# Laying the Foundation for Complete Automation in Particle Image Inference François Drielsma (SLAC) Panofsky Seminar, Feb. 22nd 2024





# **Ultimate Research Goal**





→Goal: Leverage Artificial Intelligence (AI) to automate this task

# **Neutrino Oscillations**



Neutrinos are produced as different types

• Neutrino types are a **superposition** of **quantum mass states** 

Neutrino types  $\begin{pmatrix} \nu_e \\ \nu_\mu \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \nu_1 \\ \nu_2 \end{pmatrix}$  Mass states Mixing matrix



2015





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# **Neutrino Oscillations**



Neutrinos are produced as different types

Neutrino types are a **superposition** of • quantum mass states

Neutrino types



### **Mixing matrix**

Mass wavefunctions oscillate at different rate  $\rightarrow$  mixture changes



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2015

**Baseline** 

Takaaki Kaiita

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Mahmoud

# **Neutrino Oscillations**



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Neutrino types

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2015

Mahmoud Takaaki Kaiita

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# What's Missing?



Several neutrino properties remain elusive

• Neutrino mass ordering



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- Neutrino mass ordering
- Leptonic CP-violation: origin of matter-antimatter asymmetry?



# What's Missing?



Several neutrino properties remain elusive

- Neutrino mass ordering
- Leptonic CP-violation: origin of matter-antimatter asymmetry?
- Low-energy v excess at short baseline: new type of neutrino?
- $\rightarrow$  My research will help answer these questions



# **DUNE and SBN**



### Two US-based neutrino oscillation experiments to answer these questions

Deep Underground Neutrino Experiment (DUNE), 2028-?	Short Baseline Neutrino (SBN) program, 2015-2027	
1300 km: enhance matter effects	0.6 km: observe anomalies	
<ul> <li>Mass ordering, CP violation</li> </ul>	• New type of neutrino?	
<ul> <li>DUNE-FD rate: O(10<sup>3</sup>) v / year</li> </ul>	• SBN S/B ratio: ~ O(10 <sup>-5</sup> )	
Wigon Hal USen Hal USen Ration (Construction (system)) USEN (System) (Syste	Target     SBND     MicroBooNE     ICARUS       Protons     Protons     270 ions of argon     170 ions of argon     760 ions of argon       0     110 meters     470 meters     600 meters	



**LArTPC requirements** (proposals circa 2015):

- Efficiency for v<sub>u</sub> ID: > 90 %
- Efficiency for  $v_e ID$ : ~ 80 %
- Purity for both: ~ 85-90 %





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- Efficiency for  $v_{\mu}$  ID: > 90 %
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- Purity for both: ~ 85-90 %

What if efficiency drops?

- Less effective exposure
- Less sensitivity





DUNE/SBN cannot deliver physics without a reliable reconstruction...



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- 1. The Era of Humans
  - What has been the traditional approach in particle imaging detector? Has it been successful?



DUNE/SBN cannot deliver physics without a reliable reconstruction...

### 1. The Era of Humans

- What has been the traditional approach in particle imaging detector? Has it been successful?
- 2. Cybernetic Augmentation
  - How have **Machine Learning** tools helped improve reconstruction so far?







DUNE/SBN cannot deliver physics without a reliable reconstruction...

### 1. The Era of Humans

• What has been the traditional approach in particle imaging detector? Has it been successful?

### 2. Cybernetic Augmentation

- How have **Machine Learning** tools helped improve reconstruction so far?
- 3. The Age of Machines
  - How can **Artificial Intelligence** definitively solve the issue of automation in particle imaging inference?





# 1. The Era of Humans

### **Particle Imaging Detectors**





### imaging

noun [U] • COMPUTING • specialized

**US ◀》** /ɪˈmɪdʒ.ıŋ/ **UK ◀》** /ɪˈmɪdʒ.ıŋ/

#### the process of producing an exact picture of something

https://dictionary.cambridge.org/us/dictionary/english/imaging

# **Particle Imaging Detectors**







# **Particle Imaging Detectors Reconstruction**



### **Step-by-step** approach:

- 1. Identify interesting events in pictures **by eye** 
  - a. Scanning experts
  - b. Grad students
- 2. Trace particles on paper **by hand**
- 3. Estimate particle kinematics
- 4. Review by senior physicist



# **Particle Imaging Detectors Reconstruction**



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ACCELERATOR

# **Particle Imaging Detectors Reconstruction**





### Advantages:

• Very detailed interaction

### Limitations:

- Time intensive reconstruction
- Hard to scale
  - $\circ$  Largest: 15 m<sup>3</sup>
  - Slow (~ seconds)

Neutrino interactions are **rare**... 1 LY of Pb for 50 % chance

# **Liquid Argon Time Projection Chamber**





# LArTPC: Detector used today in DUNE and SBN

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# **Liquid Argon Time Projection Chamber**





**LArTPC**: Detector used today in **DUNE** and **SBN**:

- Precision of its ancestors
- Dense (1.4 g/cm<sup>3</sup>)
- Cheap (~ 1\$/kg),
   a.k.a. scalable

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# **LArTPC** Reconstruction



Moved away from hand-scanning in the XXI<sup>st</sup> century?

# **LArTPC** Reconstruction





Not immediately...

- Papers still <u>published</u> using this technique until **2013**!
- Still time intensive to reconstruct

Viable with low rates...

# **LArTPC** Reconstruction





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Viable with low rates...

...dead on arrival at SBN and DUNE

- ICARUS: O(10<sup>4</sup>) v candidate / day!
- **DUNE-ND:** O(10<sup>6</sup>) v / day!



Grad. student nightmare...



### Why is it so challenging to automate?

• Write an algorithm based on **physics principles**...





### Why is it so **challenging to automate**?

- Write an algorithm based on physics principles...
- Realize it fails on harder topologies -
- Add new rules to handle new topology, repeat -

Years of development





### Why is it so **challenging to automate**?

- Write an algorithm based on **physics principles**...
- Realize it fails on harder topologies -
- Add new rules to handle new topology, repeat -

### Years of development



With great detail comes great responsibility

 Variety of possible neutrino interactions topologies is huge



**PandoraPFA**: particle flow algorithm developed for future e<sup>+</sup>e<sup>-</sup> colliders

- Adapted in the 2010s to be used in LArTPCs, > **10 years of development**
- Best performing traditional approach in several LArTPC experiments

Does it live up to the DUNE/SBN requirements?



**PandoraPFA**: particle flow algorithm developed for future e<sup>+</sup>e<sup>-</sup> colliders

- Adapted in the 2010s to be used in LArTPCs, > **10 years of development**
- Best performing traditional approach in several LArTPC experiments

Does it live up to the DUNE/SBN requirements? Not quite...

	SBN Proposal 1eX (hand-scanning)	MicroBooNE 1eNp0π paper (PandoraPFA)
Purity	85 %	80 %
Efficiency	80 %	15 %
	<u>arXiv:1503.01520</u>	<u>arXiv:2110.14065</u>
# 2. Cybernetic Augmentation

## **Machine Learning**



#### **Traditional Approach**



## **Machine Learning**



#### **Traditional Approach**



#### **Machine Learning**





#### **Traditional Approach**



#### **Machine Learning**





#### **Traditional Approach**



## **Machine Learning and Computer Vision**



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

- ML revolutionized accuracy on image processing tasks
- AI/ML for science: leverage those techniques in LArTPCs (image data)



















## **Physics-Informed ML Reconstruction**





## **Physics-Informed ML Reconstruction**



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

1. Separate topologically distinguishable types of activity





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





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- 4. Cluster interactions, identify particle properties in context



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 $\rightarrow$  Pixel-level

Cluster-level



#### Convolutional Neural Networks (CNN, <u>source</u>)









#### Convolutional Neural Networks (source)





#### Does it work on LArTPC data?



Specificity:

- **3D**: ICARUS = O(10) Gigapixels
- **Occupancy**: ~ 10<sup>-4</sup>, locally dense
  - Mostly meaningless space

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#### Does it work on LArTPC data?



#### Specificity:

- **3D**: ICARUS = O(10) Gigapixels
- **Occupancy**: ~ 10<sup>-4</sup>, locally dense
  - Mostly meaningless space

#### Problems:

- Memory: ~ 100 GB per image...
- Wasted computation: 99.99% empty

#### $\rightarrow$ Not viable



Solution? Sparse Convolutions!

- Only operate on **active pixels**
- Technique (<u>SCN</u>) invented at <del>Facebook</del> Meta in 2017
- Pioneered use in Physics at SLAC: <u>Quanta Magazine</u>, <u>PRD paper</u>



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Solution? Sparse Convolutions!

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- Pioneered use in Physics at SLAC: <u>Quanta Magazine</u>, <u>PRD paper</u>
- Scales with space point count only!  $O(10) \text{ GPix} \rightarrow O(1) \text{ MPix}$



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## **Semantic Segmentation**



#### Separate topologically different types of activity

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



## **Dense Fragment Formation**



Break track/shower fragment instances where they touch

• Cluster track/shower fragments at this stage





CNN: mostly sensitive to local neighborhood of pixel, but...

- EM showers: photon mean free path in LAr = 18 cm (60 pixels)
- Interactions:  $\pi^0$ ,  $K^0$ ,  $\Lambda$ , neutrons





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



<sup>• . . .</sup> 



#### Graph Neural Network (2017): develop features useful to node/edge classification



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## Particle Aggregation



Aggregate track/shower fragment instances into particles

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



## Particle Aggregation



Aggregate track/shower instances into interactions

• Find edges that connect particles that belong together



## **Reconstruction in LArTPCs**



#### End-to-end ML-based reconstruction chain

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





Realistic **Neutrino + Cosmic** ICARUS simulation as a **benchmark** 

- One (two)  $v_{\mu} (/v_{e})$  + Ar interaction/image
- ~25 cosmic interactions/image (surface detector)







- $v_{\mu}$ -CCQE Selection
  - Topology: 1µ1p
  - Simplest topology to reconstruct
  - First test that **cosmic ray removal** works
  - First test to ensure the reconstruction is working at a basic level

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## $\mathbf{v}_{u}$ selection in ICARUS





## v<sub>"</sub> selection in ICARUS





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## $v_e$ selection in ICARUS





## Invariant mass of $\pi^0$ in ICARUS





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First DUNE-FD module still 4 years away...

SBN will produce plenty of interesting physics until then:

- Short baseline **oscillation** test (MiniBooNE anomaly)
- Rich cross-section program (<u>arXiv:1903.04608</u>):
  - $\circ$  NuMI off-axis @ ICARUS: 10 k v<sub>e</sub> / year, higher energy than BNB (up to 3 GeV)
  - BNB @ SBND: 2 M v / year, O(1) k  $\Lambda^0$  /  $\Sigma^+$  hyperons, ~400 v<sub>e</sub> e scattering
- $\rightarrow$  ML chain essential to deliver on these physics goals

SBN Physics	ICARUS Michel $e^-$				
	ICARUS $\nu_{\mu}/\nu_{e}$ sel.	<b>SBND</b> $\nu_{\mu}/\nu_{e}$ sel.		End of SBN data taking	First DUNE-FD
	SBN <i>v</i>	$ u_{\mu} \rightarrow \nu_{e} \text{ appearance}$			module online
	ICARUS NuMI/SBND BNB cross-section programs				
	20	24 20	025 2026	2027	9//////X//////////////////////////////

# Scalability





#### On **ICARUS**:

- 1 s / event, leveraging GPU acceleration
  - Pandora: 40 s / event
- ~1.5 M beam events / yr

Implications:

- Fast software development (testing)
- Fast turnaround



**Outreach**: familiarize physics the community with ML tools

- Targeted ML workshops and schools
  - 2 ICARUS/SBND, 2 SLAC ML Schools, KMI Nagoya ML School (astrophysics), SSI
- Open source software stack and first public LArTPC neutrino dataset





# 3. The Age of Machines

100011111

9

10%

. . .

#### **Performance Drop on Data**





#### Automatic selection selected as 1mu+1p T\_>50 MeV 1mu + 1 p 109 1mu + 2p 9 1mu + 3p Neutrinos not contained 8 Other interactions 9 Cosmics TOTAL EVENT 135 SELECTED Purity 109/135 =>80.7% FLAT SCAN 52

Purity:

80.7 %

Efficiency: **52 %** (target: >90 %)

#### **Purity**:

ML on Data

- Handscan selected events
- Efficiency:
   Reconstruct handscanned
  - events

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#### **Domain Shift**





#### **Domain Shift**





Simulation



#### **Domain Shift**







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# Addressing the Domain Shift



What if we could train directly on data?

- Start from raw data = target domain → no domain shift!
- Reduces detector systematics



# Addressing the Domain Shift

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What if we could train directly on data?

- Start from raw data = target domain → no domain shift!
- Reduces detector systematics



**Elephant in the room:** 

• Raw data has **no obvious labels**, how can we train a network on it?

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# Self-Supervision in Large Language Models



Simple idea: mask known areas of a text, try to reconstruct it



#### Masked Self-Supervision Learning (SSL)

# Self-Supervision in Large Language Models



#### Self-supervision works incredibly well for Large Language Models (LLMs)



# Transformers



LLMs use transformers to learn correlations between words in a sentence



Words with the **same meaning** are **strongly correlated** 

# Transformers



LLMs use transformers to learn correlations between words in a sentence



# **Transformers**



LLMs use transformers to learn correlations between words in a sentence





#### Transformers can use learned correlations to guess the next word in a sequence





#### Transformers can use learned correlations to guess the next word in a sequence



#### Raw LArTPC data



#### This is what LArTPC data looks like raw...



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#### **Raw LArTPC data**



#### This is what **LArTPC data looks like raw**...



#### Language of Detectors: the Waveform



At the most basic level, most detectors produce waveforms

• Response of electronics to a charge signal (collected electrons)





At the most basic level, most detectors produce waveforms

- Response of electronics to a charge signal (collected electrons)
- Information sparse: mostly meaningless noise
- Long: 4096 samples per wire in ICARUS, O(10<sup>4</sup>) wires





Can we use **Transformers**?

- Words: waveform chunks
- Word representation: value for each tick in chunk
- Information extracted: correlations between waveform chunks



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Naive approach:

- 1. Mask one to a few ticks of the waveform
- 2. Train network to reproduce missing region(s), minimize:  $\mathcal{L} = \sum_{i \in M} (\hat{y}_i y_i)^2$

a.k.a. L2 loss



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What you get from  $\mathcal{L} = \sum_{i \in M} (\hat{y}_i - y_i)^2$ 

- 1. Cannot reproduce random noise, **baseline is the best fit**
- 2. Can reproduce signal, if visible around the mask region



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What you get from  $\mathcal{L} = \sum_{i \in M} (\hat{y}_i - y_i)^2$ 

- 1. Cannot reproduce random noise, **baseline is the best fit**
- 2. **Can reproduce signal**, if visible around the mask region
- $\rightarrow$  Learn signal shape and noise removal





#### What if the **signal is buried in noise**? What if **noise looks like signal**?



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#### What if the **signal is buried in noise**? What if **noise looks like signal**?

• We have **context!** 







What if the **signal is buried in noise**? What if **noise looks like signal**?

• We have context! It allows us to infer dead regions effectively



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In LArTPCs, we have 3 projections available

**Game**: find correlated signals across 3 planes 







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In LArTPCs, we have 3 projections available

- Game: find correlated signals across 3 planes
- Transformers are correlation machines

3 space points in 3D





In LArTPCs, we have 3 projections available

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Infer space points/segment from correlated wire signals

dx



In LArTPCs, we have 3 projections available

- Game: find correlated signals across 3 planes
- Transformers are correlation machines



Small time chunk = slice in x



Infer space points/segment from correlated wire signals



Feasibility study with GNNs: it can work (TomoGNN)

• Relied on 2D hits being built, signal-based method would not





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Self-supervised LLMs (e.g. GPT-4) have very interesting properties if

- Built on a very complex model: ~ 10<sup>12</sup> parameters
- Given a huge amount of raw training data: ~ 5 x 10<sup>9</sup> words (45 GB)


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- $\rightarrow$  Can be quickly **fine-tuned to perform specific tasks**!





Tasks

Question Answering

Information Extraction

Captioning

nstruction

Object

Recognition

Image

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## **Generic Artificial Intelligence**





Instead: give a lot of raw waveform data to a large model

Learn a **general** raw data representation useful to all reco. tasks



## **Center for Research on Foundation Models**



Unique opportunity to collaborate with and contribute to the CRFM

• Support and experts to mitigate the risks associated with this endeavor



SLAC Colloquium - "Some Building Blocks for Foundation Model Systems" by Chris Re, Stanford University

Chris Re, Stanford University, Department of Computer Science





Stanford University Human-Centered Artificial Intelligence

## Research on long sequence processing:

- FlashAttention: speed-up by localizing computations on GPU
- <u>S4/Mambda Model</u>: subquadratic implementation of a state-space model with FM properties
- HyenaDNA: 420k "words"



Waveform data is ubiquitous in science and industry

 $\rightarrow$  Successful self-supervision on raw waveform data has implications well beyond LArTPCs alone, synergies at SLAC



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Waveform data is ubiquitous in science and industry

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 $\rightarrow$  Science for AI/ML



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## Conclusions



LArTPCs are at the core of the US-based accelerator neutrino program

- **DUNE** and **SBN** cannot succeed without a **high-quality reconstruction**
- Partially automated the reconstruction from space point to interactions
  - New state-of-the-art on 3 LArTPC experiments
- Clear road-map towards foundation models in waveform data
  - Address the remaining challenges in LArTPCs and **open a new pole of research**

