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Simulation and reconstruction challenges for DUNE / LAr TPCs

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Outline

- The physics
- LAr TPCs
- Reconstruction and simulation overview
- Challenges and outlook
- Summary

Neutrino oscillations

- Standard model 3-flavor neutrino mixing

Flavor eigenstates

$$\begin{bmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{bmatrix} = \begin{bmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{bmatrix} \begin{bmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{bmatrix}$$

Mass eigenstates

Pontecorvo-Maki-Nakagawa-Sakata matrix

Neutrino oscillations

- Standard model 3-flavor neutrino mixing

$$\begin{bmatrix}\nu_e\\ \nu_\mu\\ \nu_\tau\end{bmatrix} = \boxed{\begin{bmatrix}U_{e1} & U_{e2} & U_{e3}\\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3}\\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3}\end{bmatrix}}\begin{bmatrix}\nu_1\\ \nu_2\\ \nu_3\end{bmatrix}$$

$$\overbrace{\boxed{\begin{bmatrix}1 & 0 & 0\\ 0 & c_{23} & s_{23}\\ 0 & -s_{23} & c_{23}\end{bmatrix}}\boxed{\begin{bmatrix}c_{13} & 0 & s_{13}e^{-i\delta_{CP}}\\ 0 & 1 & 0\\ -s_{13}e^{i\delta_{CP}} & 0 & c_{13}\end{bmatrix}}\boxed{\begin{bmatrix}c_{12} & s_{12} & 0\\ -s_{12} & c_{12} & 0\\ 0 & 0 & 1\end{bmatrix}}}^{\text{PMNS matrix}}$$

Atmospheric/
Accelerator

Accelerator/Reactor

Solar/Reactor

Three mixing angles:

θ_{12}, θ_{13}, θ_{23}

CP-violating phase:

δ_{CP}

Neutrino oscillation parameters

- Measure the oscillation parameters by measuring appearance and disappearance probabilities

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

$\alpha, \beta \in (\nu_e, \nu_\mu, \nu_\tau)$

DUNE: ν_e appearance + ν_μ disappearance + c.c.

Three mixing angles: θ_{12}, θ_{13}, θ_{23}

CP-violating phase: δ_{CP}

2 mass differences: Δm^2_{32}, Δm^2_{21}

+ the sign of Δm^2_{32}

Neutrino oscillation parameters

- Measure the oscillation parameters by measuring appearance and disappearance probabilities:

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

$\alpha, \beta \in (\nu_e, \nu_\mu, \nu_\tau)$

DUNE: ν_e appearance + ν_μ disappearance + c.c.

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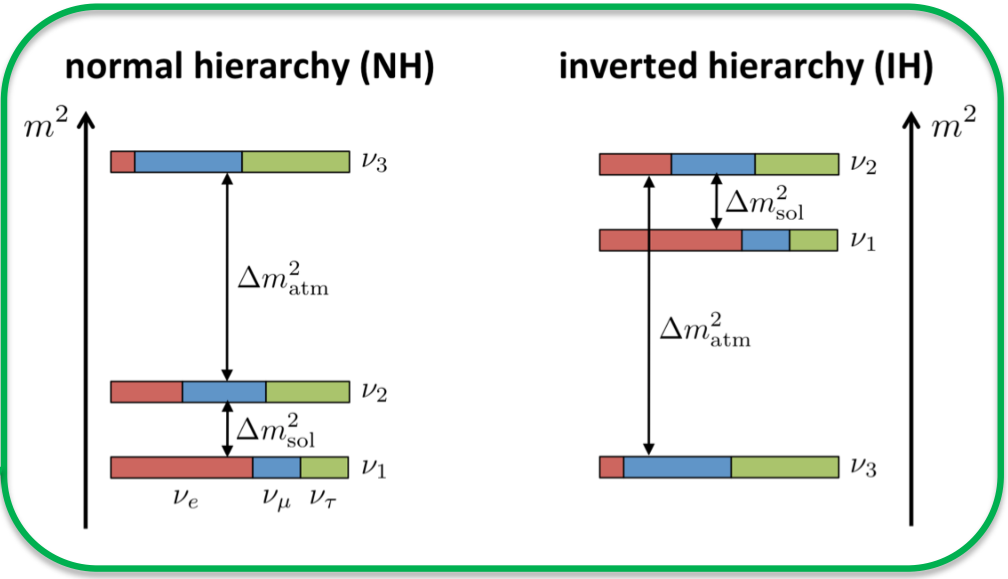


Unknown

Open questions in neutrino physics to be addressed

- What is the neutrino mass ordering?
- Is there CP violation in the neutrino sector

Long-baseline oscillation measurements

- Are there more than 3 neutrino flavors

Short-baseline oscillations

- Is our picture of neutrinos correct?

Additional goals for DUNE

- Search for neutrinos from supernovas
- Search for evidence of proton decay

Large underground detectors

Liquid argon time projection chamber experiments

- New generation of neutrino experiments based on LAr TPCs

Long baseline:

DUNE DEEP UNDERGROUND NEUTRINO EXPERIMENT

A collaboration of CERN, Fermilab,
labs and universities around the world

Short baseline:

SBN Program

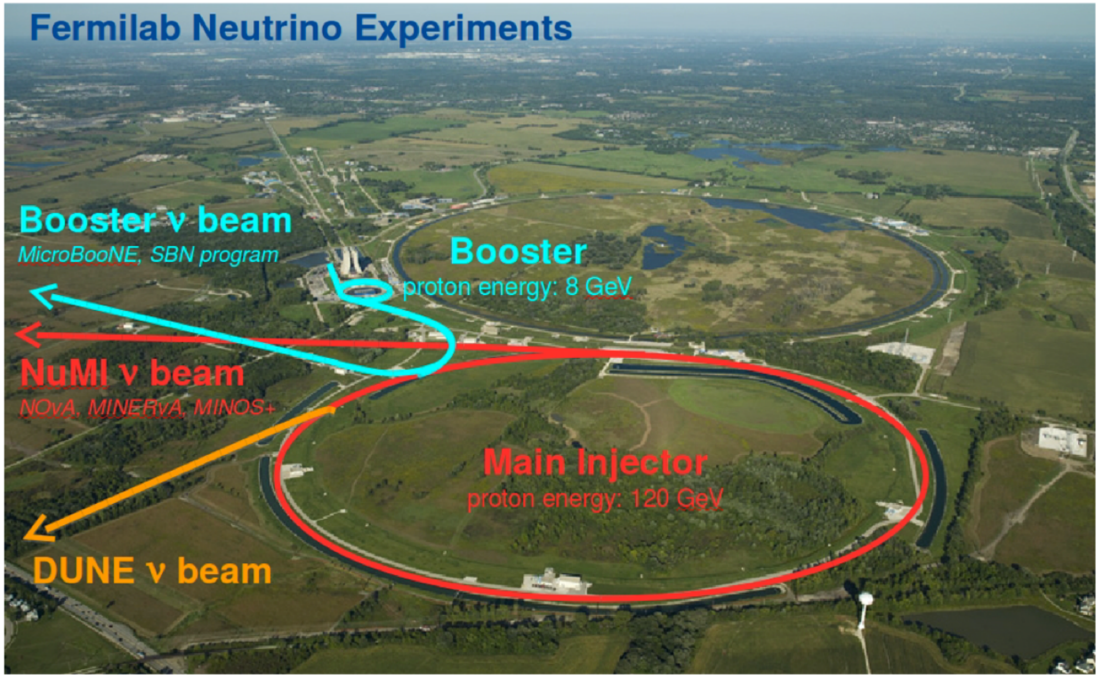
SHORT-BASELINE NEAR DETECTOR SBND

μBooNE LArTPC

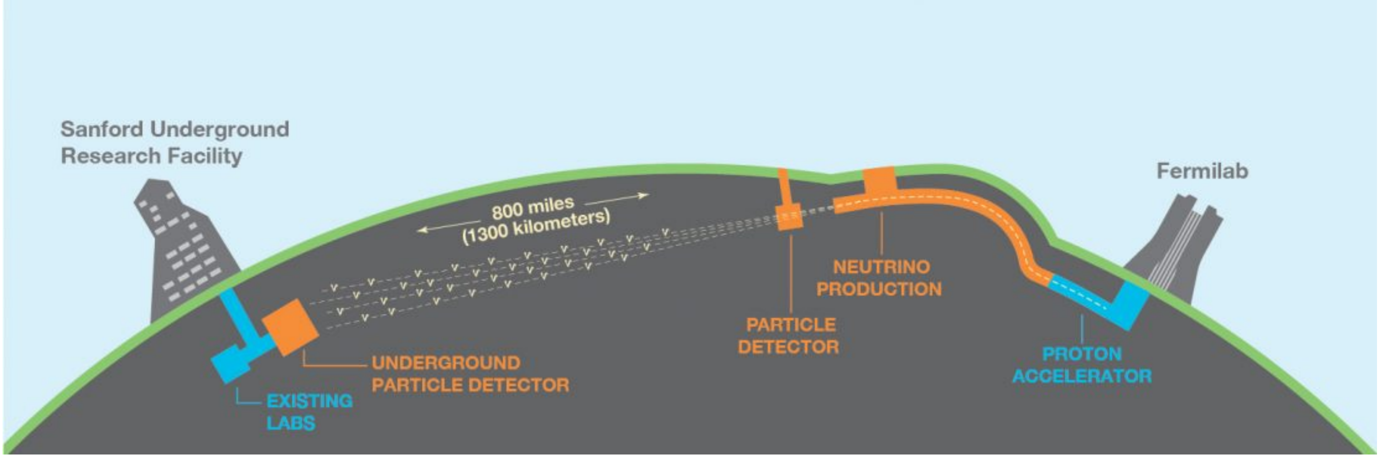
Imaging Cosmic And Rare Underground Signals

Liquid argon time projection chamber experiments

SBN Program



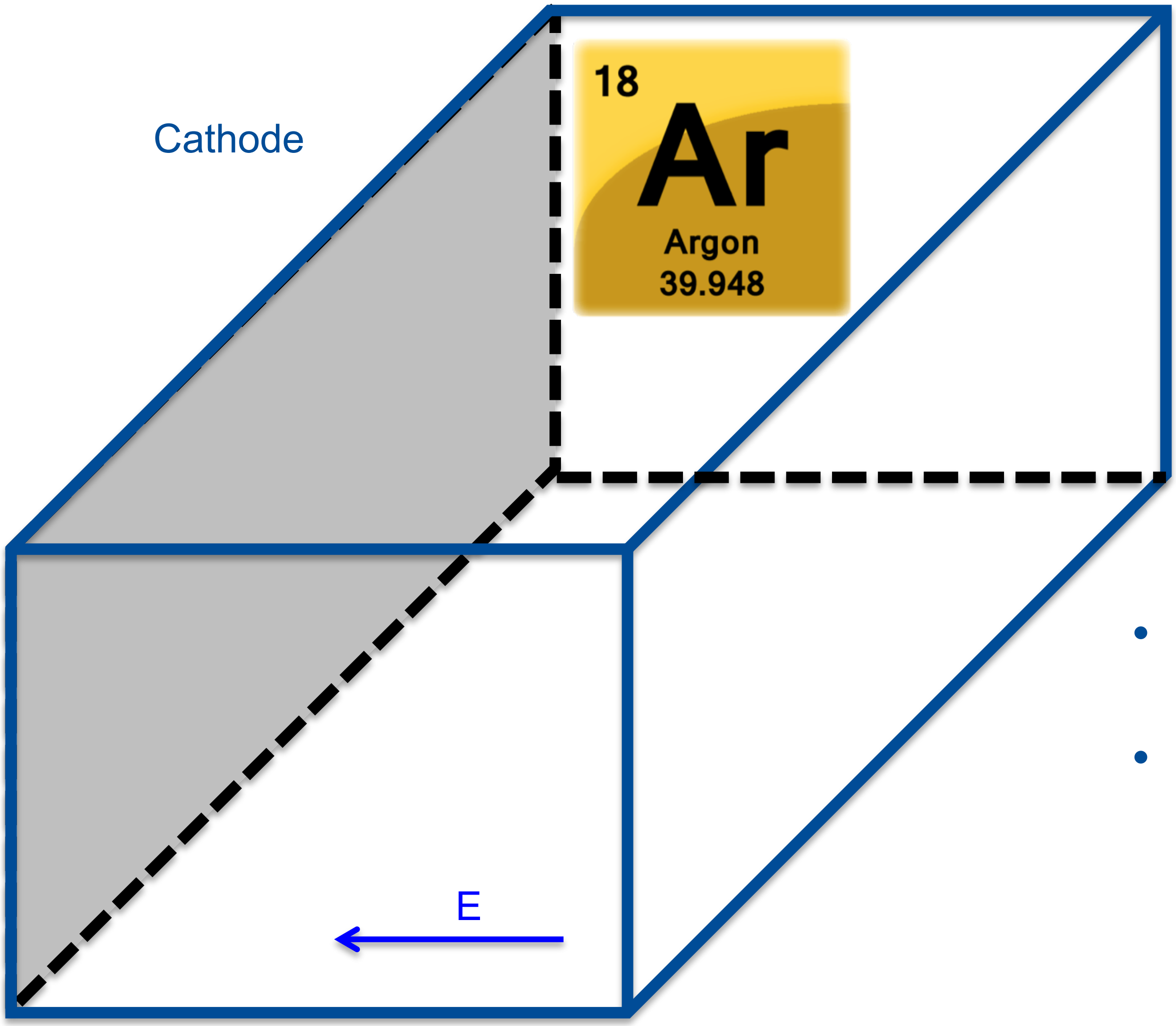
DUNE DEEP UNDERGROUND NEUTRINO EXPERIMENT



Also the ProtoDUNE demonstrator experiments at CERN

LAr TPCs

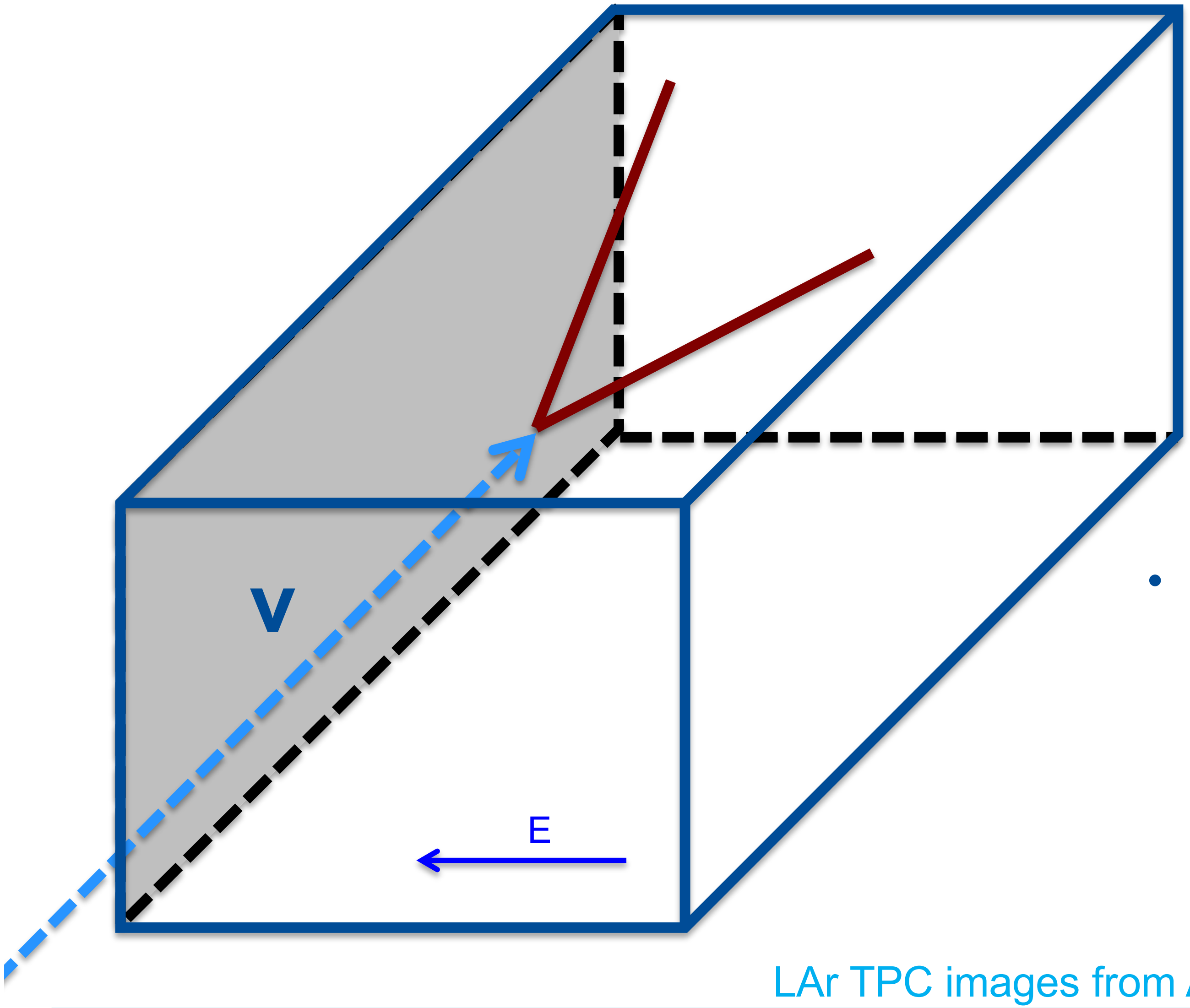
Single-phase LAr TPCs



- Large volume filled with liquid-argon
- Strong electric field

LAr TPC images from Anne Schukraft

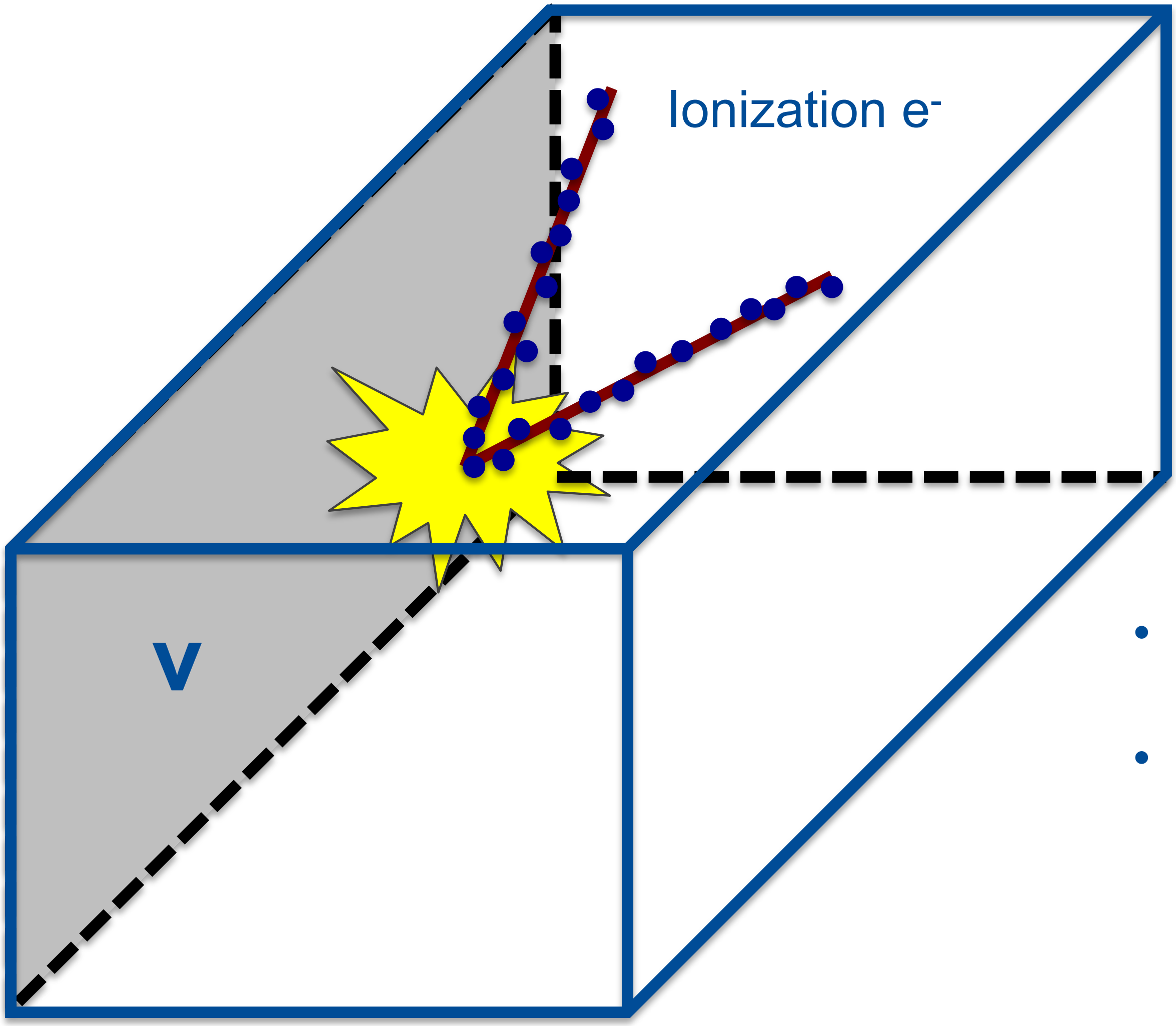
Single-phase LAr TPCs



- Neutrinos interact within the liquid argon volume

LAr TPC images from Anne Schukraft

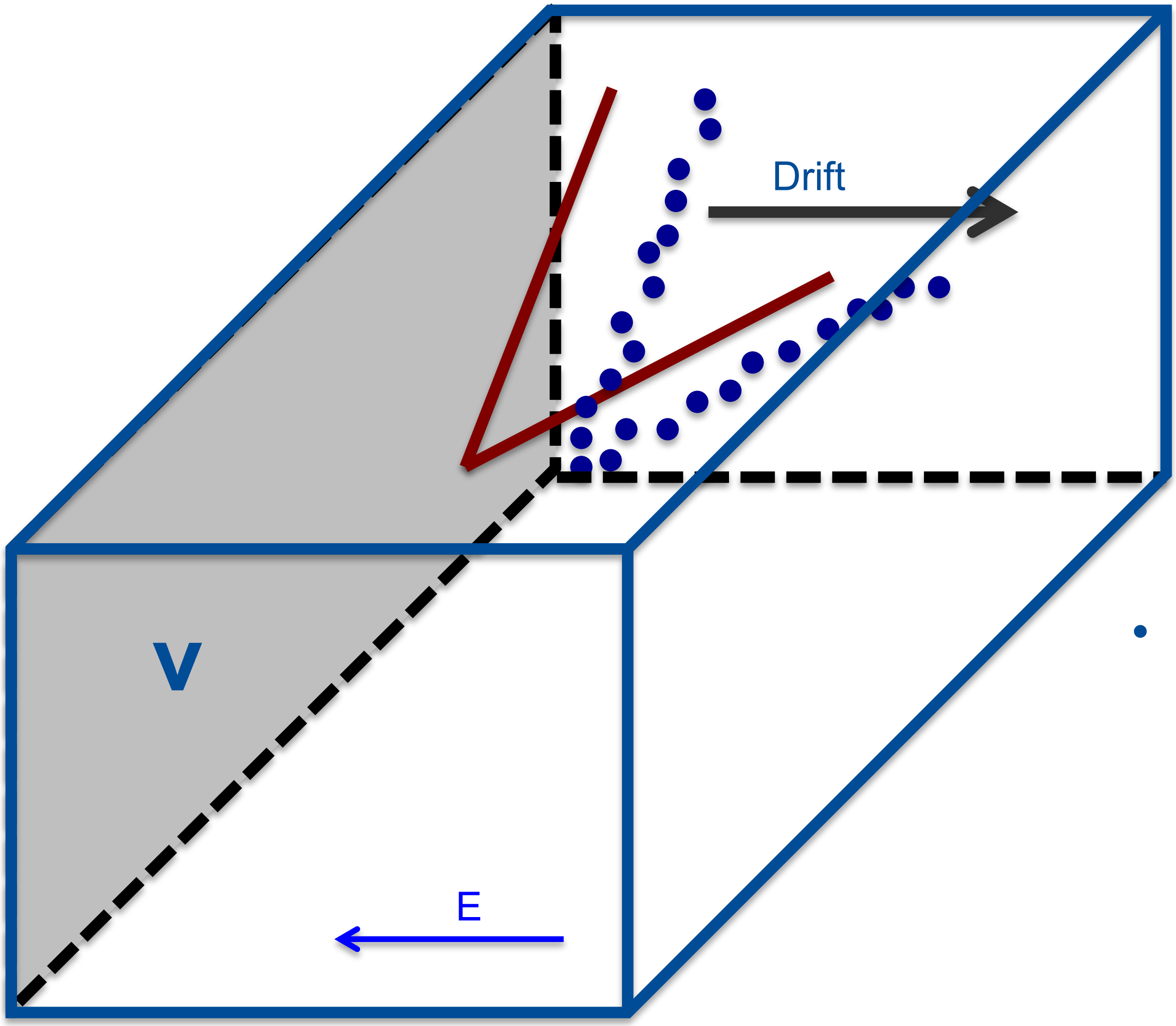
Single-phase LAr TPCs



- Charge particles produce ionization electrons
- Scintillation light production

LAr TPC images from Anne Schukraft

Single-phase LAr TPCs



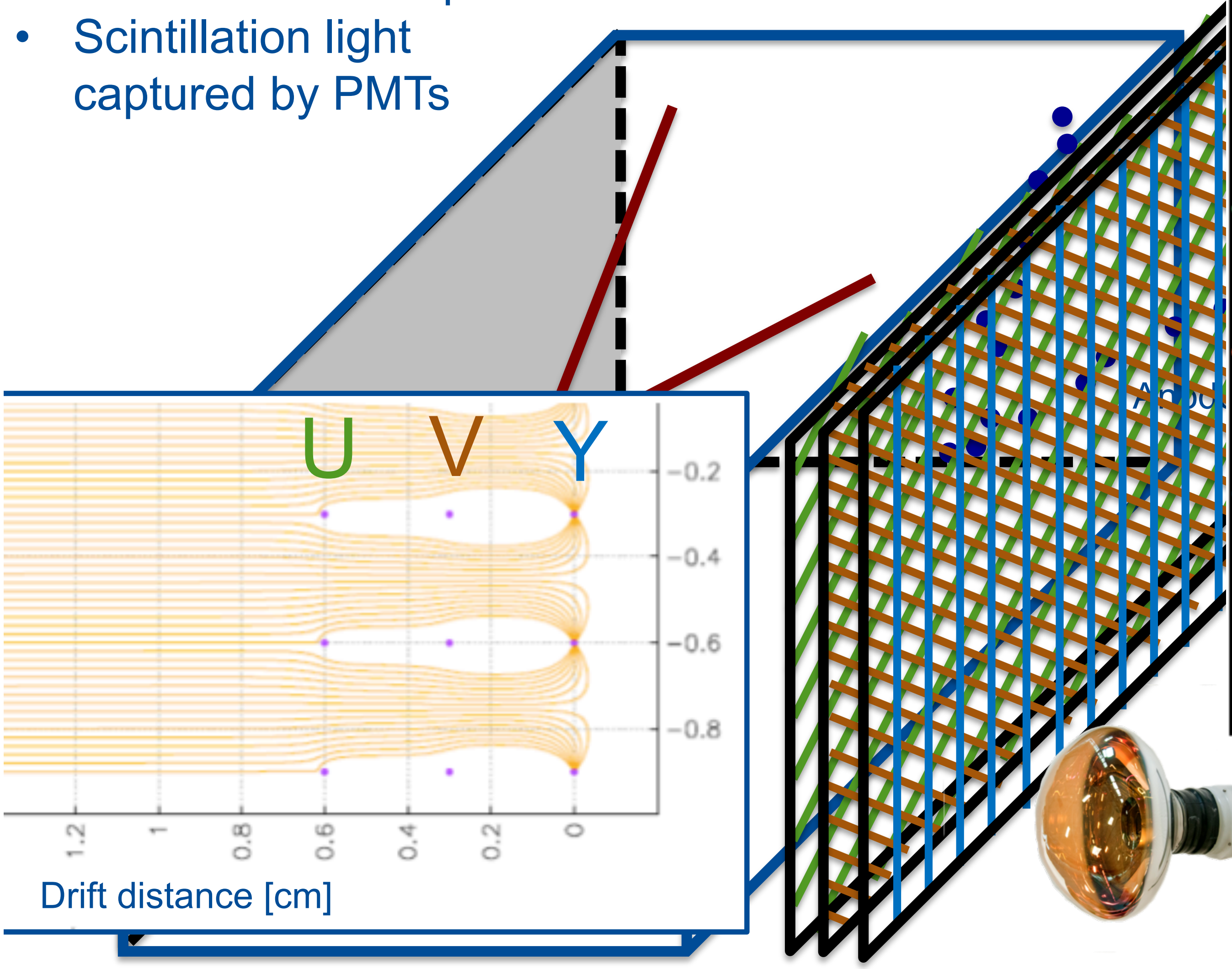
Anode

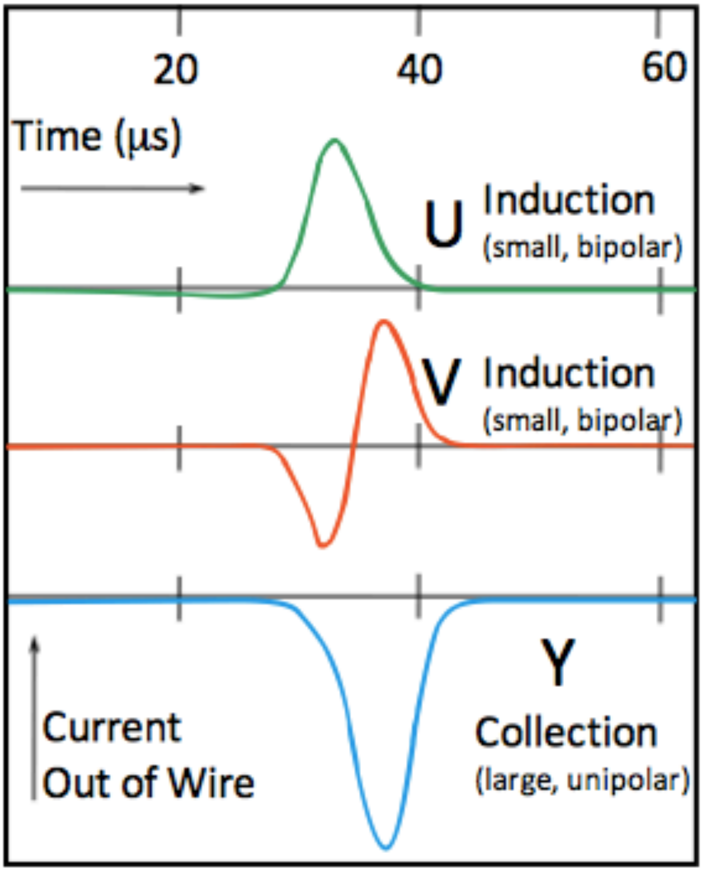
- Electrons drift towards anode plane

LAr TPC images from Anne Schukraft

Single-phase LAr TPCs

- Read out on wire planes
- Scintillation light captured by PMTs

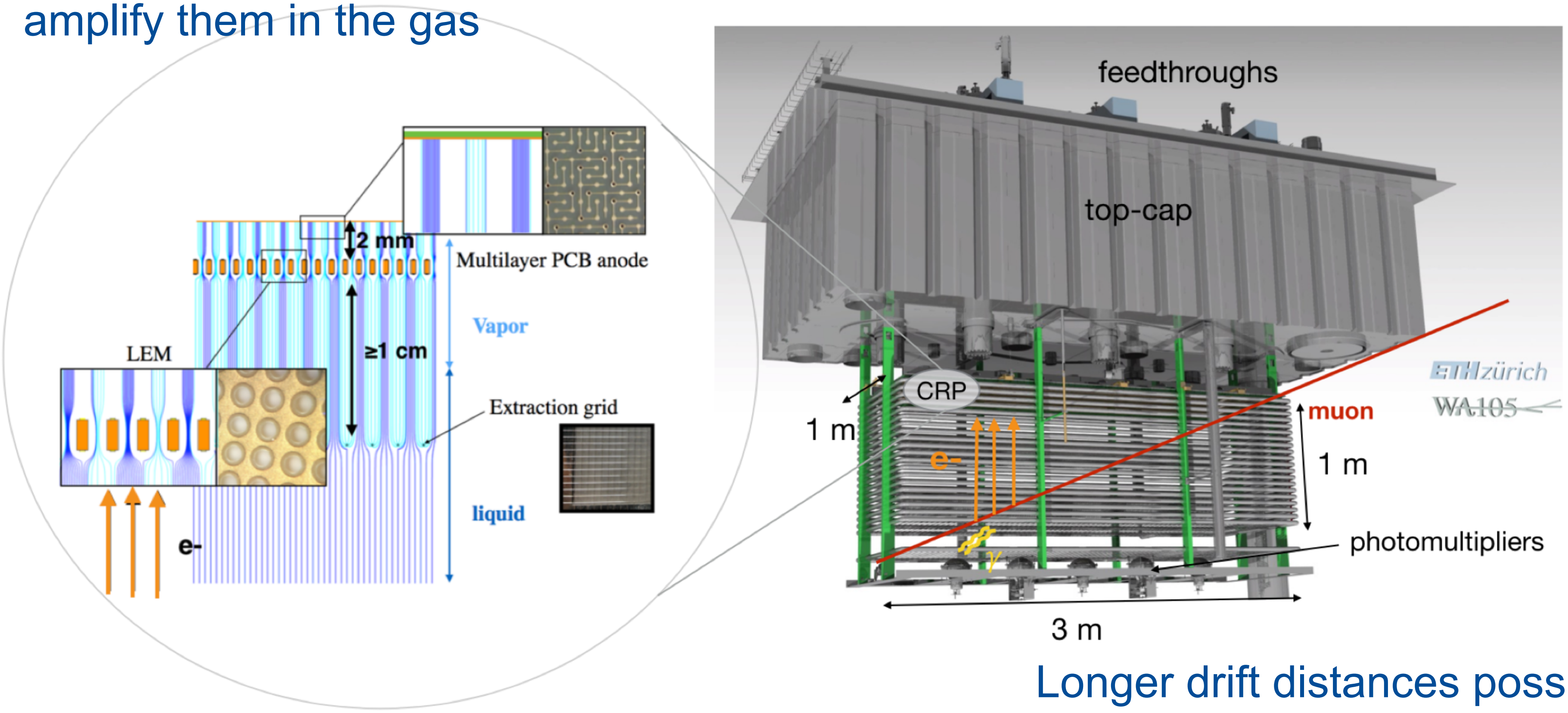




LAr TPC images from Anne Schukraft

Dual-phase LAr TPC

Extract electrons from the LAr,
amplify them in the gas



Longer drift distances possible
with very high S:N

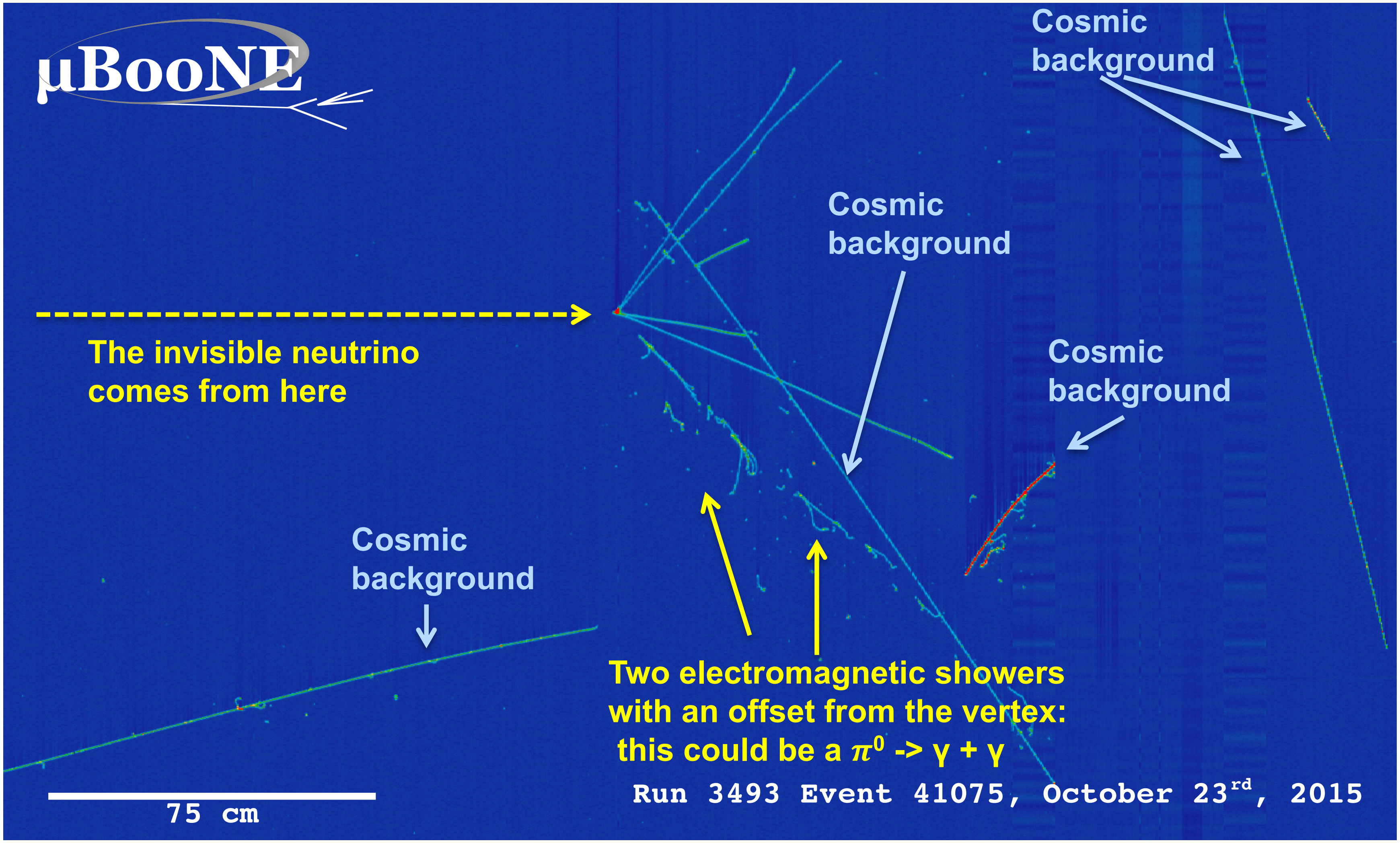
Two planes of readout strips at 90°
Both are "collection" planes with unipolar signals

Images from WA105 Collaboration, PoS ICHEP2016 (2016) 305

Future TPCs

- Other variations, e.g., for DUNE ND
  - Replace wire planes with a pixel readout plane
    - 3D space-point data directly from the detector
    - DUNE near detector, LArIAT, ArgonCube
  - HP gas Ar TPC with pixel readout

LAr TPC images



Cosmic background

Cosmic background

Cosmic background

Cosmic background

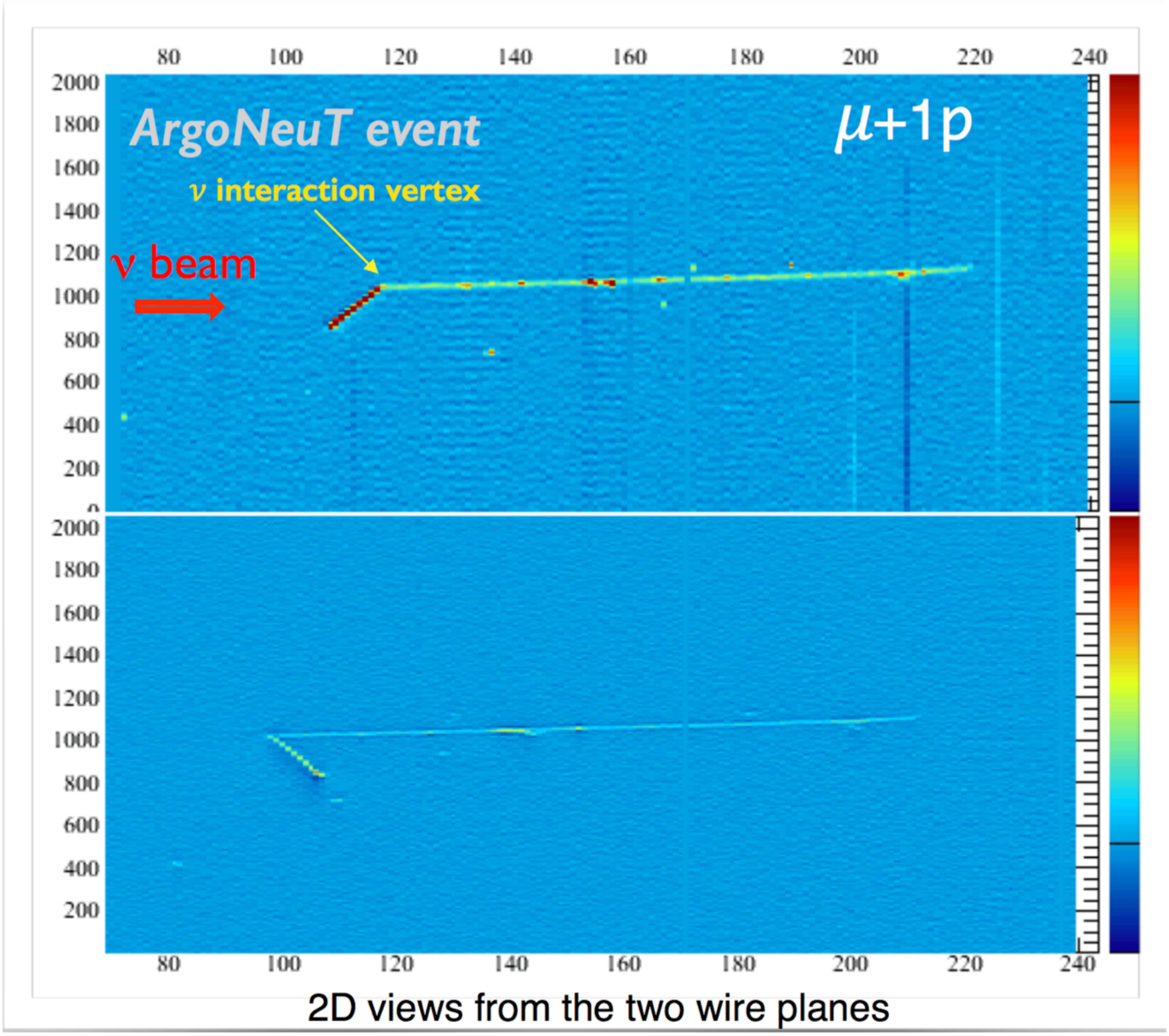
The invisible neutrino comes from here

Two electromagnetic showers with an offset from the vertex: this could be a π^0 -> γ + γ

Run 3493 Event 41075, October 23rd, 2015

LAr TPC images

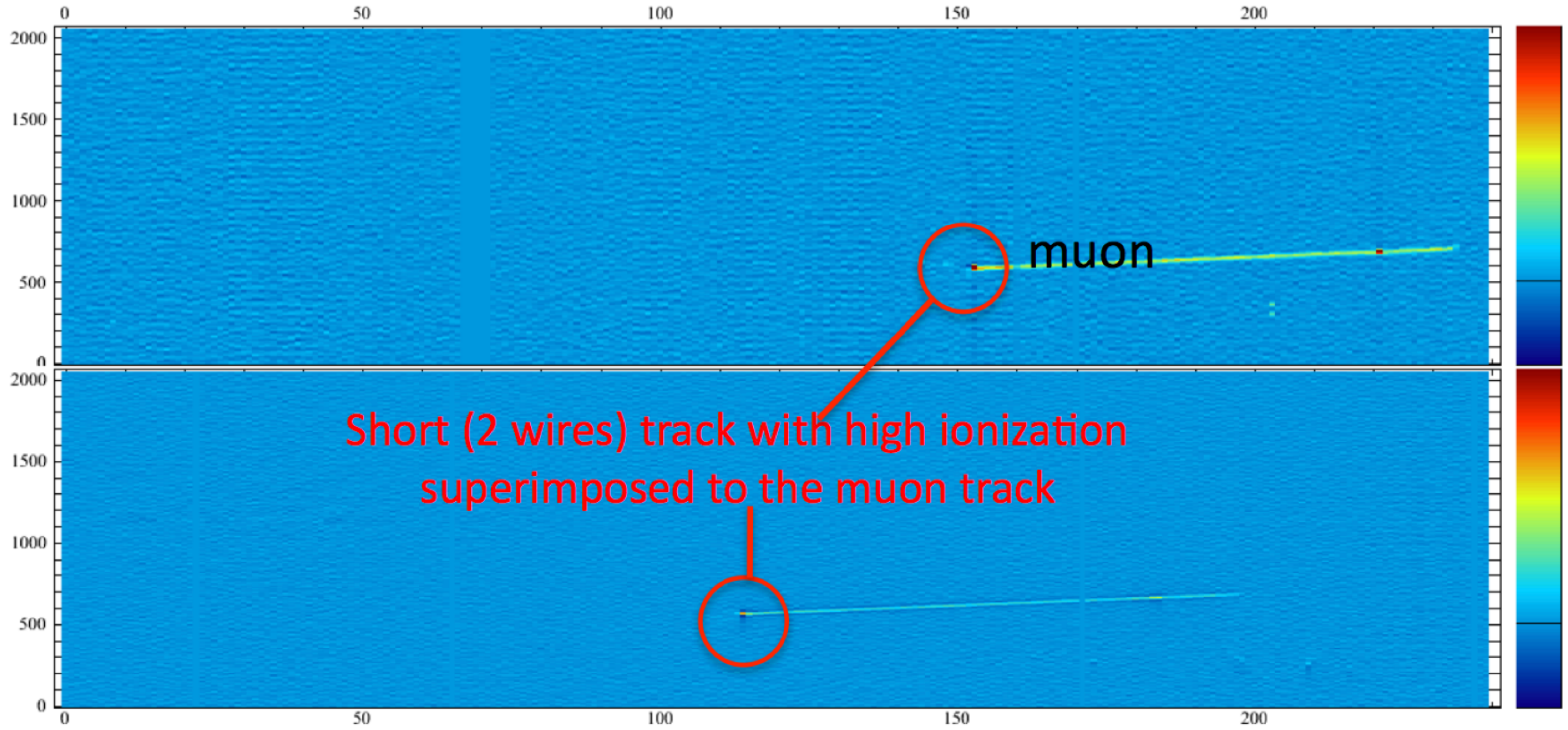
- ν_μ charged-current quasi-elastic candidate in ArgoNeuT



2D views from the two wire planes

Image from Ornella Palamara

LAr TPC images

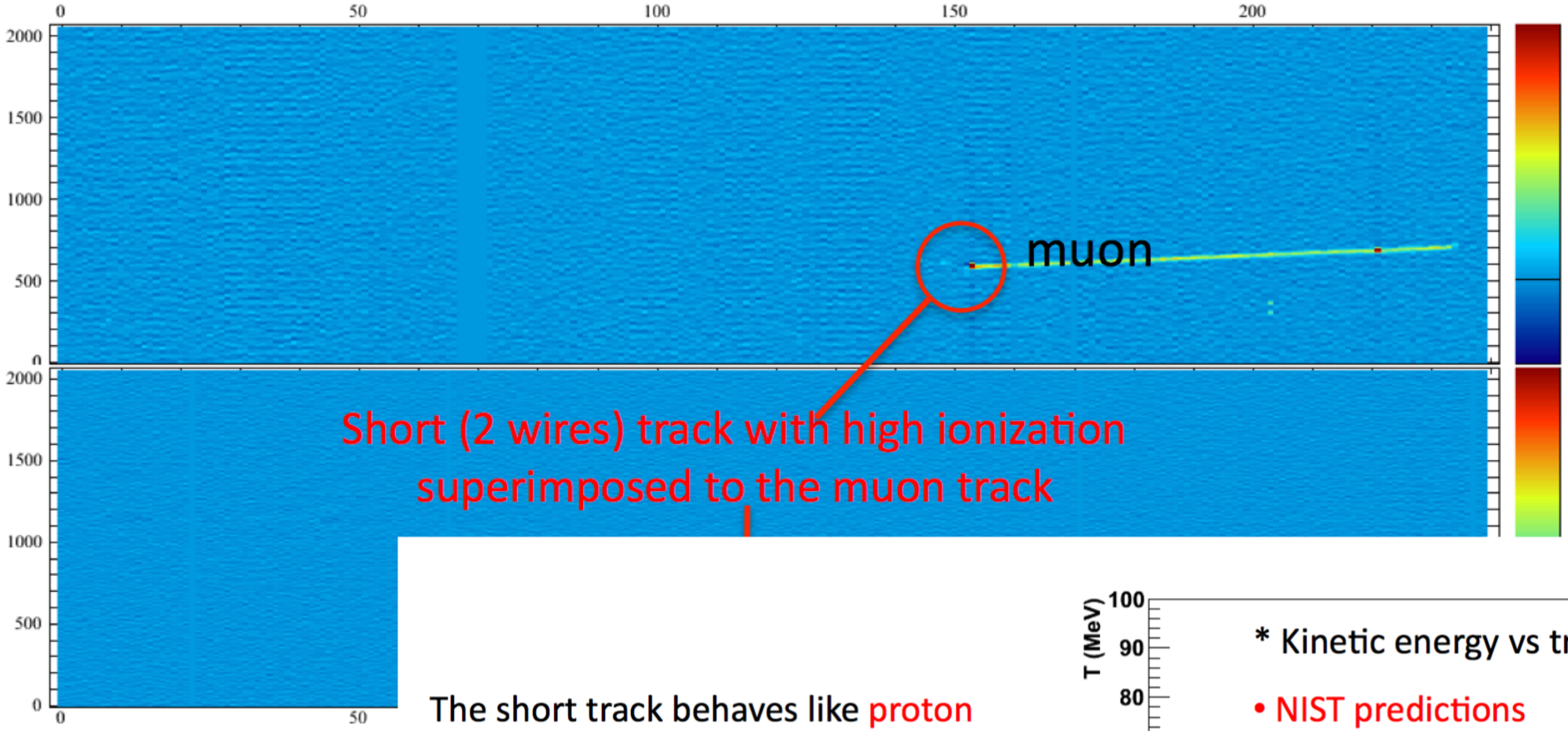


A proton is identified that touched only two wires *and* is overlaid on a muon.

Charge separated at waveform level

Images from Ornella Palamara

LAr TPC images

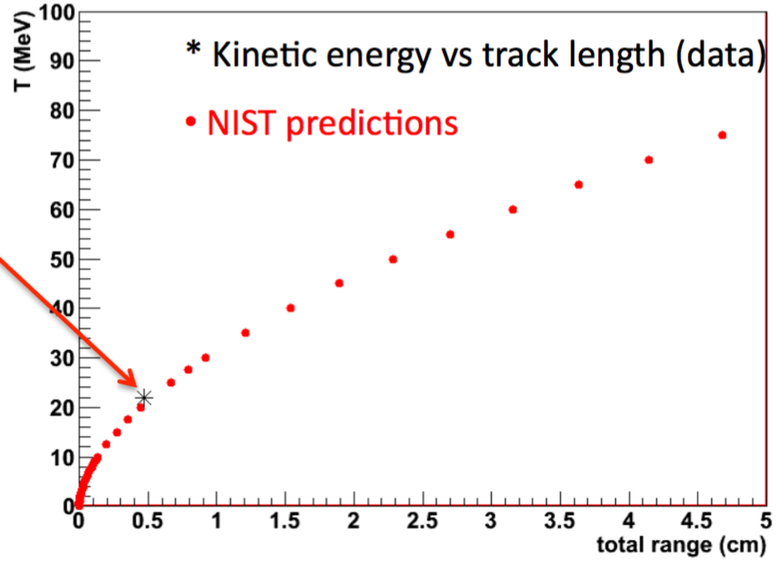


Short (2 wires) track with high ionization superimposed to the muon track

The short track behaves like proton

Length=0.5 cm

KE=22±3 MeV



Images from Ornella Palamara

LAr TPC images

Neutral current proton: ~4 cm track reconstructed, then identified using boosted decision tree algorithm

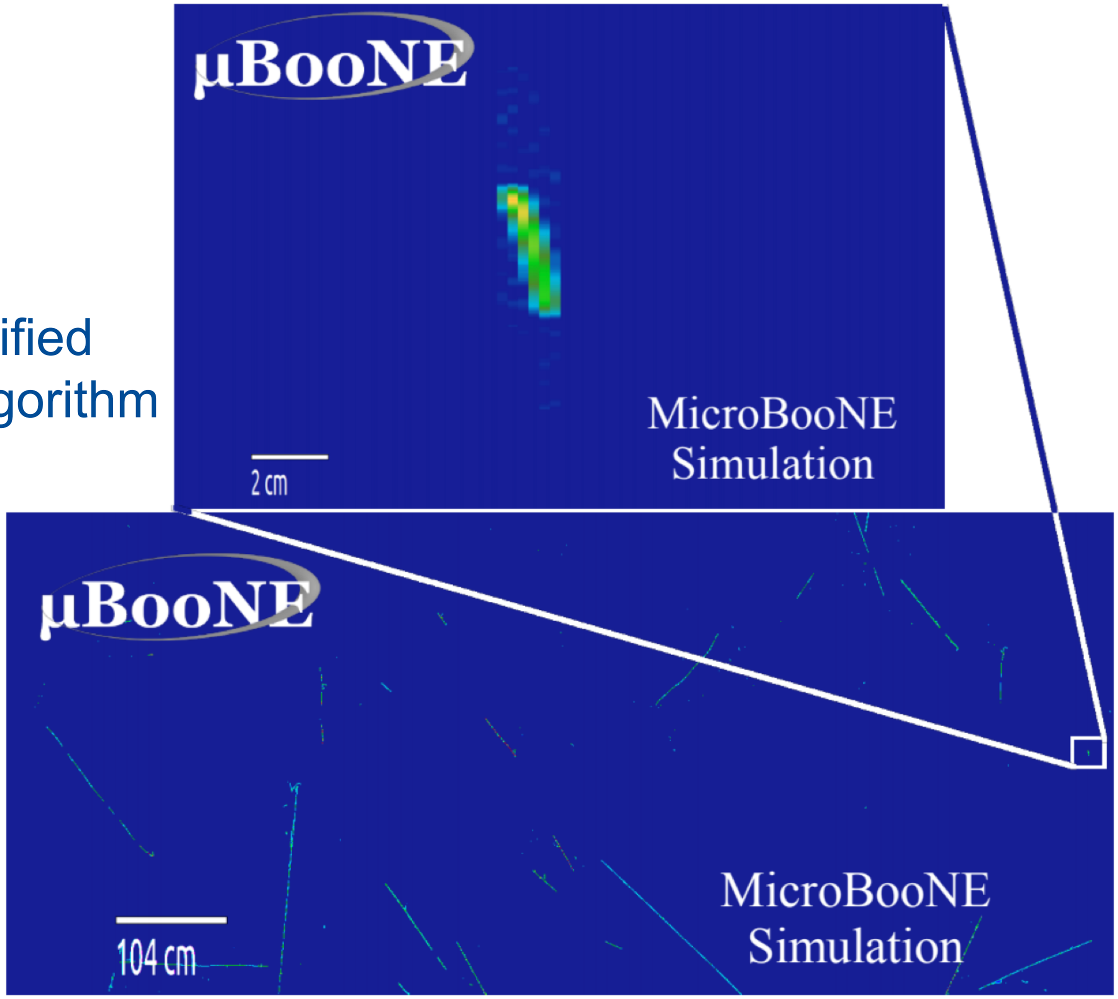
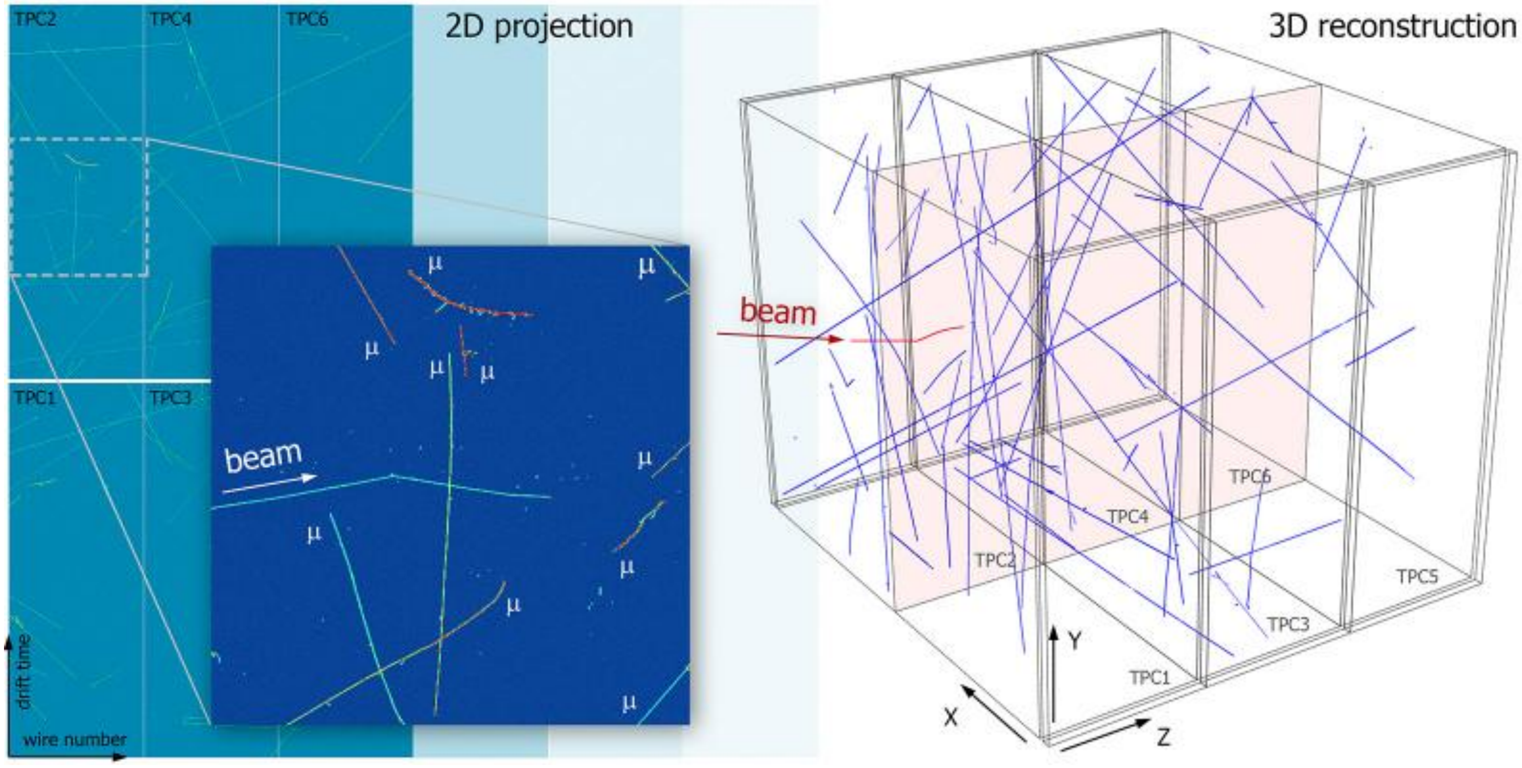


FIG. 4. 2D event display of a simulated neutral-current elastic event in MicroBooNE that was classified as a proton. The top image is a close-up event display of the simulated proton track. The bottom image shows the side view of the entire MicroBooNE TPC. All of the additional tracks are from cosmic rays.

MICROBOONE-NOTE-1025-PUB
http://microboone.fnal.gov/public-notes/

LAr TPC images

A simulated event in ProtoDUNE SP: beam particle plus cosmics

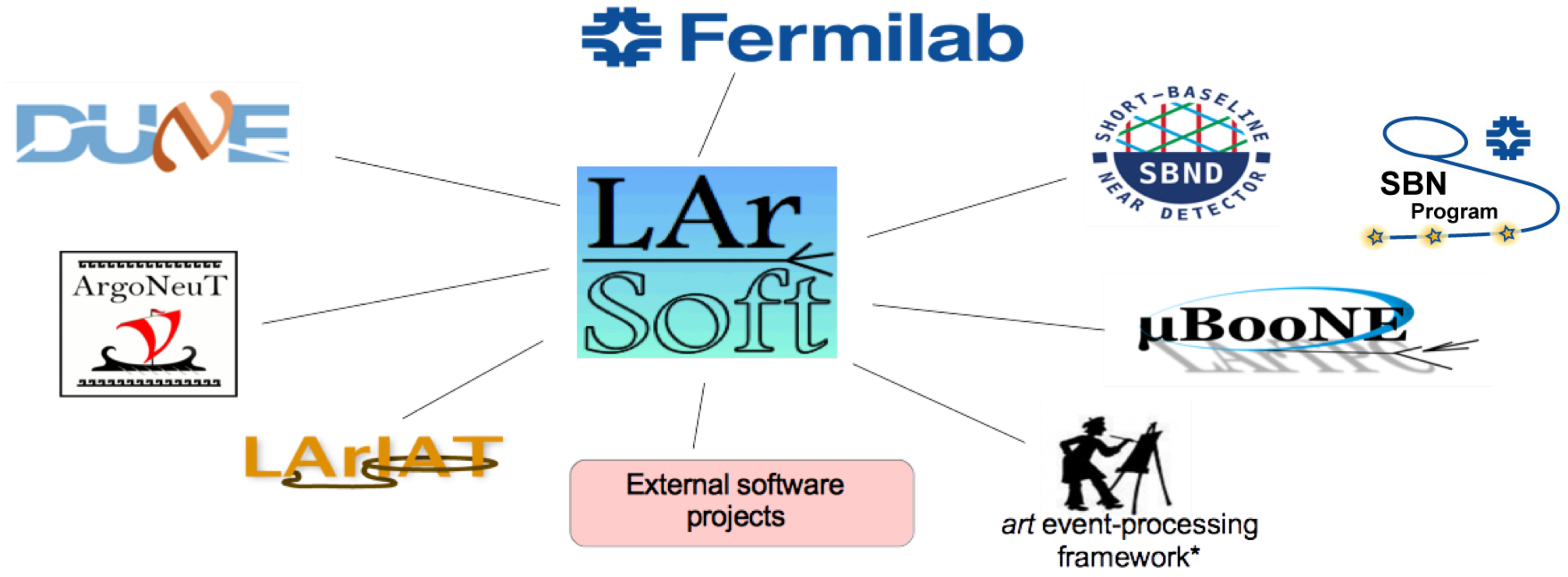


Images from www.duncescience.org

LAr TPC reconstruction and simulation

LArSoft

- A collaboration of experiments, labs, university groups and software projects



External software projects

art event-processing framework*

- Goal is to provide integrated, detector-independent software tools for the simulation, reconstruction and analysis for LAr TPC neutrino experiments

LArSoft

- External projects that coordinate with experiments and integrate code into LArSoft
  - Pandora (Cambridge University)
    - Multi-algorithm pattern recognition
    - Event topology reconstruction (particle flow)
  - Wire-cell (Brookhaven National Laboratory)
    - Signal processing / simulation
    - 3D imaging
    - 3D pattern recognition

- Production code for experiments based on LArSoft
- Significant fraction of code is shared between experiments

LAr TPC reconstruction approaches

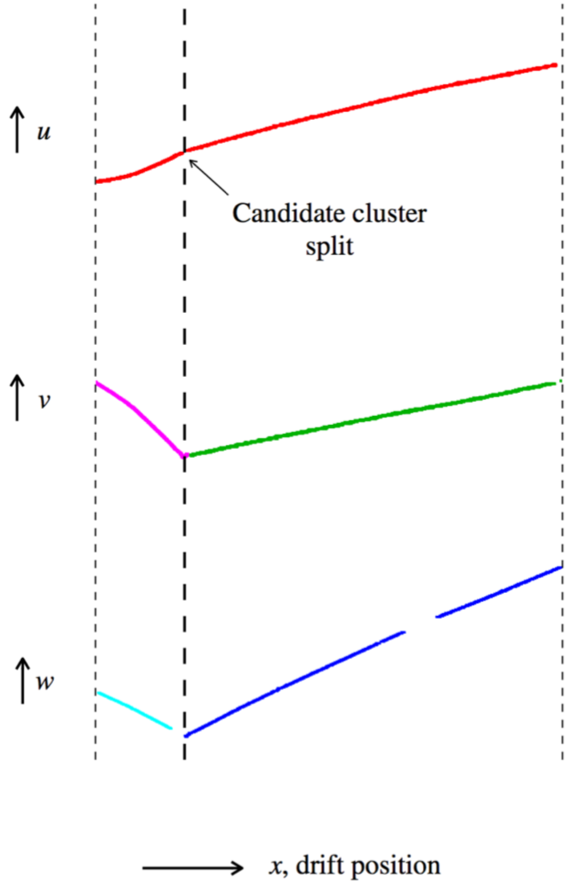
- 2D view matching
  - Perform 1D “hit-finding” in waveforms
  - Cluster hits into 2D objects within each plane
  - Match 2D objects between views: 3D tracks and showers
    - Typically uses a combination of drift time and geometrical constraints, sometimes charge, MCS

Examples: Pandora

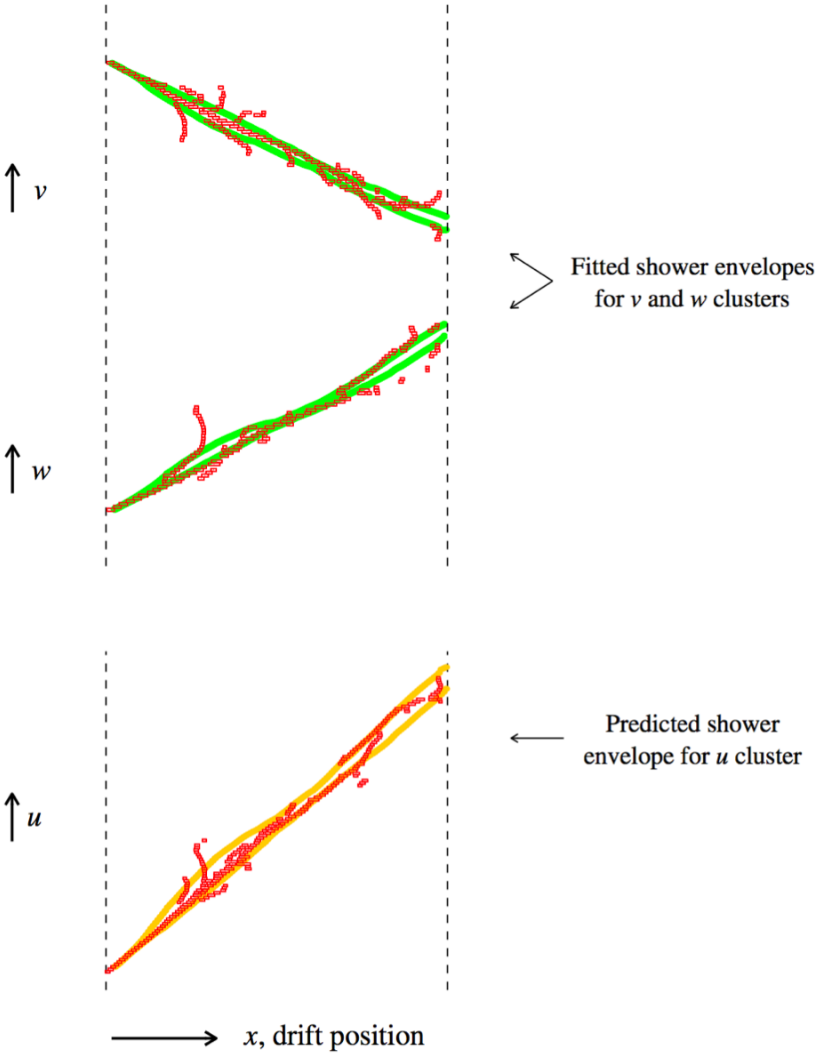
Trajectory Cluster + Projection Matching Algorithm (originally from ICARUS)

Example of Pandora track and shower view matching

Track view matching



Three views
stacked vertically



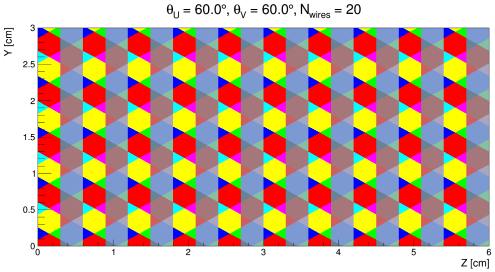
Shower view matching

From R. Acciarri, et al., Eur. Phys. J. C 78:82 (2018)

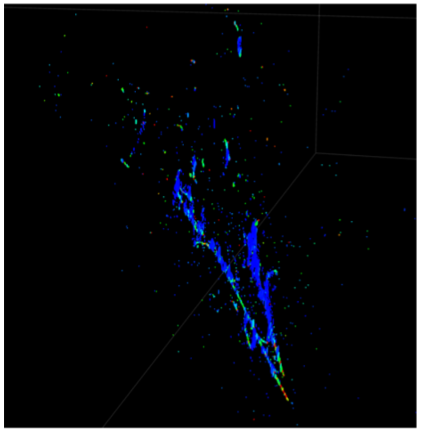
LAr TPC reconstruction approaches

- 3D reconstruction
  - Attempts to construct 3D space-points or images without first clustering in 2D views
  - Two main approaches

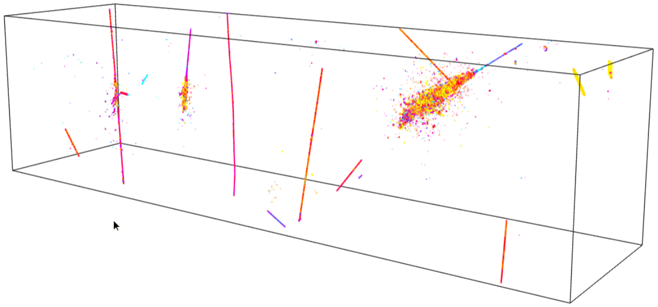
1. Wire-cell 3D imaging
   - Tomographic technique on views
   - Matches charge, other information across wire planes in time slices
   - L1 regularization to solve under-constrained problem



Tiles created by wire crossings. Wires see same charge through each tile..



3D charge deposition models for pi-zero (left), neutrino plus cosmics (right)



Images from https://www.phy.bnl.gov/wire-cell/examples

LAr TPC reconstruction approaches

- 3D reconstruction
  - Attempts to construct 3D space-points or images without first clustering in 2D views
  - Two main approaches

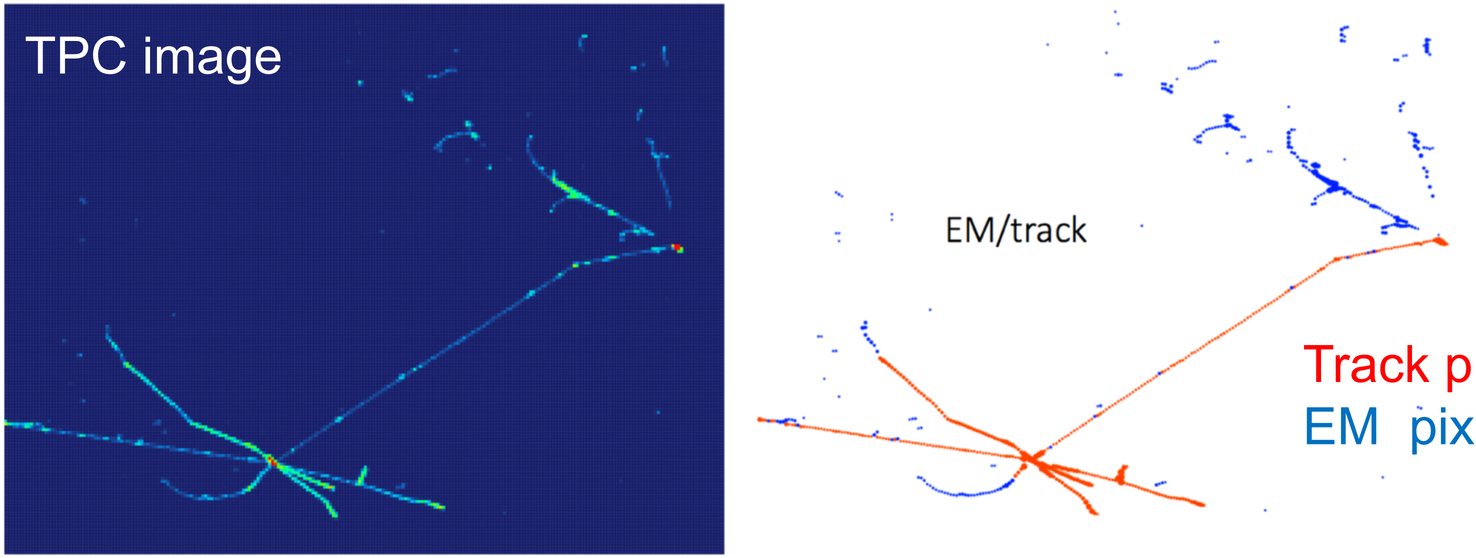
2. “Cluster 3D” (Stanford Linear Accelerator Laboratory)
   - Starts with hits found in waveforms
   - Matches across planes based on time, charge, geometry

LAr TPC reconstruction approaches

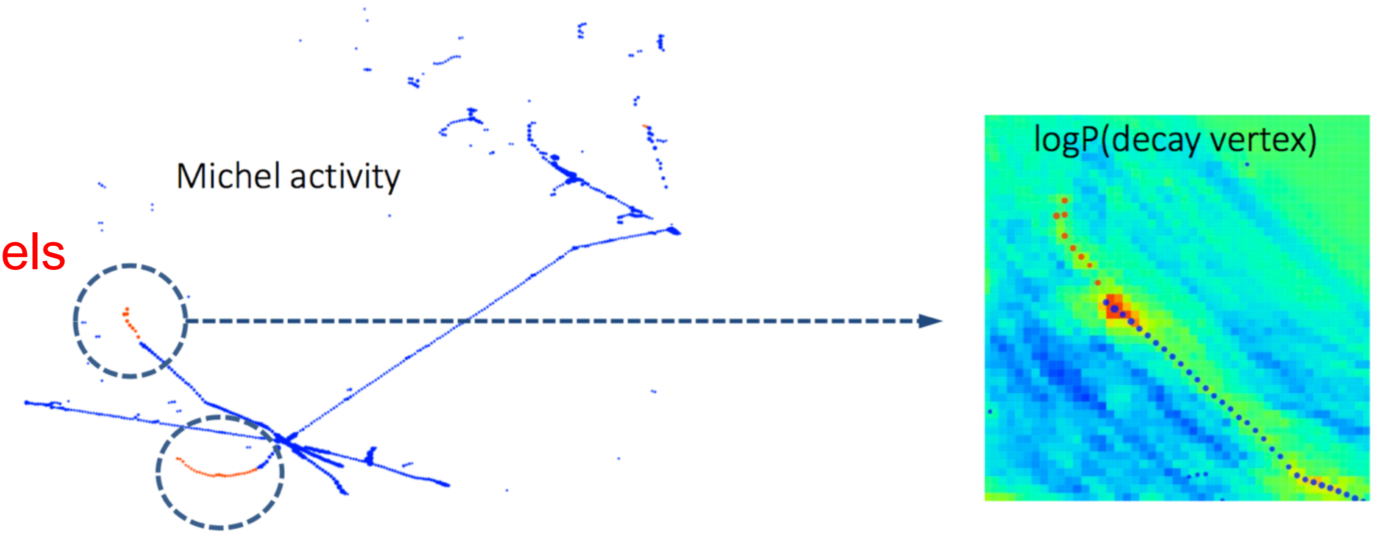
- Pixel-level image processing
  - Deep learning: convolutional neural networks
    - Can extract pixel-by-pixel classifications directly from image
      - Empty / not empty, track / shower, vertex / not a vertex, etc.
    - Usually a hybrid approach
      - DL used only for parts of the problem
      - E.g., provide well-informed hints to downstream pattern recognition

    - ProtoDUNE and MicroBooNE working extensively on this
      - DUNE using CNN for track-shower separation
        - Looking into much more
      - MicroBooNE working on full reconstruction with multiple DL steps
        - Constructing an entire chain for low energy excess analysis

CNN-based pixel classification



Track pixels in red
EM pixels in blue



Michel pixels
in red

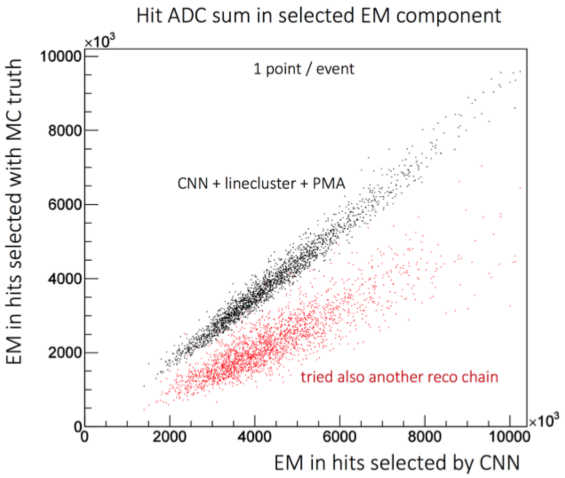
Image courtesy of Tom Junk, Robert Sulej

LAr TPC reconstruction approaches

- Pixel-level image processing
  - Other techniques taken from image processing industry
    - Combinations of blurring / contour-finding used to aid in clustering energy deposition from showers
    - DUNE and MicroBooNE have developed approaches

Algorithmic challenges

- Shower energy reconstruction
  - MicroBooNE is achieving excellent calorimetric energy resolution after calibration, but…
  - …current shower algorithms *tend* to under-cluster



Note: for illustrative purposes only!! Not a real performance test!!

Plot courtesy of Tom Junk, Robert Sulej

- Have seen steady improvements, so prospects are good for excellent shower energy resolution

Algorithmic challenges

- Track / shower separation
  - Particularly difficult at lower energies when there is minimal showering activity
  - Can lead to mis-classification of events
- Short track reconstruction
  - Efficiency falls dramatically for tracks less than ~20 cm long
- Event vertex identification
  - Easy most of the time. Surprisingly error prone at others.
  - Really hard for single pi-zero events, for instance
  - Not helped by spatial ambiguities induced by wire-plane readouts
    - Contained tracks offer lots of handles

Algorithmic challenges

- So, basically, need improvements in all areas related to observing low energy ν_e charged current quasi-elastic interactions
  - I.e., the ν_e appearance measurement need by DUNE

LAr TPC simulation

- Simulation within LArSoft
  - Geant4
    - Ray tracing
    - Material interactions, energy deposition
  - Detector simulation and digitization
    - Ionization electron / scintillation photon modeling
    - Electron drift model
    - Field response model
    - Electronics response model
    - Digitizer simulation to generate raw data
    - Parameterized photon propagation

LAr TPC simulation

- Detector modeling
  - High fidelity simulation requires charged particle step sizes ~few x 100 μm for events that can span meters
  - Some low-level modeling needs improvement
    - Good results obtained using data-driven methods at MicroBooNE
      - 2D response functions available in Wire-cell
    - Making progress on understanding ionization and scintillation
  - Even now, agreement in high-level physics distributions is more than adequate for physics (e.g., MicroBooNE)

Computing challenges

The first potential challenge: data scale

- DUNE far detector is large with high resolution data
  - 4 modules x 10kt fiducial mass
  - 384k channels in first (single phase) module
    - One drift window readout + 12 bit ADC = 3 GB / event / module
    - Anticipate 2.5 drift window readout x 4 modules ~ 25 GB / event

  - Potentially > 400 PB / year for beam data alone
  - SN and proton decay searches need a continuous stream
    - Large background from radiological decays to be suppressed

- Need to manage data rate by triggering + zero-suppression
  - E.g., beam dataset becomes manageable with 500 keV cut
  - Need to find the sweet spot without sacrificing physics

The computing challenge

- The current state
  - Neither simulation nor reconstruction are “fast”
    - Many minutes per event often in seemingly “simple” events
    - Needed physics performance gains will likely make this worse
    - With potentially huge data volumes, this needs to be addressed
  - Memory footprint often exceeds 2 GB grid slot
    - Particularly bad for simulation, which can range 6 to 8 GB
    - Multi-threading seen as a possible solution – not yet demonstrated
  - Missed opportunities for acceleration
    - Many of our algorithms lend themselves to vectorization
    - None of the code currently uses SIMD extensions that are available for use on most grid slots (TensorFlow and fftw excepted)

Where are we headed?

- Expect there to be continued demand to increase use of multi-threading on all scales to manage memory and throughput efficiently
  - Does not increase overall throughput

- Full exploitation of vectorization wherever possible
  - Make full use of SIMD capabilities on each platform
  - This will increase overall throughput

- Continue to optimize / innovate on the software algorithms
  - Many rewards to building smarter algorithms
    - Add equivalent beam as sensitivity increases
    - Add equivalent computing with resource efficiency gains

Where are we headed?

- Expect demand for machine learning algorithms to grow
  - Image data ideally suited to CNN architectures from industry
    - Already see evidence of the great promise these algorithms offer
    - Expect to build on these successes
  - Expect increasing role in production reconstruction workflows
  - Conventional algorithms will remain an important component even in this new paradigm
    - Focus ML algorithms on those that are difficult to solve using conventional coding techniques

Where are we headed?

- Open question (1): will extensive use of machine learning push demand for GPU / other HPC resources?
  - Or conversely, will availability enable this growth
  - These algorithms are highly vectorizable
    - Have seen accelerations of ~1000x on GPU machines
  - Have seen factors of 10 on grid nodes with SIMD extensions
    - …but was combined with multi-threading across cores
    - Can we do CNNs with a grid computing model in finite time? *Some* evidence the answer is yes.

My guess to the open question? Yes.

Where are we headed?

- Open question (2): will the availability of GPU / other HPC resources and the tools used for CNNs spur changes to accelerate conventional algorithms?
  - Some have speculated that many of our algorithms can be structure to obtain potentially huge gains in throughput (i.e., beyond fully availing ourselves of grid-level SIMD extensions)
    - Faster data turn-around = more physics.
  - Is it possible? Cost effective? It is worth thinking about.

Summary

- LAr TPC simulation and reconstruction poses a set of rich and complex problems

- Advanced computing technologies could play an increasingly important role in simulation and reconstruction solutions
  - Still an open question whether HPC is needed

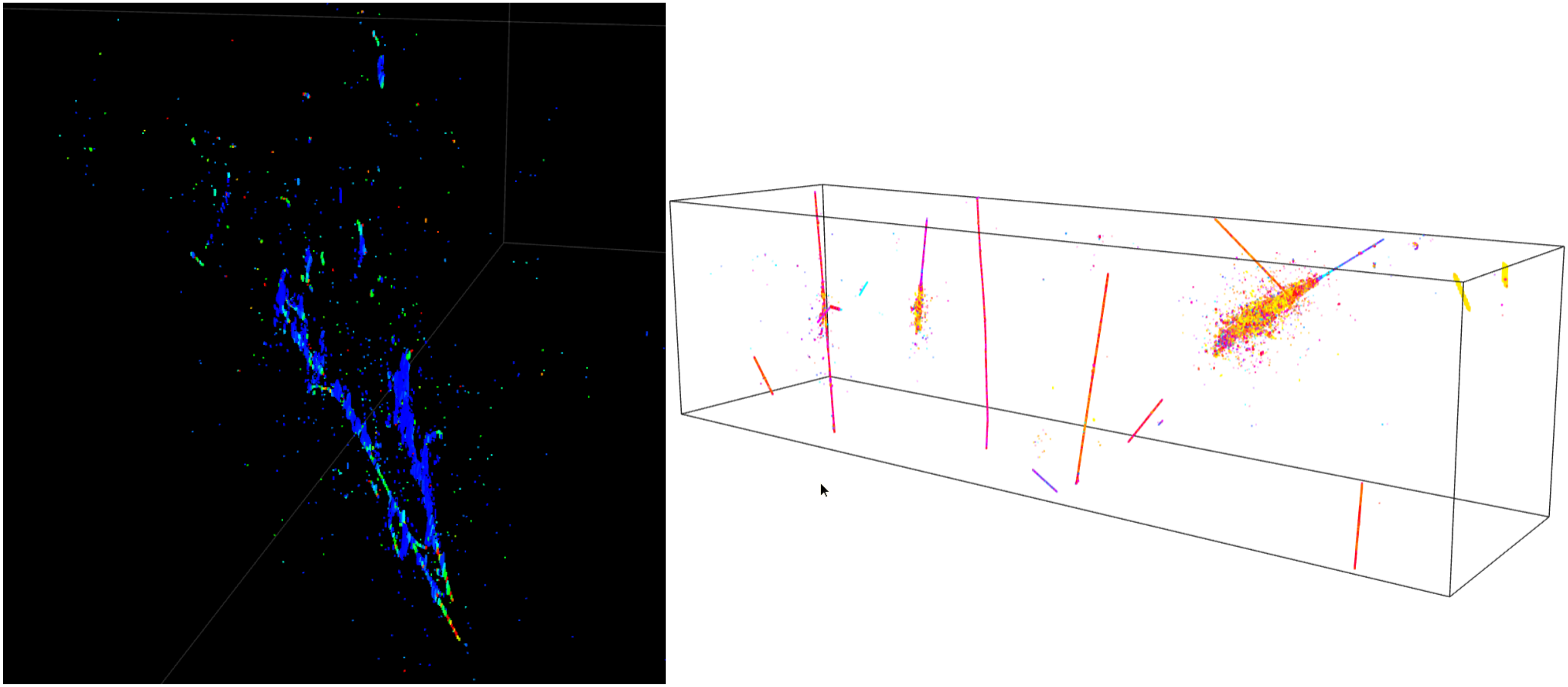
- DUNE is well advanced in algorithm development
  - A major contributor to and consumer from the community

- Based on existing experiments, fully expect LAr TPCs to deliver on their promised performance

BACKUP

Example wire-cell 3D images

3D charge deposition models for pi-zero (left), neutrino plus cosmics (right)



Images from https://www.phy.bnl.gov/wire-cell/examples

- Picture of nue event – an important part of signal for DUNE

Reconstruction dashboard

Taken from DUNE CDR benchmarks

Good to go!

Not yet demonstrated (that I’ve seen…)

- For mass ordering and CP violation
  - Muon reconstruction efficiency > 99%
  - Electron reconstruction efficiency: >90%
- For nucleon decay search
  - Kaon reconstruction efficiency (up to 200 MeV) > 80%
  - Muon reco efficiency (muons around 150 MeV) > 99%
  - Michel electron reconstruction efficiency > 99%
- For supernova neutrino search
  - Low energy (~10 MeV) electron neutrino reco efficiency > 90%

Promising results so far

The computing challenge

- Current strategy
  - Exploit vectorization wherever gains can be made
    - Accelerates computing on existing grid resources
    - Possibly transferrable to other platforms
  - Multi-thread to address the issue of growing memory demand
    - The major gains will be from multi-threading within an event
      - The harder thing to do well…
  - Continue to optimize / innovate on the software algorithms
    - Many rewards to building smarter algorithms
      - Add equivalent beam as sensitivity increases
      - Add equivalent computing with resource efficiency gains

Parallelization efforts

- Where are we?
  - LArSoft based on art event processing framework
    - Work to support multi-threading is nearly complete
    - Have started architectural changes in core LArSoft code to ensure thread-safety
  - Vectorization
    - Work on first demonstration targets is proceeding (see talk on Wednesday)
    - Demonstrated gains from vectorization in TensorFlow based CNN inference stages for DUNE track-shower classification