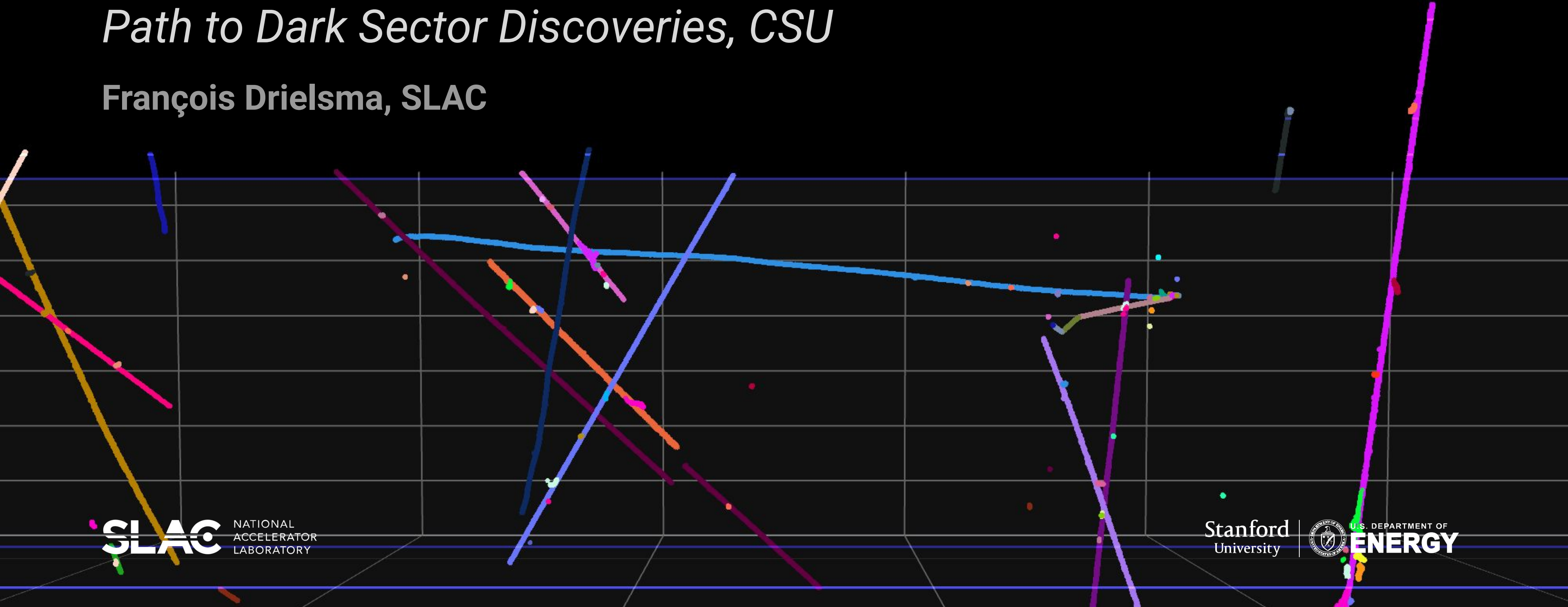
Scalable, End-to-end, ML-Based Reconstruction Chain in LArTPCs

Path to Dark Sector Discoveries, CSU

François Drielsma, SLAC



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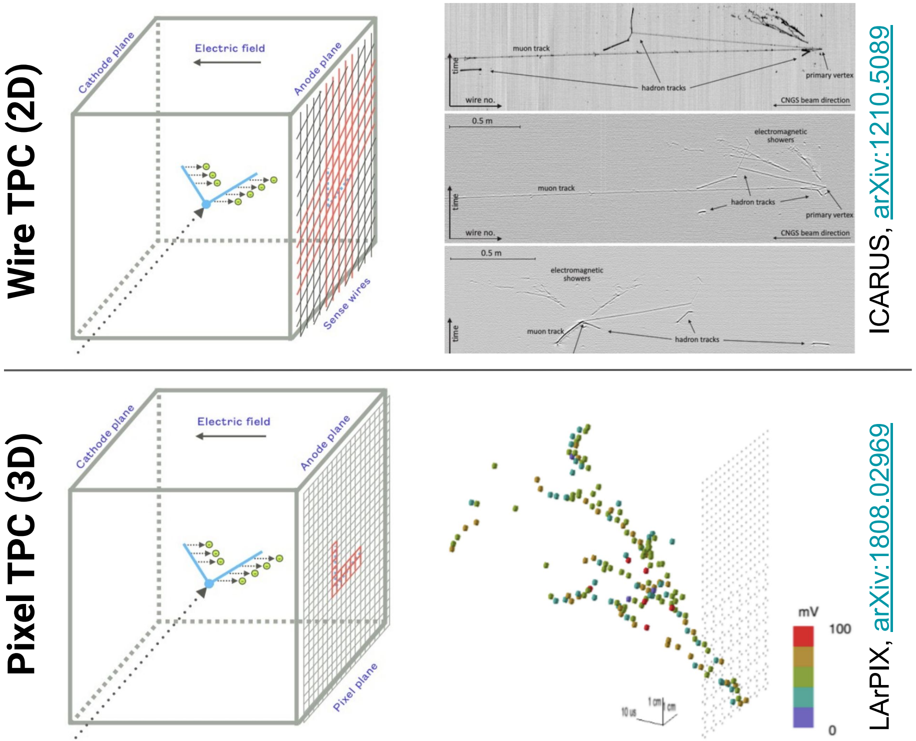
Stanford University | U.S. DEPARTMENT OF ENERGY

Liquid Argon Time-Projection Chambers

The modern Particle Imaging Detector



LArTPC are at the center stage of **beam ν physics** in the US

Short Baseline Neutrino program

- µBooNE, **ICARUS**, SBND

DUNE long-baseline experiment

- **Wire**: DUNE FD
- **Pixel**: DUNE ND-LAr

Advantages:

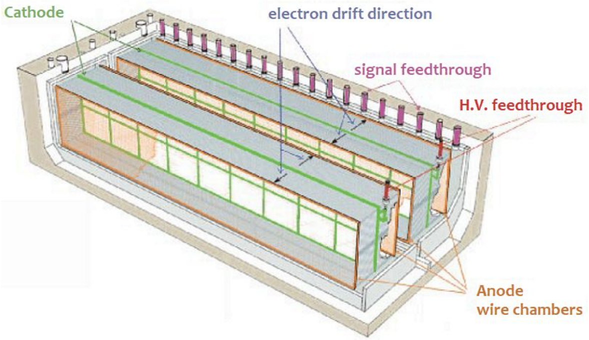
- **Detailed:** O(1) mm resolution, precise calorimetry
- **Scalable**: Up to tens of kt

Liquid Argon Time-Projection Chambers

Case study: Detector

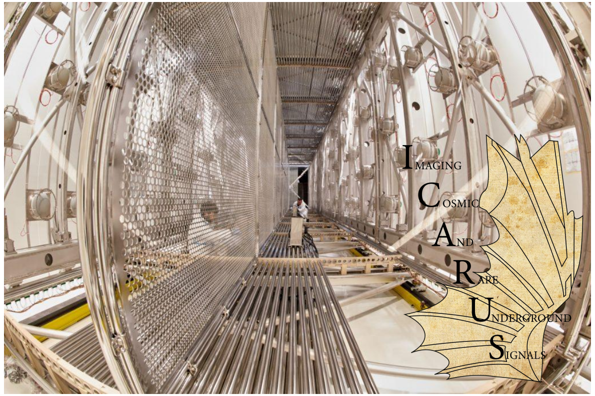
The **largest LArTPC** in operation is **ICARUS**

- **Surface**-level detector
- **500 t** fiducial mass (2 cryos, 4 TPCs)
- **Physics**: sterile neutrinos (MiniBooNE / Neutrino-4), cross sections, BSM



Event rates

- BNB beam: ~ 0.03 Hz neutrinos
- NuMI off-axis: ~ 0.015 Hz neutrinos
- In-time cosmic activity: ~ 0.25 Hz



Low-rate neutrino experiment with a **significant cosmic background**

Liquid Argon Time-Projection Chambers

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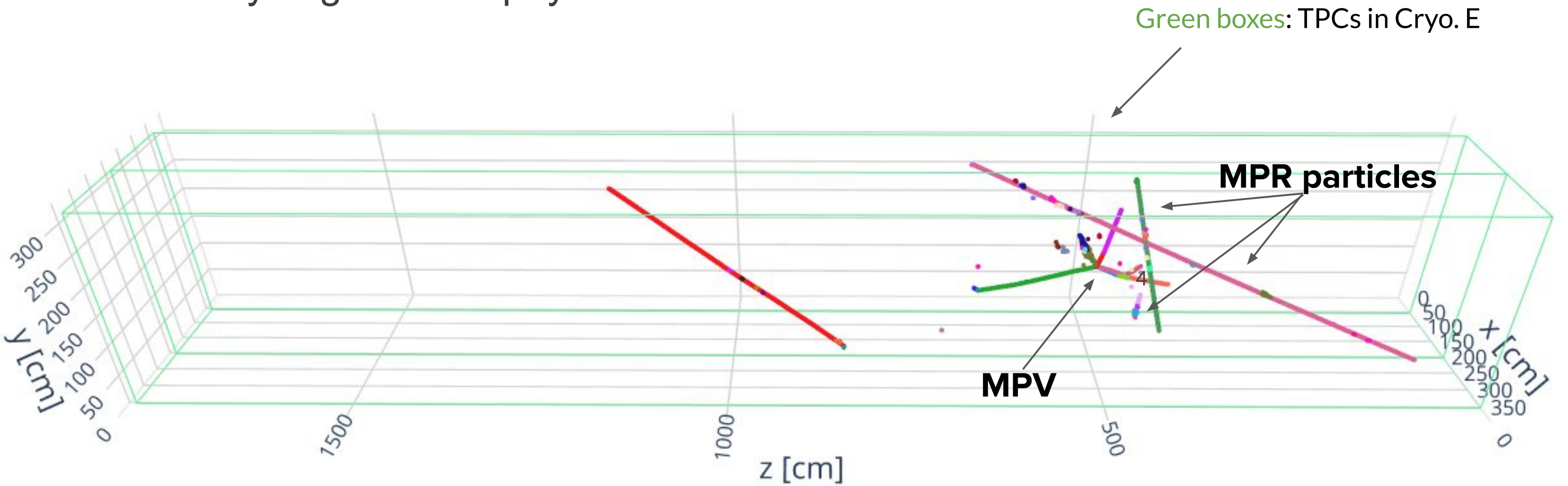
Case study: Datasets

Generic **simulated** dataset used for **optimization** and **testing**:

- Isotropic mix of 1 set of particles sharing a vertex + 5-9 localized single particles
  - **Covers phase-space** of neutrino interactions + cosmics, but…
  - … stays agnostic to physics → unbiased



Liquid Argon Time-Projection Chambers

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Case study: Datasets

Generic **simulated** dataset used for **optimization** and **testing**:

- Isotropic mix of 1 set of particles sharing a vertex + 5-9 localized single particles
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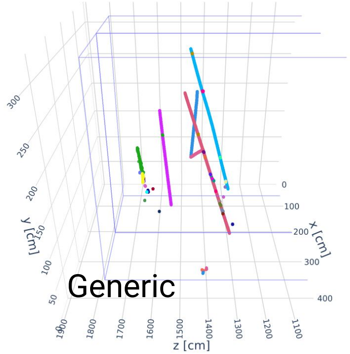
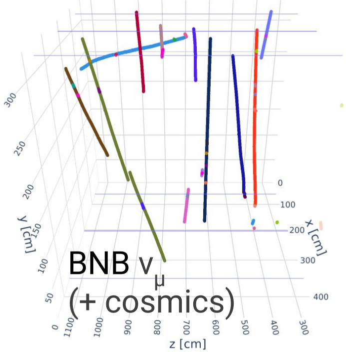
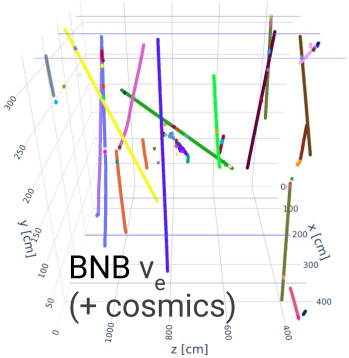
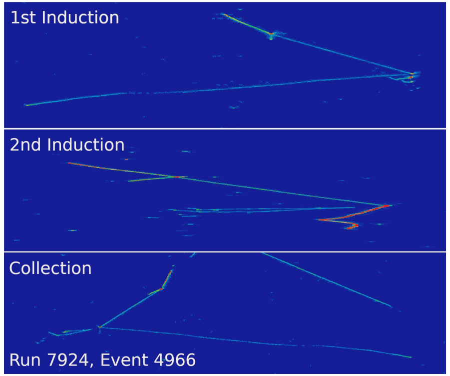
Specific datasets used for **validation**:

- Simulated **BNB ν_μ** and **BNB ν_e** + **hand-scanned data events** (C. Farnese et al.)





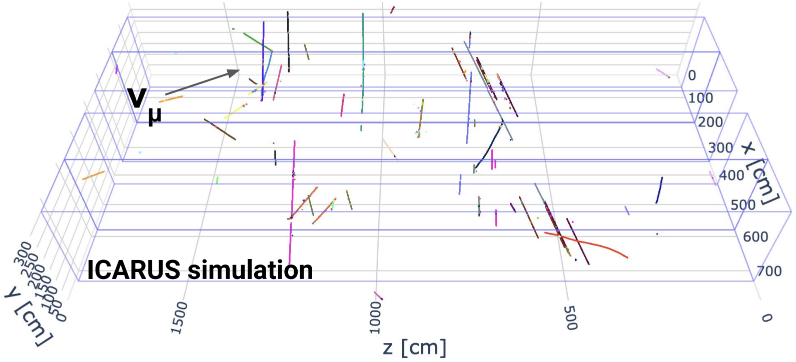


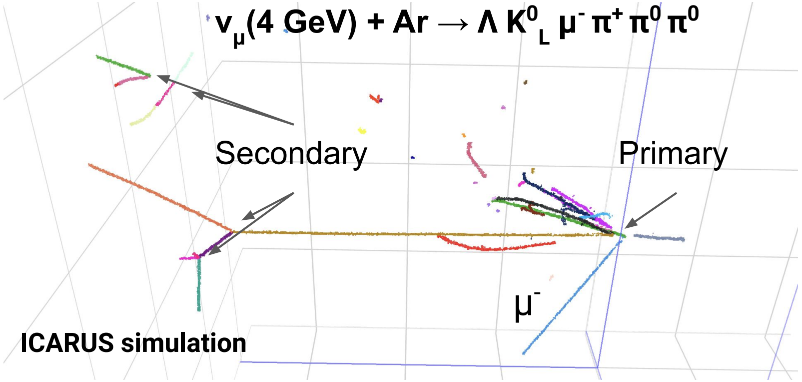


Reconstruction in LArTPCs

Challenges with LAr

Dense medium → Slow	High Z material → Messy
Electron drift velocity O(1) mm/μs • **Long** (O(1) ms) readout **window** • Need **light association** for timing	Argon has a large nucleus (Z=18) • **Complicated** nuclear physics • **Secondary** interactions





Reconstruction in LArTPCs

Machine Learning Group at SLAC

LArTPC ML effort **started** at SLAC by **K. Terao**

- Funded by **DoE ECA and ML grants**, many synergies with **ML initiative**
- **Primary Goal**: Implement **full** ML-based reco. **chain** for LArTPCs
- **Experiments**: µBooNE, **ICARUS**, pDUNE-SP, **pDUNE-ND**, DUNE-ND

ML Convener

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F. Drielsma
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L. Dominé
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DUNE

Y-J. Jwa
ICARUS

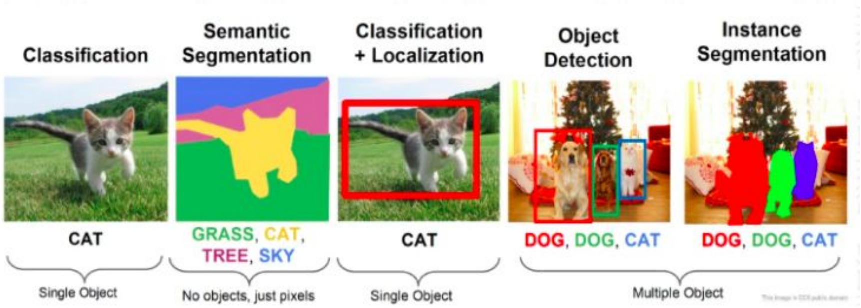
D.H. Koh
ICARUS

Z. Hulcher
DUNE-ND

Machine Learning in Computer Vision (CV)

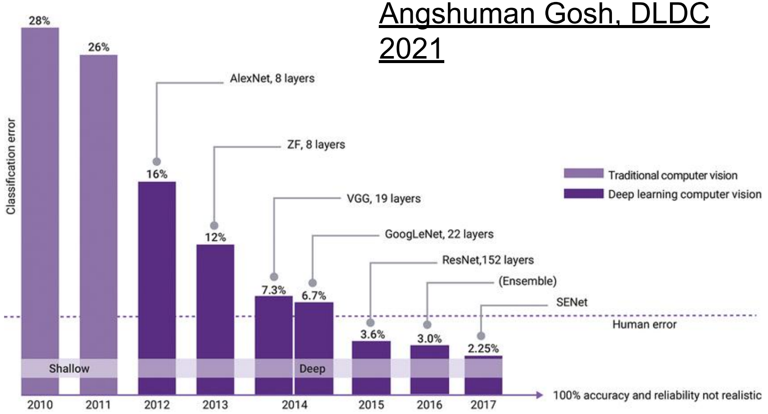
ML is the state-of-the-art in CV, i.e. extracting high level information from images

- ML revolutionized accuracy on image processing tasks
- Should **leverage those techniques in HEP**



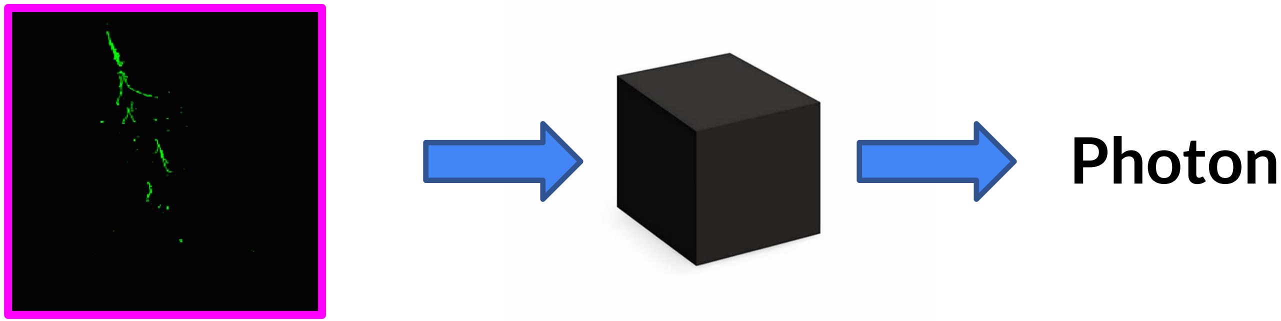
Stanford, CS231

Angshuman Gosh, DLDC 2021



Reconstruction in LArTPCs

Neural Network Primer



Reconstruction in LArTPCs

Neural Network Primer

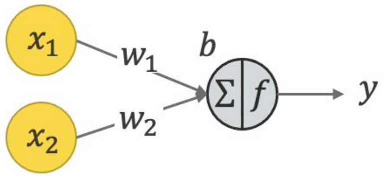
$$\mathbf{x} = \begin{bmatrix} 0 & 20.78 & \cdots & 0 \\ 0 & 56.34 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 86.3 \end{bmatrix} \Rightarrow F(\underbrace{\mathbf{x}}_{\text{Input}}, \underbrace{\mathbf{w}}_{\text{Parameters}}) \Rightarrow \mathbf{y} = \begin{array}{cc} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} & \begin{array}{c} \gamma \\ e \\ \mu \\ \pi \\ p \end{array} \end{array}$$

Reconstruction in LArTPCs

Neural Network Primer

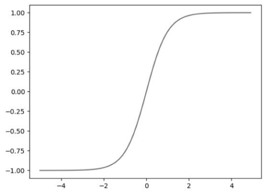
$$\mathbf{x} = \begin{bmatrix} 0 & 20.78 & \cdots & 0 \\ 0 & 56.34 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 86.3 \end{bmatrix} \Rightarrow F(\mathbf{x}, \mathbf{w}) \Rightarrow \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} \gamma \\ e \\ \mu \\ \pi \\ p \end{matrix}$$

What is **F ?** In ML, typically a **neural network (NN)**, a **universal function approximator**



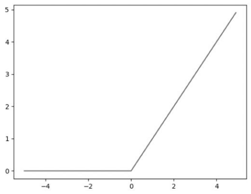
$$y = f(w_1 x_1 + w_2 x_2 + b)$$
$$f = \text{Tanh, ReLU, ...}$$

Tanh

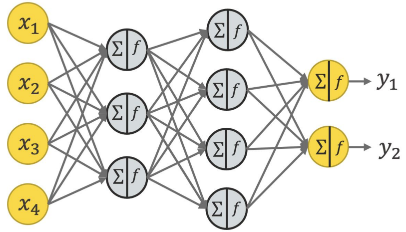


$$f(a) = \frac{e^{2ha} - 1}{e^{2ha} + 1}$$

Rectified Linear Unit (ReLU)



$$f(a) = max\{0, ha\}$$



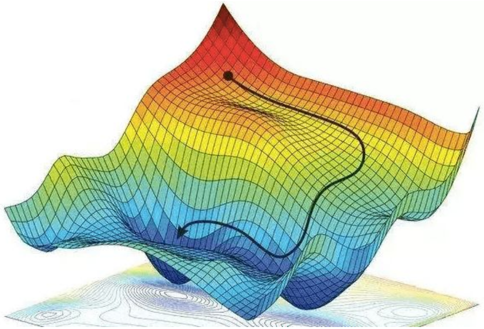
Machine Learning

Brief Primer

$$\mathbf{x} = \begin{bmatrix} 0 & 20.78 & \cdots & 0 \\ 0 & 56.34 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 86.3 \end{bmatrix} \Rightarrow F(\mathbf{x}, \mathbf{w}) \Rightarrow \mathbf{y} = \begin{array}{cc} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} & \begin{array}{c} \gamma \\ e \\ \mu \\ \pi \\ p \end{array} \end{array}$$

How does it learn ? NN are fully differentiable. Define loss, optimize by **gradient descent**

$$L = ||F(\mathbf{x}, \mathbf{w}) - \mathbf{y}|| = \begin{bmatrix} 0.8 \\ 0.18 \\ 0.01 \\ 0.01 \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

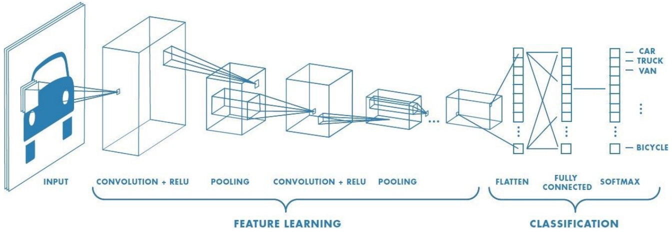


$$\mathbf{w}_i = \mathbf{w}_{i-1} - \alpha \nabla_{\mathbf{w}} L$$

Reconstruction in LArTPCs

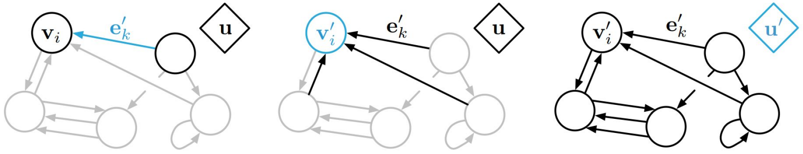
Convolutional Neural Network (CNN)

- Receptive field (kernel): **pixel neighborhood**
- Kernel shared in image: **translation**



Graph Neural Network (GNN)

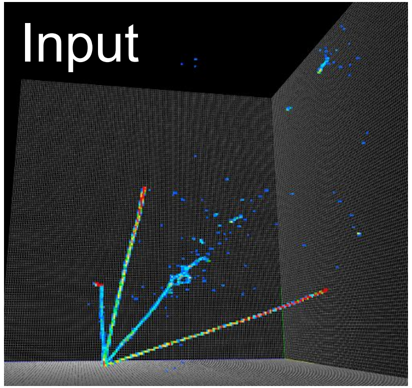
- Receptive field: **graph neighborhood**
- Agnostic to ordering: **permutation invariant**

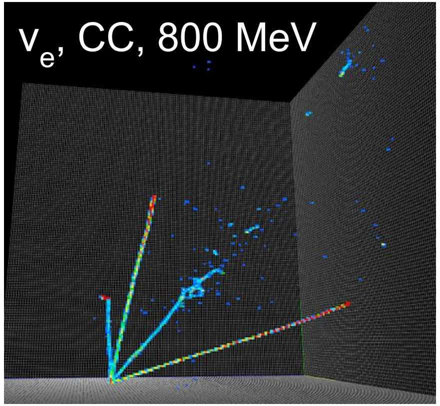


(a) Edge update (b) Node update (c) Global update

Reconstruction in LArTPCs

Hierarchical feature extraction





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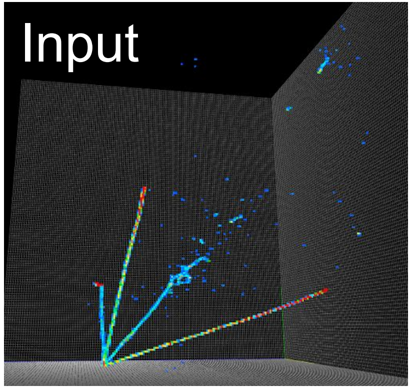
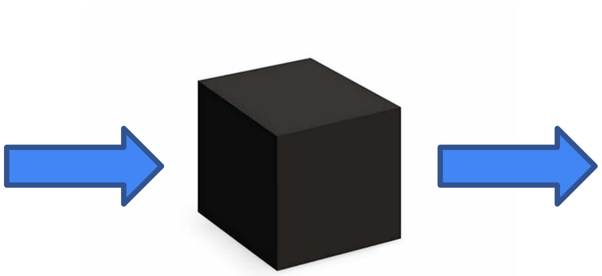
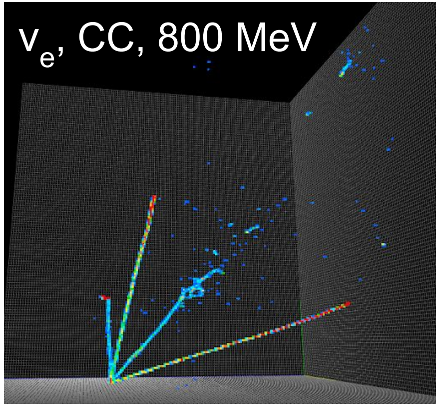


Image Classifier (CNN)





Reconstruction in LArTPCs

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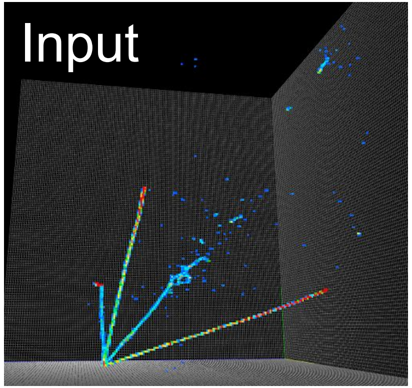

Image Classifier (CNN)

- What to do with > 1 interaction ?
- What if it fails ? Why ?
- What behavior if unknown interaction?

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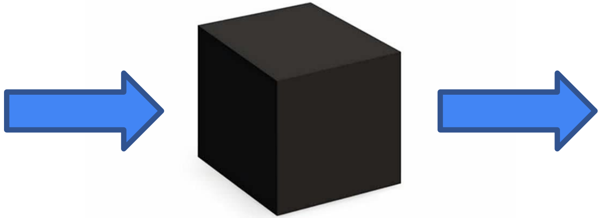
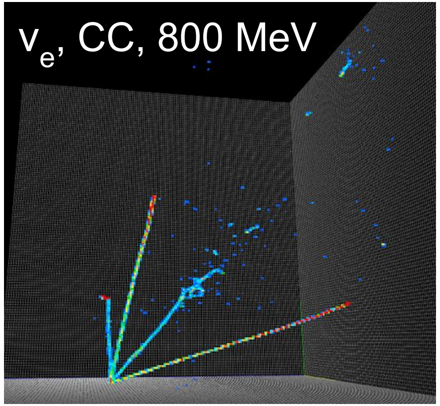
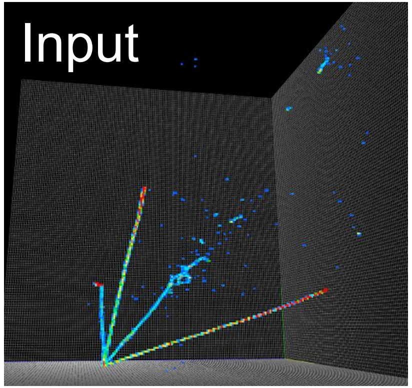




Reconstruction in LArTPCs

Hierarchical feature extraction

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

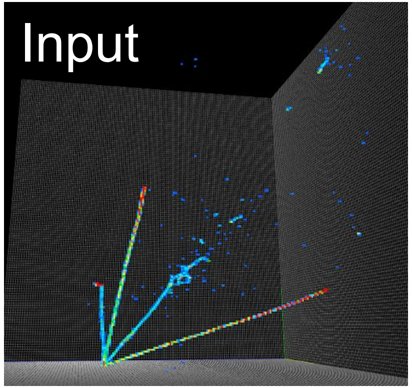


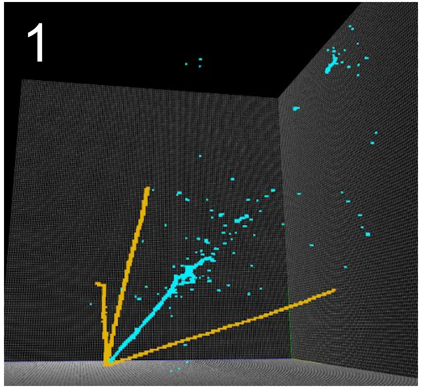
Reconstruction in LArTPCs

Hierarchical feature extraction

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

1. Separate topologically distinguishable **types of activity**



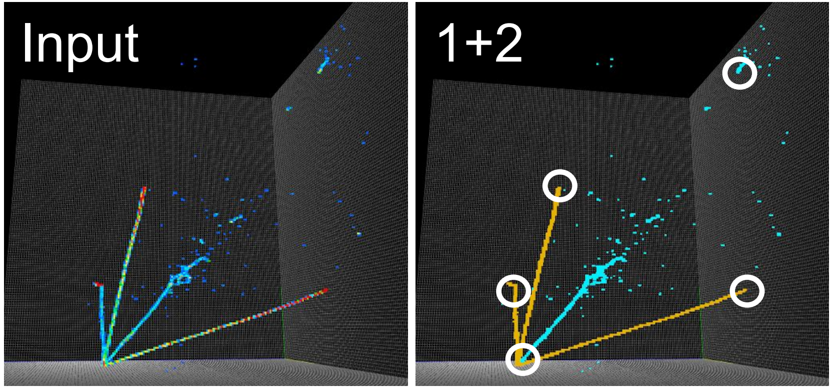


Reconstruction in LArTPCs

Hierarchical feature extraction

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

1. Separate topologically distinguishable **types of activity**
2. Identify **important points** (vertex, start points, end points)



Reconstruction in LArTPCs

Hierarchical feature extraction

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

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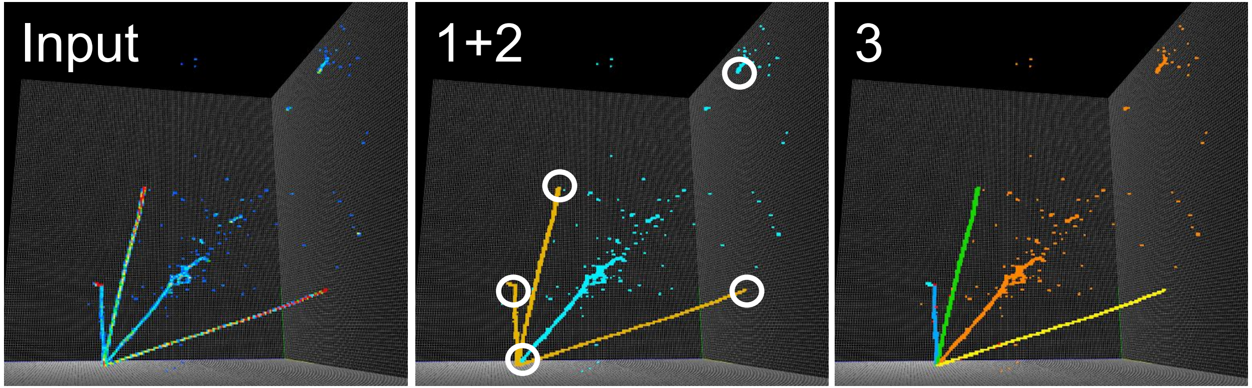

Reconstruction in LArTPCs

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Hierarchical feature extraction

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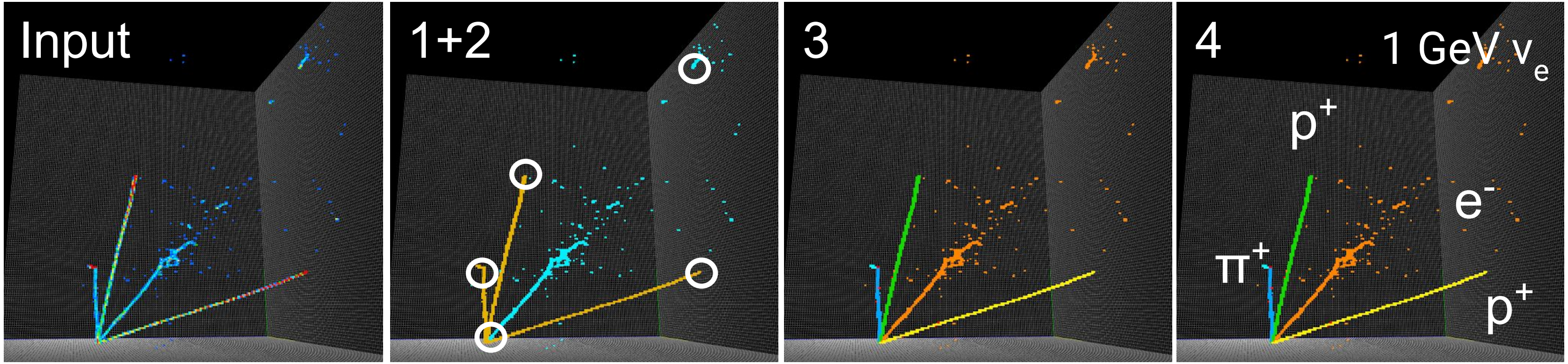
4. Cluster **interactions**, identify **particle properties** in context



Reconstruction in LArTPCs

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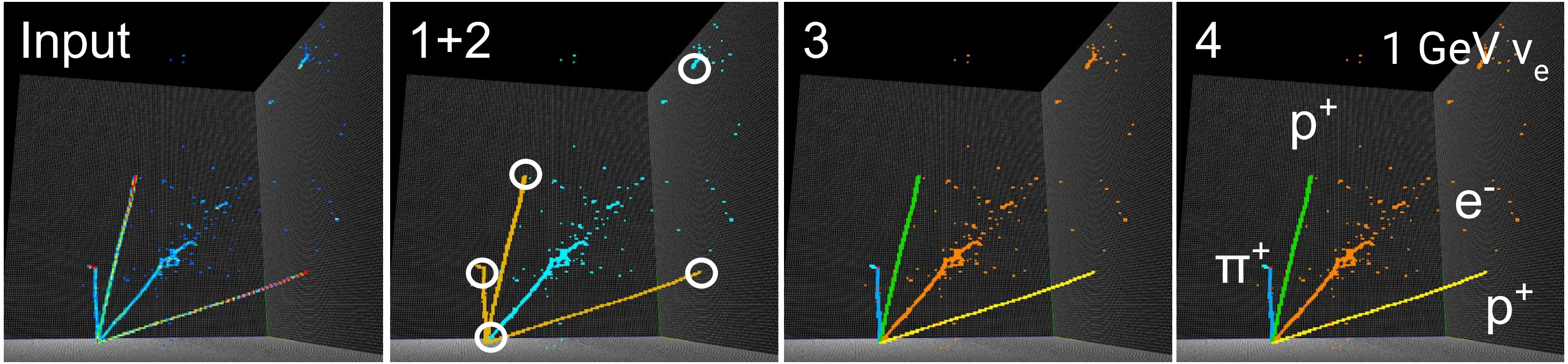
Pixel-level (1–2)

Cluster-level (3–4)

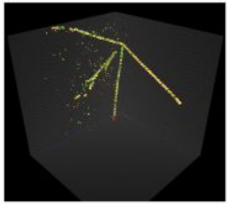


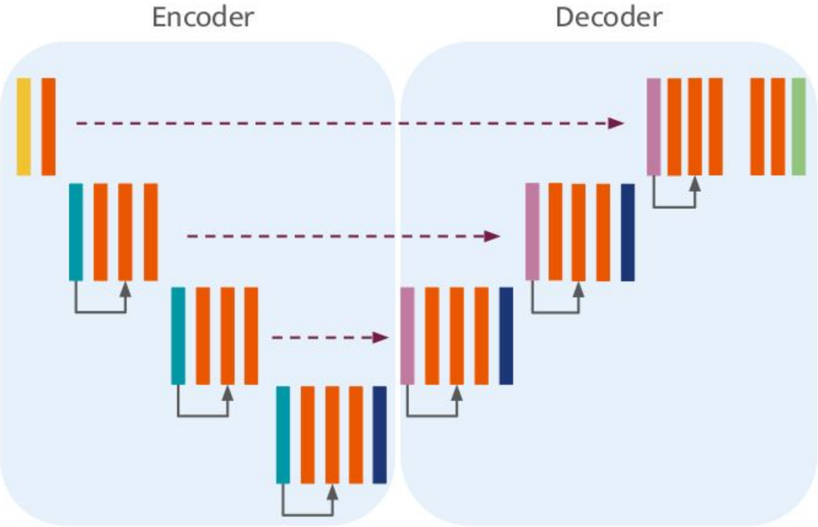
Pixel-Level Feature Extraction

Backbone

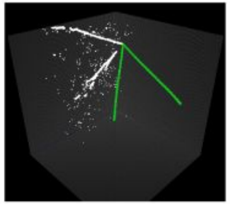
UResNet (UNet + ResNet + Sparse Conv.) as the **backbone feature extractor**

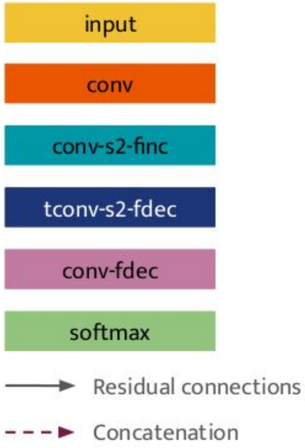
Input





Features





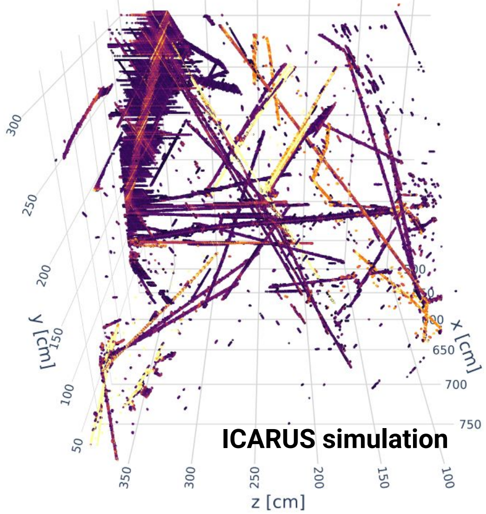
Paper: PhysRevD.102.012005

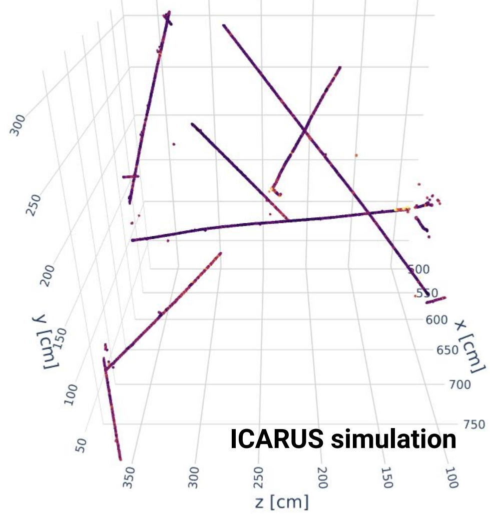
Tomographic Reconstruction

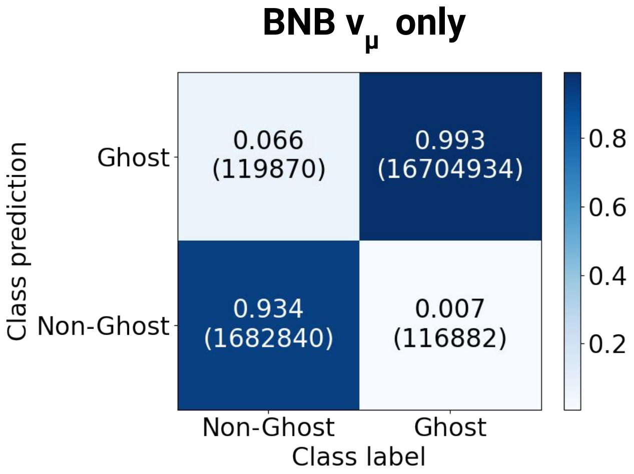
Ghost buster

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

- Find **valid combinations of 2D hits**: legitimate + artifacts (**ghosts**)
- Classify artificial space points as such: **ghost removal** (busting)





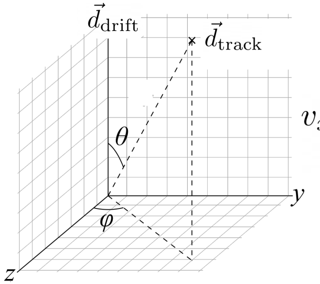


Tomographic Reconstruction

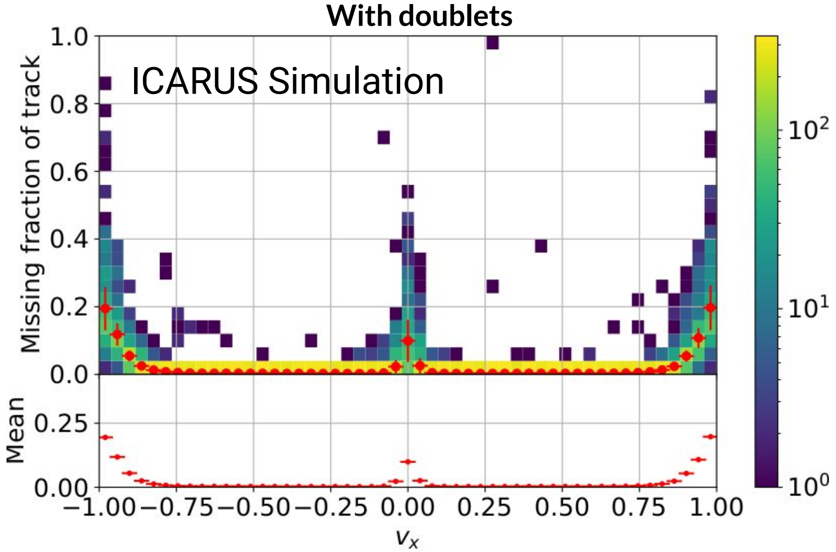
Track completeness

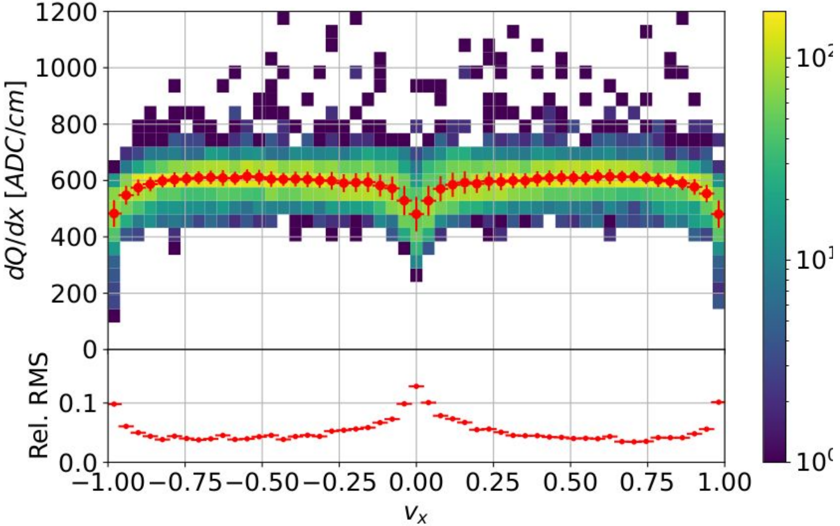
Definition: (total length of gaps)/(length of track)

- **Excellent track completeness with doublets**
- Overall **dQ/dx mostly flat w.r.t. angle**



$$v_x = \vec{d}_{\rm track} \cdot \vec{d}_{\rm drift} = \cos\theta$$





Semantic Segmentation

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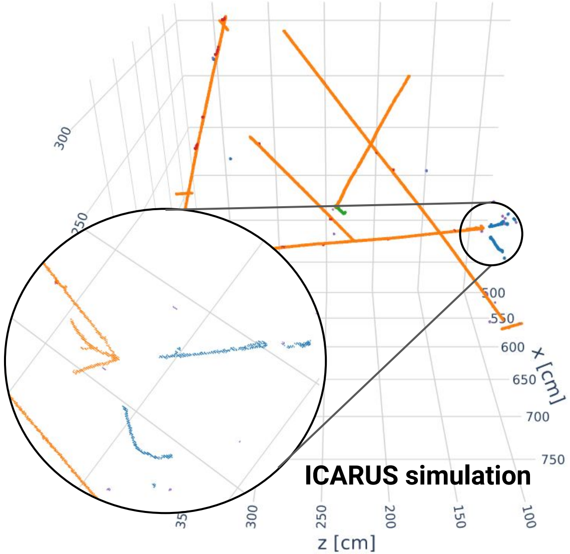
Particle voxel class classification

Separate **topologically different** types of activity

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



BNB ν_μ only

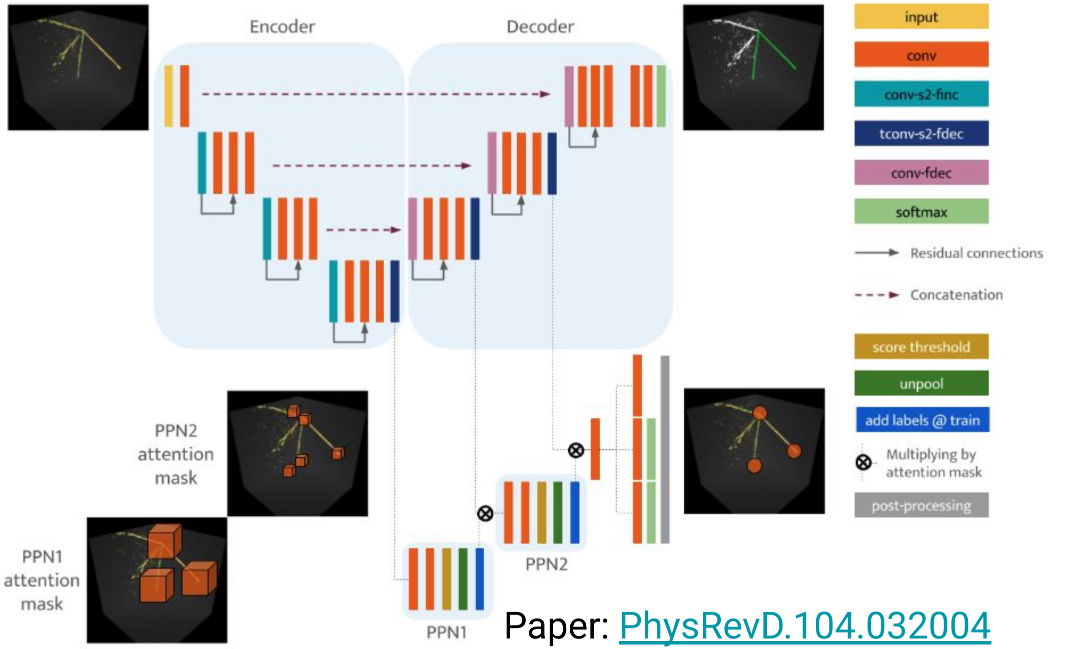
Paper: PhysRevD.102.012005

Point Proposal Network (PPN)

Architecture

The Point Proposal Network (PPN) uses decoder features:

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



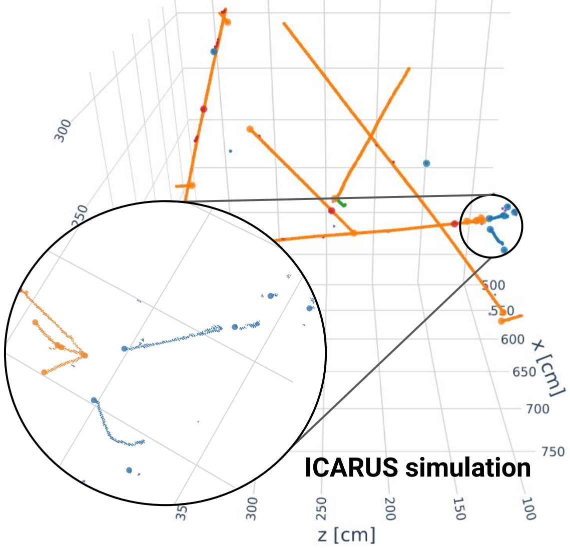
Paper: PhysRevD.104.032004

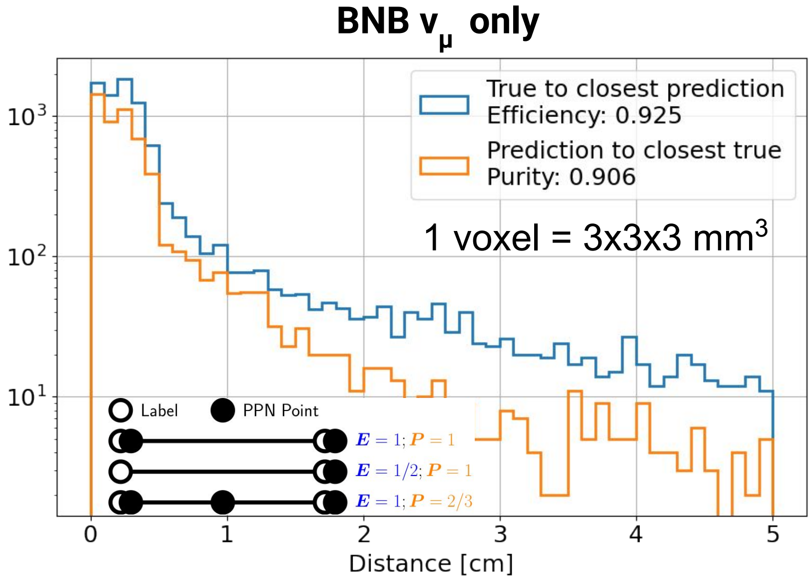
Point Proposal Network (PPN)

Points of interest

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

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

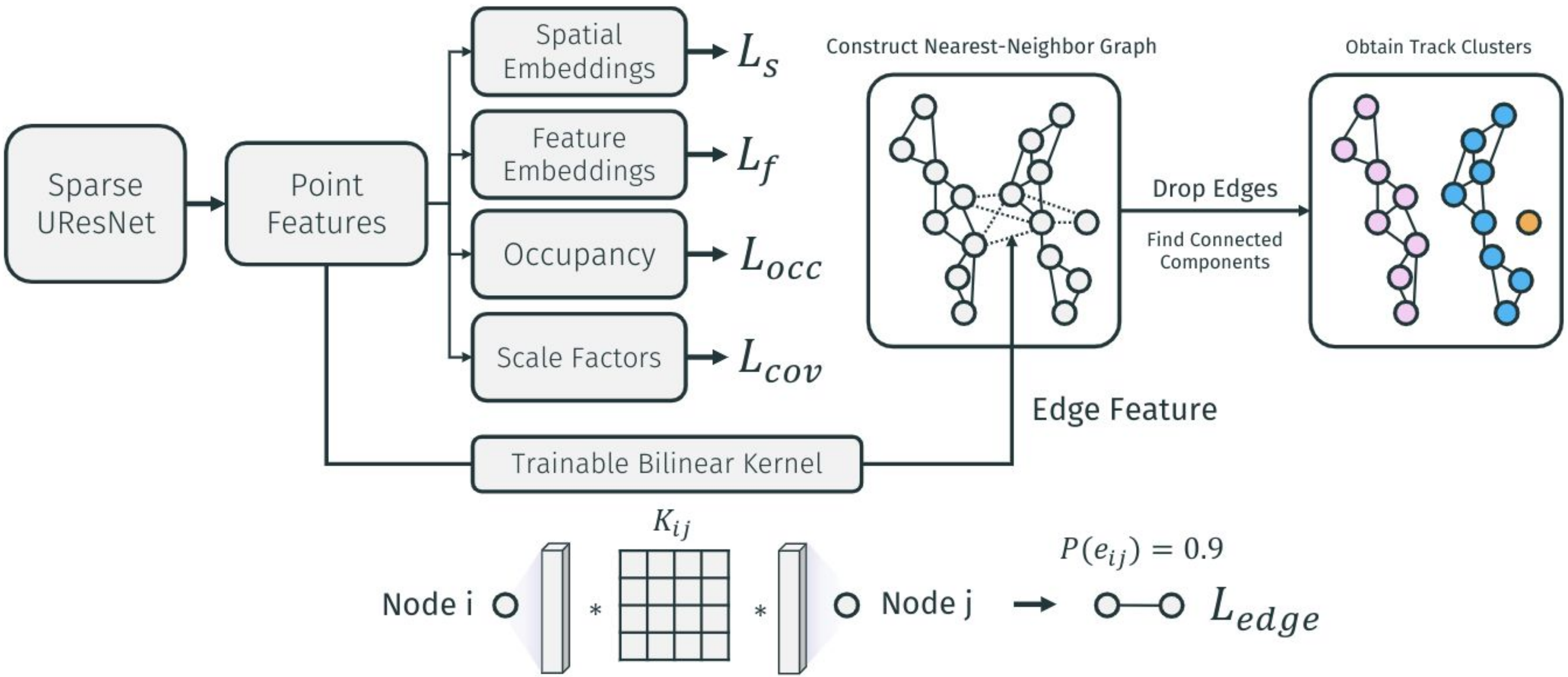




Paper: PhysRevD.104.032004

Graph-SPICE

Architecture

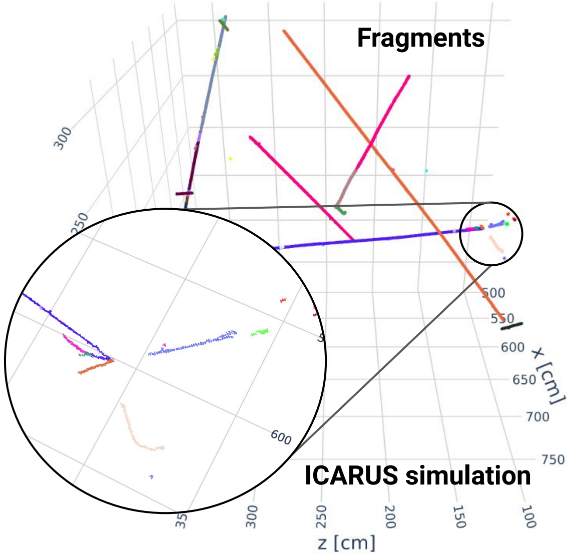


Dense Fragment Formation

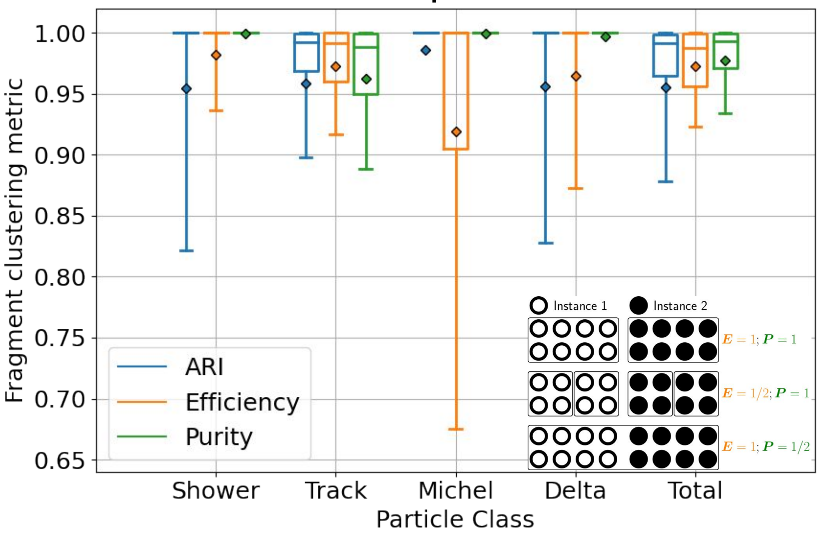
Spatial embedding transformation

Transform coordinates to an space in which tracks are spatially separated

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



BNB ν_μ only

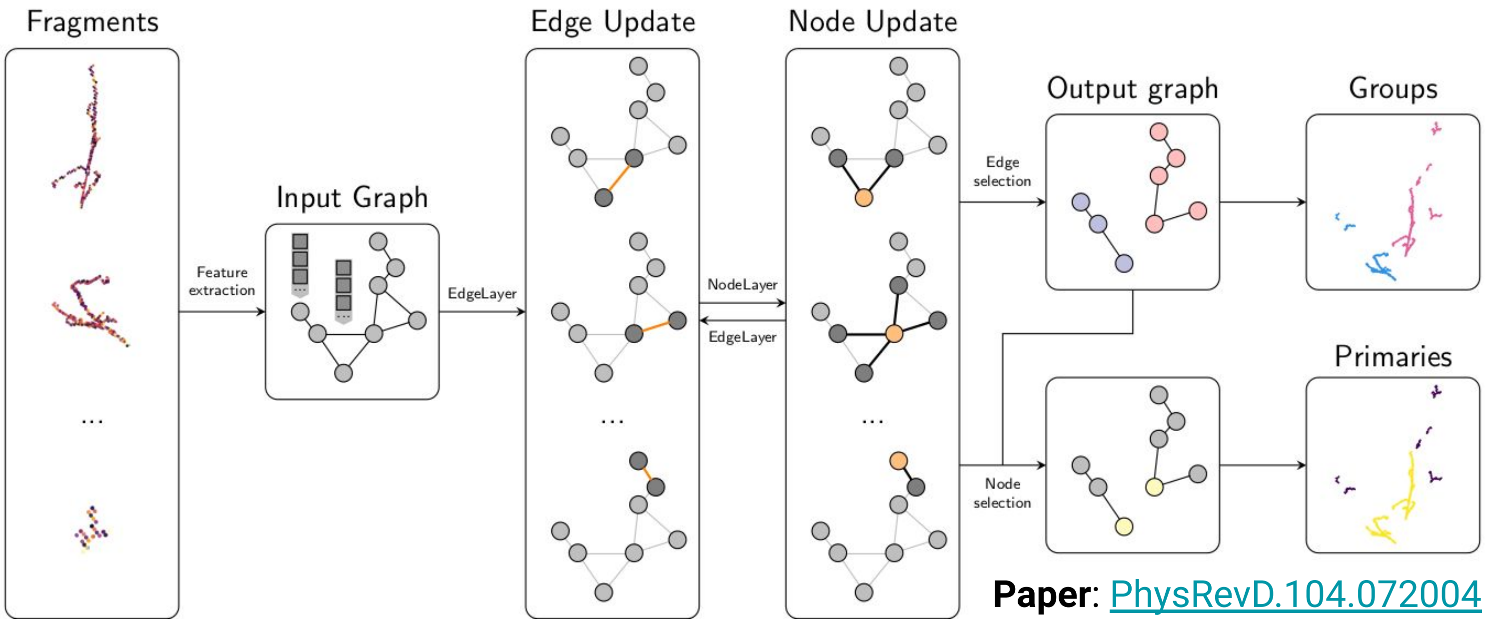


Paper: arXiv:2007.03083

Particle-Level Aggregation

Graph Particle Aggregator (GrapPA)

Graph Neural Network: fragments/particles (**nodes**), correlations (**edges**)



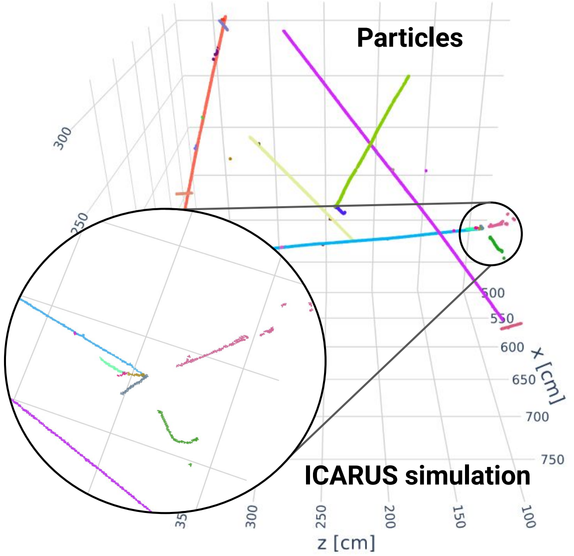
Paper: PhysRevD.104.072004

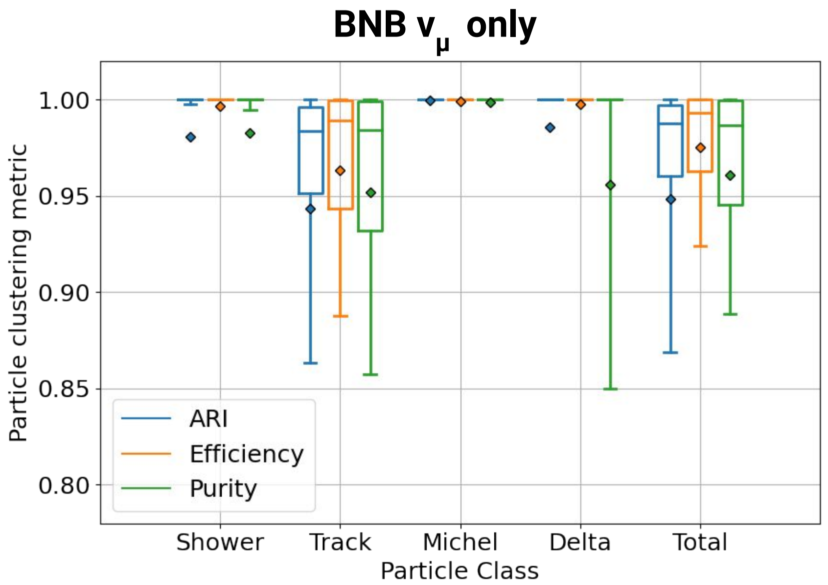
Aggregation

Graph edge classification

Two aggregation steps: **fragments** → **particles** → **interactions**

- **Select edges** in the graph that minimize loss, find **connected components**





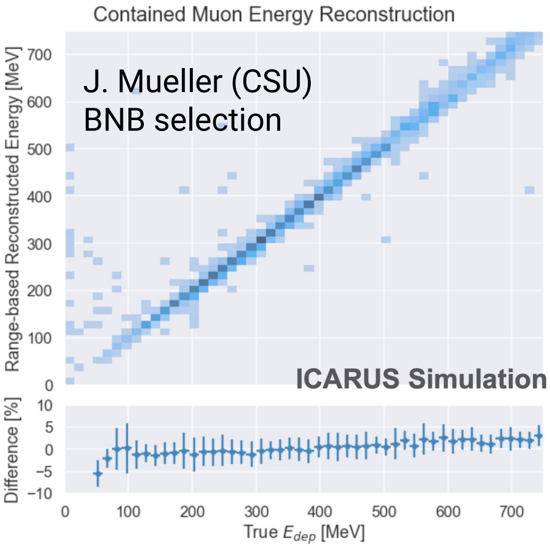
Paper: [PhysRevD.104.072004]

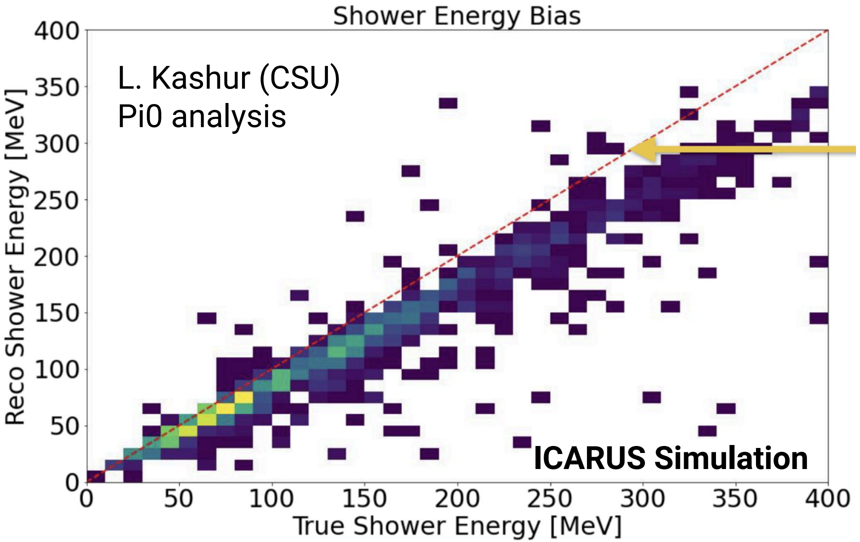
Energy reconstruction

Traditional techniques

Played around with regression NNs, but…

- **Range-based** momentum estimation of tracks is hard to beat
- **Calorimetric** energy reconstruction of showers is also hard to beat





Offset is an overall scaling factor (tiny fragments missing)

Aggregation

Graph edge classification

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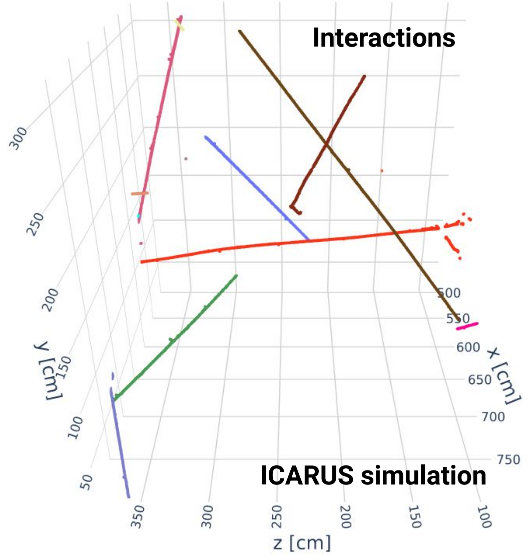
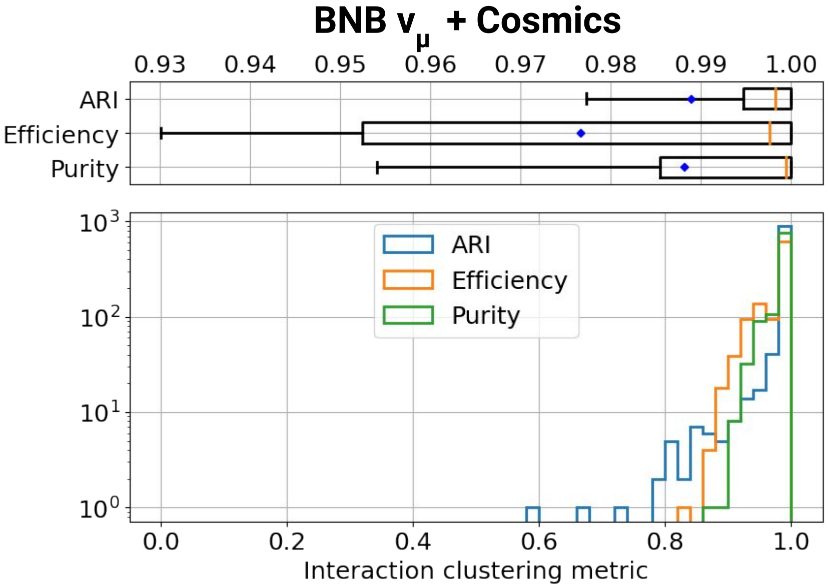
- **Select edges** in the graph that minimize loss, find **connected components**





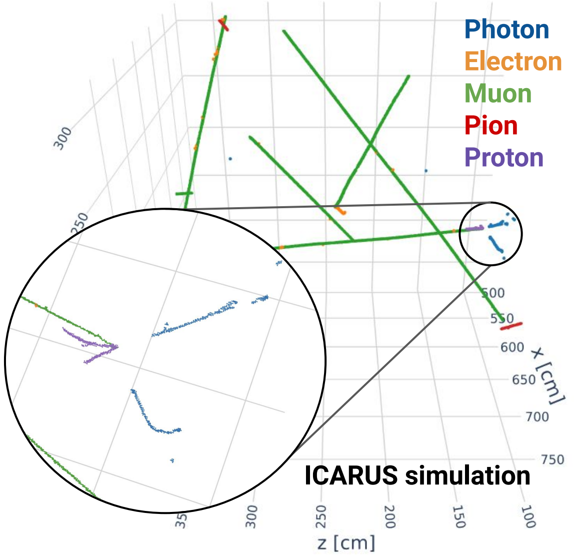
Paper: PhysRevD.104.072004

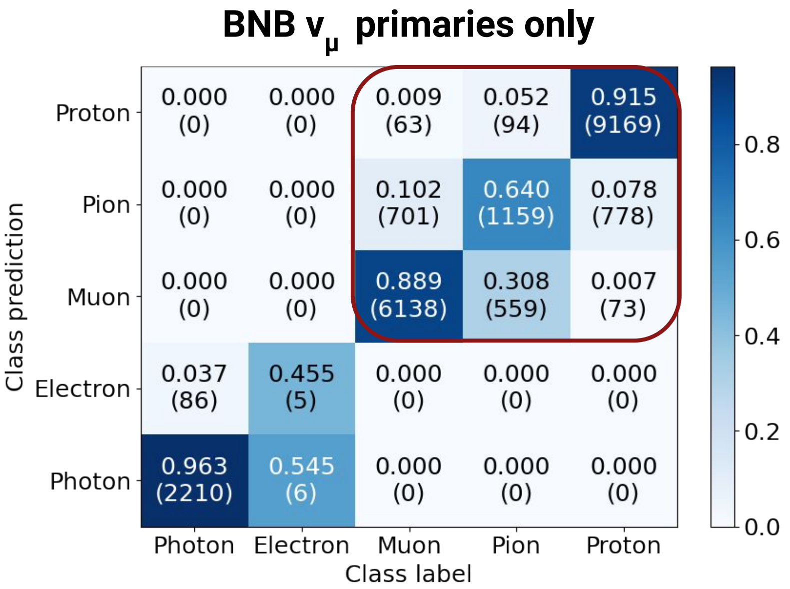
Particle Identification

Graph node classification

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

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





Particle Identification

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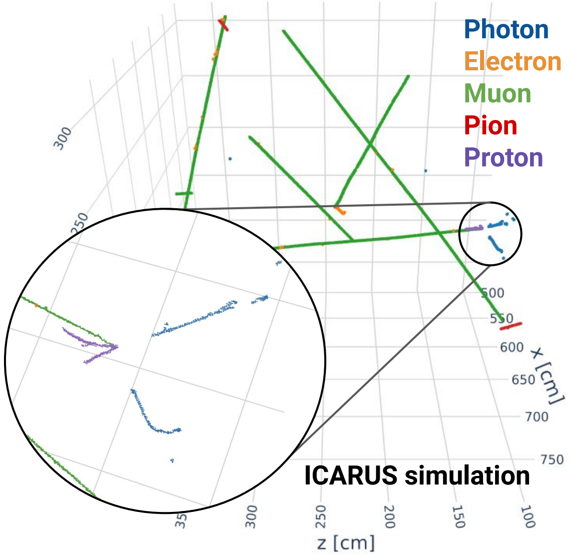
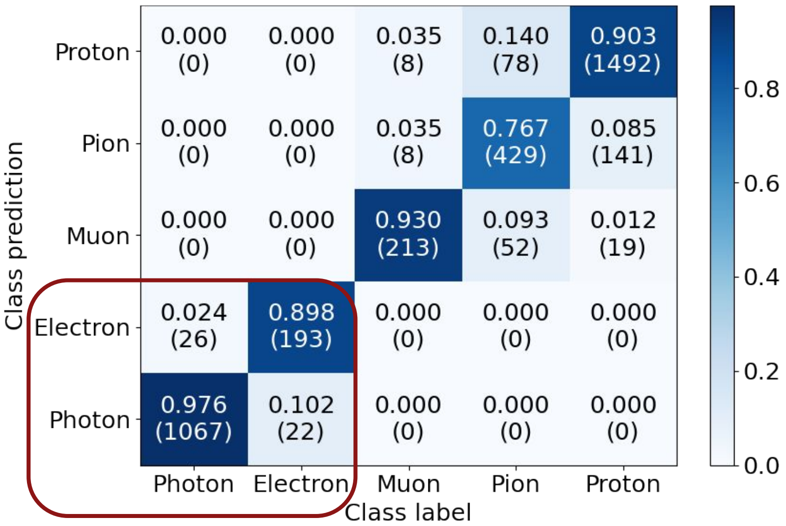


Generic dataset (particle bombs)

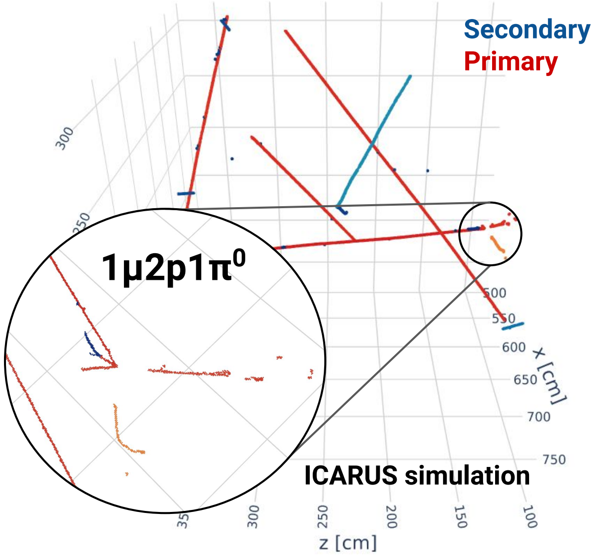


Primary Identification

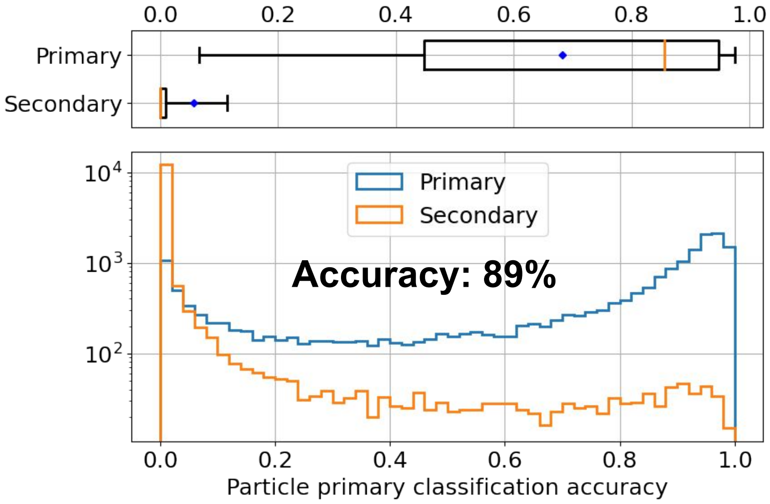
Graph node classification

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

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



BNB ν_μ primaries only

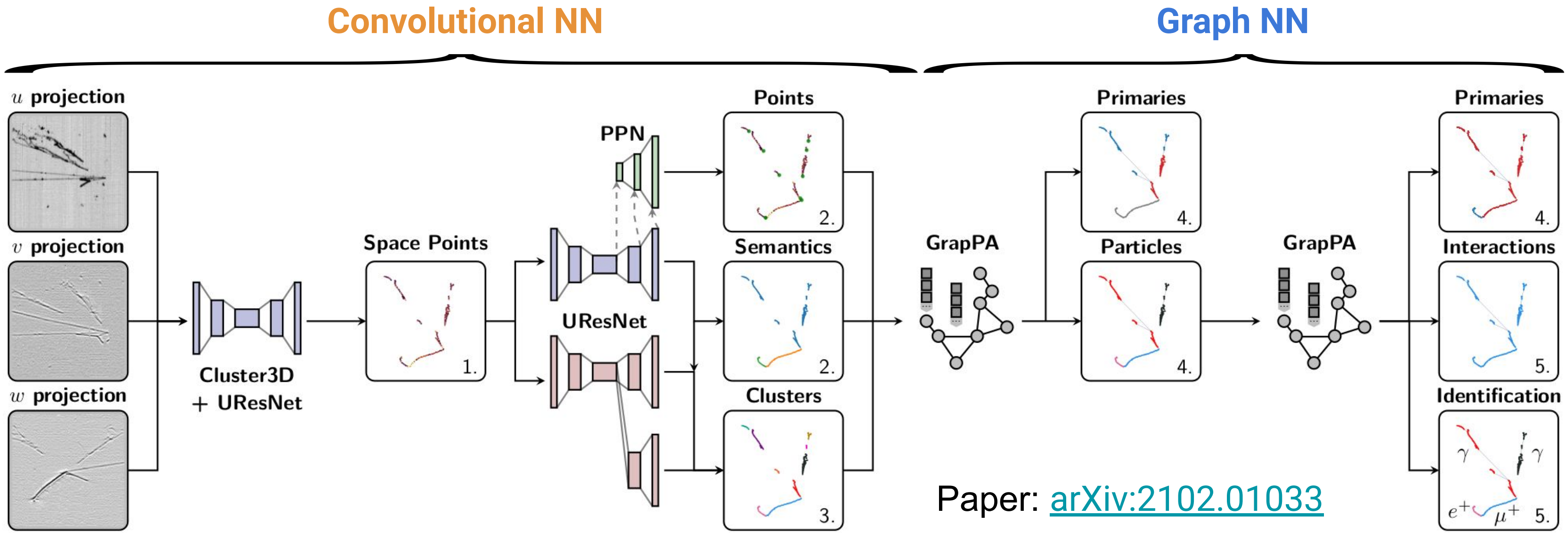


Reconstruction in LArTPCs

Full Reconstruction Chain Architecture

End-to-end ML-based reconstruction chain

- **UResNet** for pixel feature extraction, **GrapPA** for superstructure formation



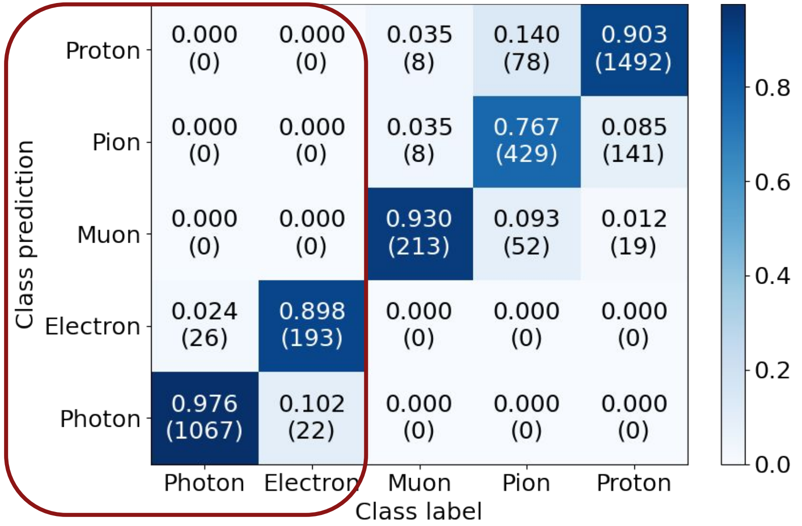
Paper: [arXiv:2102.01033](https://arxiv.org/abs/2102.01033)

S->ee searches

Challenges

What do we need for this search?

- Shower ID, e/gamma separation
  - Previous analyses see p->e confusion, **none in this ML scheme**

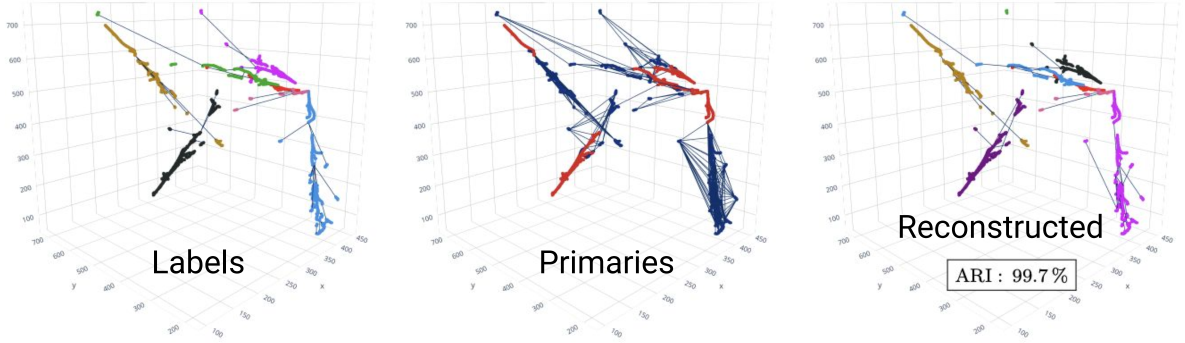


S->ee searches

Challenges

What do we need for this search?

- Shower ID, e/gamma separation
  - Previous analyses see p->e confusion, none in this ML scheme
- Reliable shower clustering (collinear showers are hard)
  - Need a dedicated study to see how far we can take it (J. Dyer)
  - Previous studies on pile-up indicate we do well at this



Generic simulation
6 showers in 10 m^3

Paper:
PhysRevD.104.072004

Low Energy Searches

Early days

Not much on this:

- Need to study blip reco. efficiency (secondary for oscillations)
- Some handle on low energy using Michel reconstruction as a benchmark
  - Currently much better than other techniques on the market

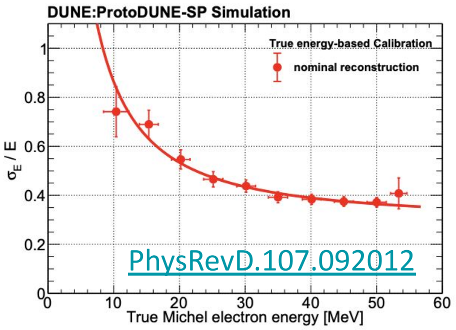
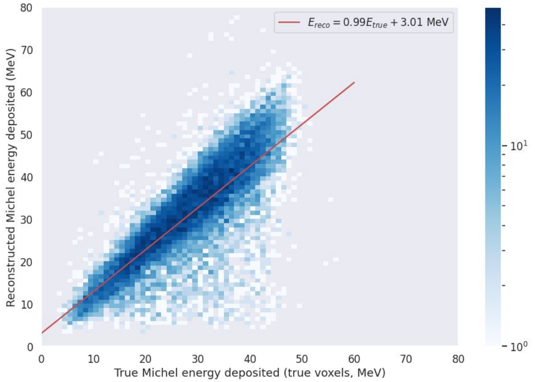
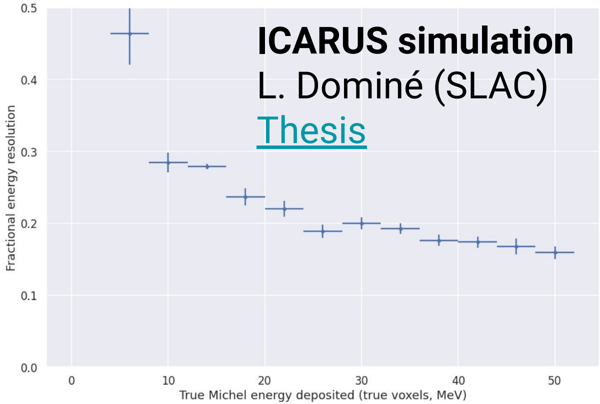


FIG. 10: Michel electron energy resolution as a function of Michel electron true energy using muon-based calibration (top); and the Michel electron energy resolution as a function of Michel electron true energy using true energy-based calibration (bottom).





ICARUS simulation
L. Dominé (SLAC)
Thesis

Reconstruction in LArTPCs

Scalability

A fair bit of work invested in speeding up the execution speed. On **ICARUS**:

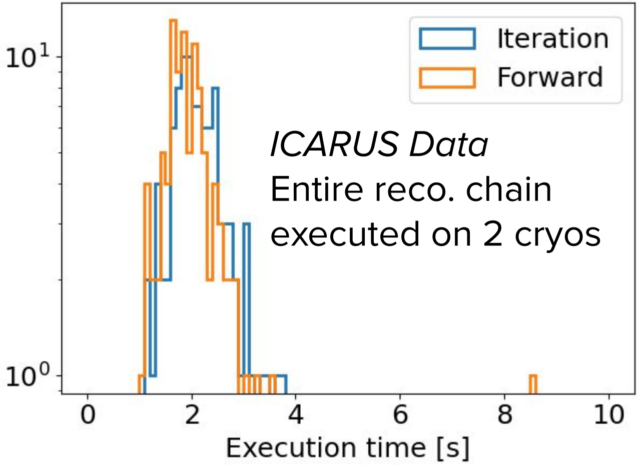
- ~2 M input space points/event
- O(1) M edges in the aggregator graphs
- **TPC reco: 2 s/event on an A100**

Very cheap to run on large datasets:

- **1 year of ICARUS beam-on data** can be reconstructed **in 1 day** with <200 A100s
- Perlmutter (NERSC): > 6000 A100s

Only **scales** with **space point count**

- Very cheap to run on DUNE-FD

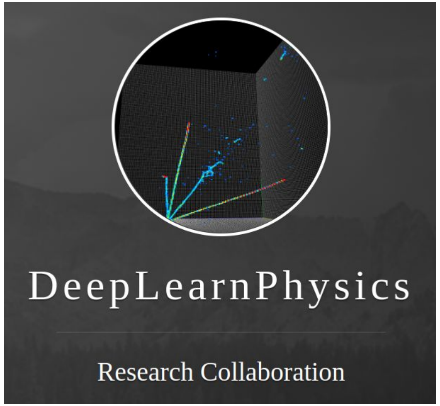


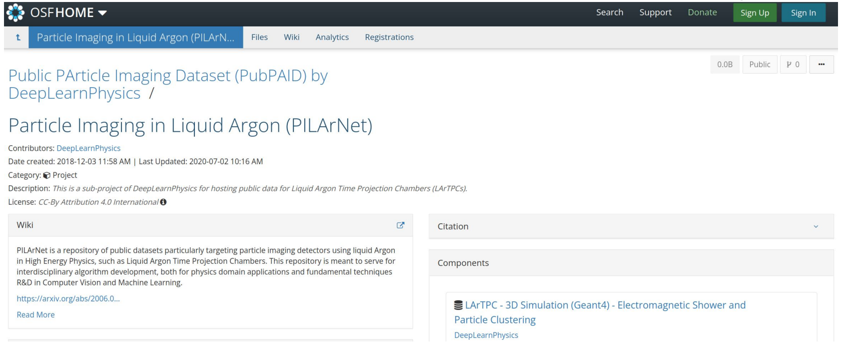
Reconstruction in LArTPCs

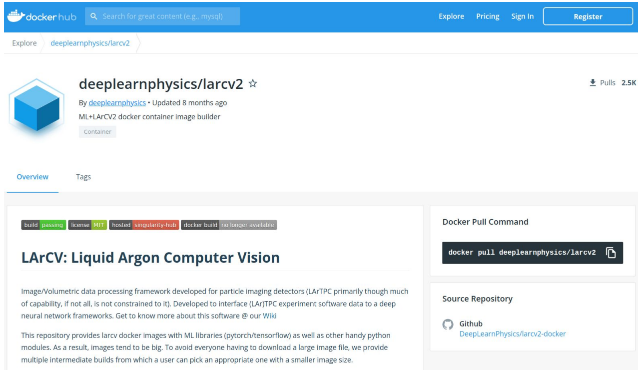
Open-source ecosystem

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
- Fully **reproducible results**
  - Readers have reproduced PhysRevD.102.012005







Other ML reconstruction efforts in LArTPCs

Very brief overview of the landscape

Many specific-purpose ML algorithms sprinkled in many places:

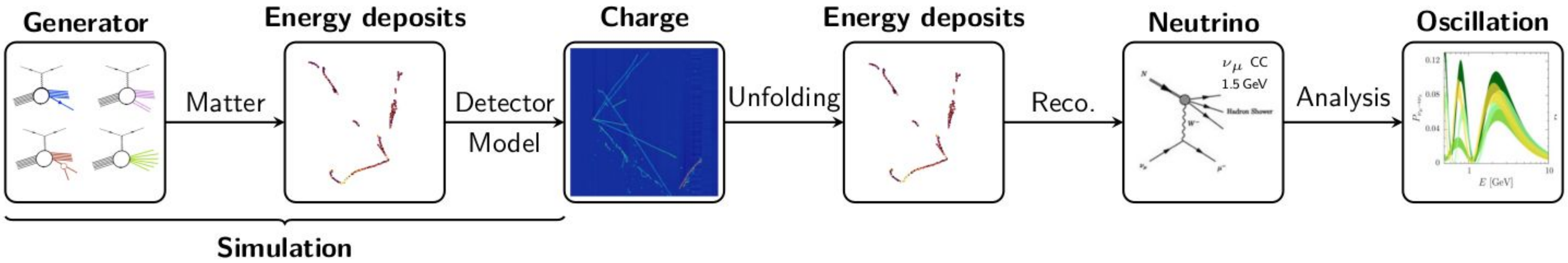
- BDTs are commonplace for S/B separation, particle type, etc.
- Some targeted ML-based effort to reconstruct the vertex location using CNNs
- Semantic segmentation in 2D in uBooNE (used in one of the LEE analyses)
- MPID algorithm based on CNNs in uBooNE (particle composition)
- CVN for image classification at the DUNE-FD

V. Hewes at U. Cincinnati leading another end-to-end effort based on GNNs from hits

- Early days, performance on semantic segmentation promising but worse
- Small networks (GNNs are shallower)
- Fast inference speed
- Nothing yet on clustering

Non-Reconstruction ML Efforts in LArTPCs

Future prospects



So far, we have tackled the **reconstruction challenge**, what's next?

- Can we go beyond “most likely” prediction and **quantify an uncertainty** ?
- Can we **mitigate differences** between simulation and data ?
- Can we **optimize detector modeling from data** and remove the issue altogether ?
- Can we **unfold detector effects** directly ? Yes, **learn inverse function automatically!**
- Can we **learn physics** (generators) **from data** ? Yes and no

Conclusions

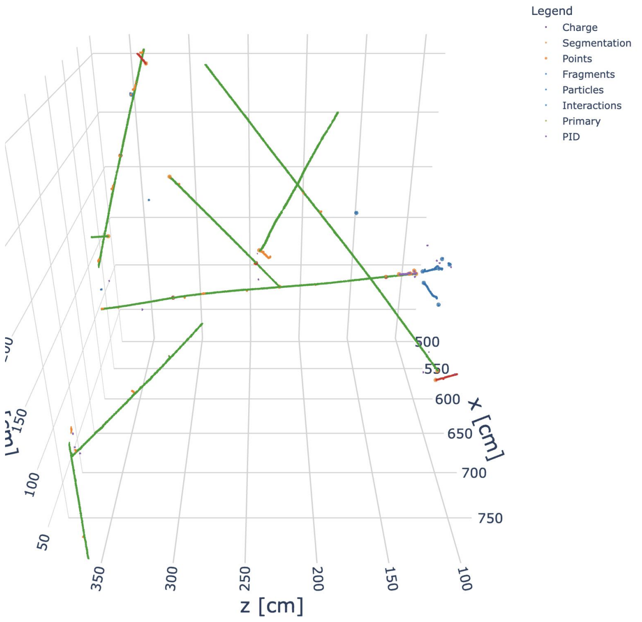
Takeaways

End-to-end ML-based reconstruction chain mature and functional

- Used on **ICARUS** sim./data and **DUNE-ND** (high neutrino pileup) sim. **today**
- Check out this ICARUS [interactive reconstructed event] !

In need of people to study performance on specific dark searches targets

- Promising early results on adjacent issues
- Many thanks to Jamie for her pioneering work in the ICARUS ML group



Backup Slides

GrapPA Aggregation Method

Edge selection procedure

What the network gives you:

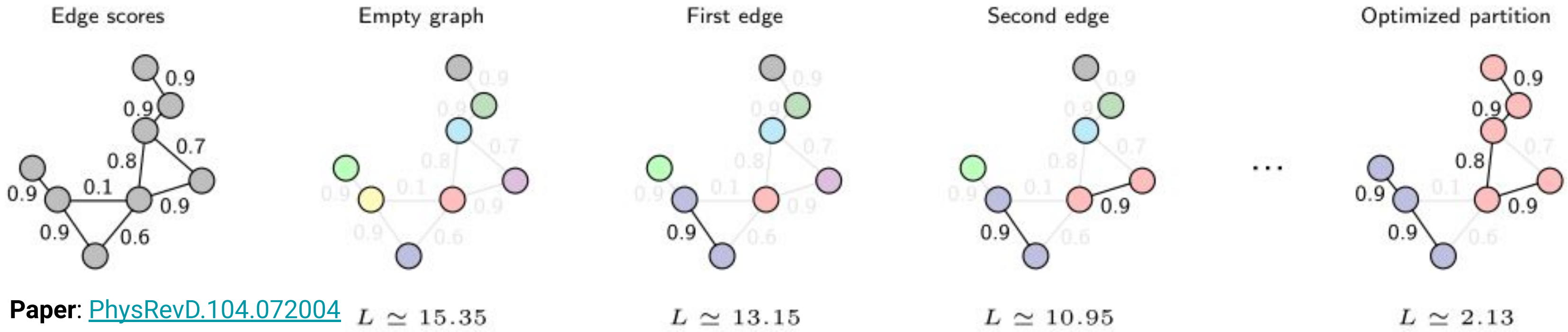
- Likelihood that an edge connects two objects in the same group

Target:

- Find the optimal partition

Method:

- Iteratively add the most likely edge to optimize CE loss



Paper: PhysRevD.104.072004

GrapPA Aggregation Method

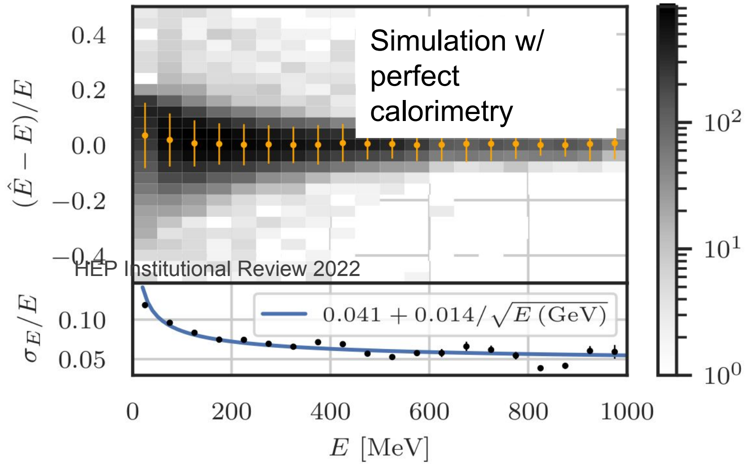
Shower energy reconstruction

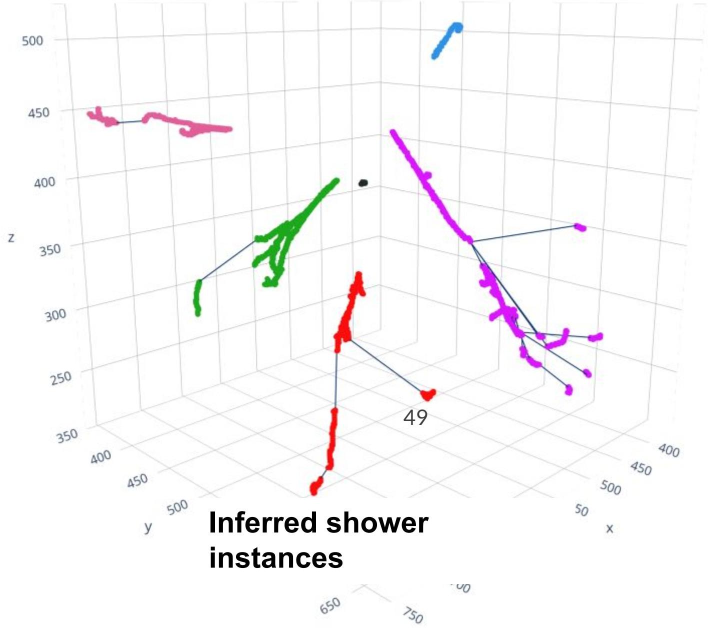
Identify **correlations** between shower fragments, **aggregate** them, identify **primaries**

Paper:

- [PhysRevD.104.072004]

Energy resolution at 1GeV: 5.5 %





Inferred shower instances

GrapPA Aggregation Method

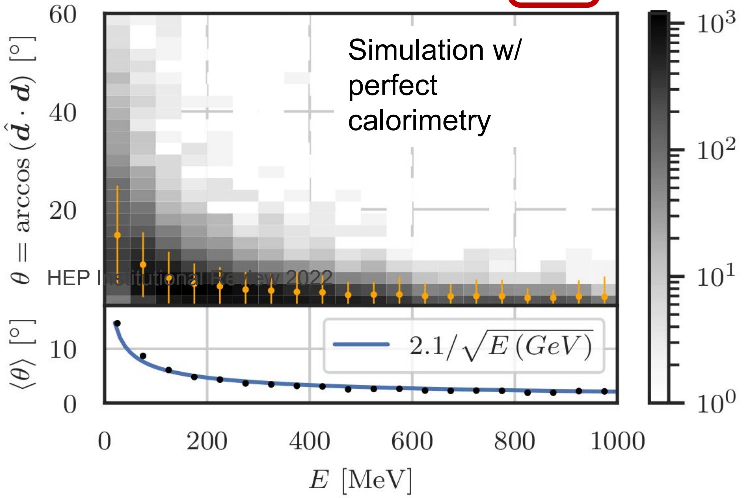
Shower angle reconstruction

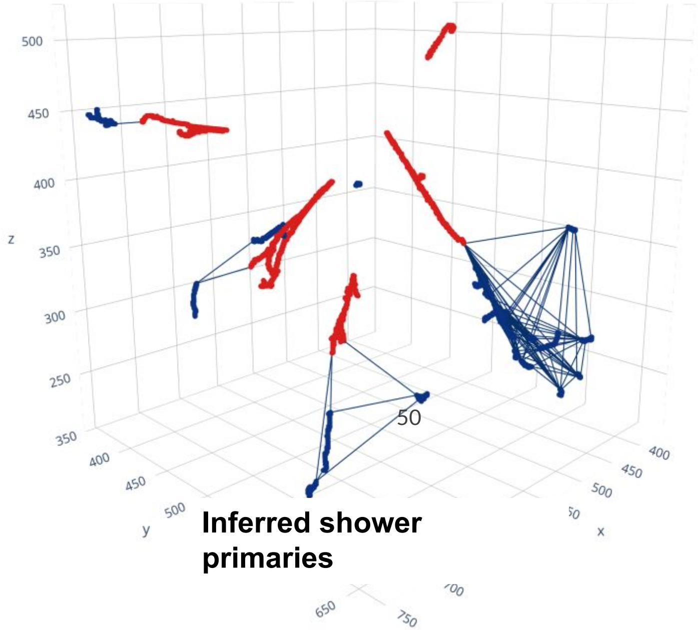
Identify **correlations** between shower fragments, **aggregate** them, identify **primaries**

Paper:

- [PhysRevD.104.072004]

Angular resolution at 1GeV: $\boxed{2.1°}$



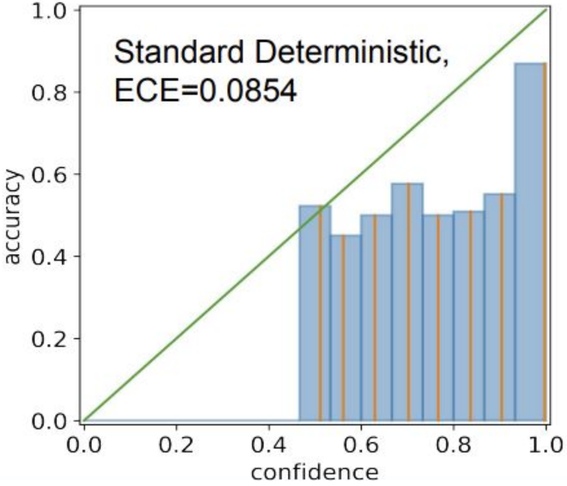


Uncertainty Quantification

Overview

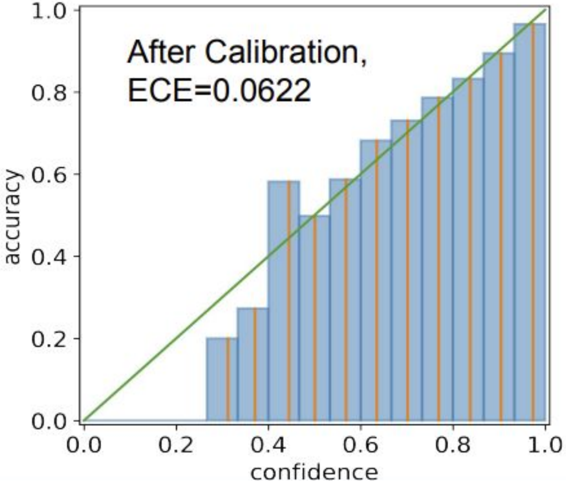
Goals of Uncertainty Quantification in Probabilistic Models:

- **Calibration**: Score p in [0,1] <=> probability p to be correct
- **Error detection**: Low confidence <=> large uncertainty



$$\hat{p}(x,T) = \max_i \frac{e^{l_i(x)/T}}{\sum_j e^{l_j(x)/T}}$$

Temperature Scaling



Uncertainty Quantification

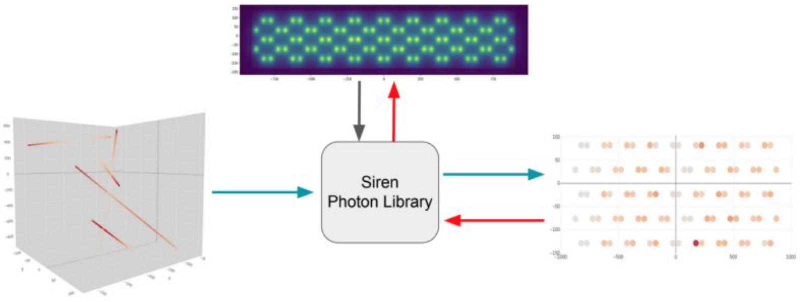
Photon visibility map

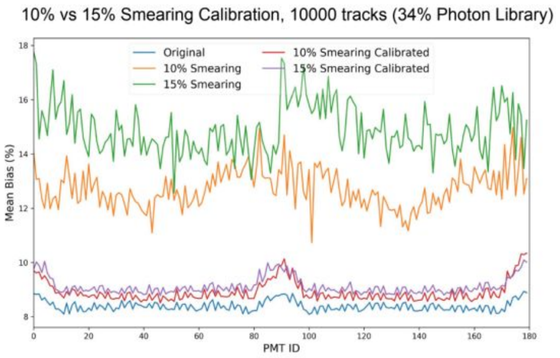
Can we make the **light simulation** differentiable ?

- Photon library maps x = (x, y, z) to visibility in each PMT (number of photons)
- Learn photon library using **scene representation** (SIREN): F (x, θ) differentiable

Calibration process: bias in library (offset in the actual visibility): θ ' = θ + δ

- Compare observed visibility to predicted visibility, use gradient descent to find θ ' !



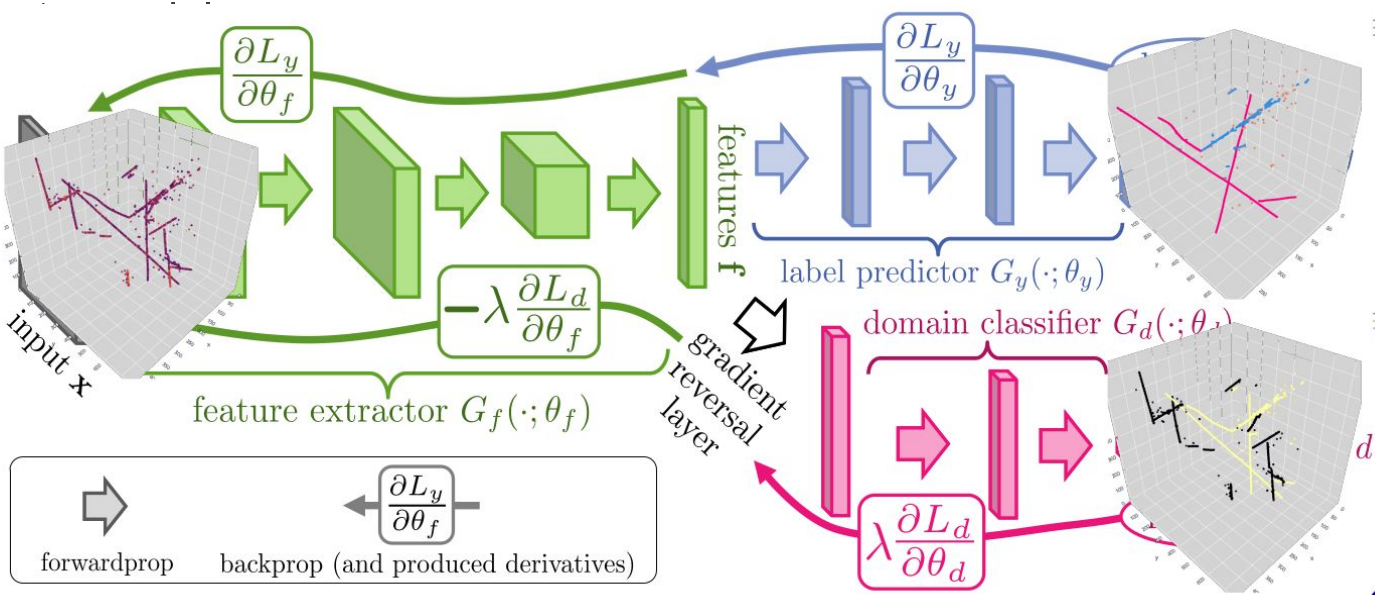


Domain Adversarial Training

Overview

Basics of **Domain Adversarial Networks**:

- Penalized for producing features that are different between

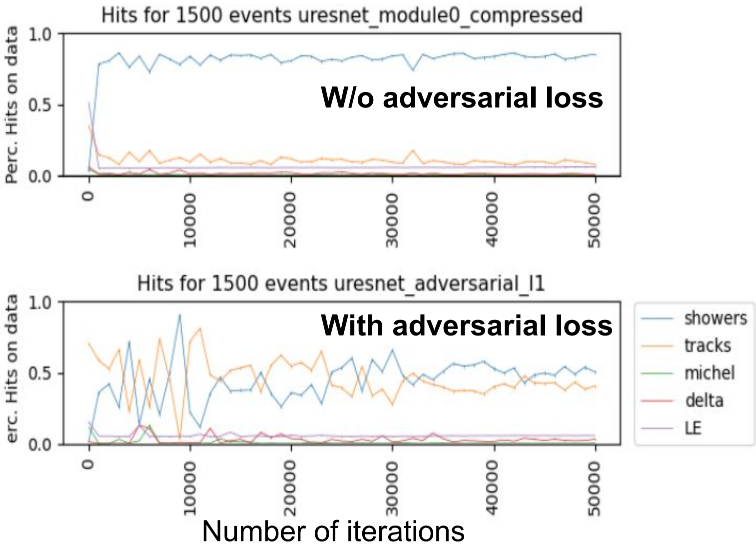


Domain Adversarial Training

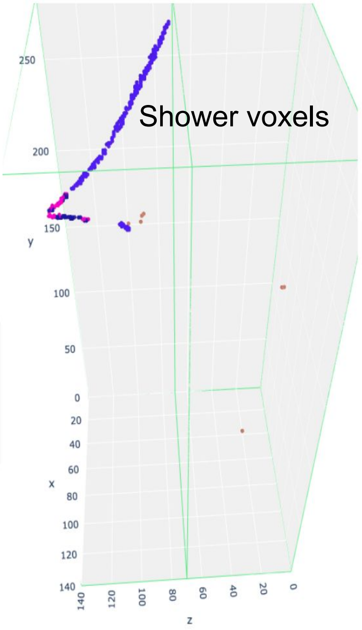
Overview

Basics of **Domain Adversarial Networks**:

- Penalized for producing features that are different between sim. and data



W/o adversarial loss



With adversarial loss