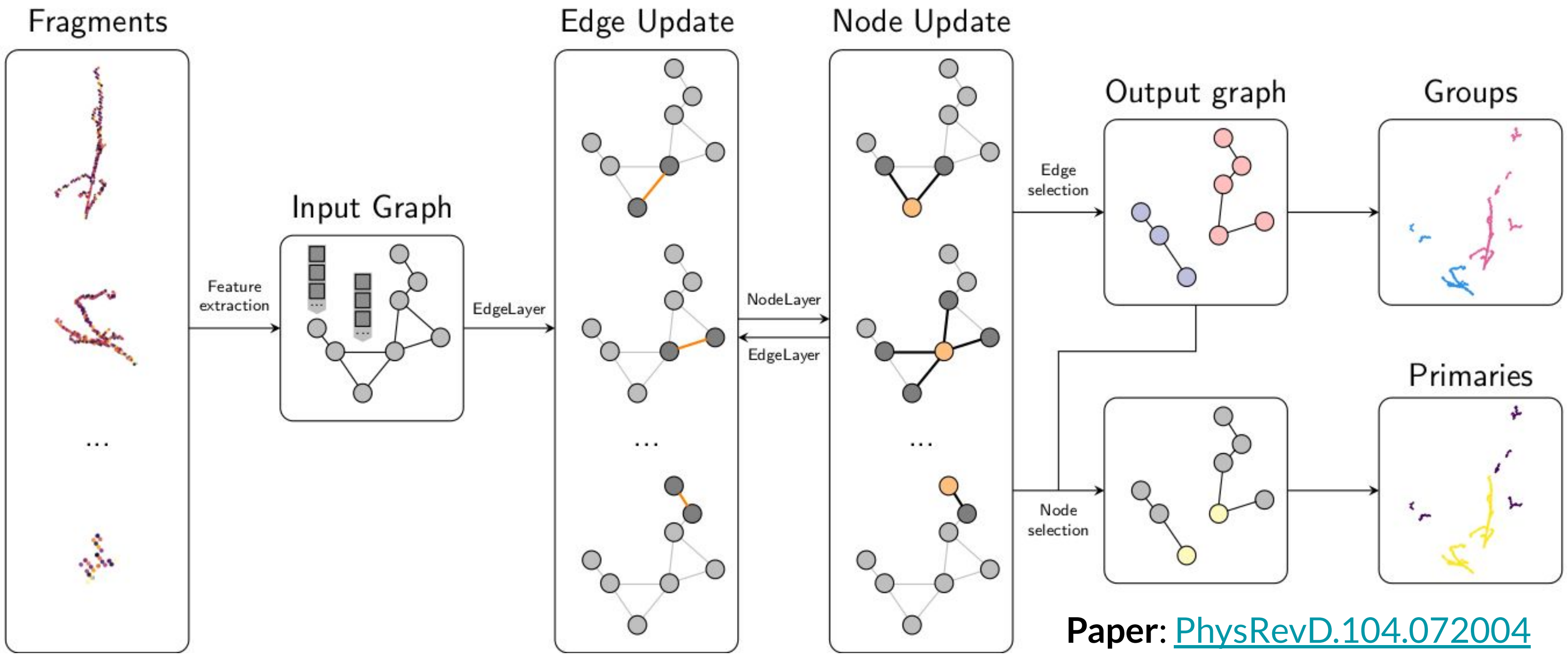
Graph Neural Network: develop features useful to node/edge classification



Paper: PhysRevD.104.072004

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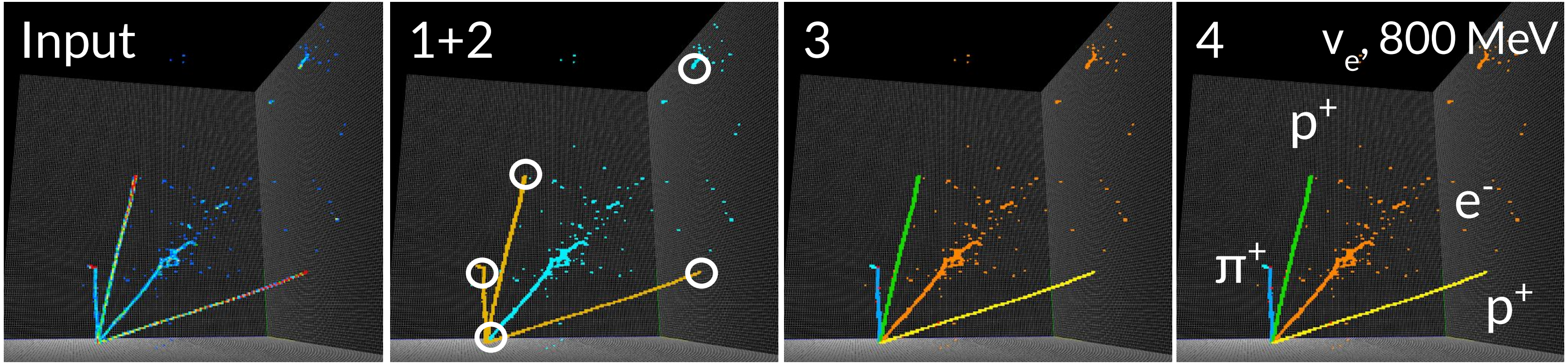
3. Cluster individual **particles** (tracks and full showers)
4. Cluster **interactions**, identify **particle properties** in context



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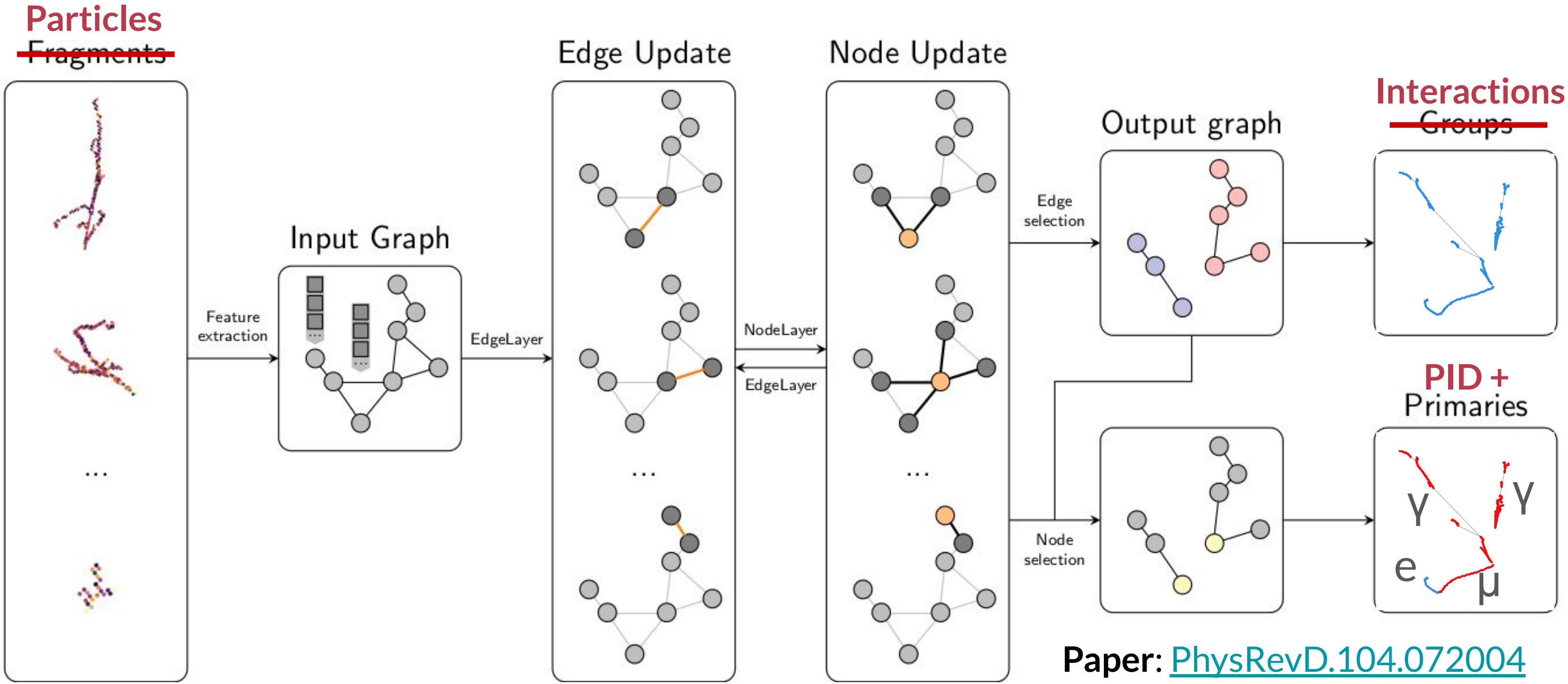

Paper: PhysRevD.104.072004

Reconstruction in LArTPCs

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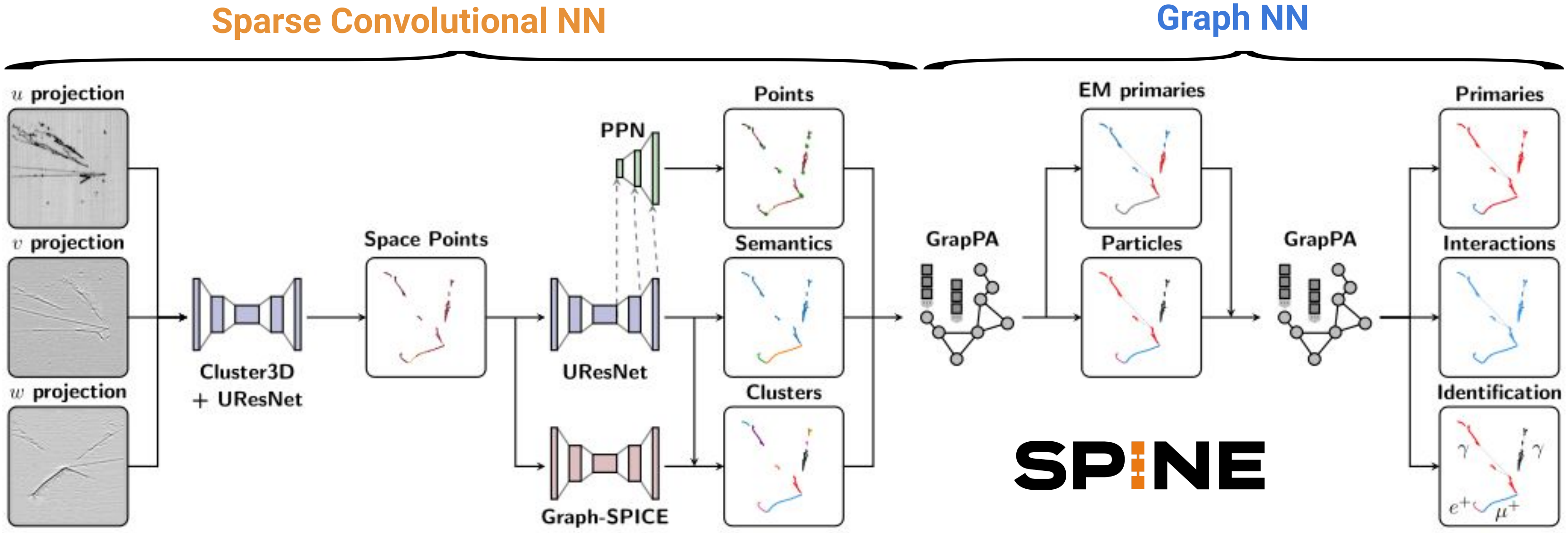
End-to-end ML-based reconstruction chain

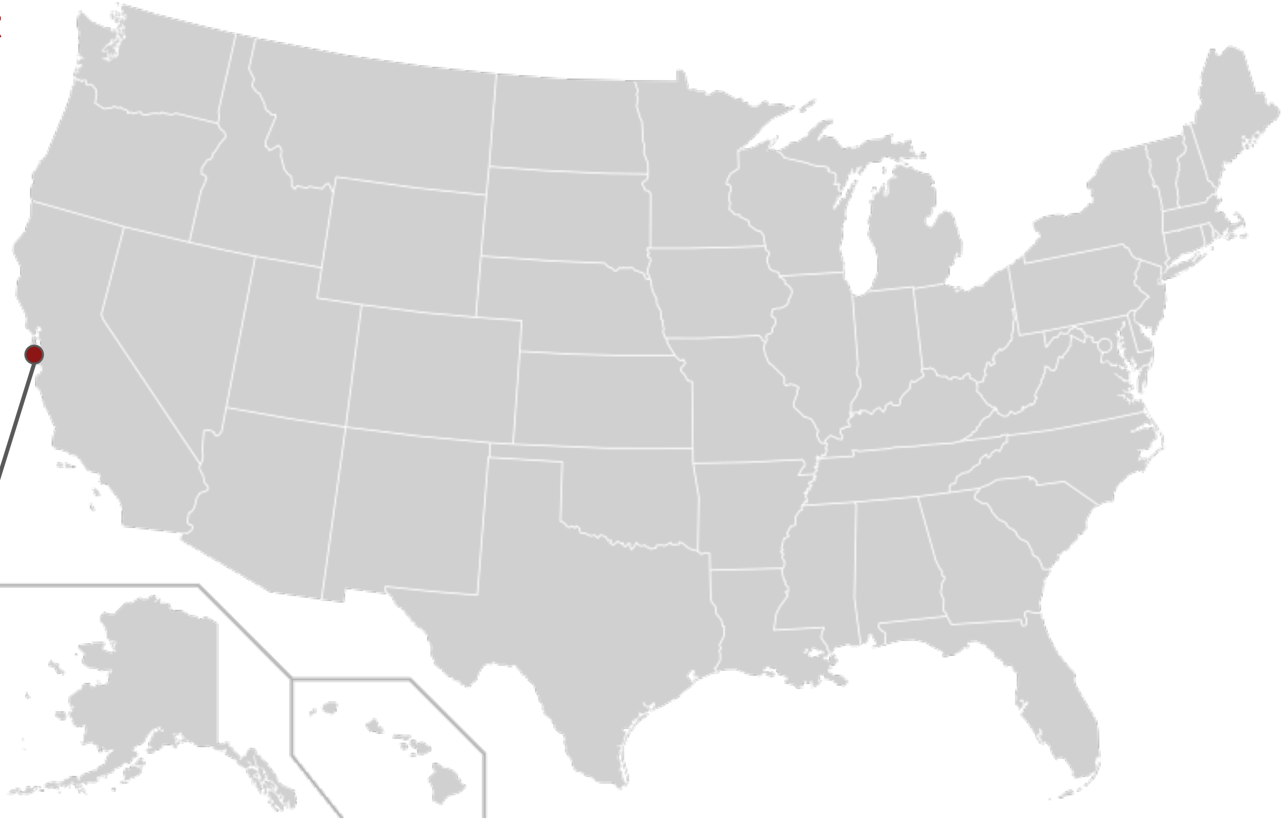
- **Sparse CNN** for pixel-level features, **GrapPA** for superstructure formation

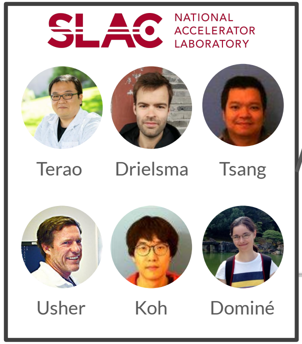


Paper: arXiv:2102.01033

SPINE “Network”

Effort starts at SLAC in 2019





SPINE "Network"

ICARUS ML group formed in 2020

Reconstruction Highlights at ICARUS

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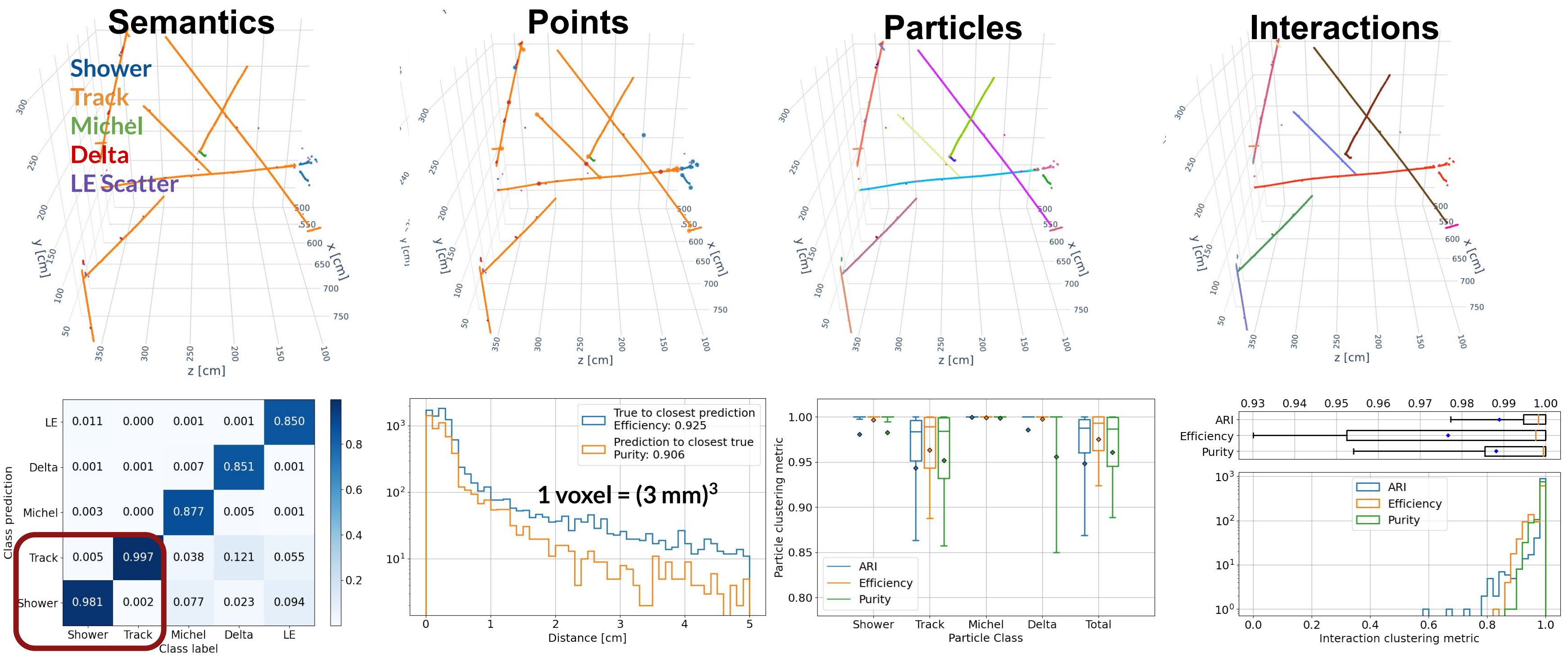
Excellent performance on a **realistic BNB ν + Cosmic sample in ICARUS** ([NPML ‘23]())

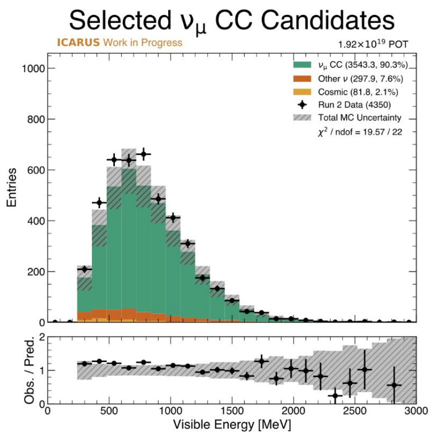


Scalable Particle Imagining with Neural Embeddings, F. Drielsma

Applications at SBN

Several **physics analyses** using **SPINE** on the way within **ICARUS:**

- **BNB ν_μ** selections (J. Mueller, L. Kashur), see Dan's talk yesterday



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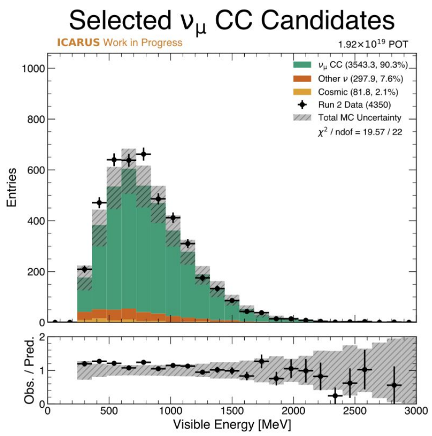

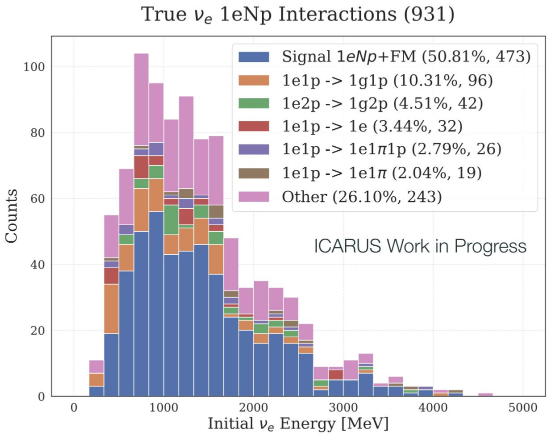

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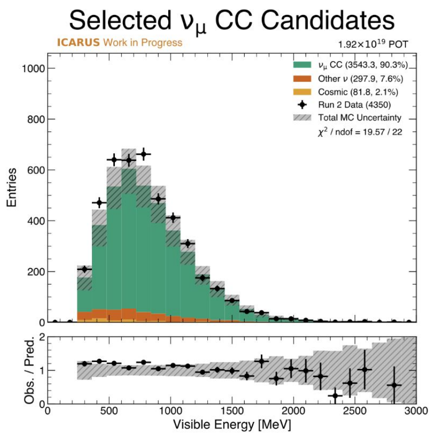
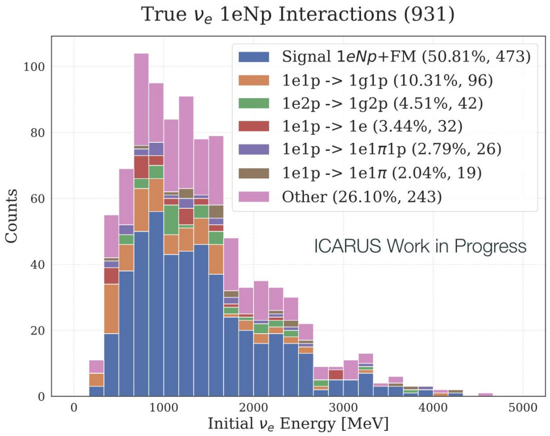
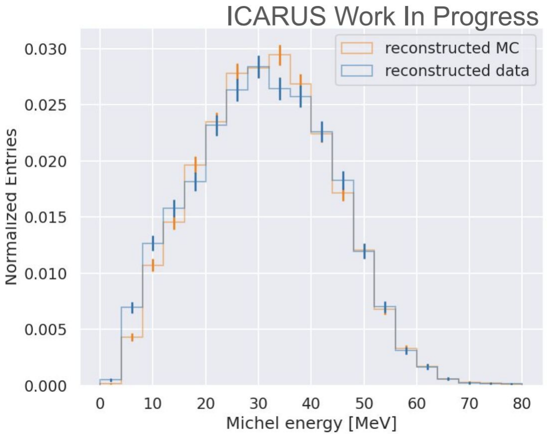
- **Michel electron** reconstruction (Y. Jwa), see Yeon-Jae's talk today

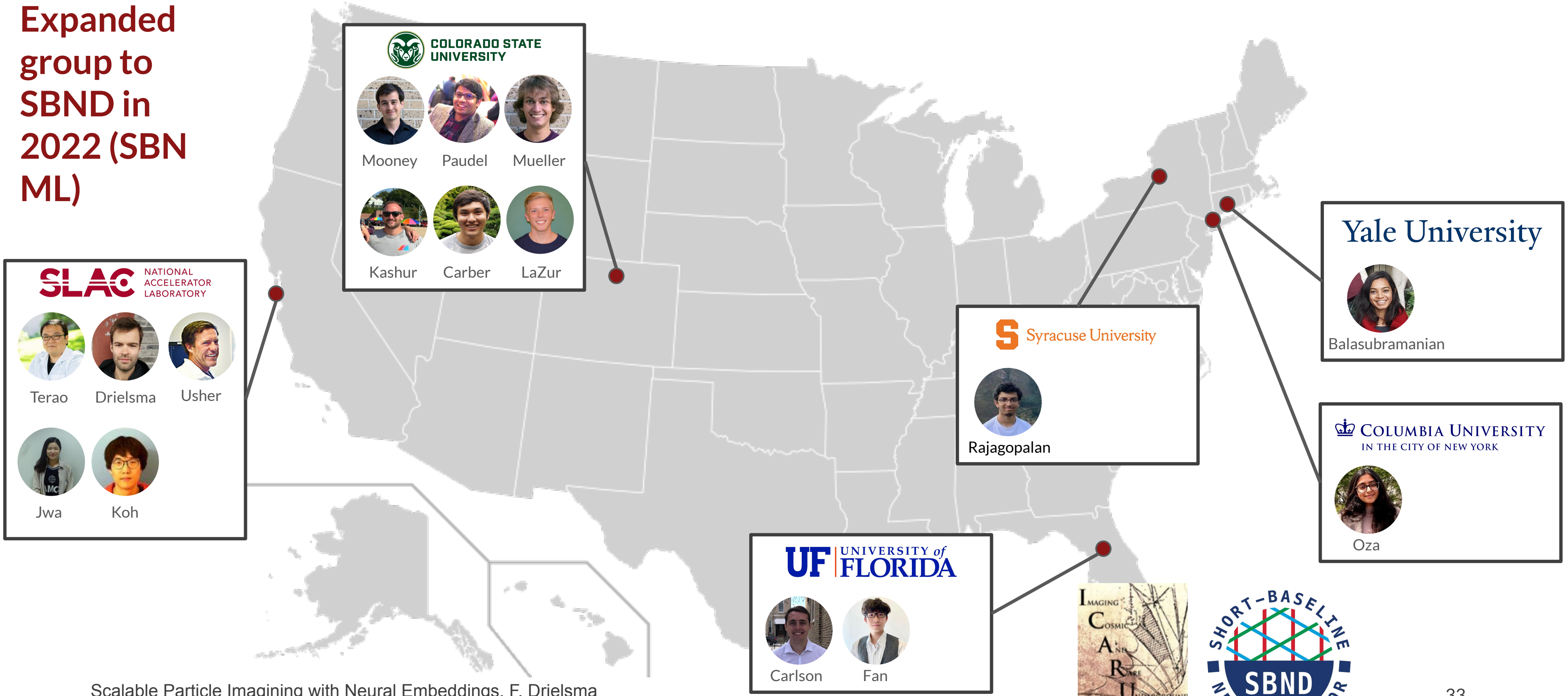






SPINE "Network"

Expanded group to SBND in 2022 (SBN ML)



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- **Michel electron** reconstruction (Y. Jwa), see Yeon-Jae's talk today

Excellent work to port the chain to **SBND:**

- Early **BNB ν_μ** selection (B. Carslon, C. Fan), see Bear's talk today
- **Michel electron** reconstruction (N. Oza)

SPINE “Network”

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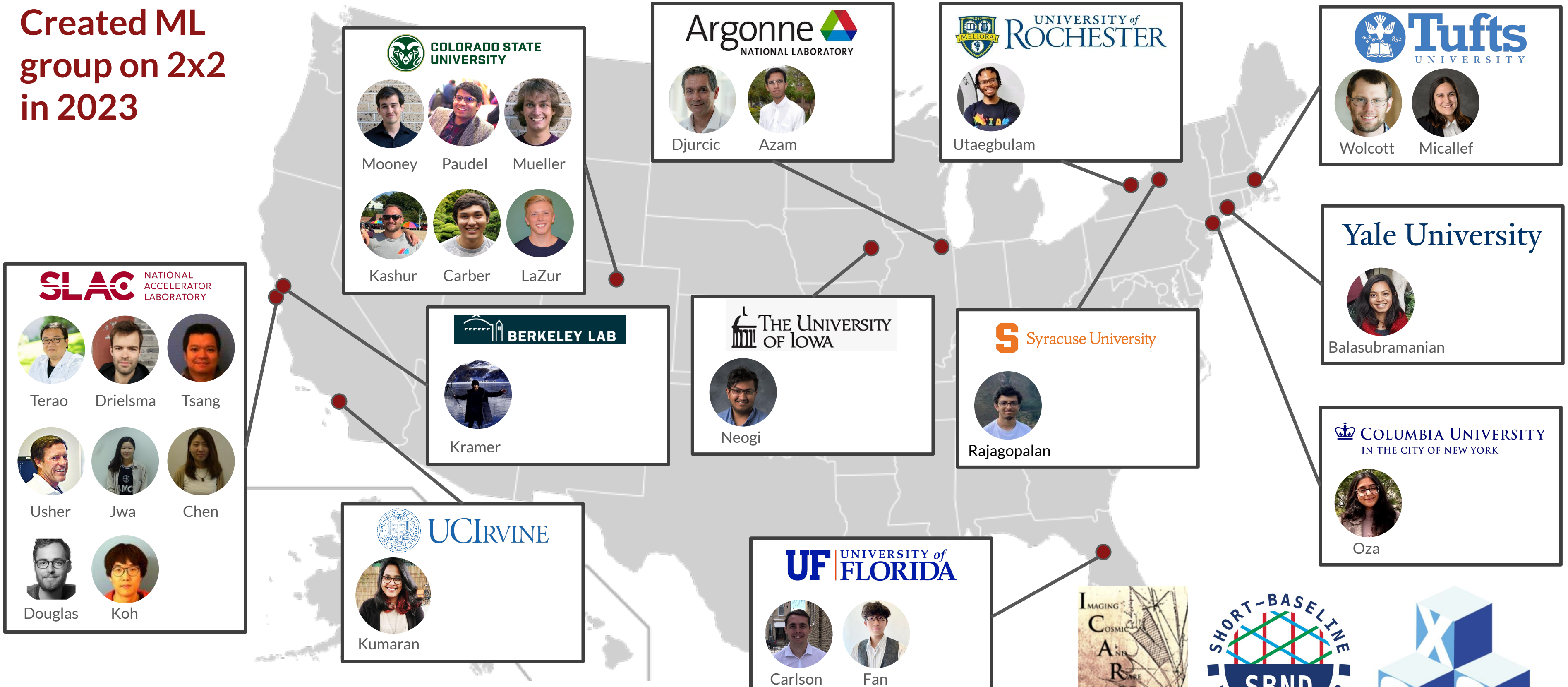
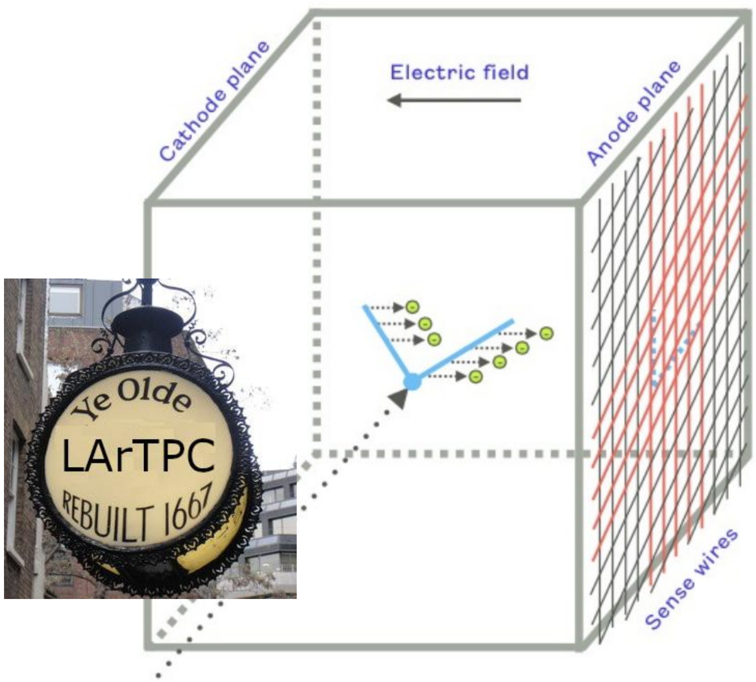
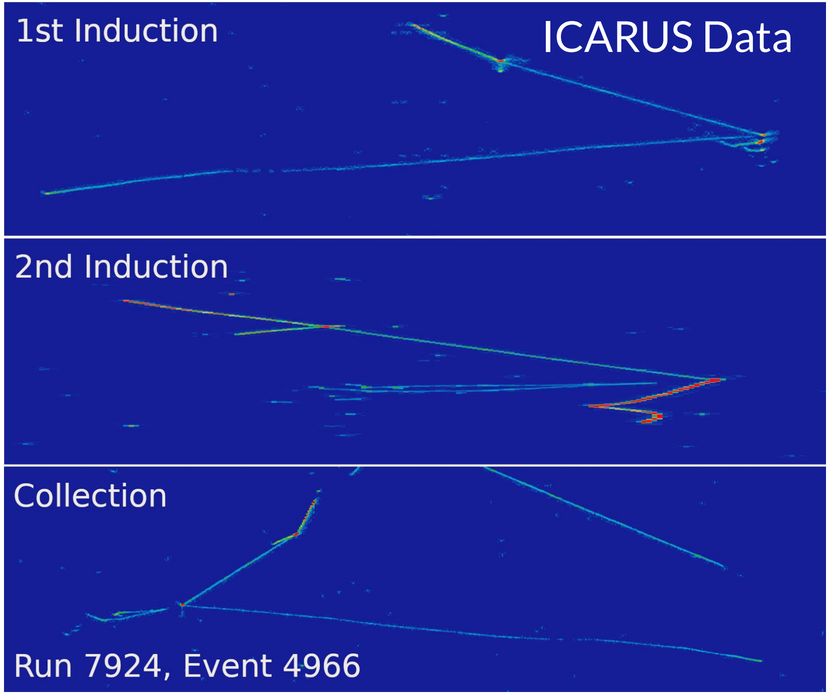
Created ML group on 2x2 in 2023



LArTPC Technologies

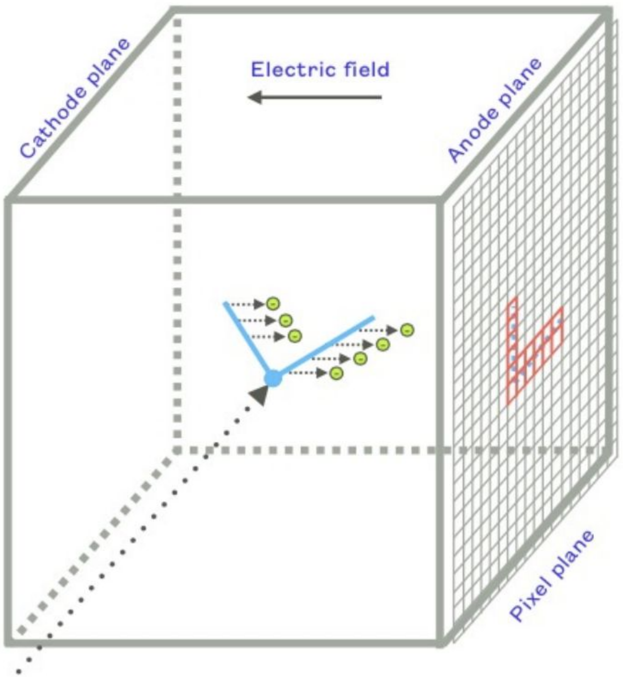
Wire planes → Set of **2D projections (SBND, ICARUS, µBooNE, DUNE-FD)**

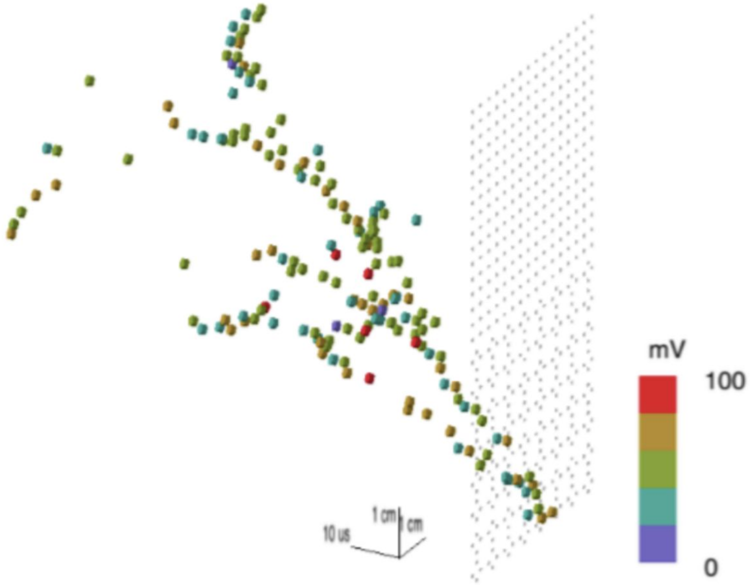




LArTPC Technologies

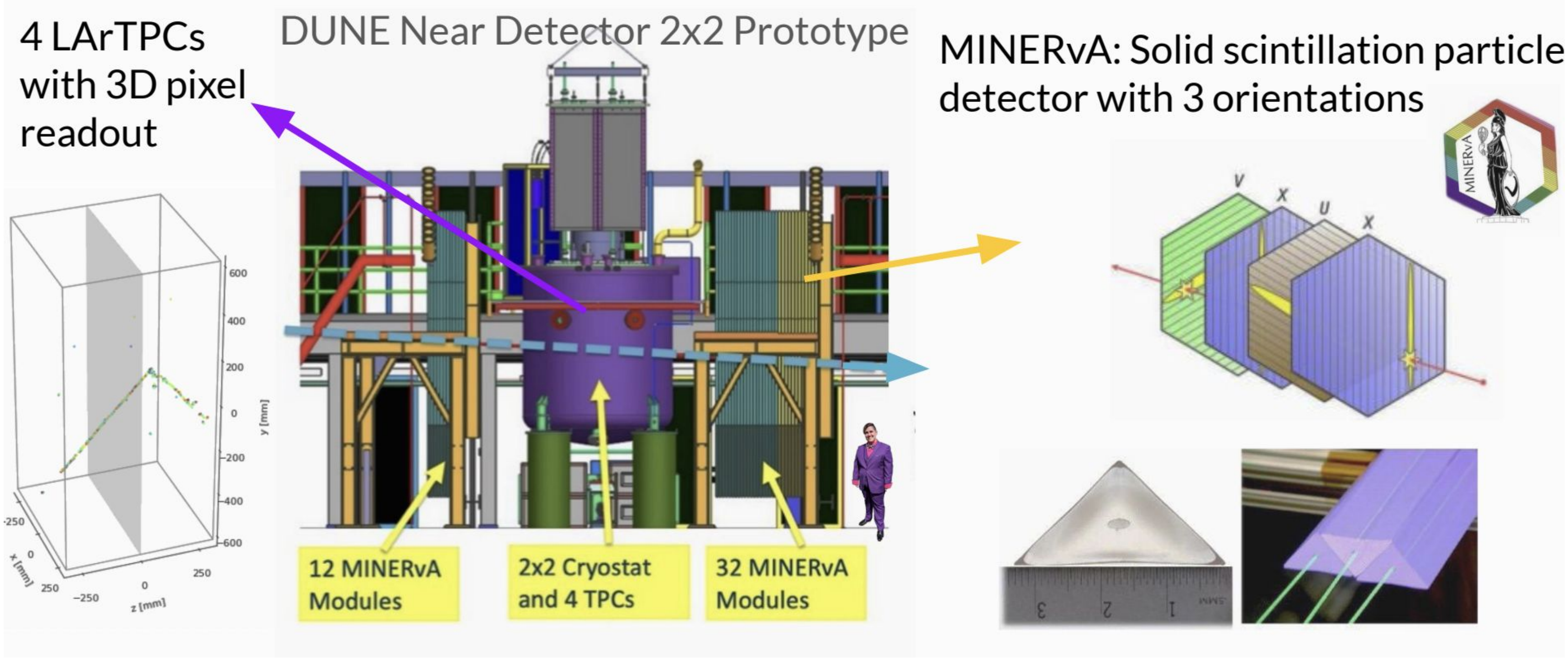
Pixel plane → Single natively 3D image **(DUNE-ND, 2x2 prototype)**





LArPIX, arXiv:1808.02969

The DUNE-ND prototype

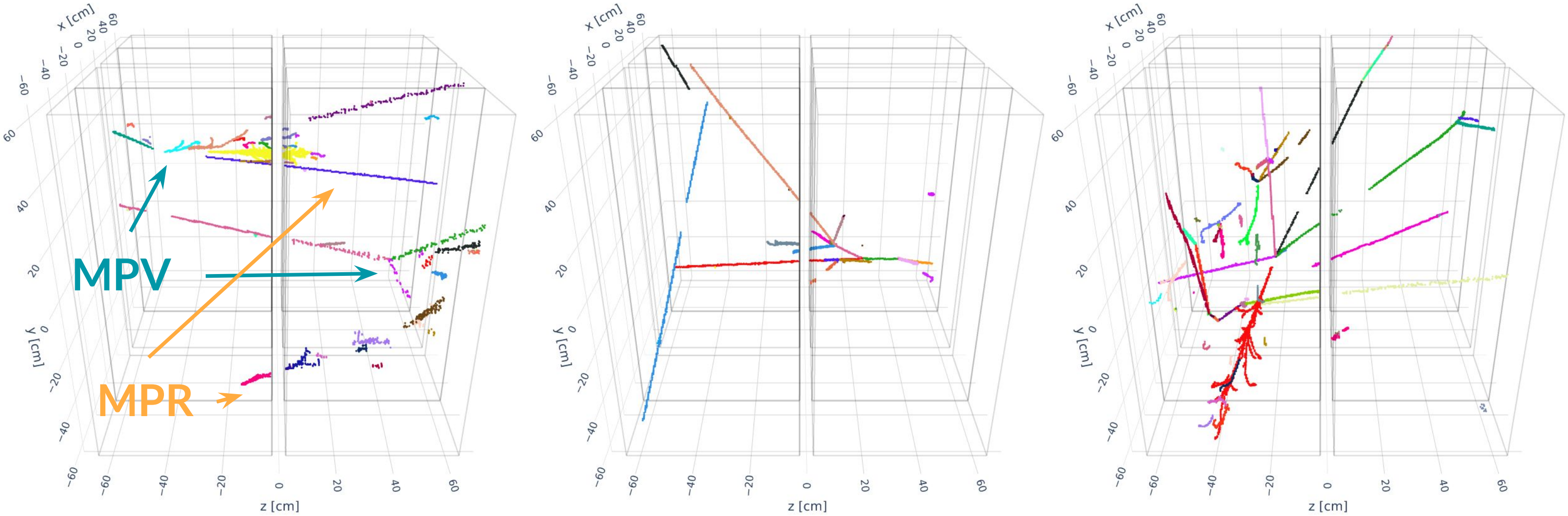


Credit: J. Micallef

Training/Validation sample

Training sample generated using the [DeepLearnPhysics generator]

- 1-3 **particle bombs** (multi-particle vertex, aka MPV)
- 1-5 **single particles** (multi-particle rain, aka MPR)



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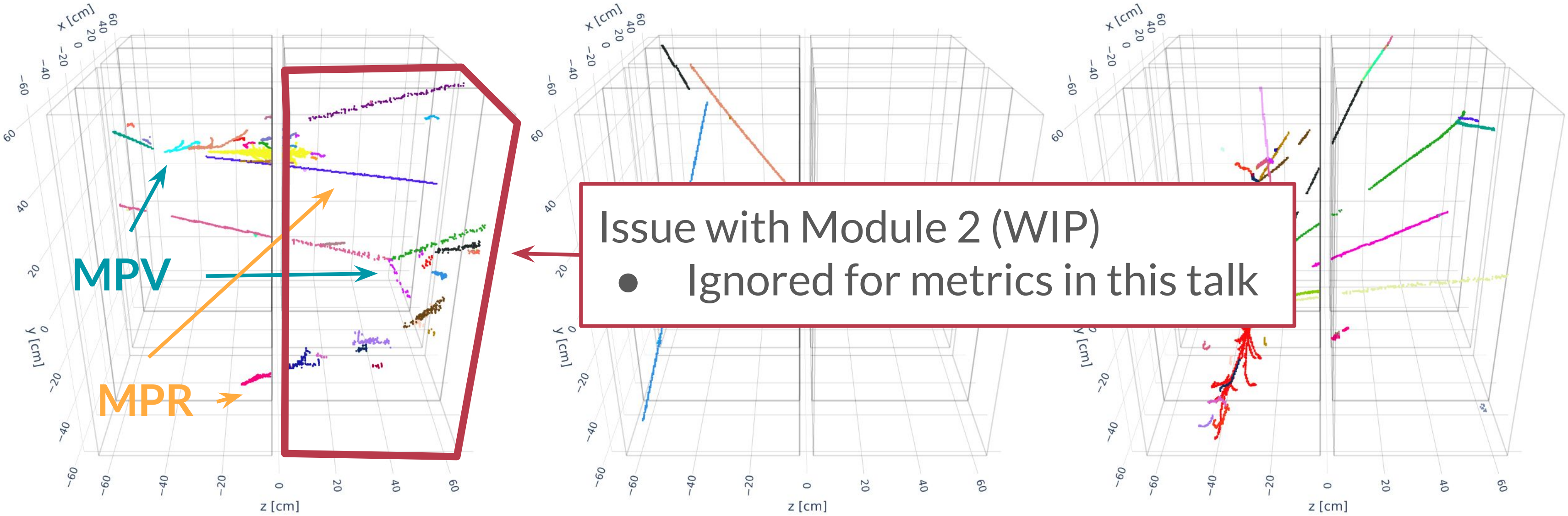

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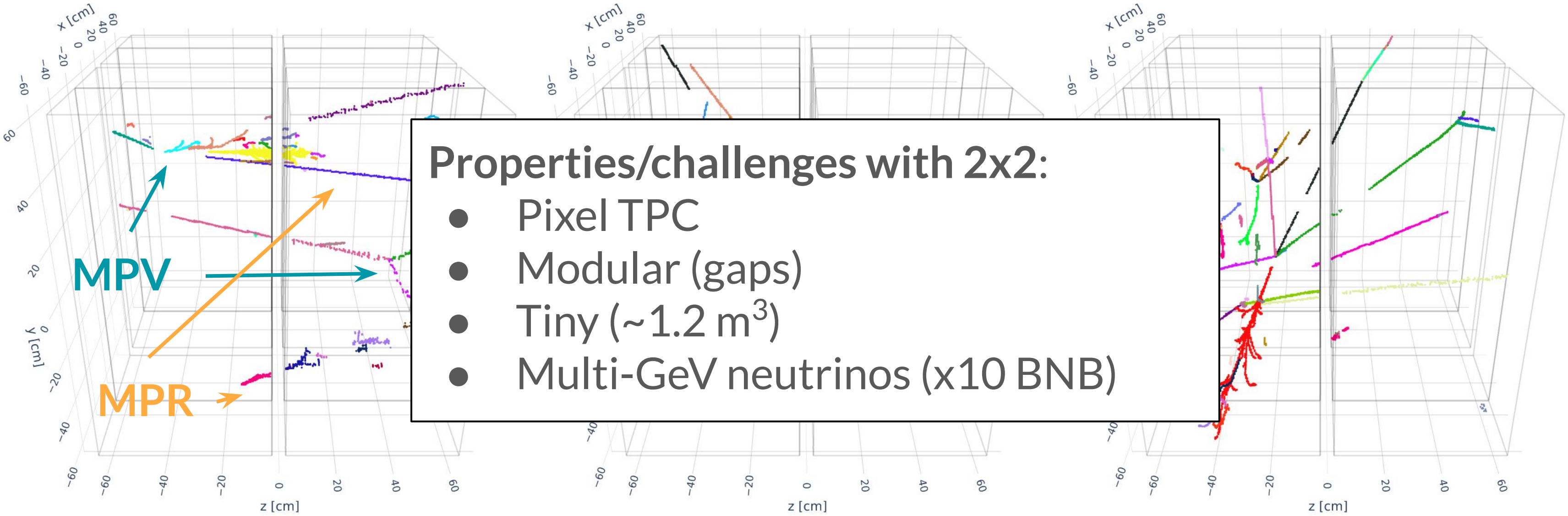
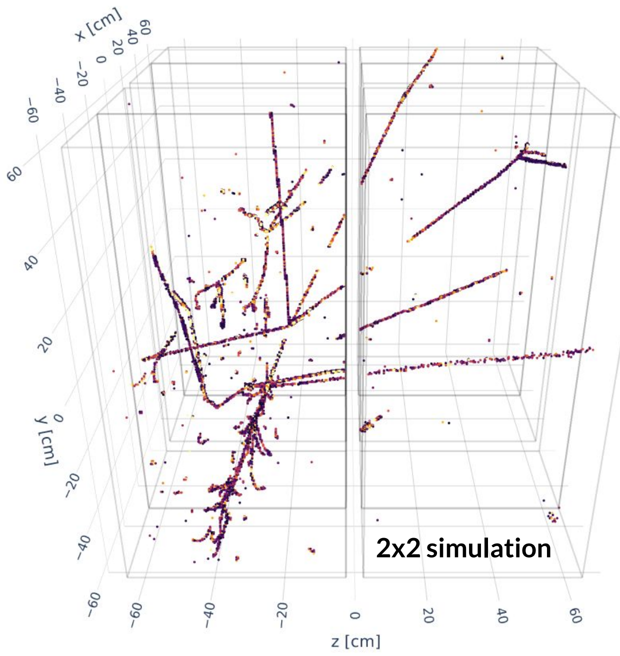


Properties/challenges with 2x2:
- Pixel TPC
- Modular (gaps)
- Tiny (~1.2 m^3)
- Multi-GeV neutrinos (x10 BNB)

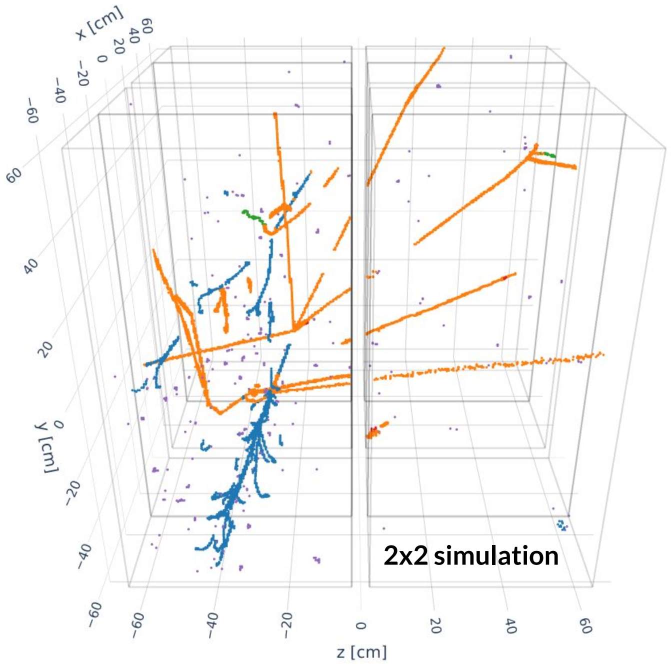
Semantic Segmentation

Separate **topologically different** types of activity

- Tracks, Showers, delta rays, Michel electrons, low energy blips



Classify pixels into categories with UResNet



Paper: PhysRevD.102.012005

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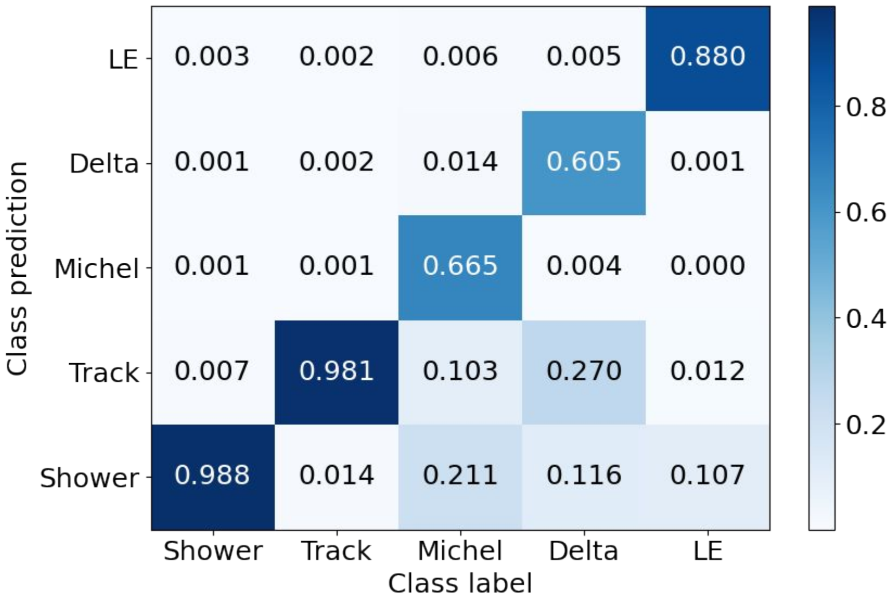
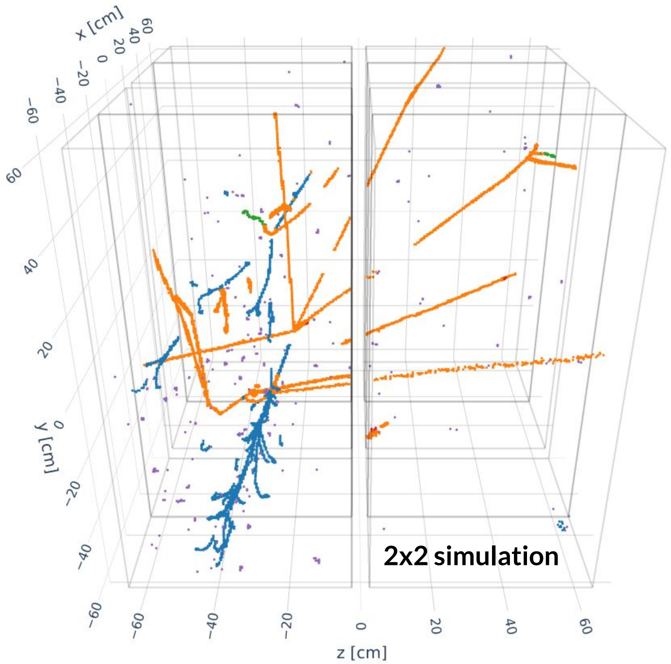
Separate **topologically different** types of activity

- Tracks, Showers, delta rays, Michel electrons, low energy blips



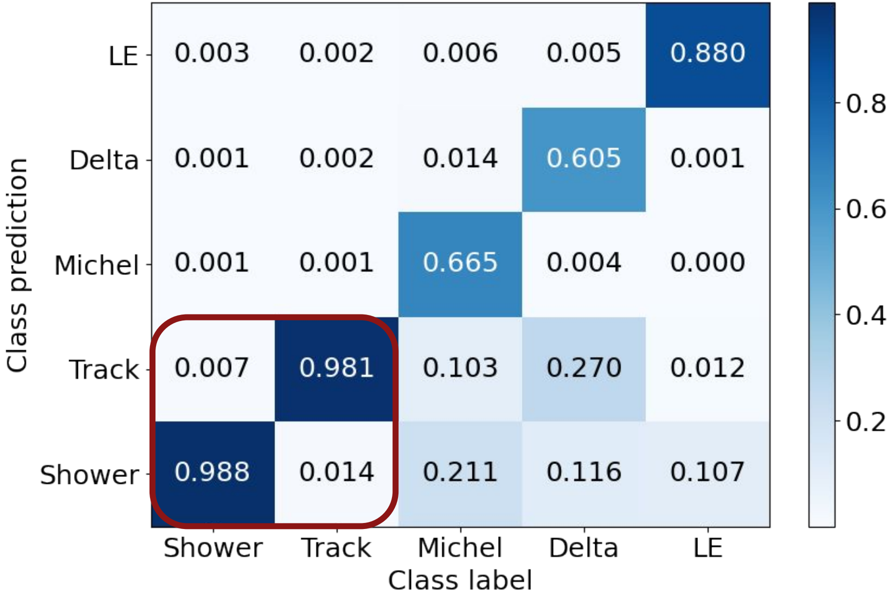


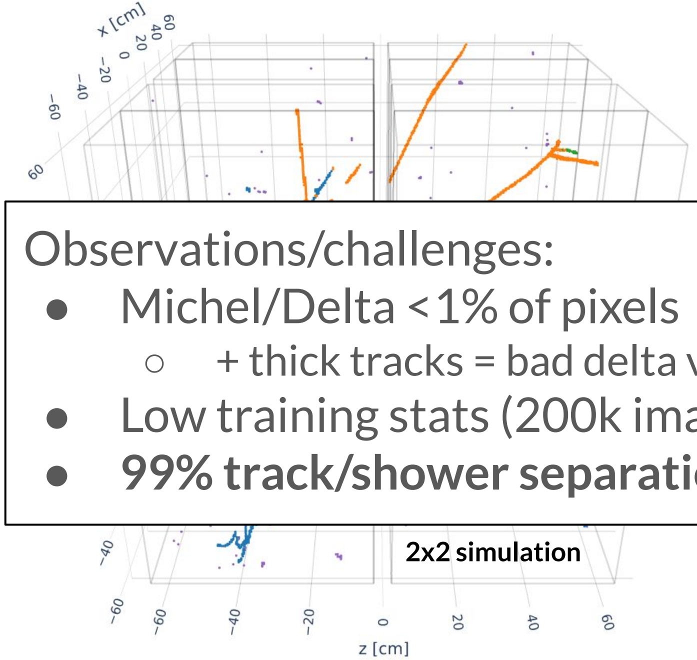
Paper: PhysRevD.102.012005

Semantic Segmentation

Separate **topologically different** types of activity

- Tracks, Showers, delta rays, Michel electrons, low energy blips





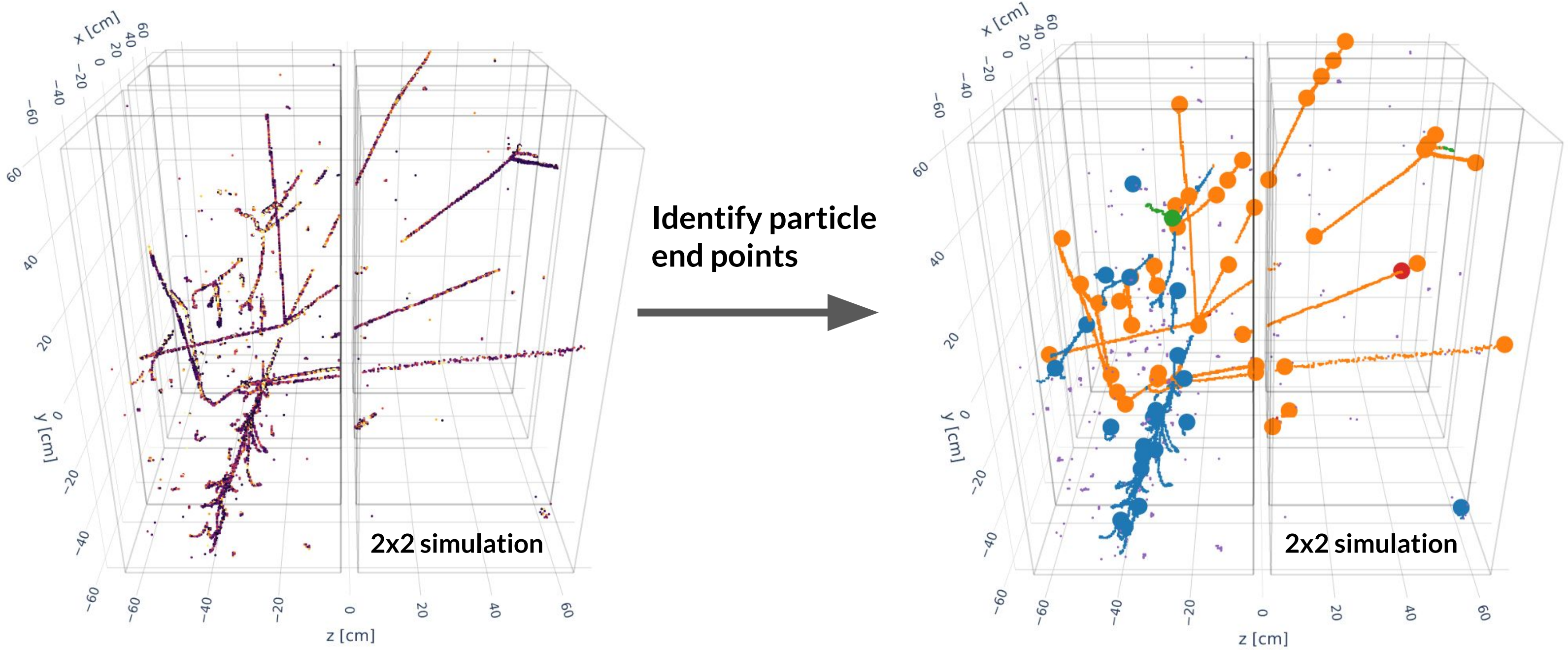
Observations/challenges:
- Michel/Delta <1% of pixels
  - + thick tracks = bad delta visibility
- Low training stats (200k images)
- **99% track/shower separation**

Paper: PhysRevD.102.012005

Points of Interest

Identify start points of showers and end points of tracks

- Tracks, Showers, delta rays, Michel electrons, low energy blips



Paper: PhysRevD.102.012005

Points of Interest

SLAC NATIONAL ACCELERATOR LABORATORY

Identify start points of showers and end points of tracks

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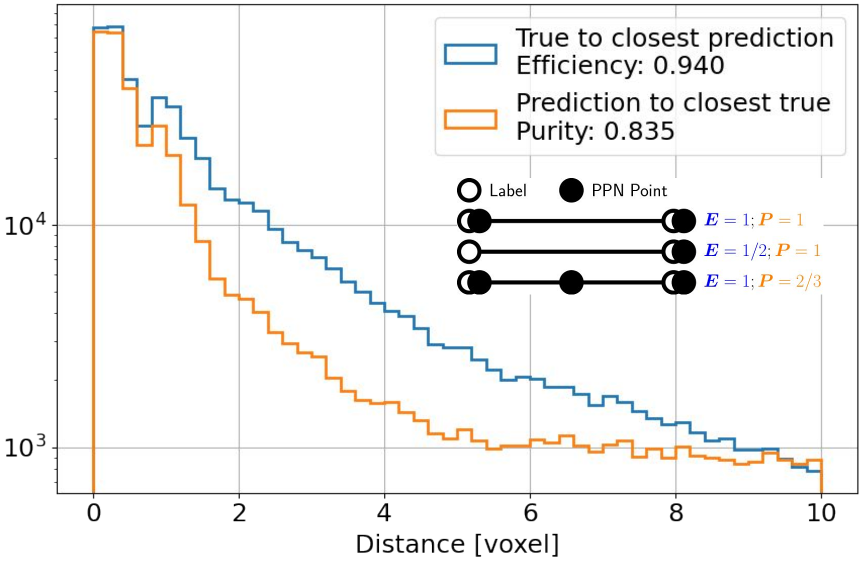

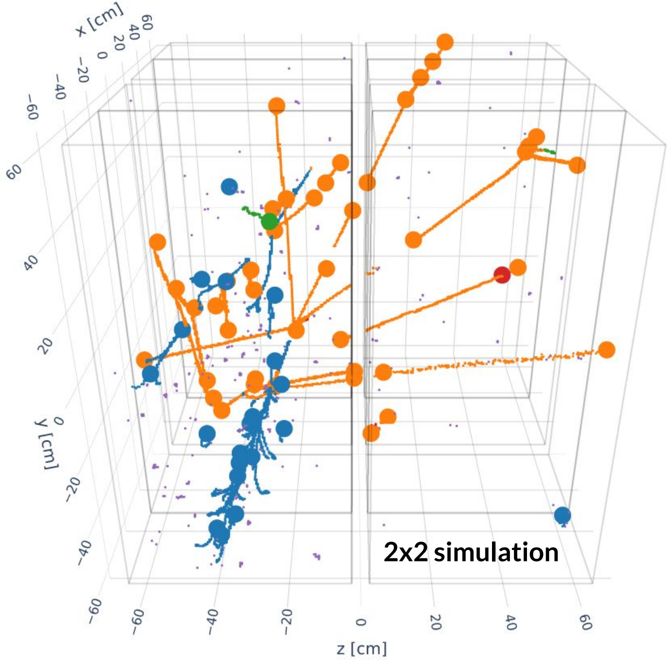

Paper: [PhysRevD.102.012005]

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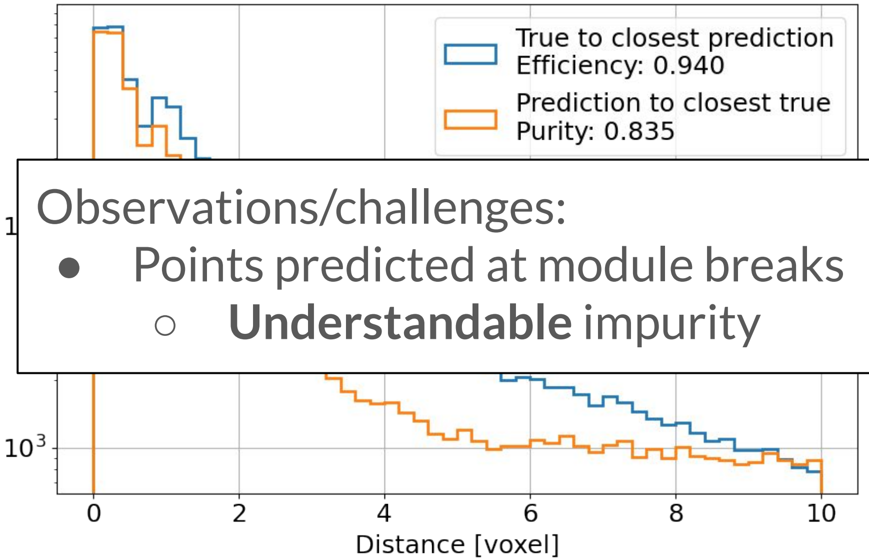
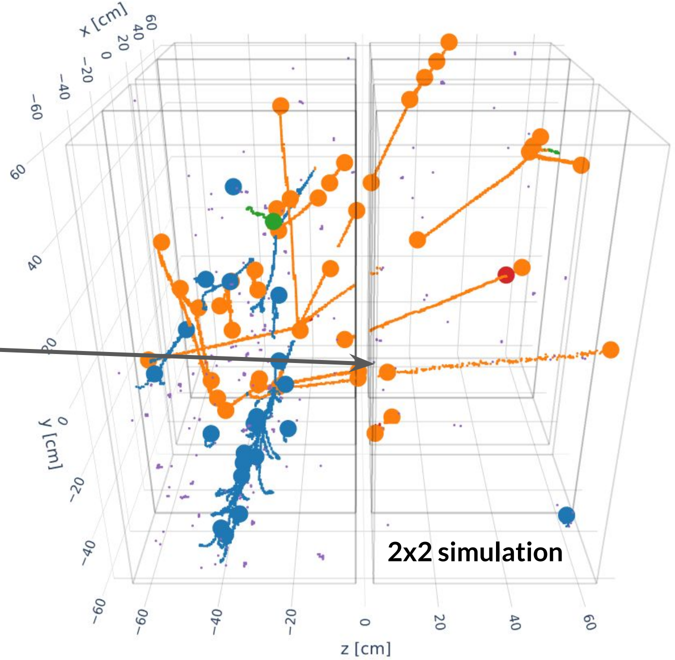


Observations/challenges:
- Points predicted at module breaks
  - **Understandable** impurity

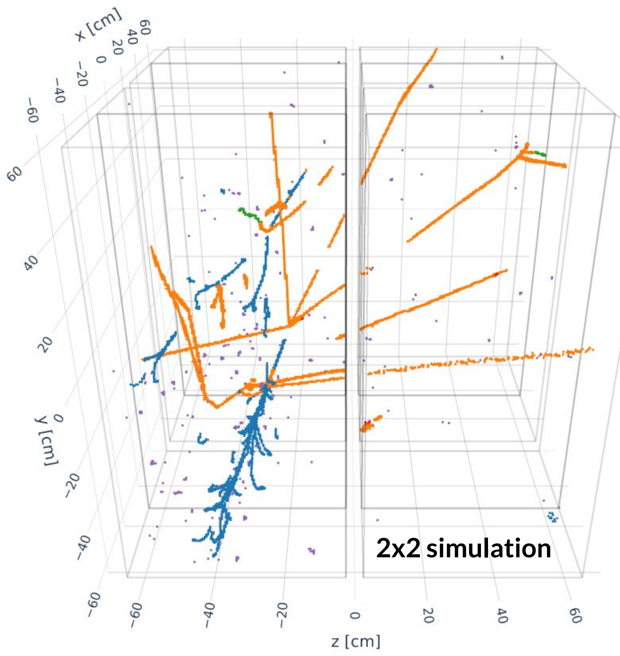


Paper: [PhysRevD.102.012005]

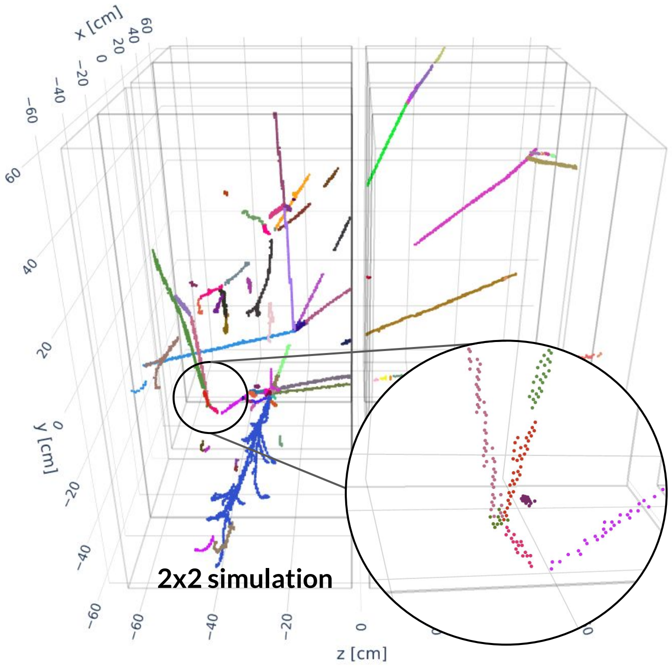
Dense Fragment Formation

Break track/shower fragment instances **where constituent pixels touch**

- Cluster track/shower **fragments** at this stage



Classify pixels into dense clusters

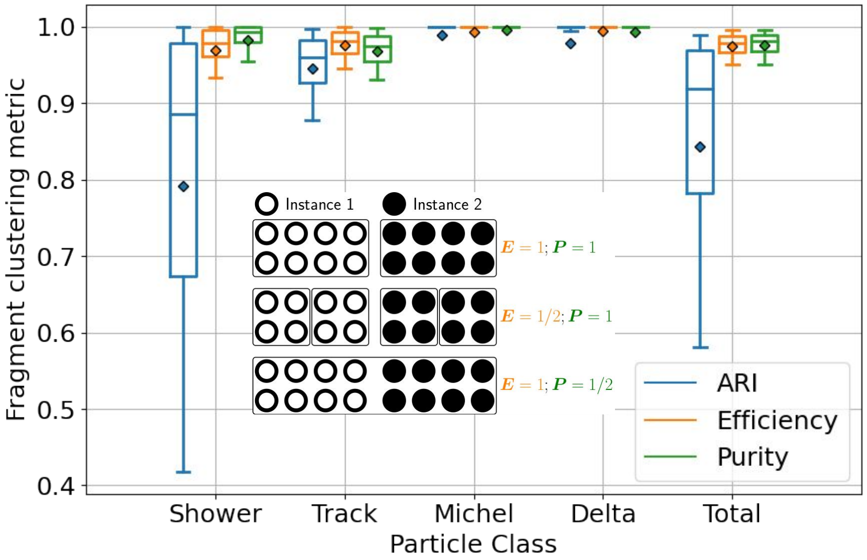


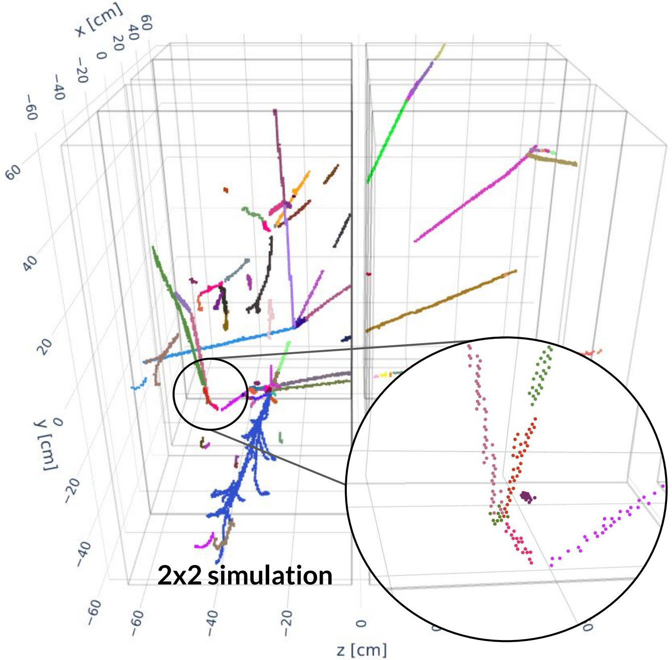
Paper: [arXiv:2007.03083](https://arxiv.org/abs/2007.03083)

Dense Fragment Formation

Break track/shower fragment instances **where constituent pixels touch**

- Cluster track/shower **fragments** at this stage





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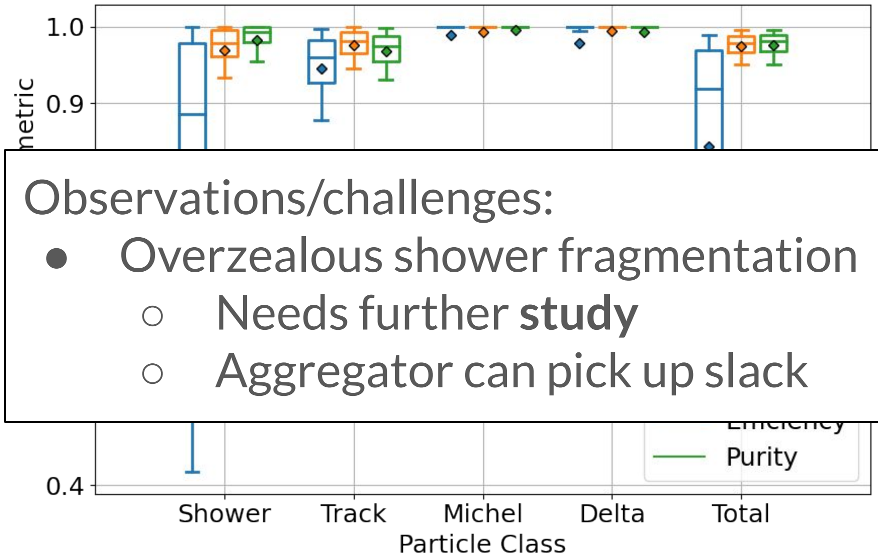
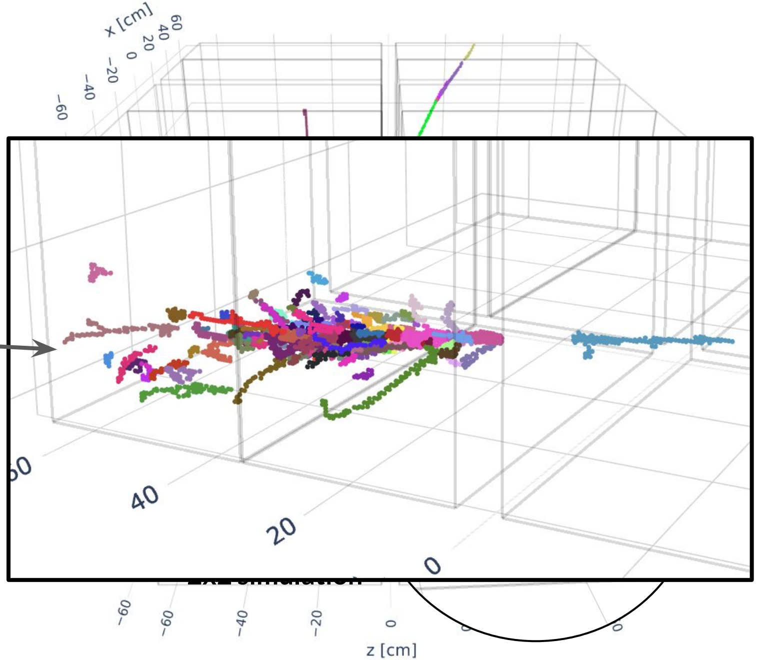


Observations/challenges:

- Overzealous shower fragmentation
  - Needs further **study**
  - Aggregator can pick up slack

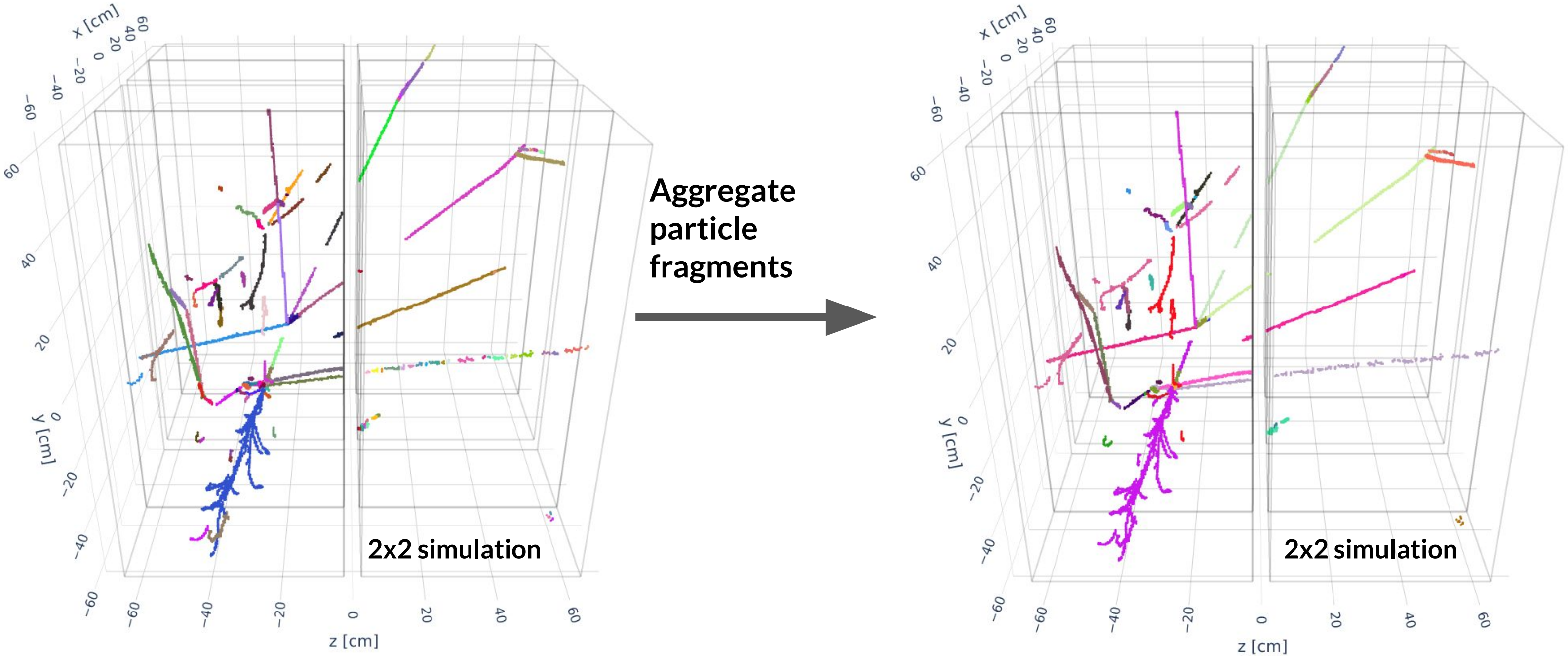


Paper: [arXiv:2007.03083](https://arxiv.org/abs/2007.03083)

Particle Aggregation

Aggregate track/shower fragment instances into **particles**

- Find edges that connect **fragments that belong together**



Paper: [PhysRevD.104.072004]

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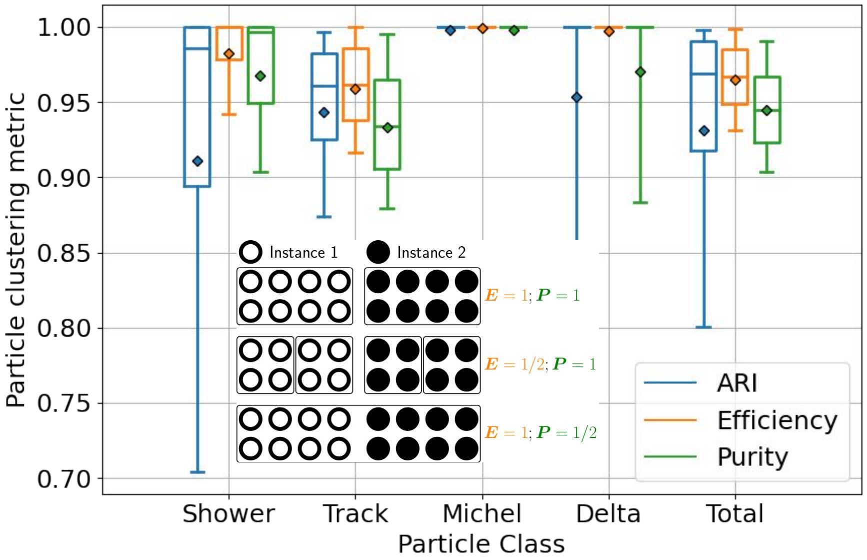

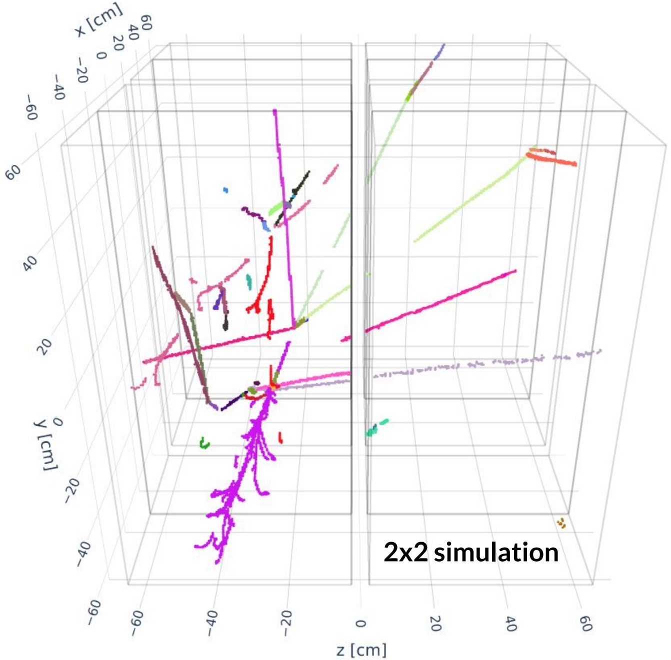

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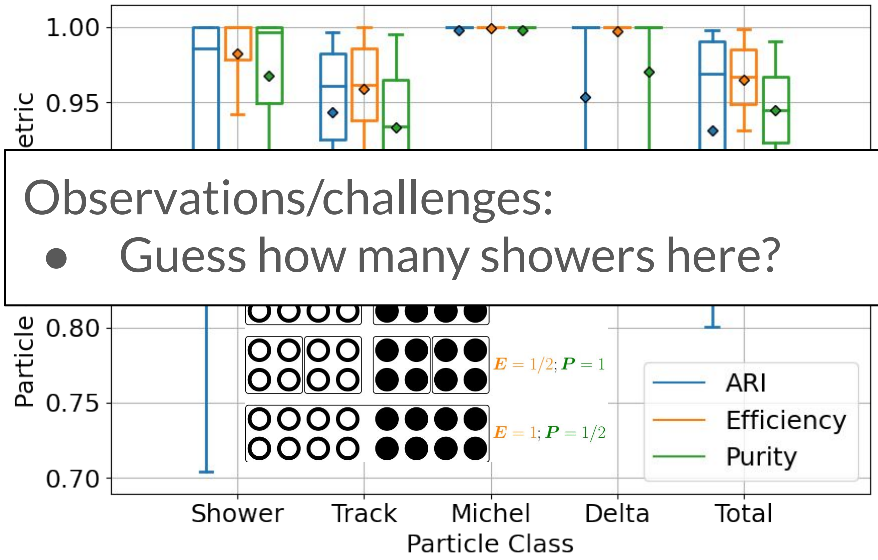
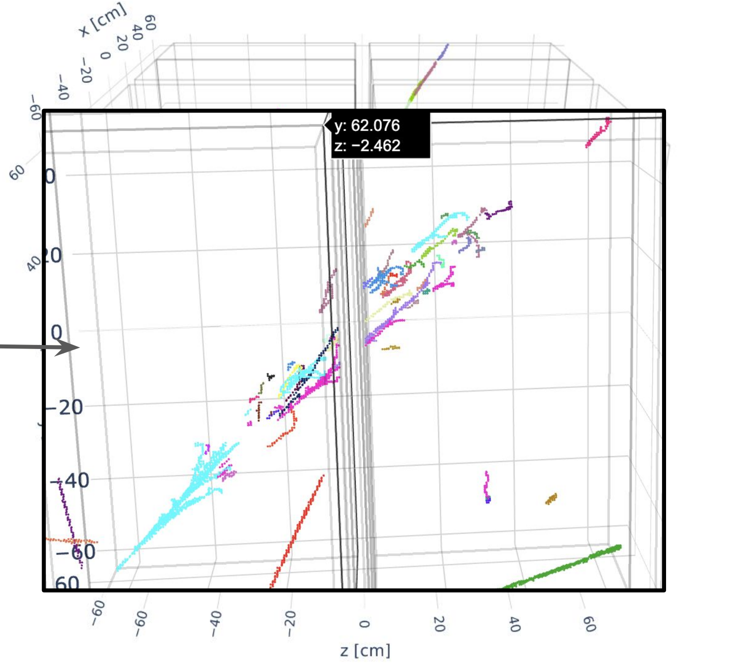


Observations/challenges:

- Guess how many showers here?



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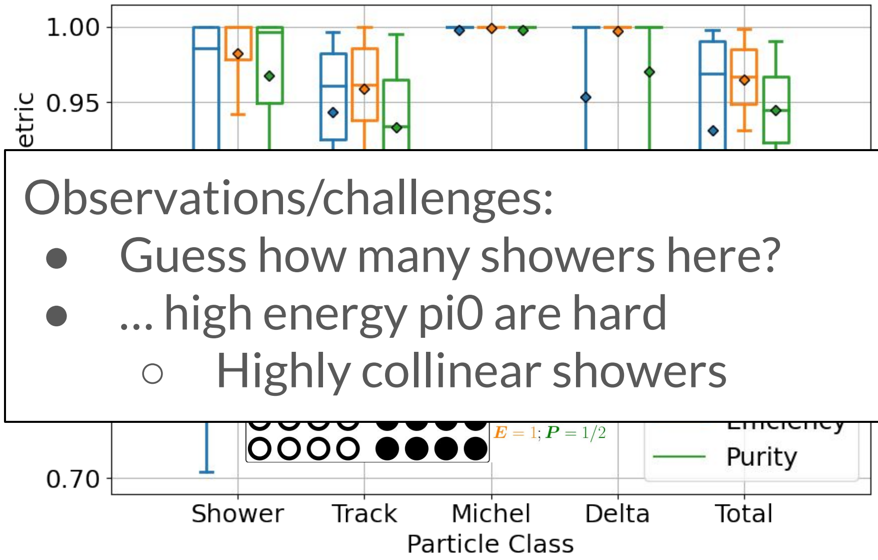
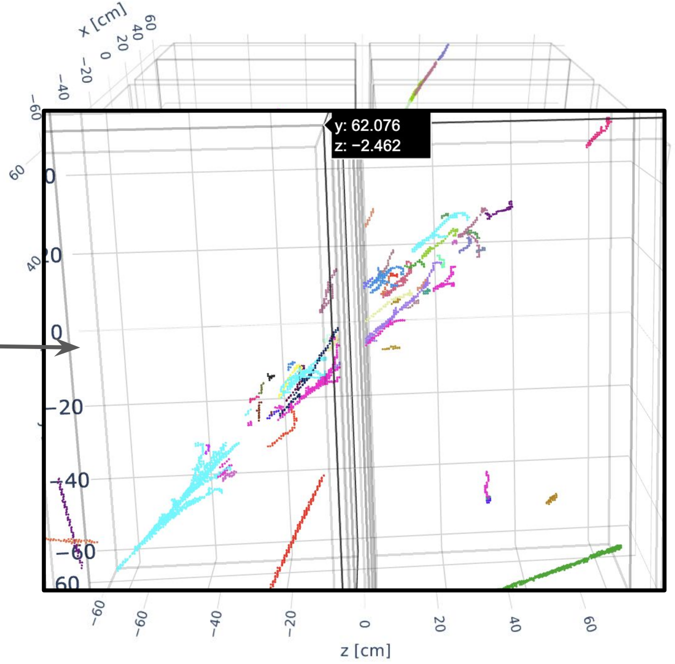


Observations/challenges:

- Guess how many showers here?
- … high energy pi0 are hard
  - Highly collinear showers

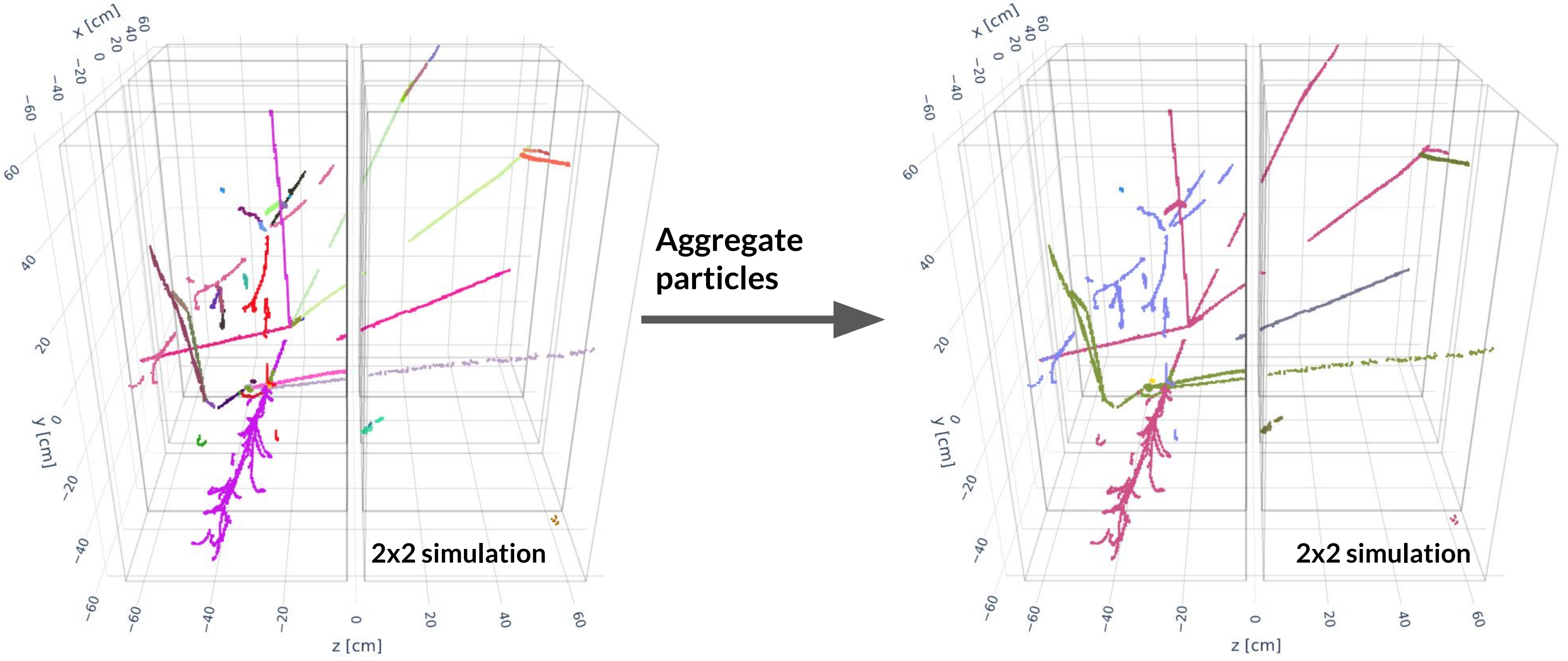


Paper: PhysRevD.104.072004

Interaction Aggregation

Aggregate track/shower instances into **interactions**

- Find edges that connect **particles that belong together**



Paper: PhysRevD.104.072004

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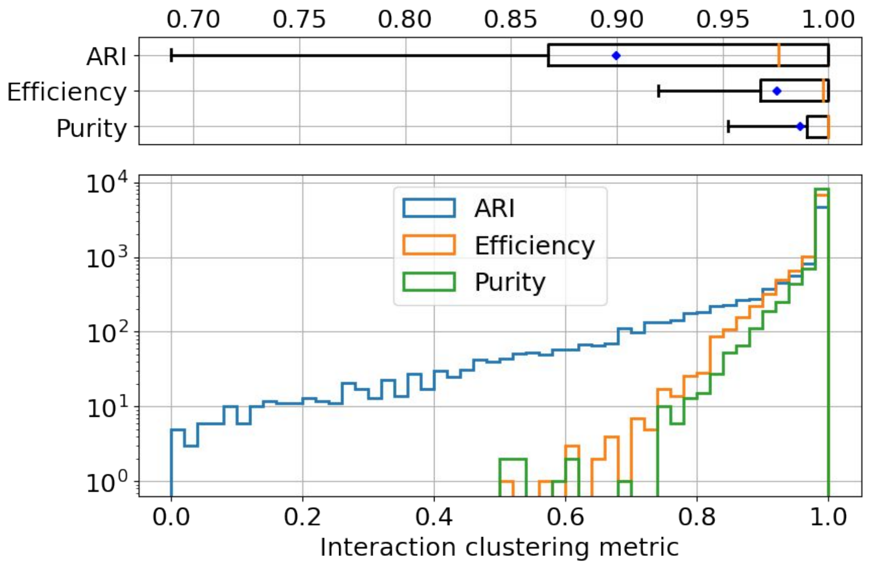

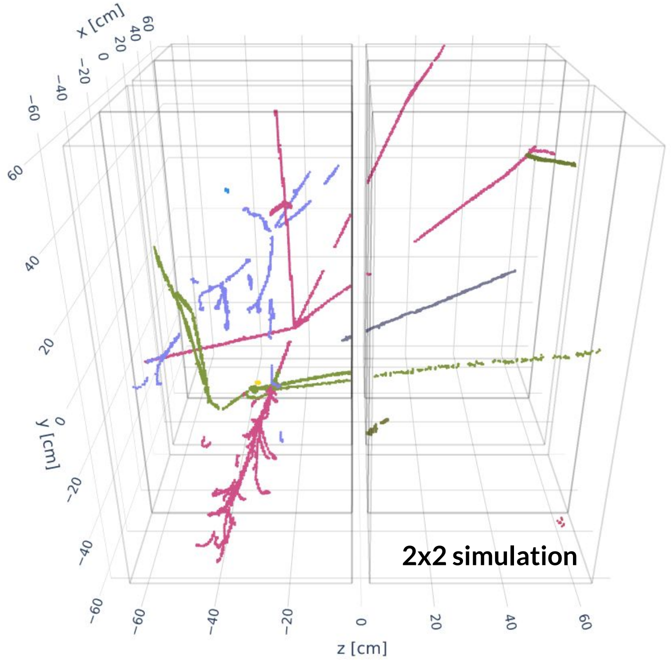

Paper: [PhysRevD.104.072004]

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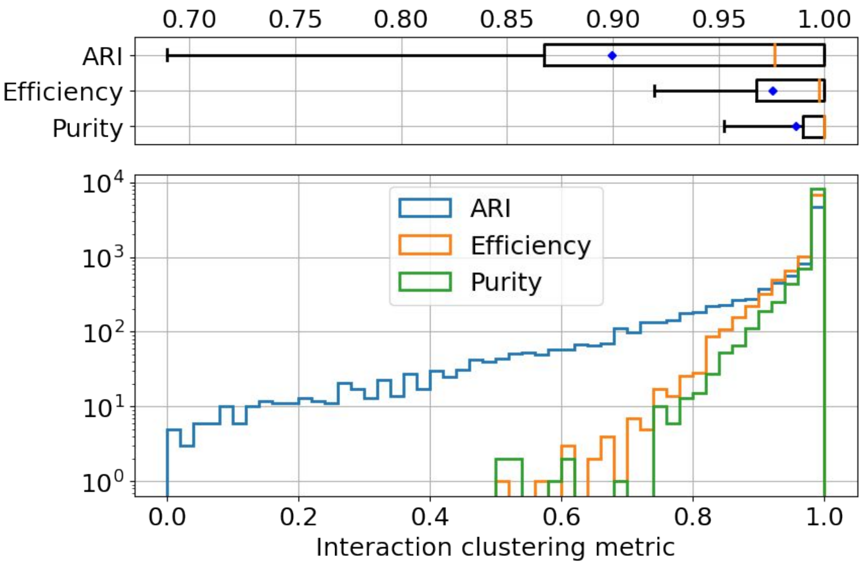

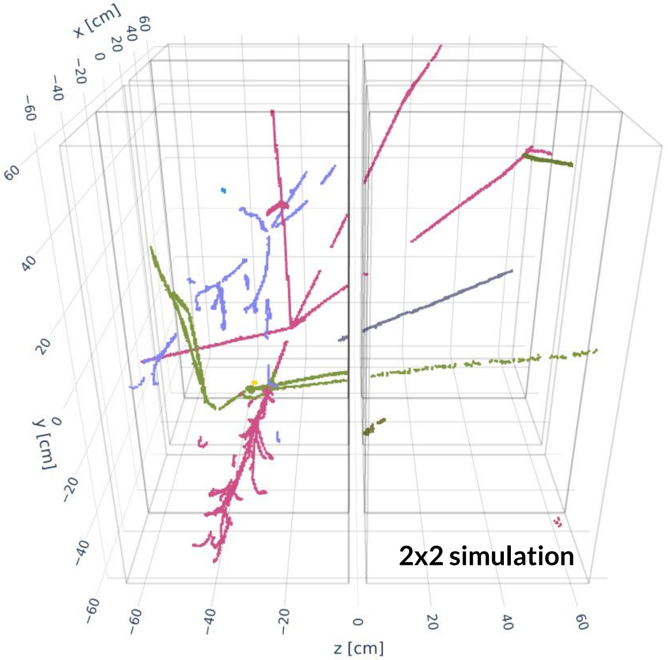

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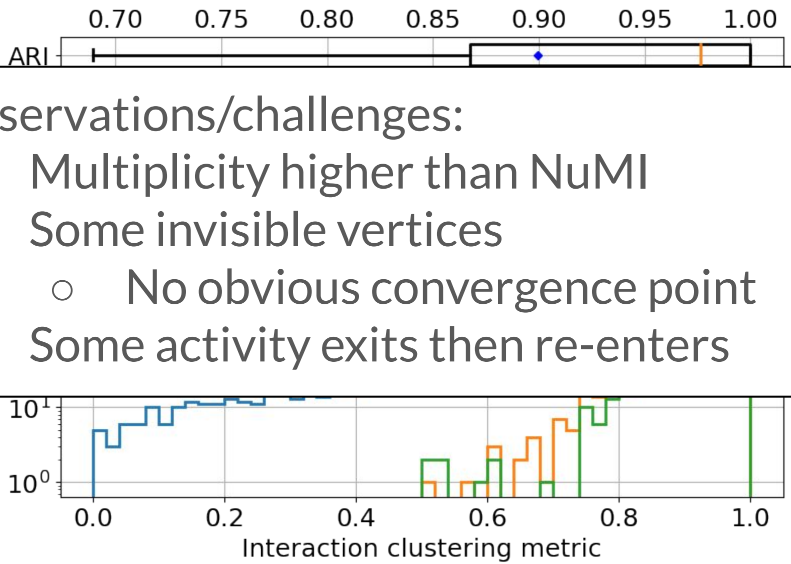
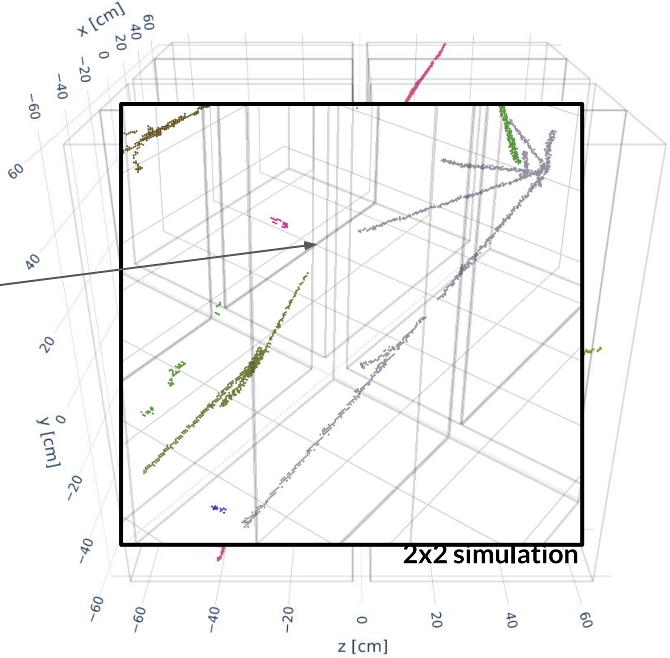


Observations/challenges:

- Multiplicity higher than NuMI
- Some invisible vertices
  - No obvious convergence point
- Some activity exits then re-enters

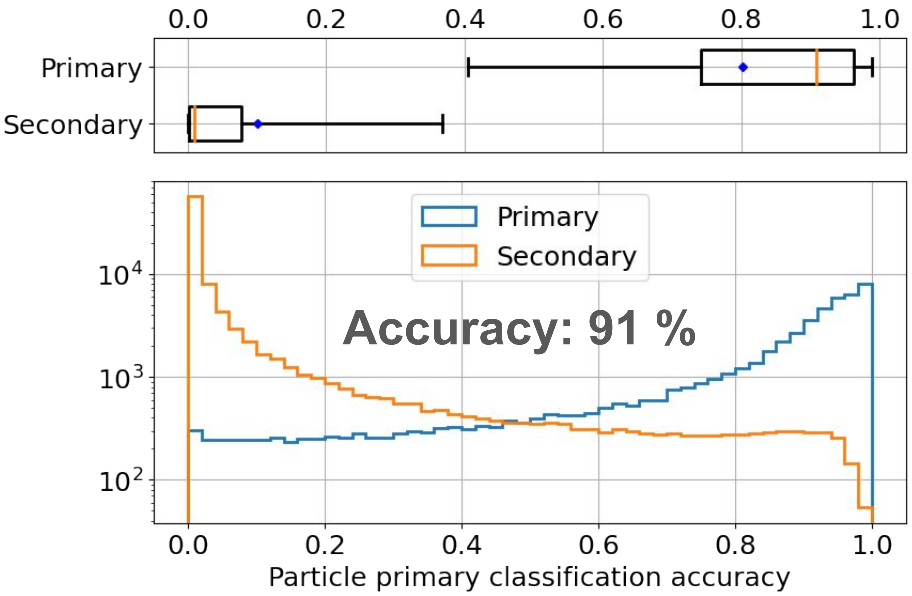


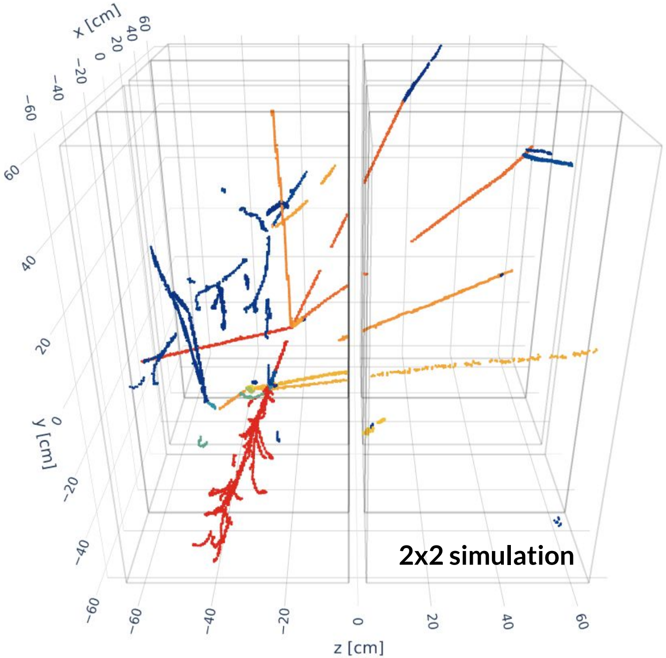
Paper: PhysRevD.104.072004

Primary Identification

Identify particle originating from the primary vertex

- Secondaries – Primaries



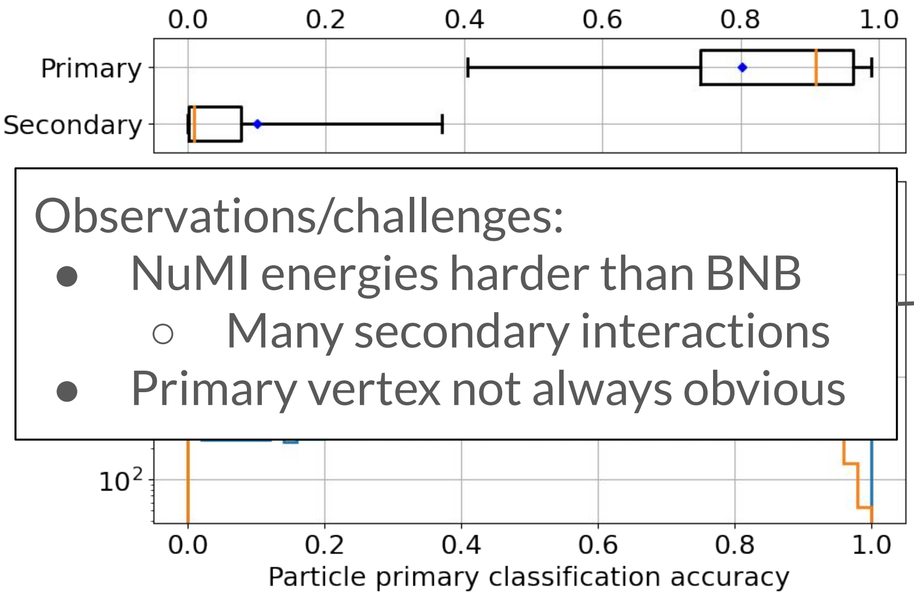


Paper: PhysRevD.104.072004

Primary Identification

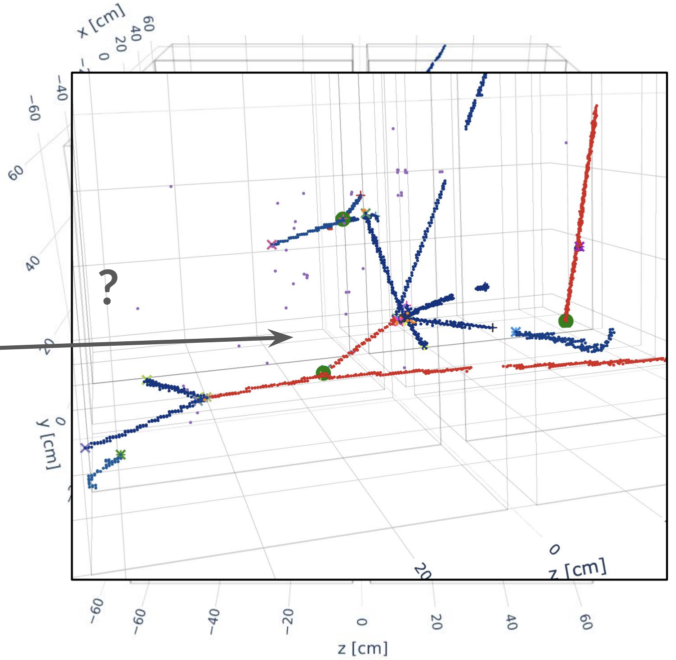
Identify particle originating from the **primary vertex**

- Secondaries — Primaries



Observations/challenges:

- NuMI energies harder than BNB
  - Many secondary interactions
- Primary vertex not always obvious

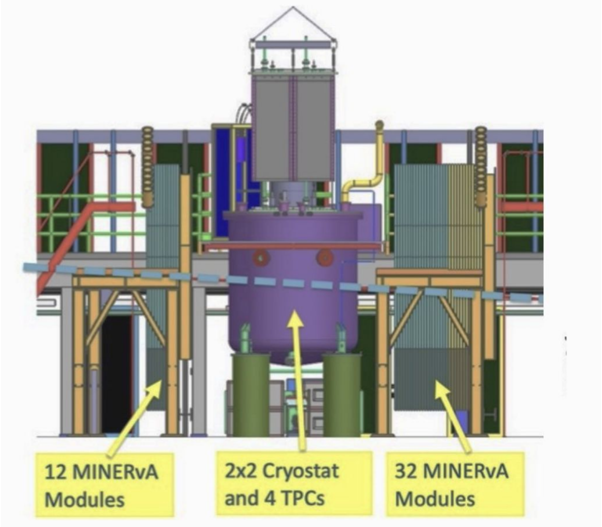


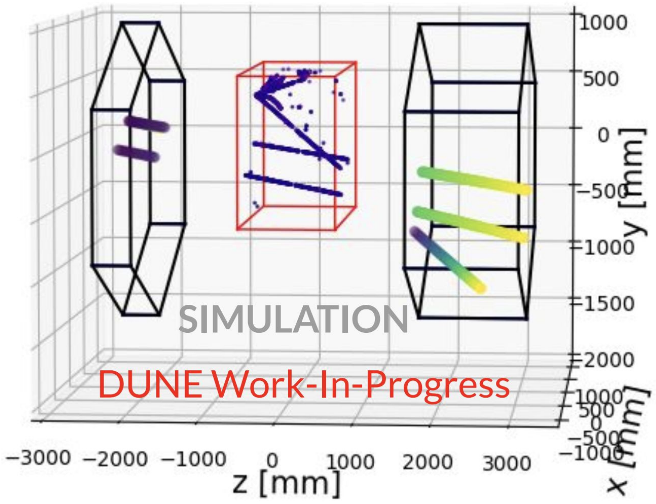
Paper: PhysRevD.104.072004

Beyond LArTPCs

Multi-detector training:

- J. Micallef looking into Minerva integration, see her talk later today!
- This would be directly apply to ND-LAr + TMS!



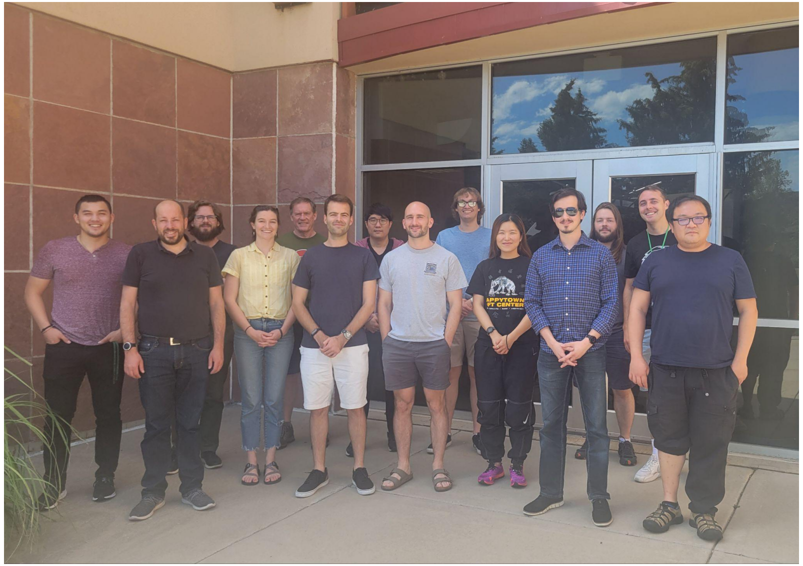


SBN-2x2 Joint ML Workshop

Goal: Familiarize analyzers with the inner workings of the ML-based reco. chain

Where: Tufts University, Boston, MA

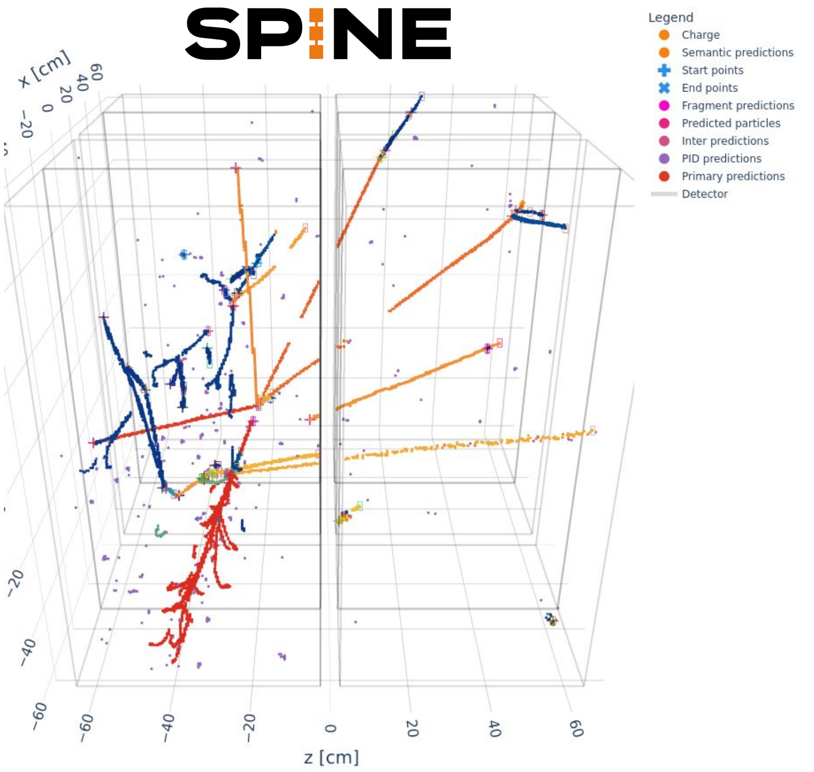
When: 22-26 July, join us!!! https://indico.slac.stanford.edu/event/8926/



Conclusions

SPINE keeps progressing:

- **Sparse-UResNet** for pixel-level features + **GNNs** for aggregation
- **ICARUS** on the cusp of multiple **physics papers** using this pipeline
- **SBND** and **2x2** (high neutrino energy) simulation studies **progressing fast**! Stay tuned…
- Check out this brand new **2x2** [interactive reconstructed event]!

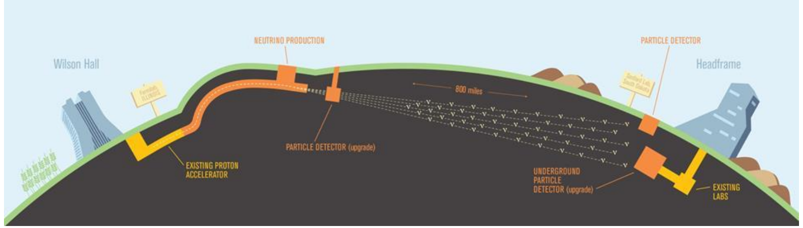


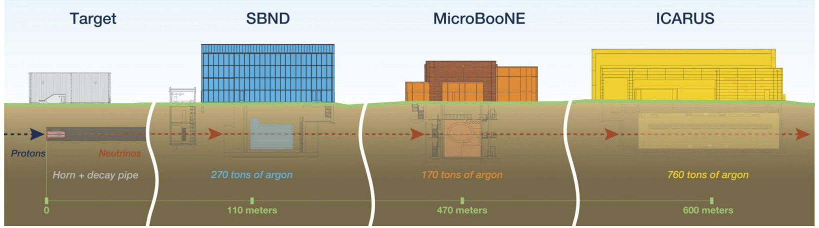
Backup Slides

DUNE and SBN

Two **US-based neutrino oscillation experiments** use/will use **LArTPCs**

Deep Underground Neutrino Experiment (DUNE), 2028-?	Short Baseline Neutrino (SBN) program, 2015-2027
1300 km: **enhance matter effects** ● Mass ordering, CP violation ● **DUNE**-FD rate: **O(10^3) ν / year**	0.6 km: **observe anomalies** ● New type of neutrino? ● **SBN** S/B ratio: **~ O(10^{-5})**





Neutrino Oscillations

Neutrinos **oscillate** (change flavor states)

- Observed in **many experiments**
  - Atmospheric, beams, reactors, solar
- **They must have mass** (≠ minimal SM)

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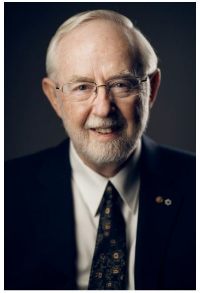
Takaaki Kajita



© Nobel Media AB. Photo: A. Mahmoud
Arthur B. McDonald

$$P_{\nu_\alpha\to\nu_\beta}(t) = \delta_{\alpha\beta} - 4\sum_{i>j}\Re(\boxed{U^*_{\alpha i}U_{\beta i}U_{\alpha j}U^*_{\beta j}})\sin^2\left(\frac{\boxed{\Delta m^2_{ij}}\,\boxed{L}}{\boxed{4E}}\right)$$

$$+\,2\sum_{i>j}\Im(\boxed{U^*_{\alpha i}U_{\beta i}U_{\alpha j}U^*_{\beta j}})\sin\left(\frac{\Delta m^2_{ij}L}{4E}\right),$$

Mass splitting

Baseline

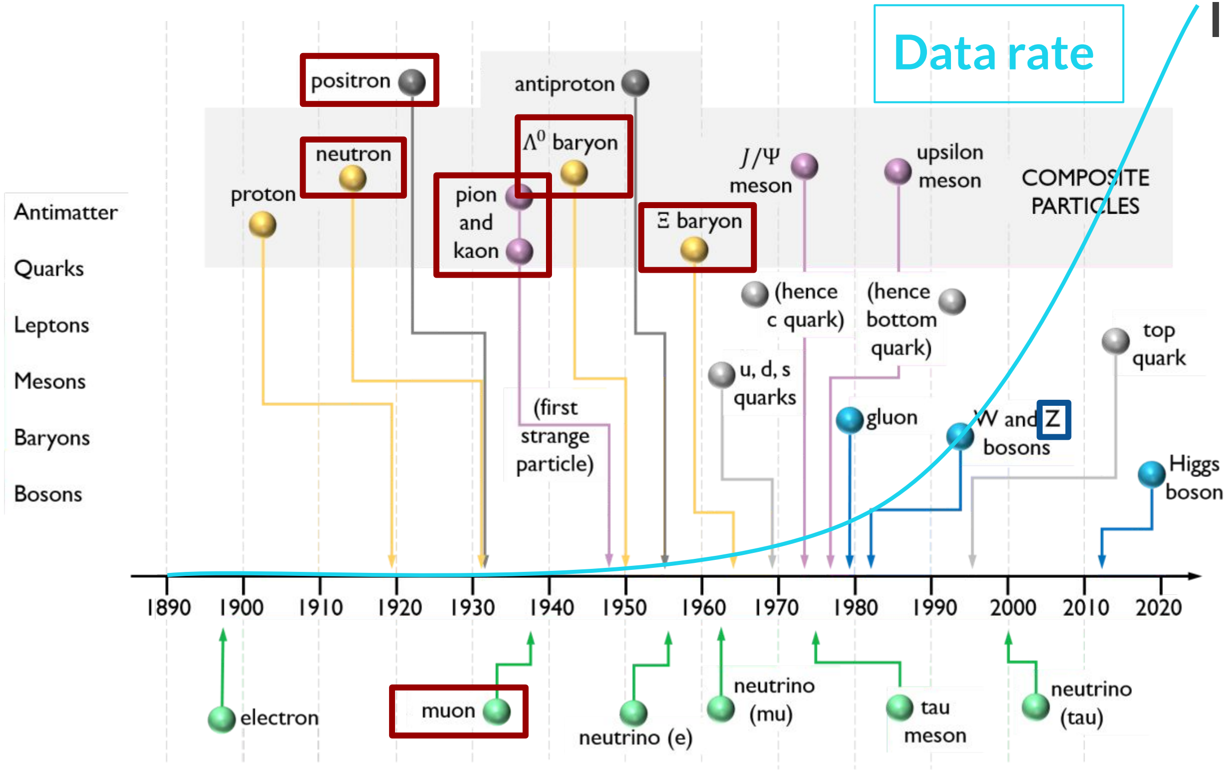
Neutrino energy

Choice of experiment

$$\begin{pmatrix}\nu_e\\ \nu_\mu\\ \nu_\tau\end{pmatrix} = \begin{pmatrix}1 & 0 & 0\\ 0 & c_{23} & s_{23}\\ 0 & -s_{23} & c_{23}\end{pmatrix}\begin{pmatrix}c_{13} & 0 & s_{13}e^{-i\delta_{CP}}\\ 0 & 1 & 0\\ -s_{13}e^{i\delta_{CP}} & 0 & c_{13}\end{pmatrix}\begin{pmatrix}c_{12} & s_{12} & 0\\ -s_{12} & c_{12} & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\nu_1\\ \nu_2\\ \nu_3\end{pmatrix}$$

Mixing matrix

Particle Imaging Detectors



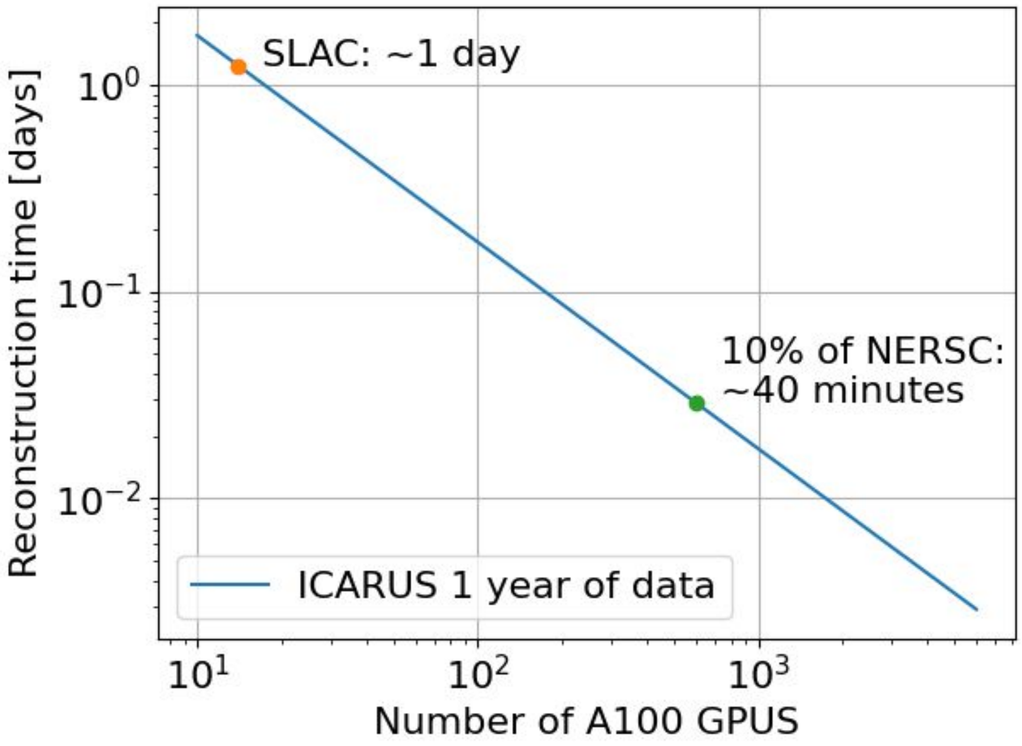
Illustrious History

- Crucial tool for particle discoveries since the 1930s
- How does reconstruction work?

Cloud chamber

Bubble chamber

Scalability



On **ICARUS**:

- **1 s / event,** leveraging **GPU acceleration**
- ~1.5 M BNB beam events / yr

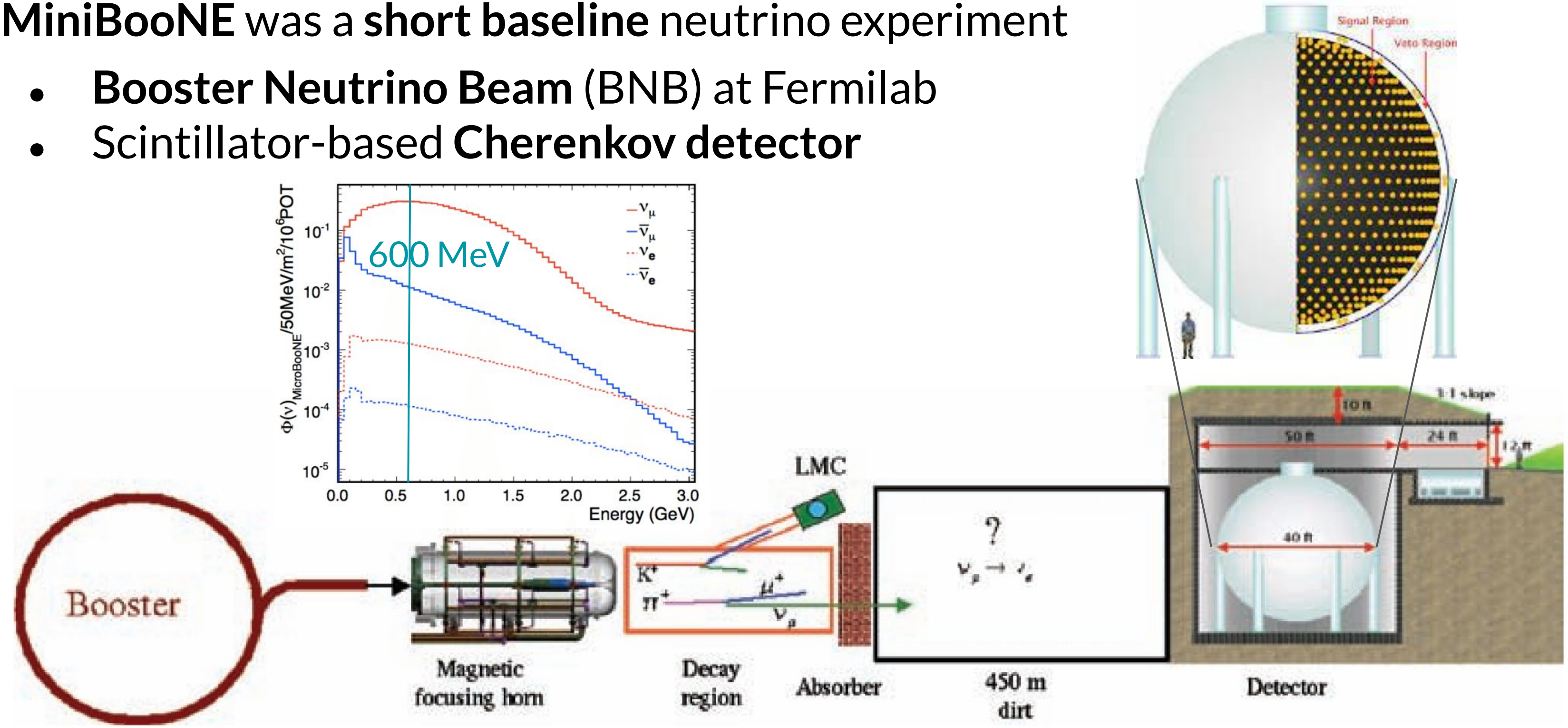
Implications:

- Fast **software development** (testing)
- Fast **turnaround**

The MiniBooNE Low Energy Excess

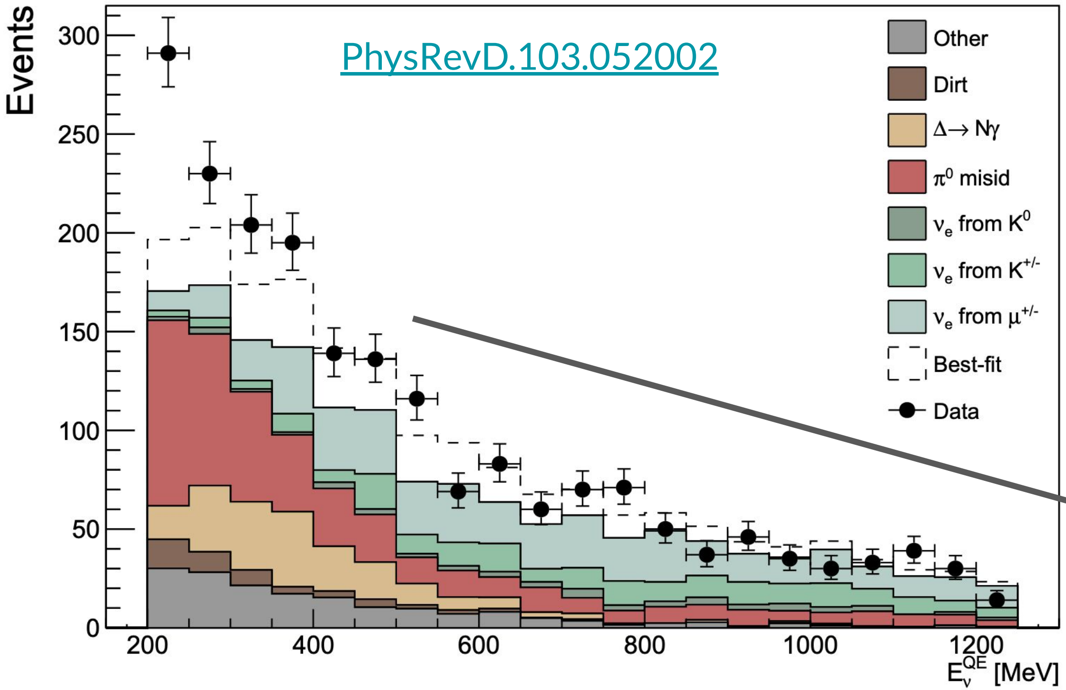
MiniBooNE was a **short baseline** neutrino experiment

- **Booster Neutrino Beam** (BNB) at Fermilab
- Scintillator-based **Cherenkov detector**



The MiniBooNE Low Energy Excess

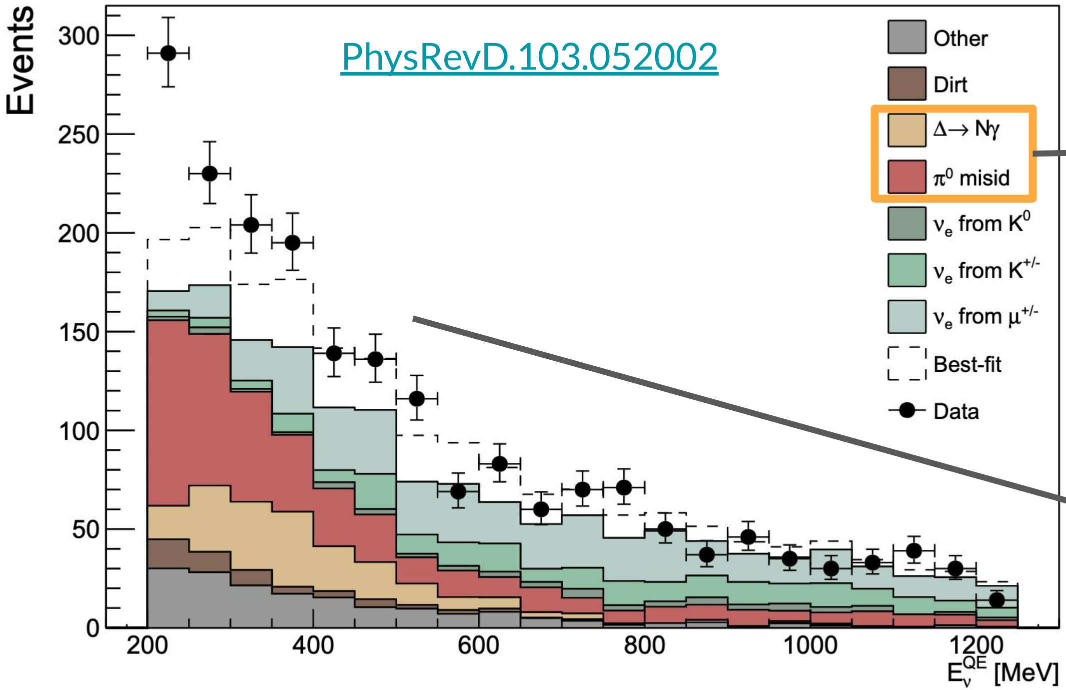
MiniBooNE observed **excess** of “**electron-like**” **neutrino events** (LSND-like)



4.8 sigma excess…

The MiniBooNE Low Energy Excess

Other interpretation: we just don't understand neutrino cross-sections…

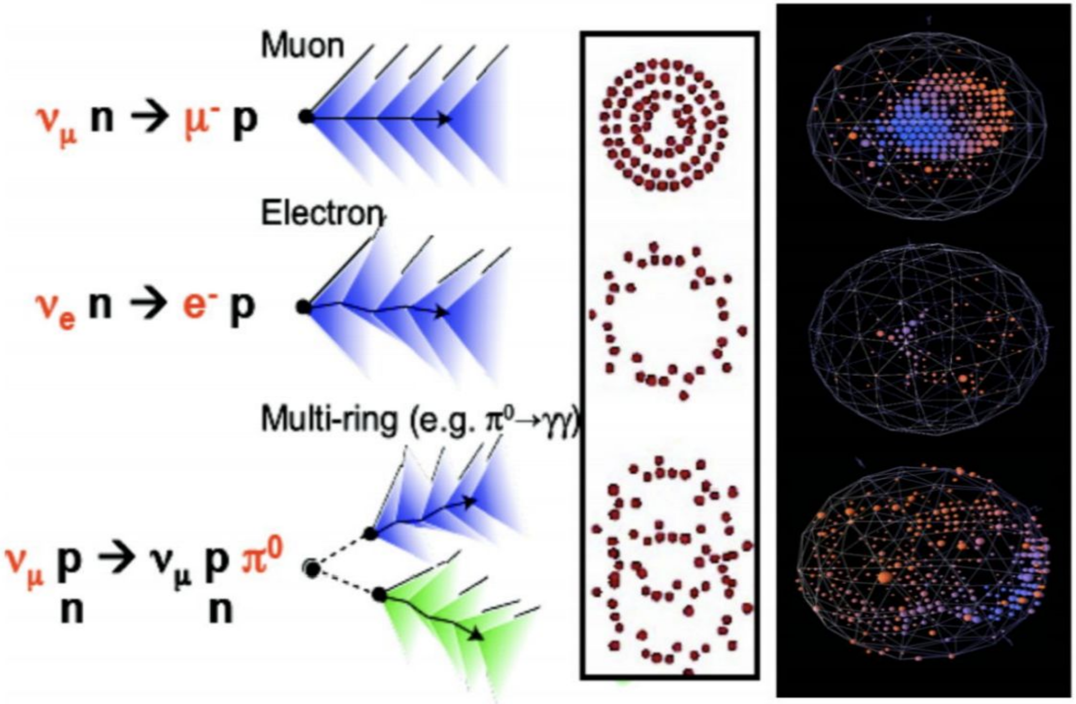


Low-energy "electron-like" events **dominated by ν_μ NC-γ and CC-π^0 background**

4.8 sigma excess…

The MiniBooNE Low Energy Excess

MiniBooNE's limitations: Cannot tell electrons from photons



μ/e separation **reliable**

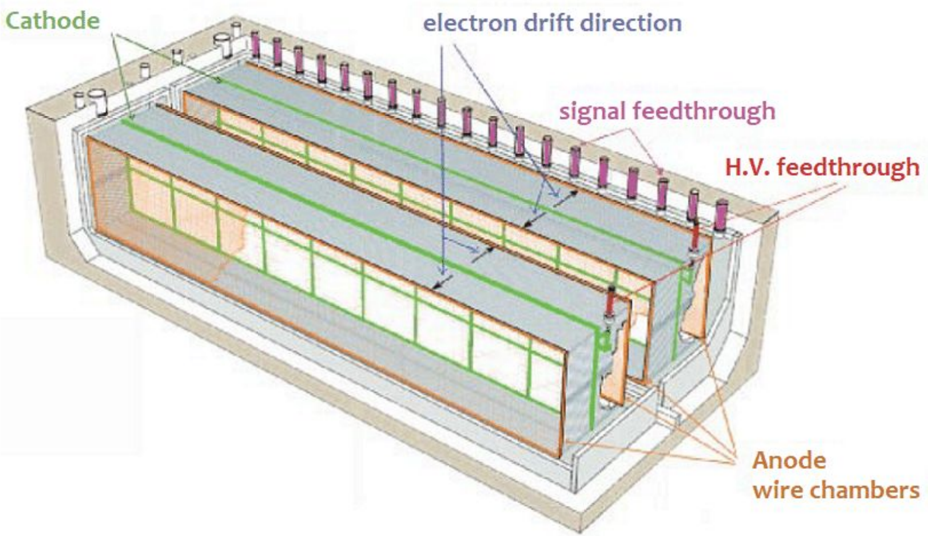
Single e and single-γ events **indistinguishable**

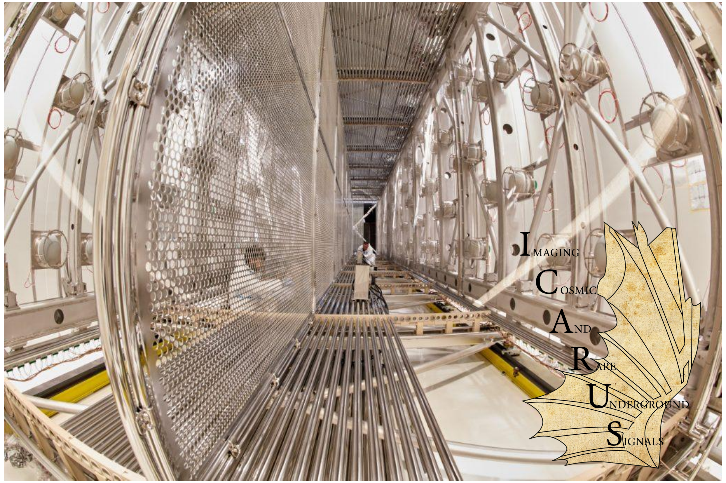
$\pi^0 \to \gamma\gamma$ events **indistinguishable** from e if one gamma missing

The ICARUS Detector

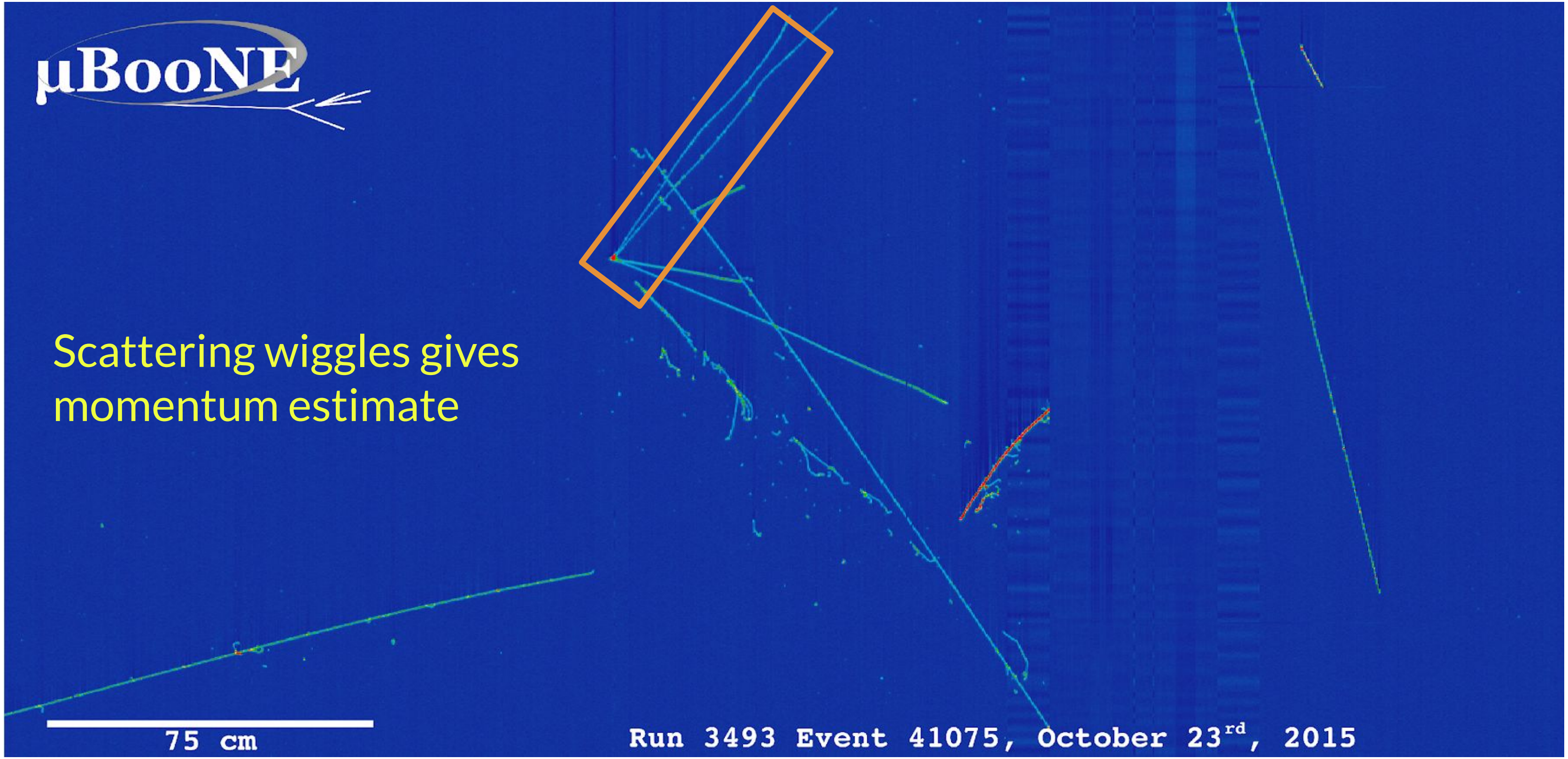
The **largest LArTPC** in operation is **ICARUS**

- **500 t** fiducial mass (2 cryos, 4 TPCs)
- First operation in early 2000s underground (CNGS), at FNAL since 2018

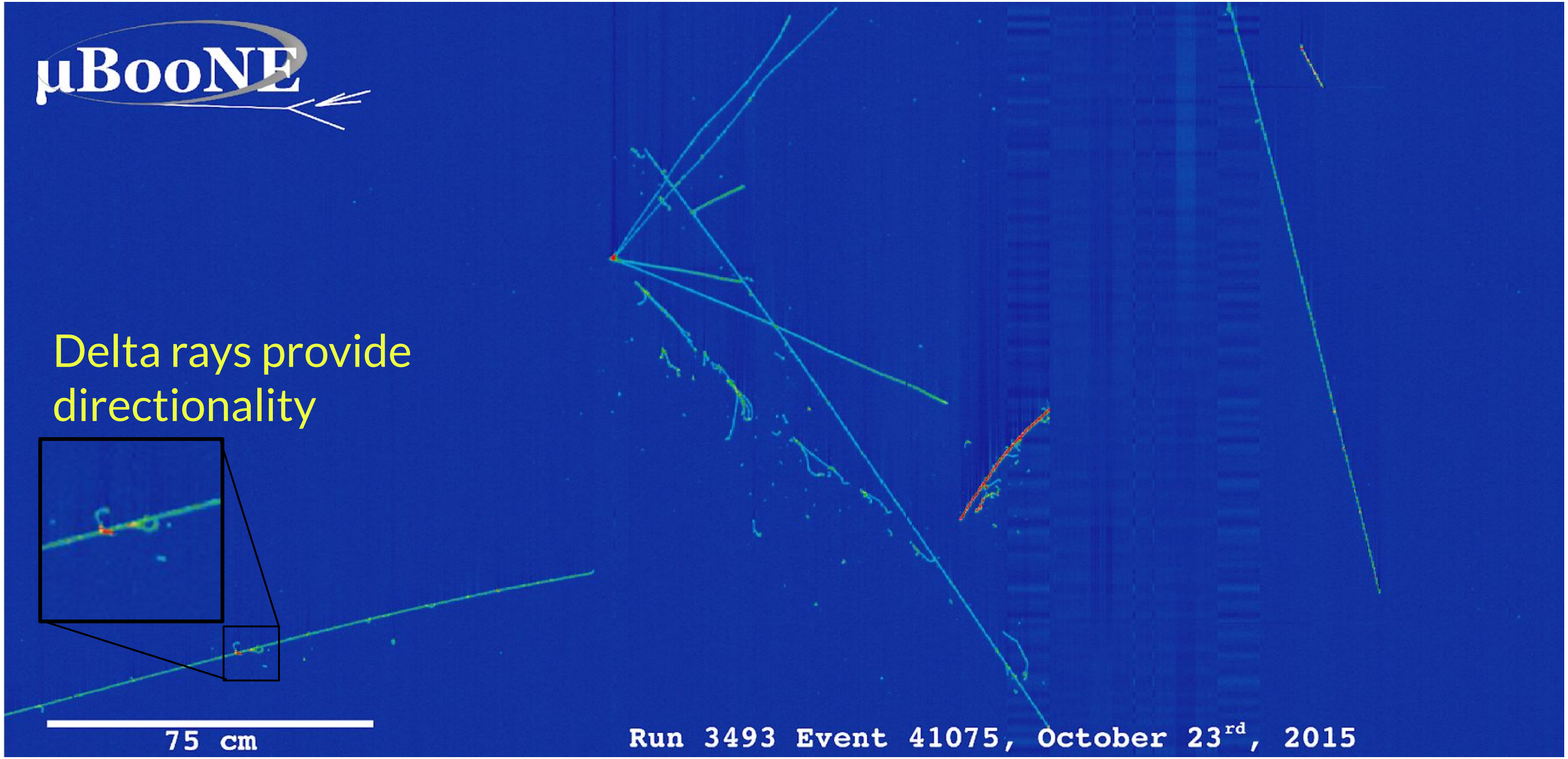




LArTPC Image



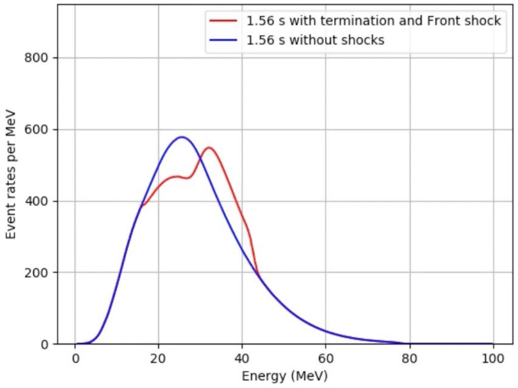
LArTPC Image



The Weight of Expectations

Honorable mention: **EM showers from low energy**

- Crucial for solar + supernovae physics
- Particular interest at SLAC: **A. Friedland et al.**



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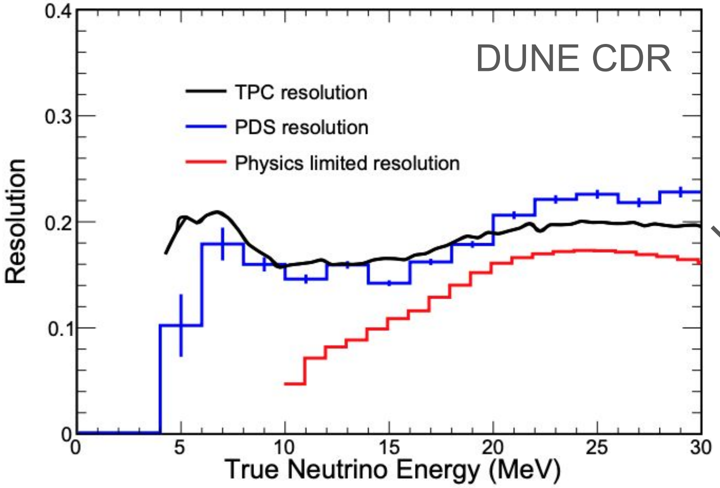
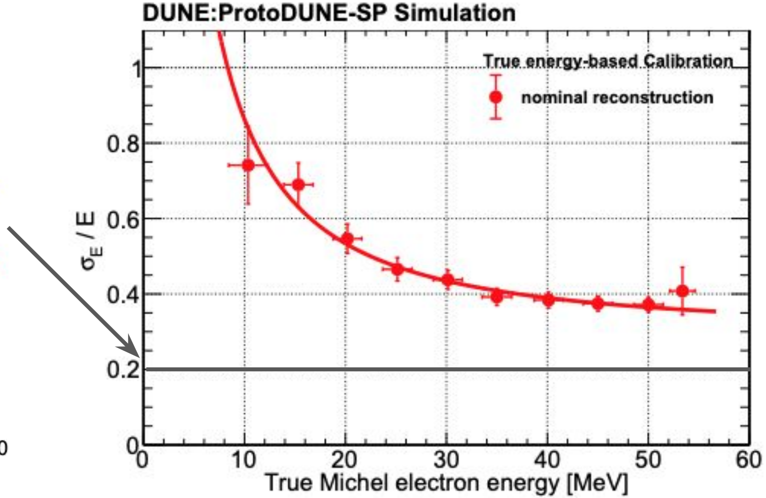
Expectation



arXiv:2008.06647

Reality

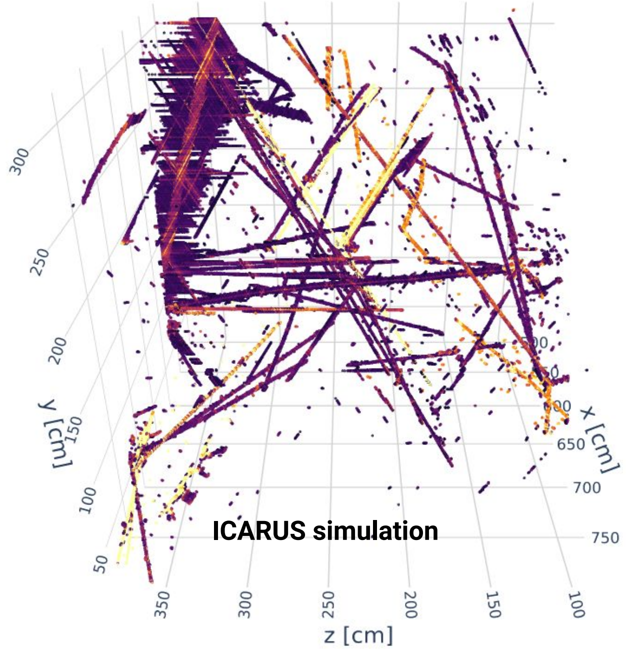


arXiv:2211.01166

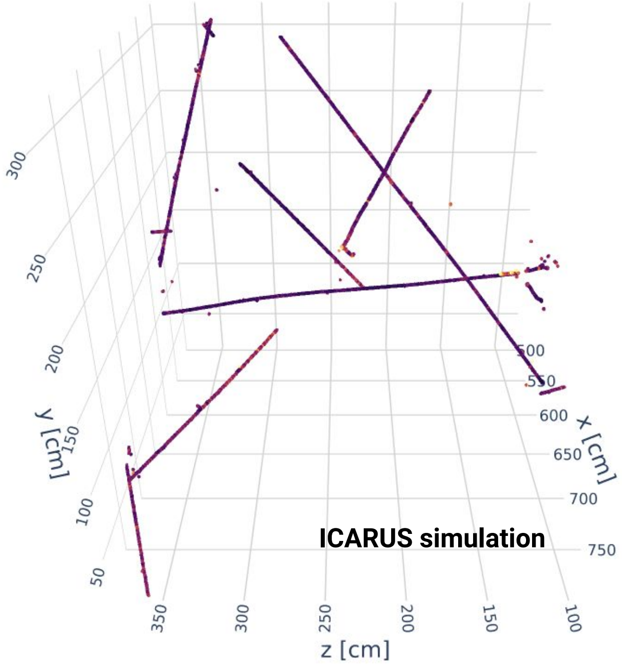
Tomographic Reconstruction

In a **wire TPC**, we do not get 3D images, but rather 3 x 2D projections

- First task: **combine projections into one 3D image**



Remove artifacts with UResNet



Tomographic Reconstruction

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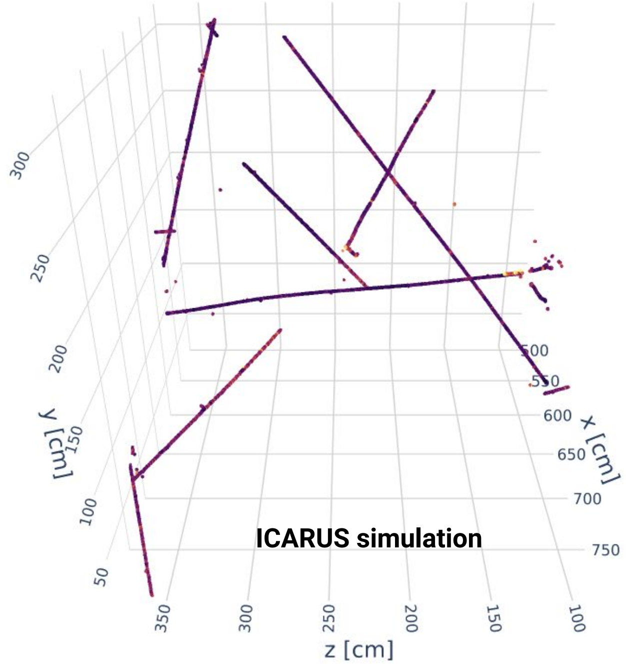
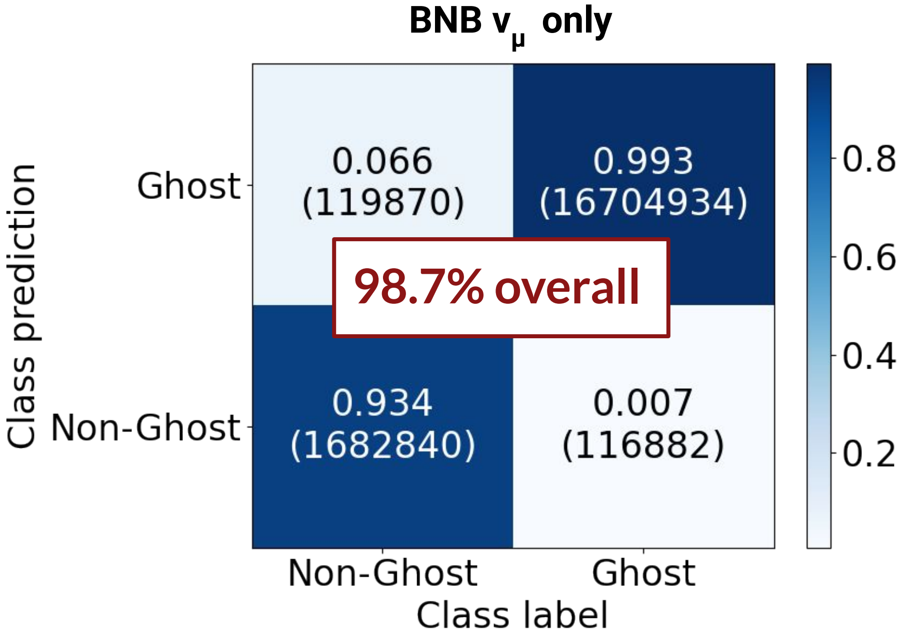
In a **wire TPC**, we do not get 3D images, but rather 3 x 2D projections

- First task: **combine projections into one 3D image**





Message passing

Two **feature update steps**

1. **Edge update**

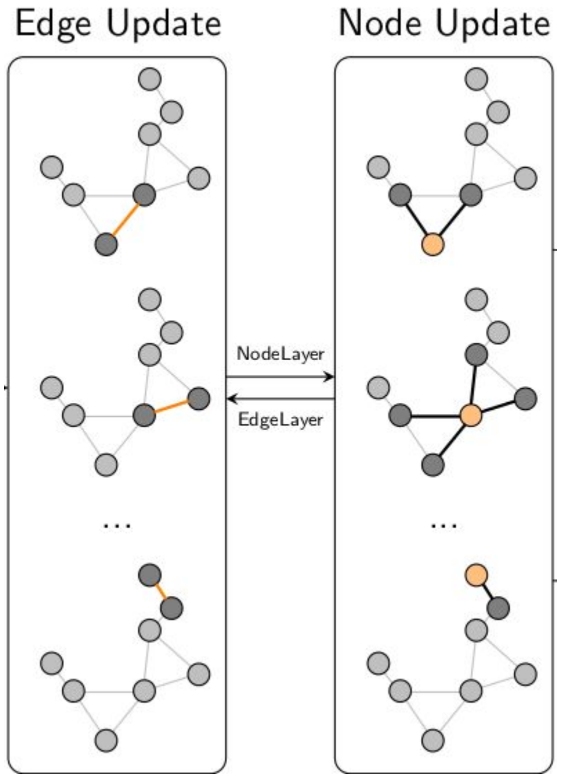
$$\mathbf{e}'_{ij} = \phi_\Theta(\mathbf{x}_i,\, \mathbf{x}_j,\, \mathbf{e}_{ij})$$

2. **Node update**

$$\mathbf{m}_{ji} = \chi_\Theta(\mathbf{x}_j,\, \mathbf{e}_{ji})$$

$$\mathbf{x}'_i = \psi_\Theta(\mathbf{x}_i,\, \square_{j\in\mathcal{N}(i)}\mathbf{m}_{ji})$$

Repeat **n** times (depth)



Edge Selection

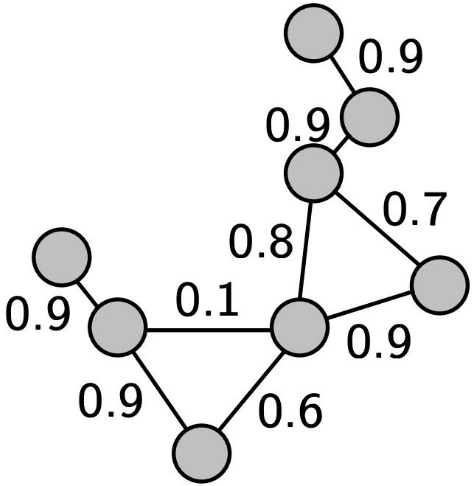
The GNN gives you a list of **edge scores**, not a partition

For the **best partition**, ĝ, we must select edges which minimizes the **partition CE loss**

Classification at the partition level!

$$\mathcal{L}_{\hat{g}} = -\frac{1}{N_e} \sum_{(i,j)\in E} \Big[\delta_{\hat{g}_i,\hat{g}_j} \ln(s_{ij}) + (1-\delta_{\hat{g}_i,\hat{g}_j}) \ln(1-s_{ij})\Big]$$

Edge scores

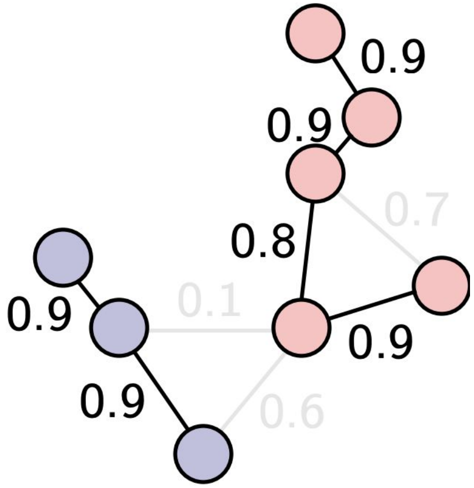


Edge Selection

Instead, **iterate:**

1. Compute partition **loss** for the empty graph
2. Add the **most likely edge**, compute loss again
3. If $L_{n+1} < L_n$, **update partition**
4. Repeat until the next best edge has $s_{ij} < 0.5$

Optimized partition

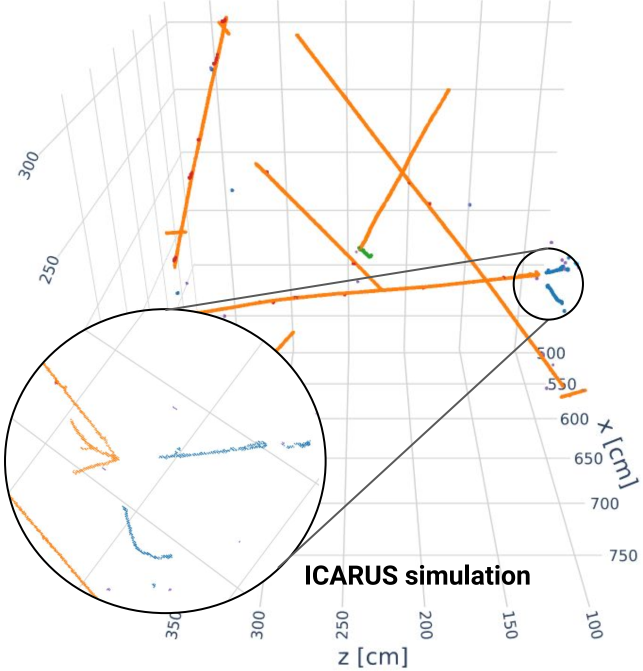


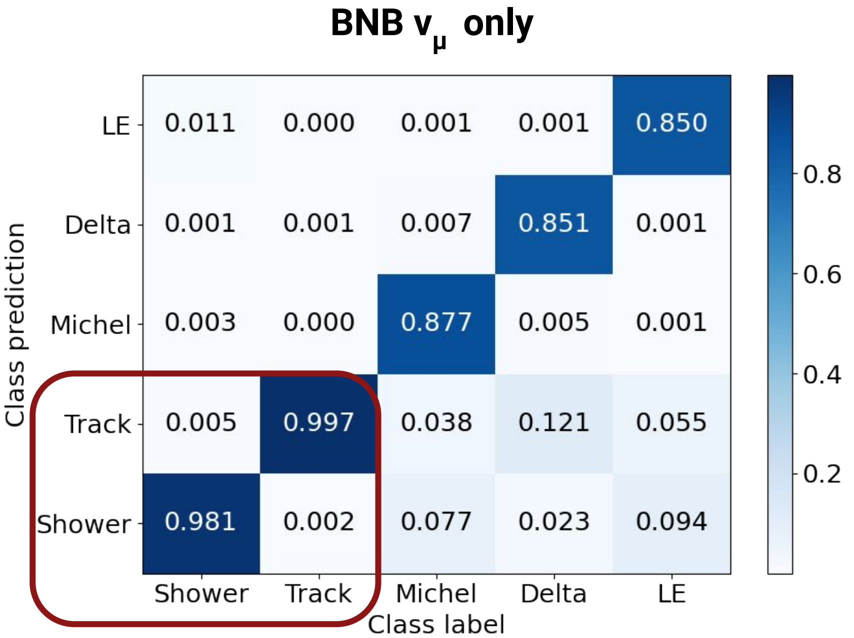
$L \simeq 2.13$

Semantic Segmentation

Separate **topologically different** types of activity

- Tracks, Showers, delta rays, Michel electrons, low energy blips





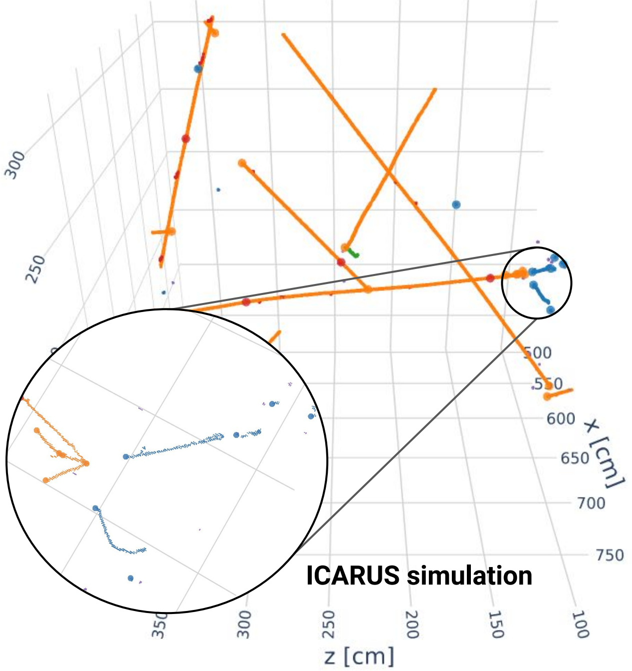
Paper: PhysRevD.102.012005

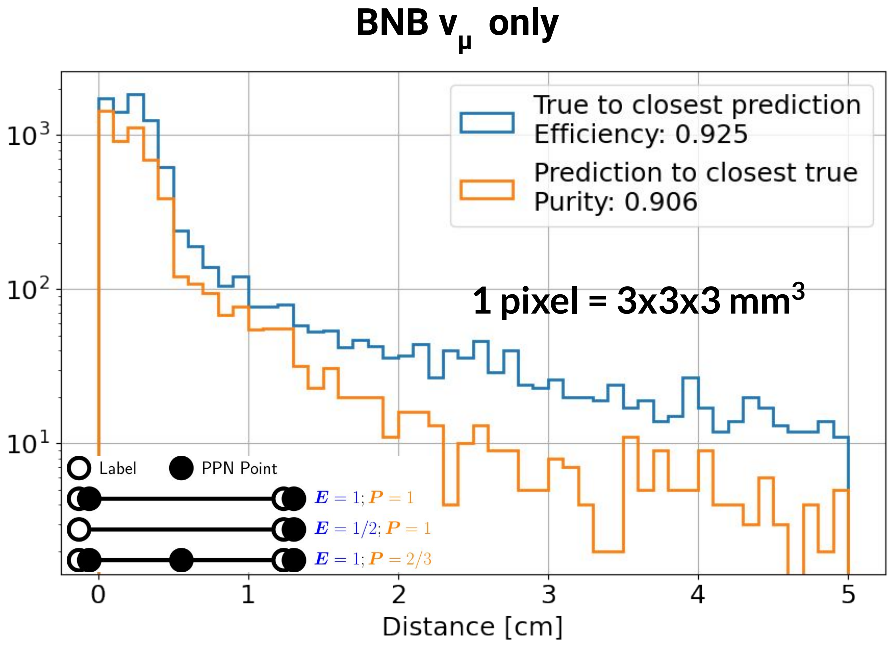
99.1% overall

Points of Interest

Narrow down a region proposal all the way to a **point**

- Predict **masks** at different scales with UResNet, predict **position** in pixel



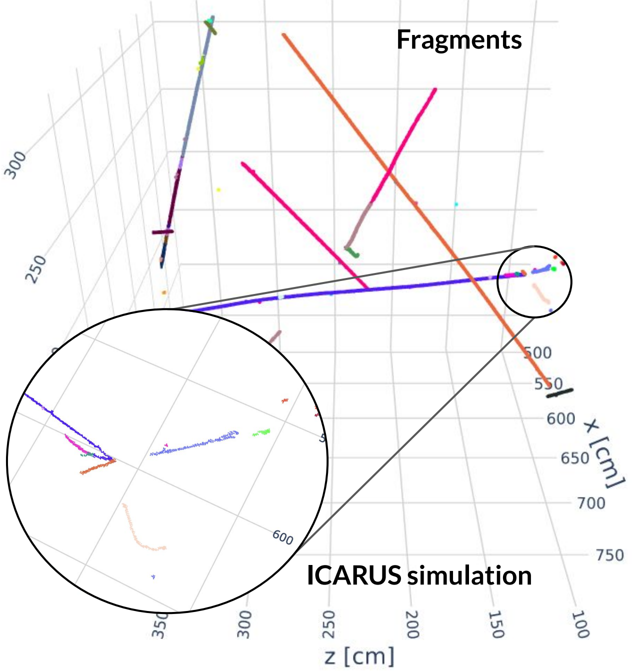


Paper: PhysRevD.104.032004

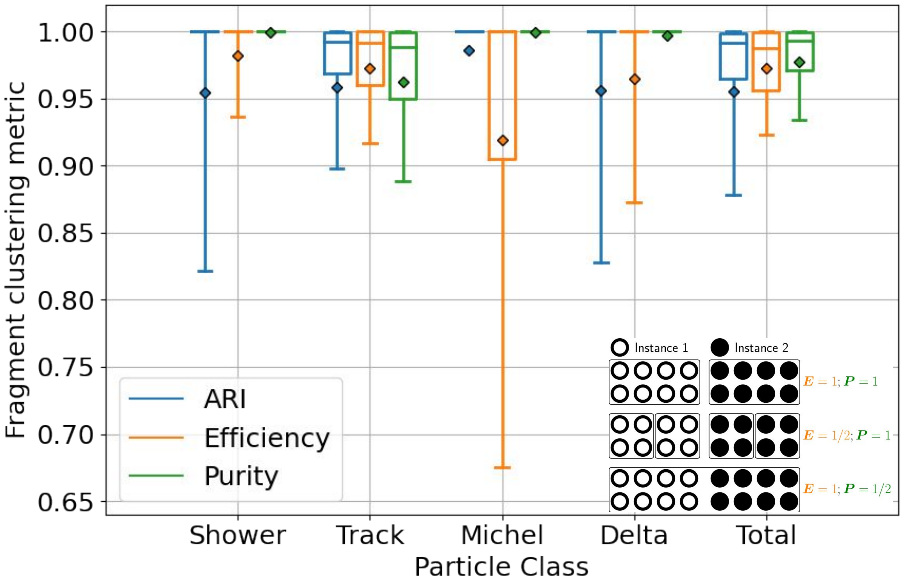
Dense Fragment Formation

Break track/shower fragment instances **where they touch**

- Cluster track/shower **fragments** at this stage



BNB ν_μ only

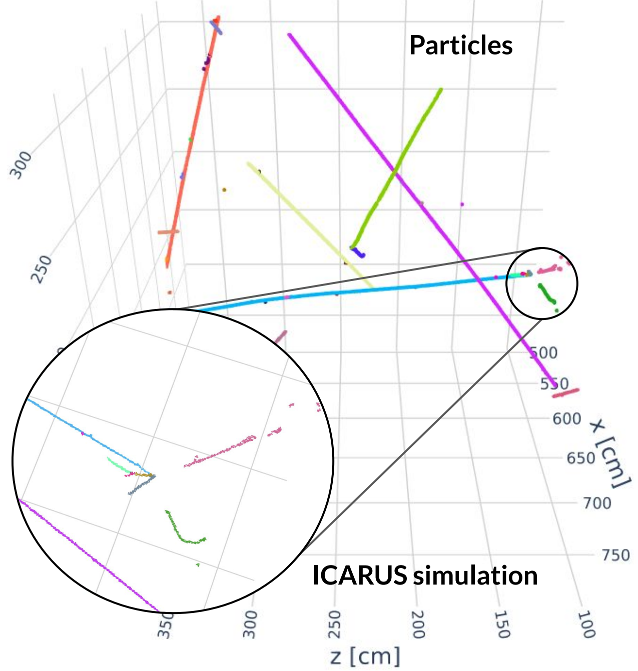


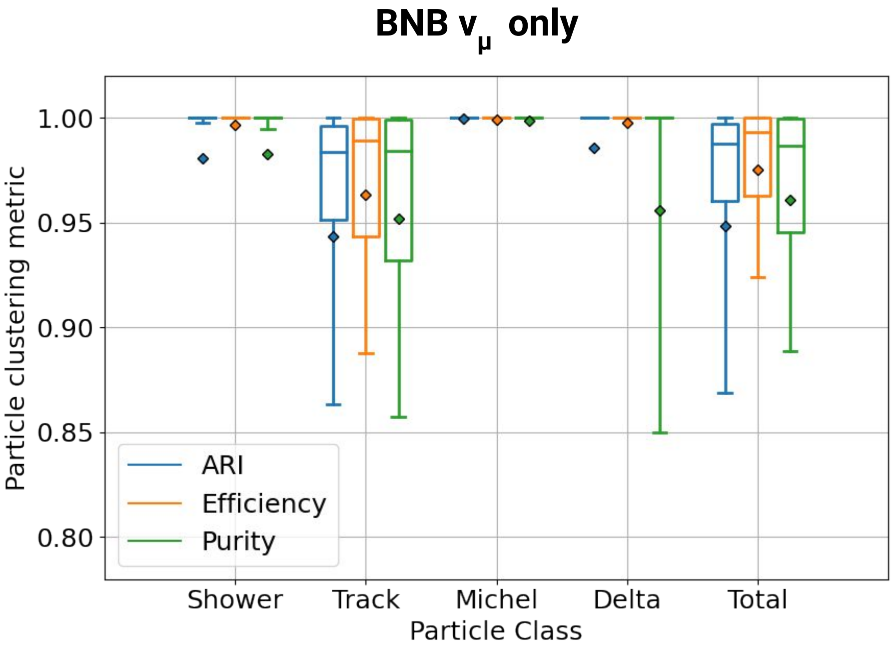
Paper: arXiv:2007.03083

Particle Aggregation

Aggregate track/shower fragment instances into **particles**

- Find edges that connect **fragments that belong together**



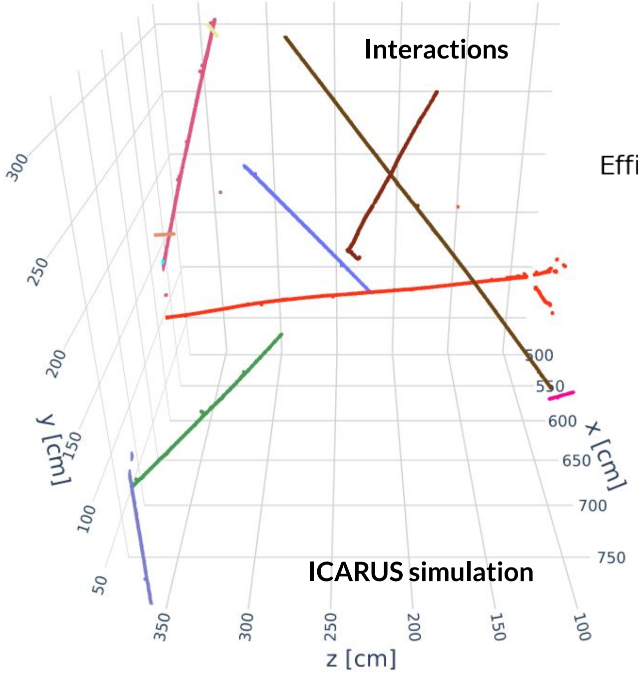


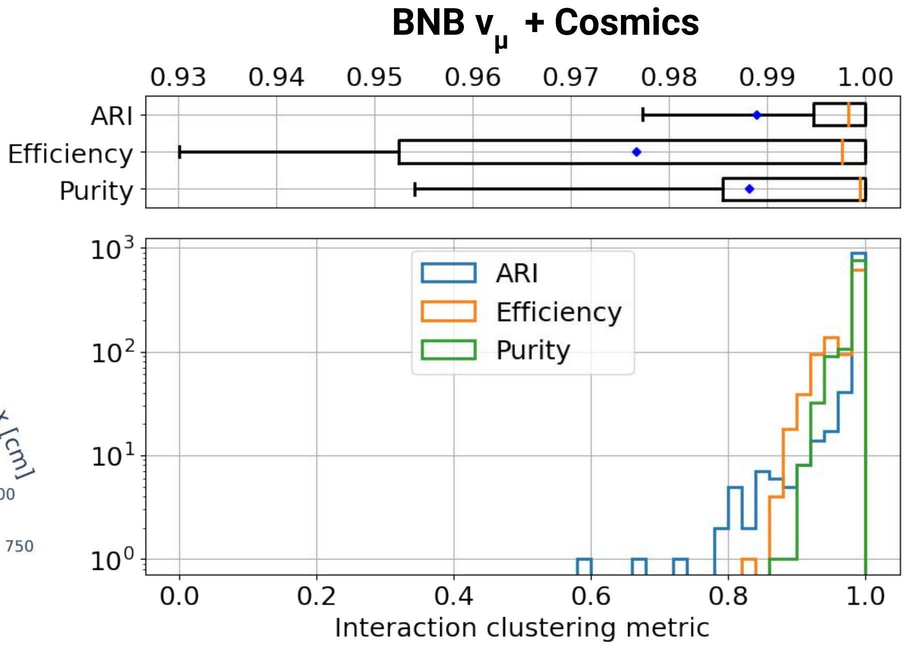
Paper: PhysRevD.104.072004

Interaction Aggregation

Aggregate track/shower particle instances into **interactions**

- Find edges that connect ~~fragments~~ **particles that belong together**



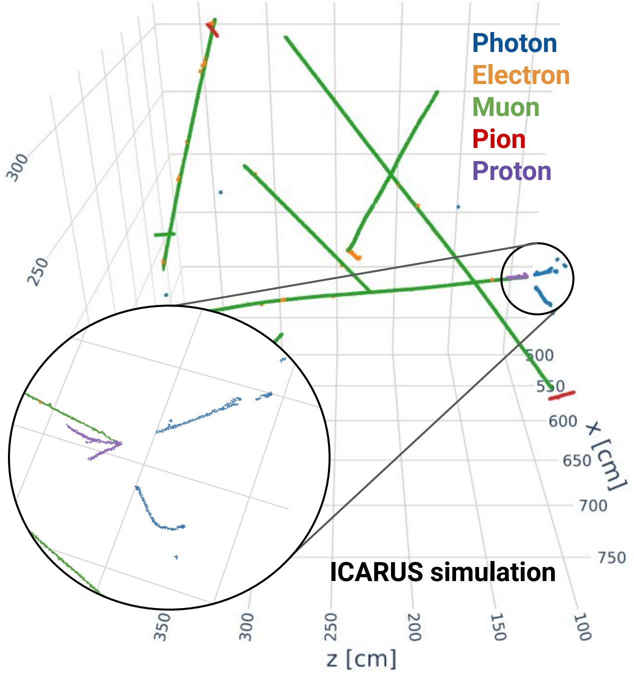


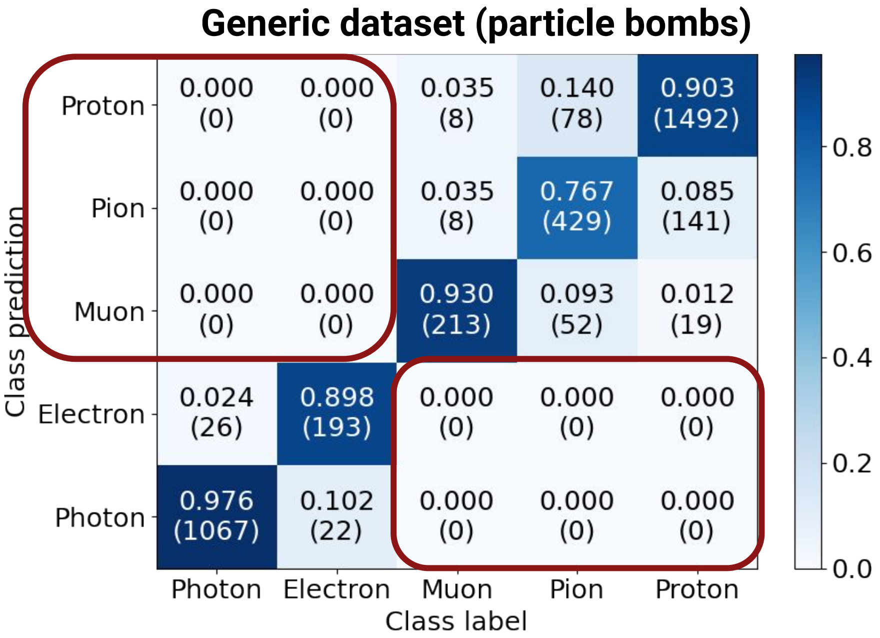
Paper: PhysRevD.104.072004

Particle Identification

Particle species much easier to **infer in context**

- Michel decays, secondary hadrons, shower conversion gaps, etc.





Particle Identification

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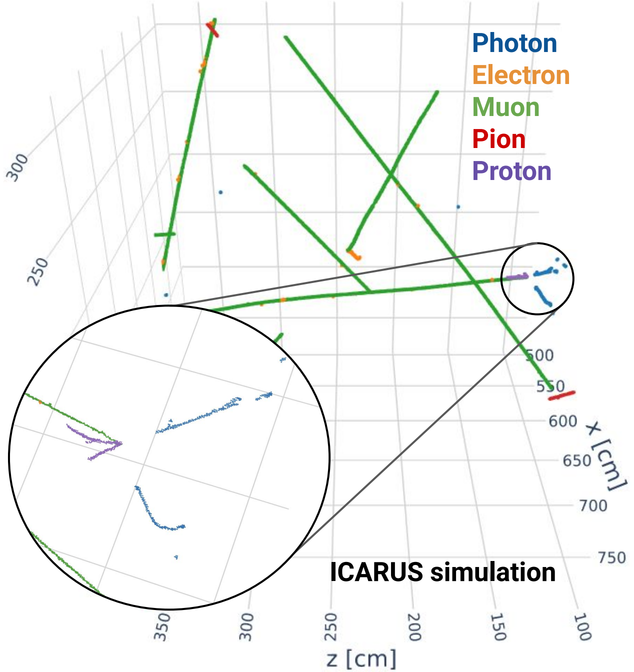


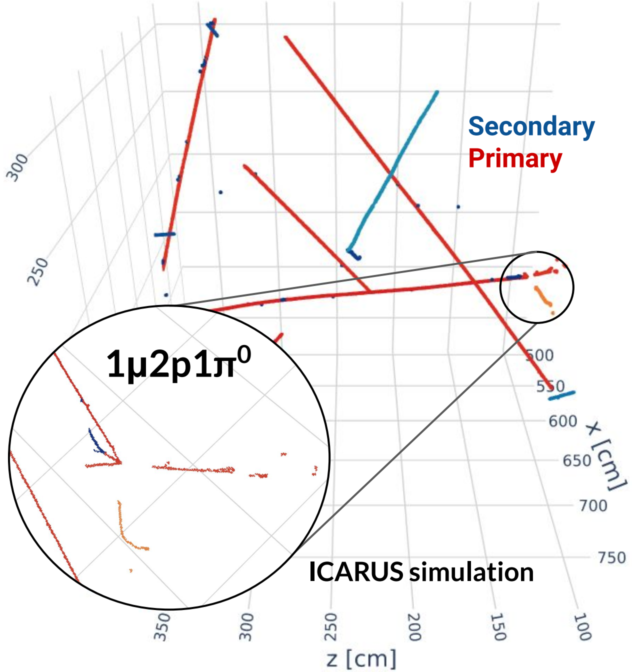
Generic dataset (particle bombs)

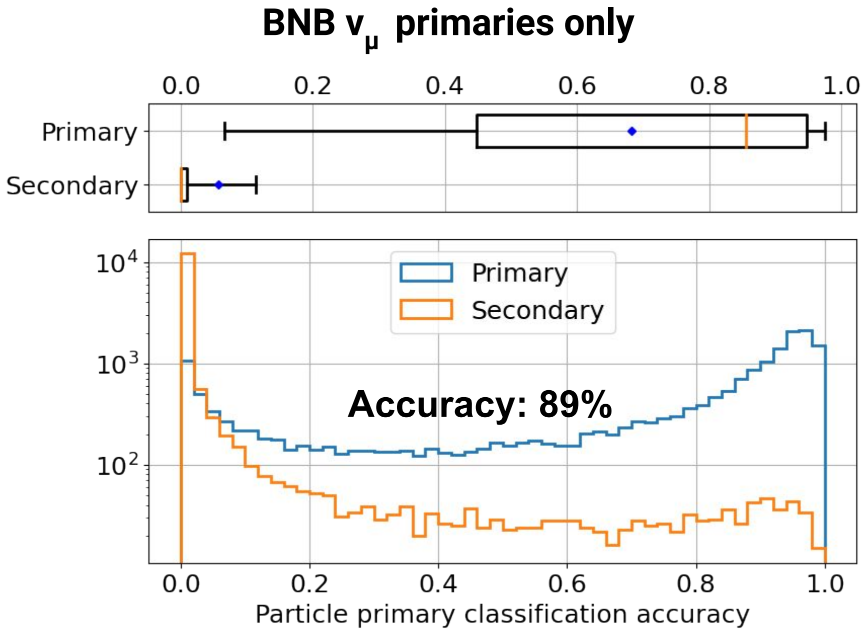
Class prediction \ Class label	Photon	Electron	Muon	Pion	Proton
Proton	0.000 (0)	0.000 (0)	0.035 (8)	0.140 (78)	0.903 (1492)
Pion	0.000 (0)	0.000 (0)	0.035 (8)	0.767 (429)	0.085 (141)
Muon	0.000 (0)	0.000 (0)	0.930 (213)	0.093 (52)	0.012 (19)
Electron	0.024 (26)	0.898 (193)	0.000 (0)	0.000 (0)	0.000 (0)
Photon	0.976 (1067)	0.102 (22)	0.000 (0)	0.000 (0)	0.000 (0)

Primary Identification

Important to know **which particle originate from the vertex**

- Central to any **exclusive analysis** (study specific interaction channels)

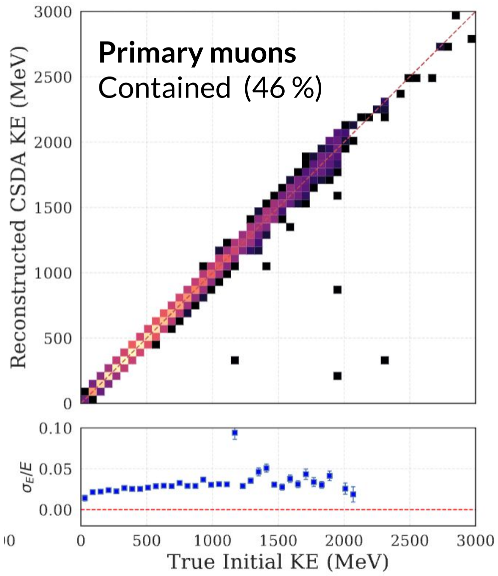


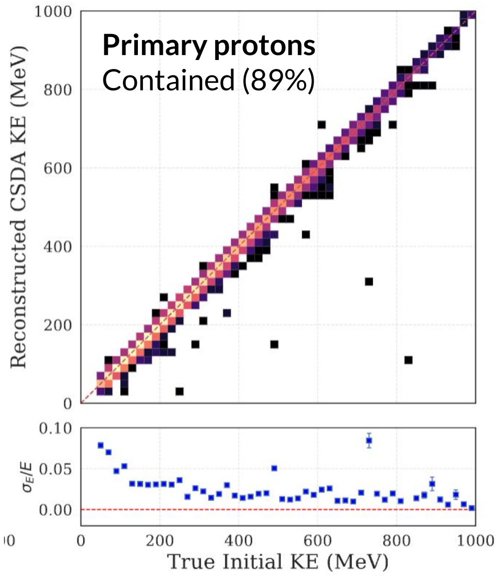


Particle energy reconstruction

Currently using **traditional techniques** for particle **energy reconstruction**:

- Range-based energy reconstruction of muons and protons



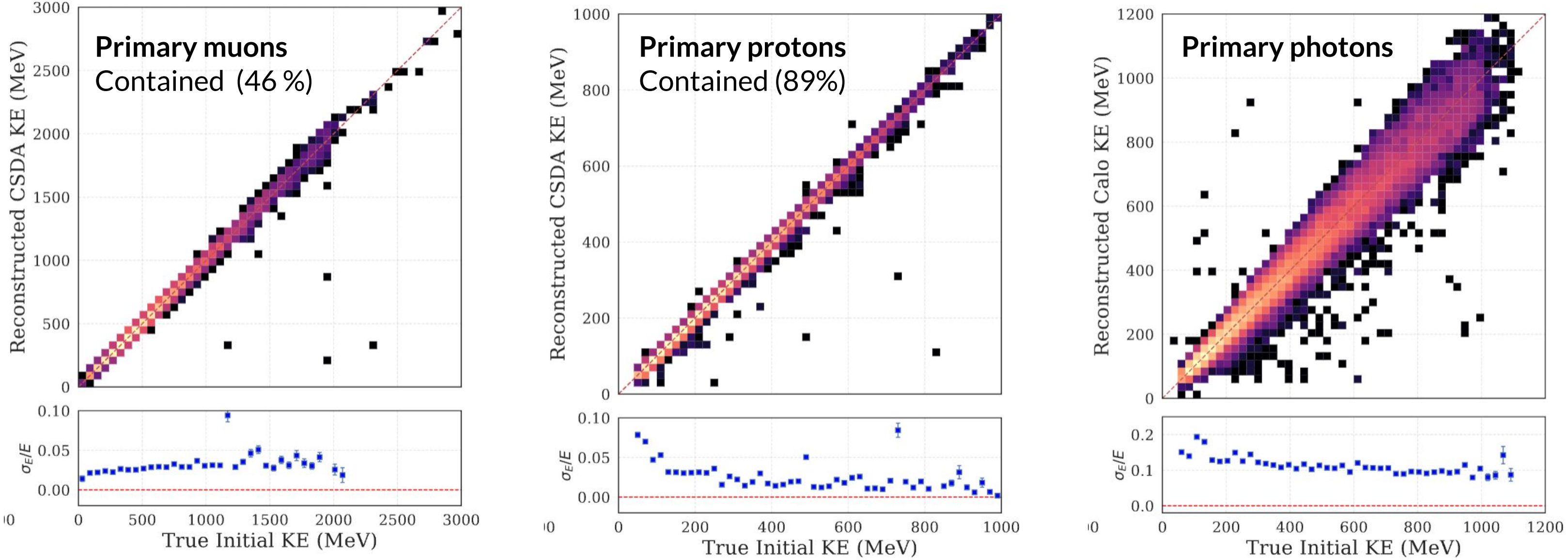


D. Koh et al.

Particle energy reconstruction

Currently using **traditional techniques** for particle **energy reconstruction**:

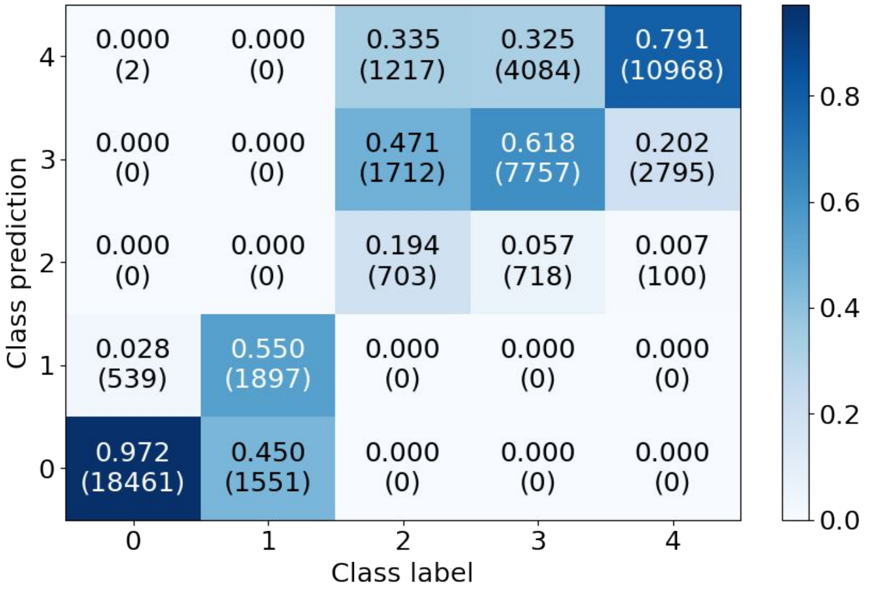
- Range-based energy reconstruction of muons and protons
- Calorimetric energy reconstruction of electrons

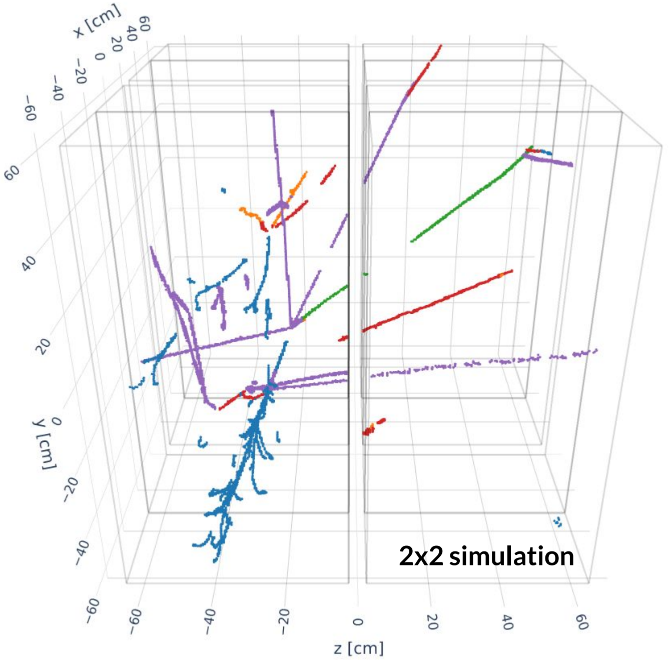


Particle Identification

Classify **particles** within interactions into different species

- Electron, Photons, Muons, Pions, Protons





Paper: PhysRevD.104.072004

Particle Identification

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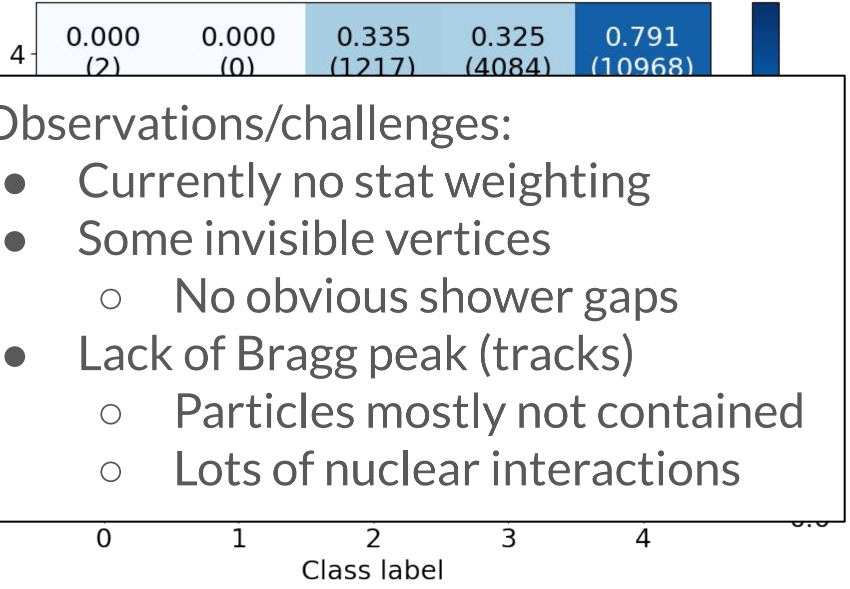
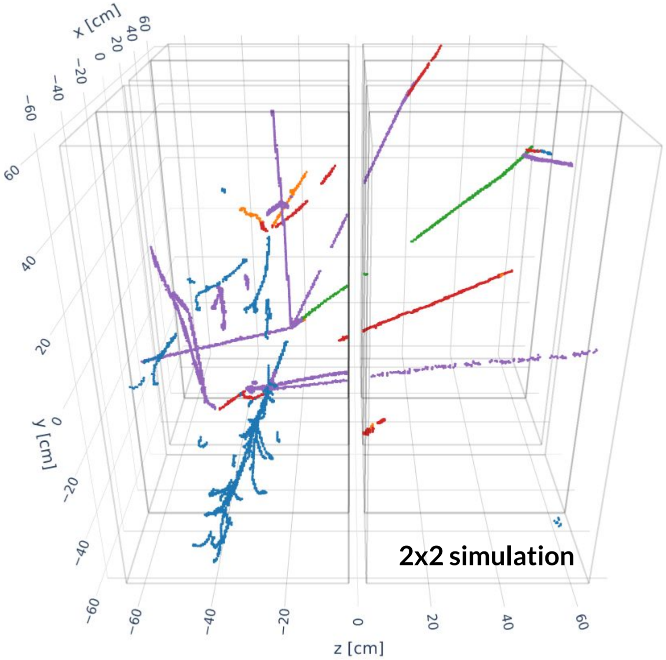


Observations/challenges:

- Currently no stat weighting
- Some invisible vertices
  - No obvious shower gaps
- Lack of Bragg peak (tracks)
  - Particles mostly not contained
  - Lots of nuclear interactions



Paper: PhysRevD.104.072004

Open Source

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DeepLearnPhysics collaboration (ML techniques R&D)

- Public LAr simulation
  - Potential for open real data from prototypes
- Shared software dependencies with Docker/Singularity
- Open reconstruction software on GitHub
- Reproducible results: PhysRevD.102.012005