Implicit Neural Representation for Modeling the Photon Transportation in a LArTPC

Patrick TSANG (SLAC)
CIDeR-ML Collaboration
Jun 28, 2024

Neutrino Physics and Machine Learning 2024 @ ETH Zurich

CIDeR-ML: Who are we?

SLAC

Calibration and **I**nference of **De**tector **R**esponse with **M**achine **L**earning

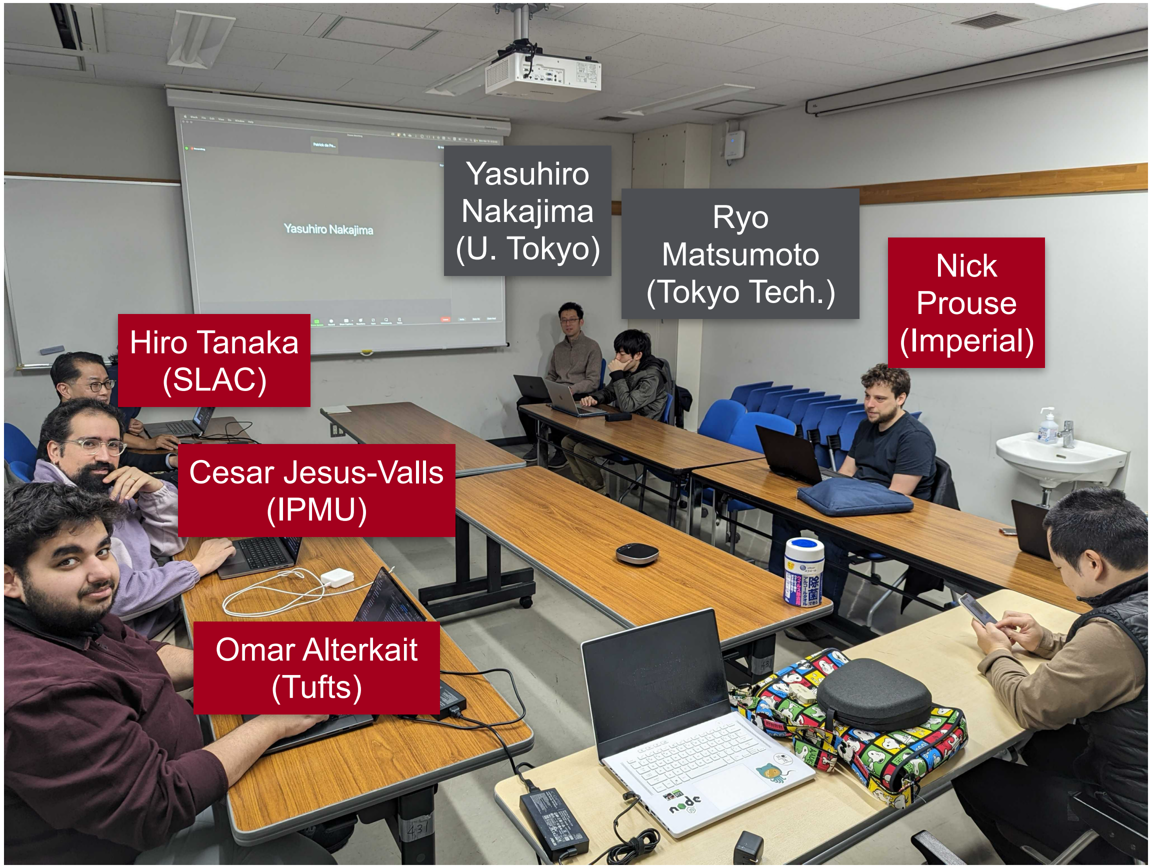
A US-Japan collaboration to develop

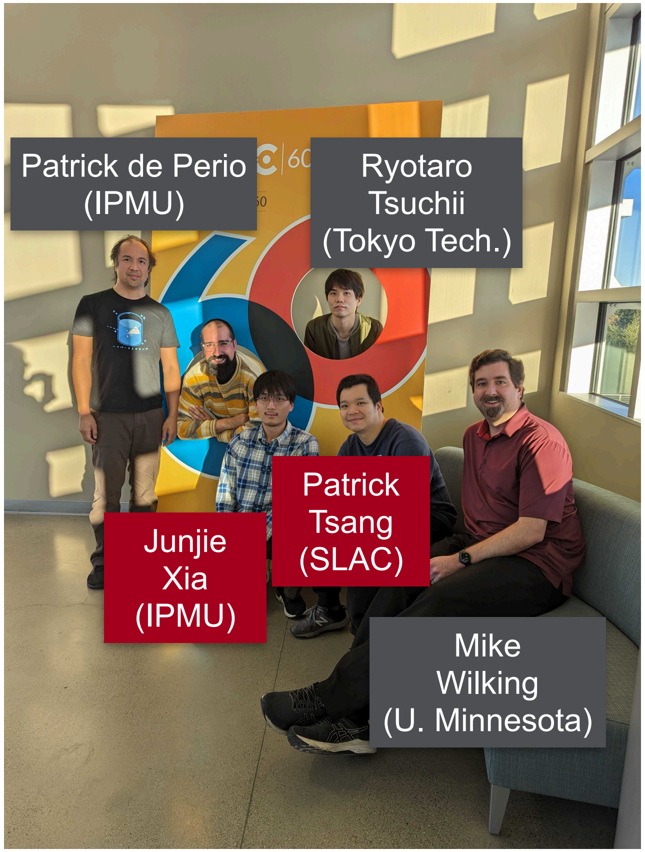
- differentiable detector simulator,
- data-driven optimization methods,
- detector inverse solver

for neutrino experiments (e.g. LArTPC & Water Cherenkov).

To provide common softwares, tutorials/examples and open dataset to the neutrino community for the above tasks.

CIDeR-ML Collaboration





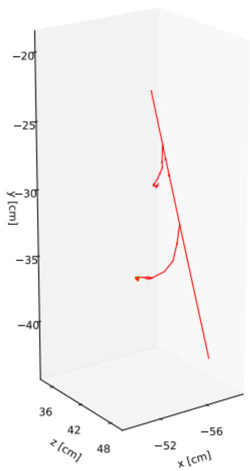
Not in pictures:
Yifan Chen, Kazu Terao, Zhe Zhang (SLAC),
Carolyn Smith, Sam Young (Stanford),
Ka Ming Tsui (IPMU), Masaki Ishitsuka (Tokyo U. of Sci.)

*** Present in NPML**

Introduction

Input

List of points/segments of a particle trajectory w/ positions & energy depositions



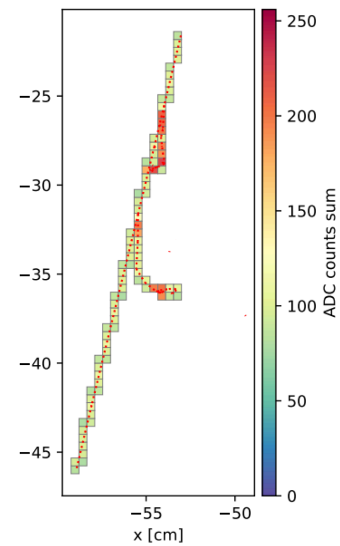
Parameters

- Physics (Ab, kb, …)
- Detector (pixel/wire response, …)

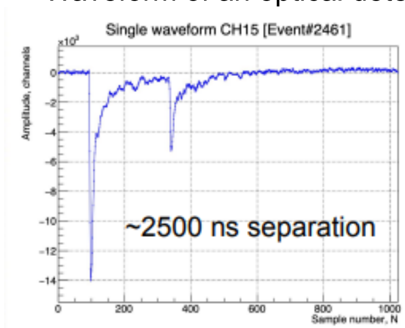
Model

Output

Digitized output of pixel readout



Waveform of an optical detector



1. Simulation, ***F*** : Input → Output
2. Reconstruction, ***F***$^{-1}$: Output → Input
3. Calibration & model tuning: Output → Parameters

Use of <u>gradient-based</u> optimization for automated, simultaneous optimization of model parameters, and inference of input or upstream physics that are not directly accessible. **Condition:** ∇F exists and well defined.

Figures adopted from the paper "*Highly-parallelized simulation of a pixelated LArTPC on a GPU*" and *larnd-sim* software.

How to implement a differentiable model?

SLAC

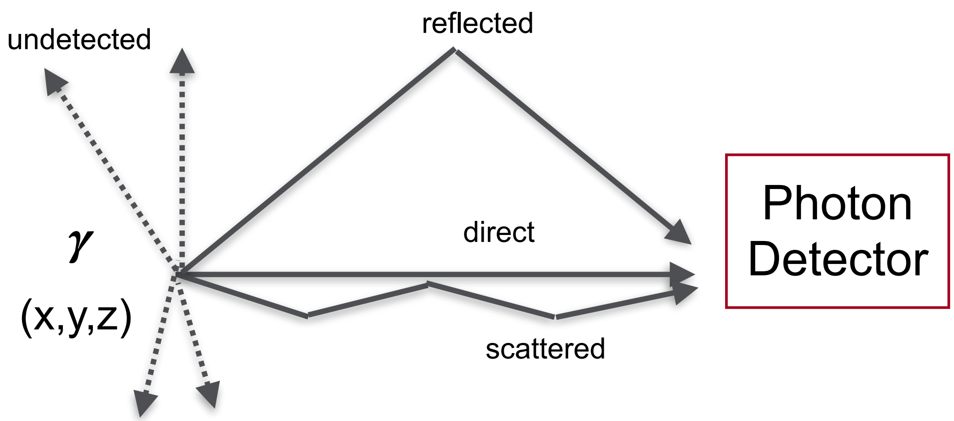
	Title	Speaker	Location	Time
2	**Implicit Neural Representation for Modeling the Photon Transportation in a LArTPC**	*Patrick Tsang*	*HCI J4, ETH Zurich*	09:00 - 09:25
	Q/A		*HCI J4, ETH Zurich*	09:25 - 09:35
1	**Simultaneous high-dimensional calibration with differentiable simulation towards data application**	*Yifan Chen*	*HCI J4, ETH Zurich*	09:35 - 10:00
	Q/A		*HCI J4, ETH Zurich*	10:00 - 10:10
1	**A differentiable simulator for LArTPCs: from proof-of-concept to real applications**	*Pierre Granger*	*HCI J4, ETH Zurich*	10:10 - 10:35
	Q/A		*HCI J4, ETH Zurich*	10:35 - 10:45
	Coffee break		*HCI J4, ETH Zurich*	10:45 - 11:15
2	**Differentiable Physics Emulator for Water Cherenkov Detectors**	*Junjie Xia*	*HCI J4, ETH Zurich*	11:15 - 11:30
	Q/A		*HCI J4, ETH Zurich*	11:30 - 11:40
1	**Advancing Detector Calibration and Event Reconstruction in Water Cherenkov Neutrino Detectors with Analytical Differ...**	*César Jesús-Valls*		

11:00

1. **Differentiable simulator**
   - explicit handling of model parameters w/ differentiable functions

2. **Surrogate model**
   - functional representation of the model

Scintillation Light Propagation Model



Traditional Approach (as a lookup table)

- divide the detector volume into voxels of ~cm in size
- for each voxel, simulate and propagate millions of photons
- count the number of detected photons
- **visibility** at (x,y,z) = # detected photons / # generated photons

- Limited by memory usage
- *Not scalable* for large detector
- Simulation-based, difficult to calibrate

Sinusoidal Representation Network (SIREN)

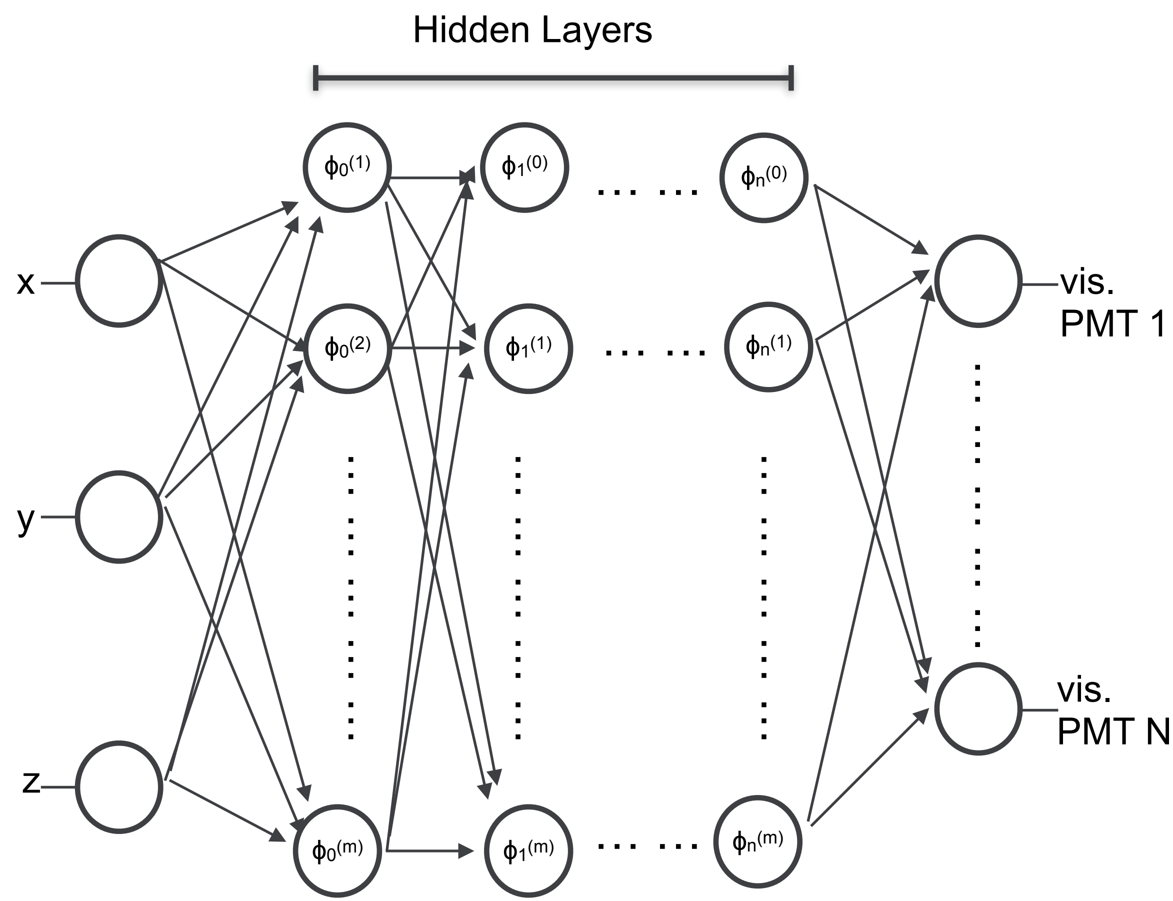
Implicit Neural Representation

Parameterize signals as *continuous* functions via *neural networks*, which are trained to map the domain the signal (e.g. spatial coordinates) to the target outputs (e.g. signal at those coordinates).

$$f: R^M \rightarrow R^N$$

SIREN

a simple multilayer perceptron (MLP) network architecture along with periodic *sine* function activations (Sitzmann et al., arXiv:2006.09661)



$$\mathbf{\Phi}(\mathbf{x}) = \mathbf{W}_n(\phi_{n-1} \circ \phi_{n-2} \circ \cdots \circ \phi_0)(\mathbf{x}) + \mathbf{b}_n,$$
$$\phi_i(\mathbf{x}_i) = \sin(\mathbf{W}_i \mathbf{x}_i + \mathbf{b}_i),$$

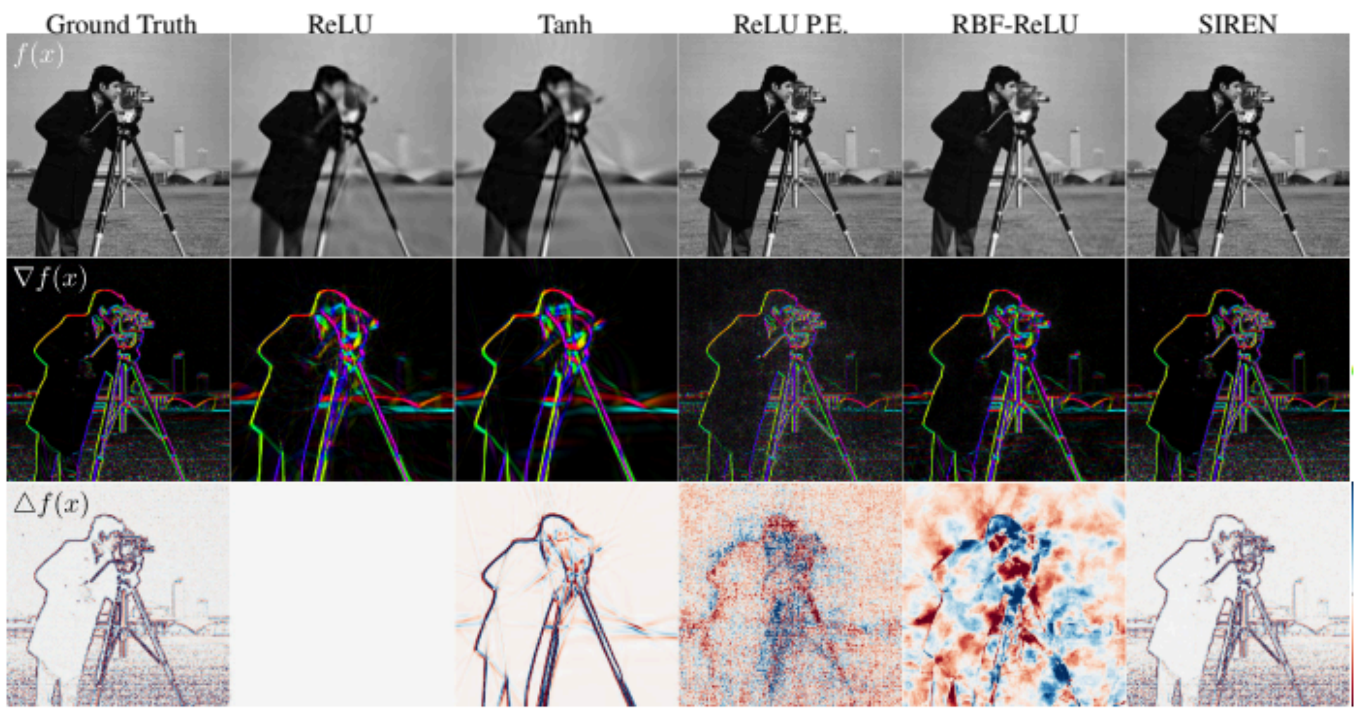
Why SIREN?

By construction, SIREN is a continuous, differentiable signal representations
=> modeling signals with fine detail, AND
=> representing smooth gradient surface (and higher order of derivatives)

f(x)

1st derivative

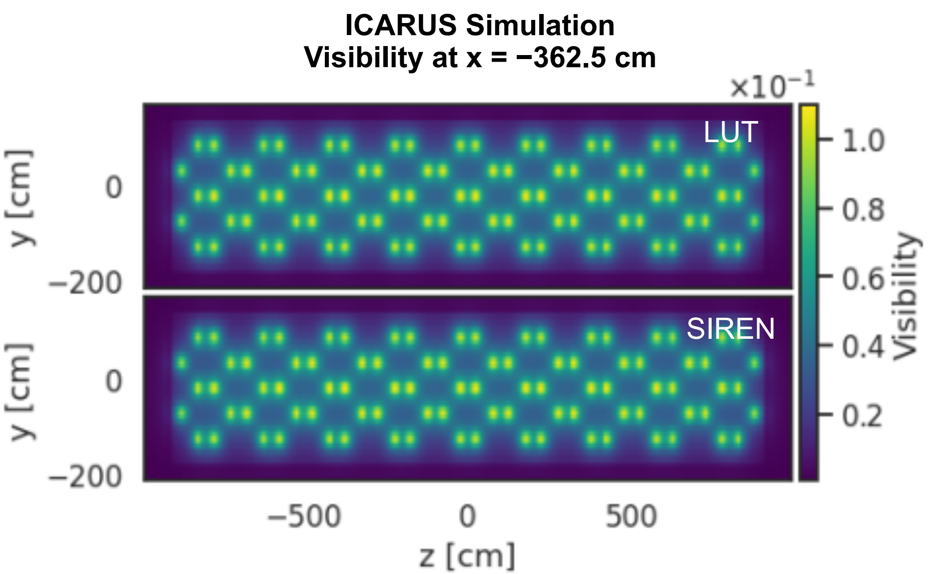
2nd derivative

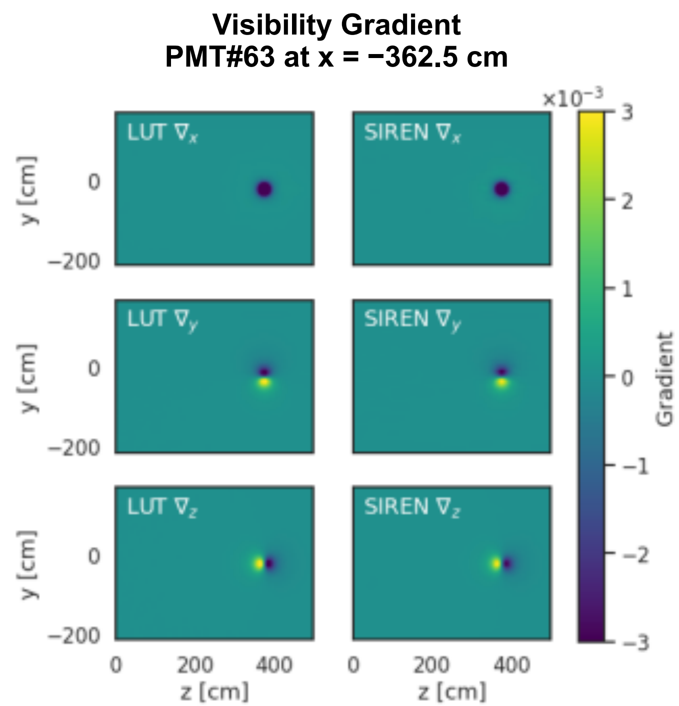


SIREN (arXiv:2006.09661)

Allows wide range of applications from gradient-based algorithms, solving differential equation, optimizing on the derivative … etc

Visibility: SIREN v.s. LUT





LUT (top)

- $74 \times 77 \times 394$ = 2.2 M voxels (5 cm in size)
- 180 PMTs = ~404 M parameters

SIREN (bottom)

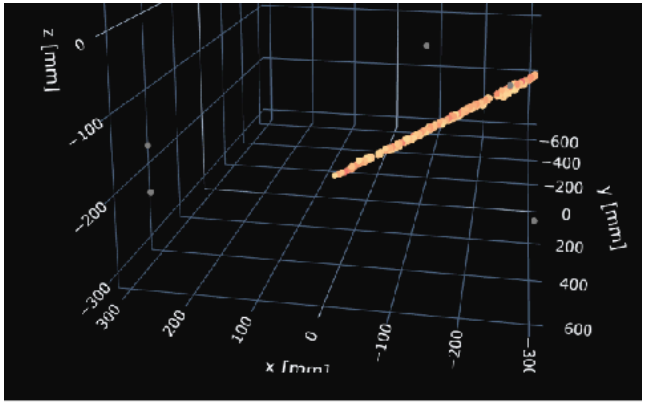
- 5 hidden layers, 512 hidden features
- ~1.5 M parameters

SIREN can reproduce both *values* and *gradients* of the visibility LUT with much smaller number of parameters.

Tsang et al., arXiv:2211.01505

SIREN: Data Driven Calibration

3D Image of an anode-cathode crossing track from charge readout

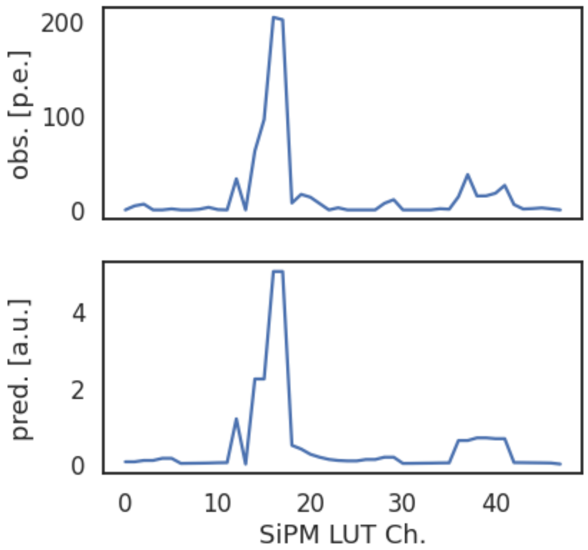


Light Signal
~ $\sum Q_i * vis(r_i)$

Sum charge (Q_i) over the track image

visibility at charge coordinates r_i

Observed and Predicted Light Signal



- point-like source, i.e. visibility at (x,y,z), is not accessible in data
- infer light signal from physics objects (e.g. tracks)

Poisson Likelihood

$$\mathcal{L}_{\text{track}} = \prod_{j=1}^{N} \text{Pois}(n_j|\lambda_j).$$

product of all PMTs

Observed p.e. for j-th PMT

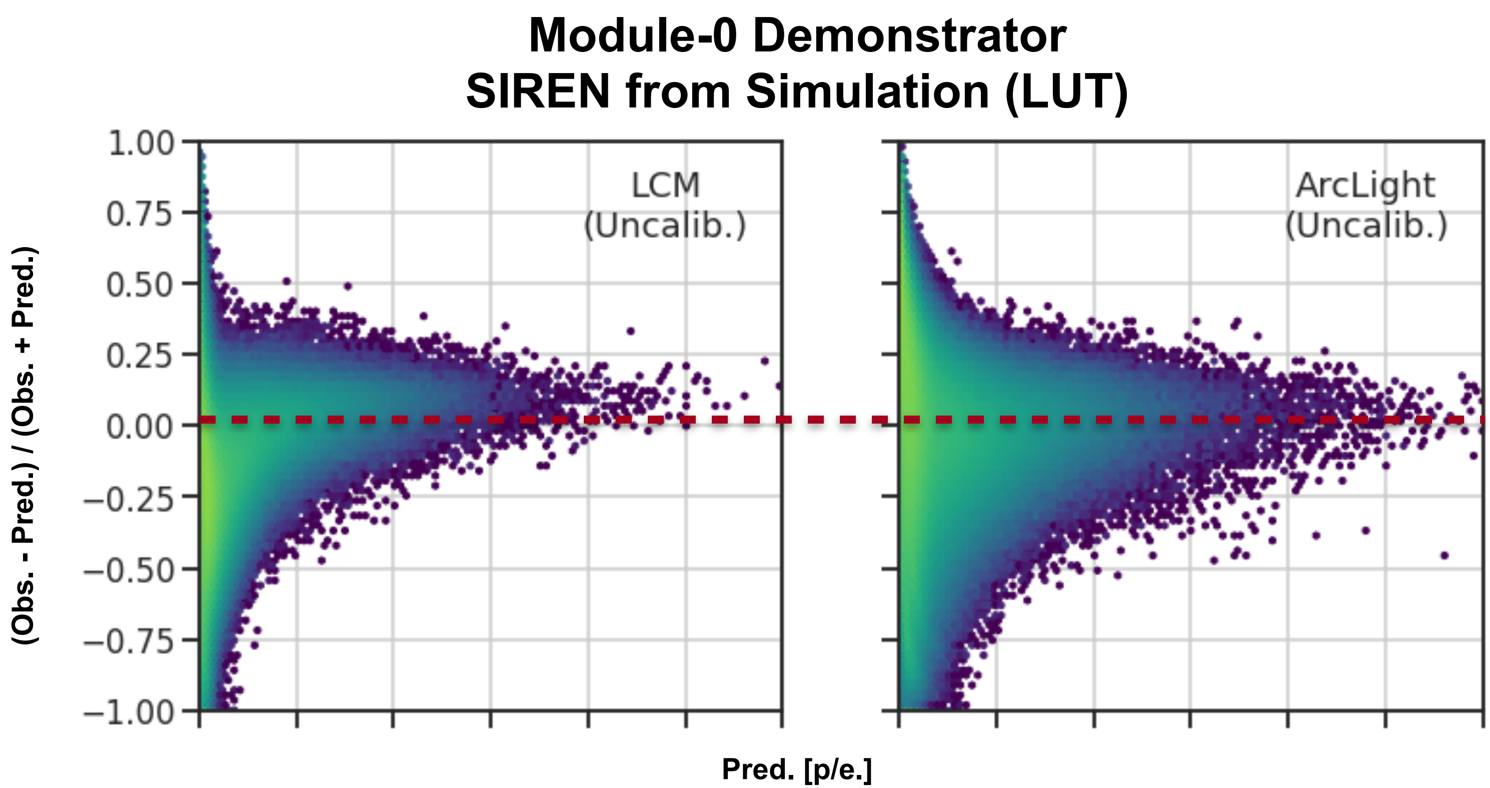
Predicted light signal

Optimize SIREN parameters using track data

For the rest of the talk, I will show some real world applications of SIREN using cosmic rays data from <u>*Module-0 Demonstrator*</u>.

Figures extracted from *Tsang @CHEP2023.*

Module-0: SIREN from Simulation

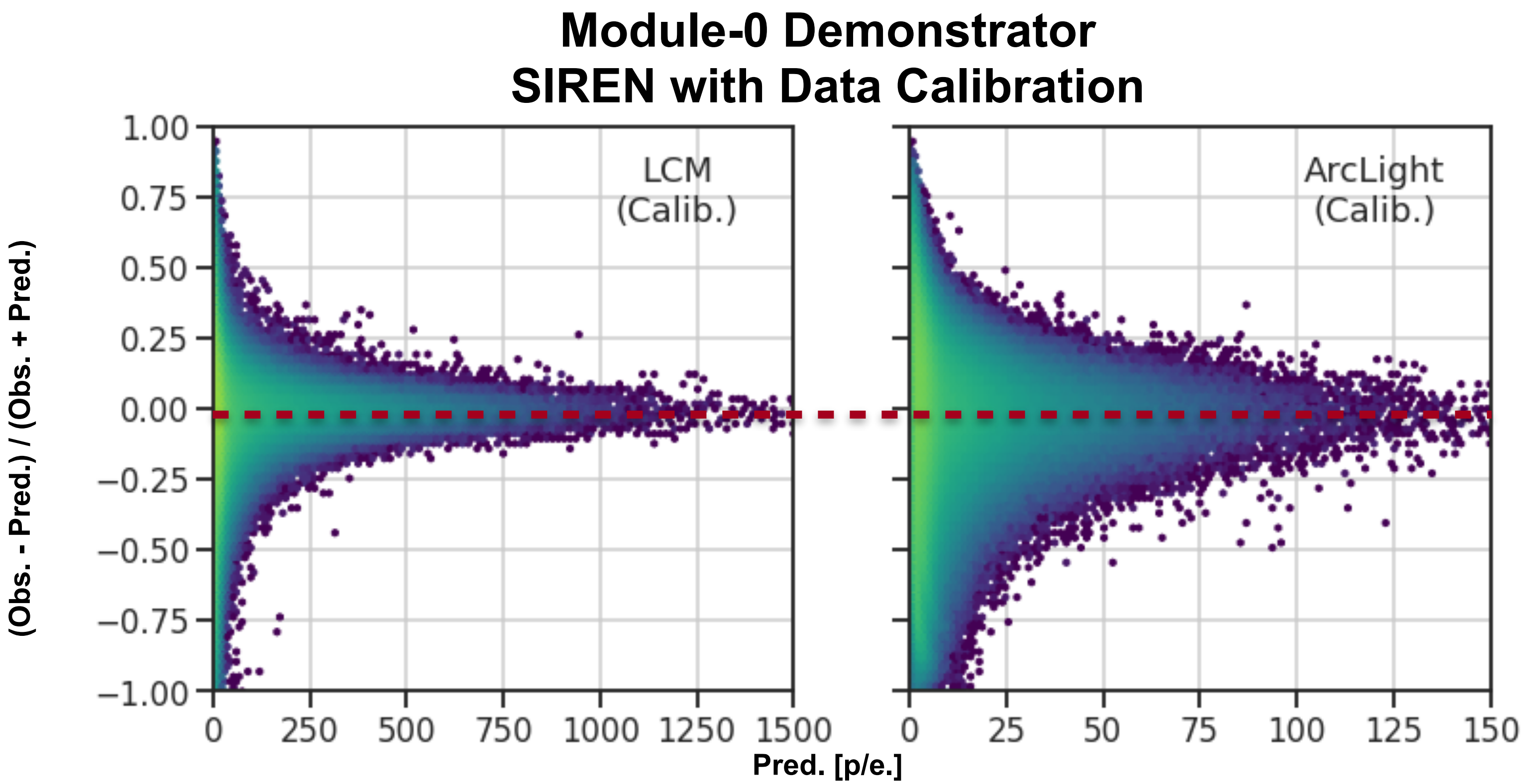


Before Calibration

- train SIREN with LUT from simulation (uncalibrated)
- ~10% discrepancy between observed and predicted light signals

Simulation is reasonable, but not perfect. Need *calibration*.

Module-0: SIREN after Calibration

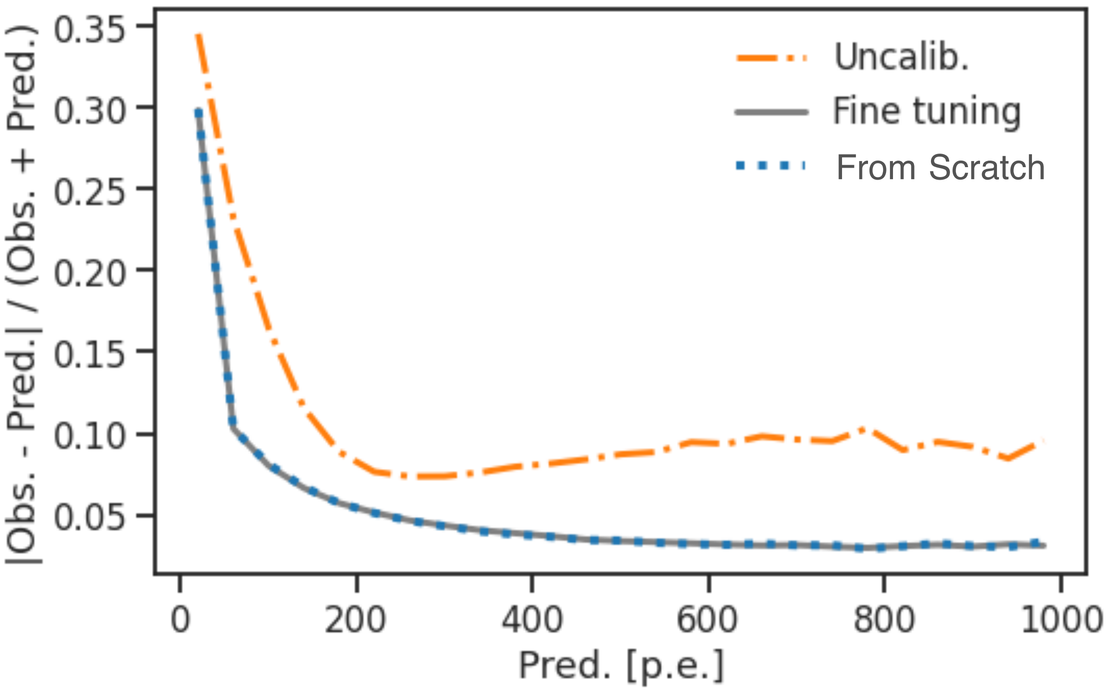


After Calibration

- re-optimize SIREN parameters with tracks
- no bias and smaller variance

SIREN can be calibrated to remove data-simulation discrepancy.

Build a SIREN Model Directly from Data



Uncalibrated

- SIREN trained from LUT (simulation)
- suffer from data-MC discrepancy

Fine Tuning

- use uncalib. SIREN model as initial parameters
- re-optimize with tracks (calibration)

From Scratch

- random initialization of SIREN parameters
- optimize with tracks

SIREN model can be constructed from data alone, without prior knowledge from simulation.

Example Events

Only one chamber TPC-0 is presented in this study.
Grayed out points (unclustered or in TPC-1) are excluded.

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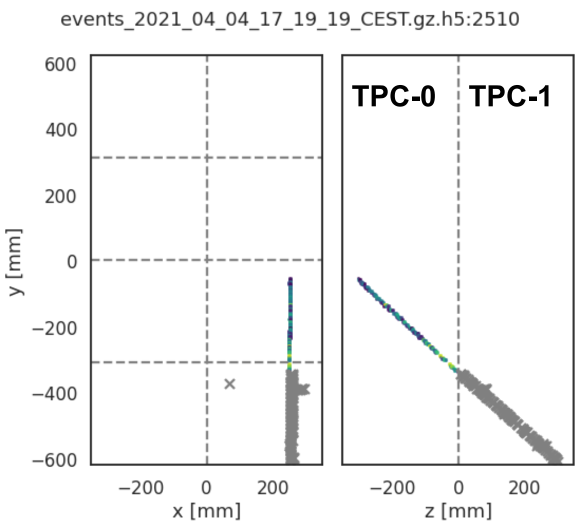
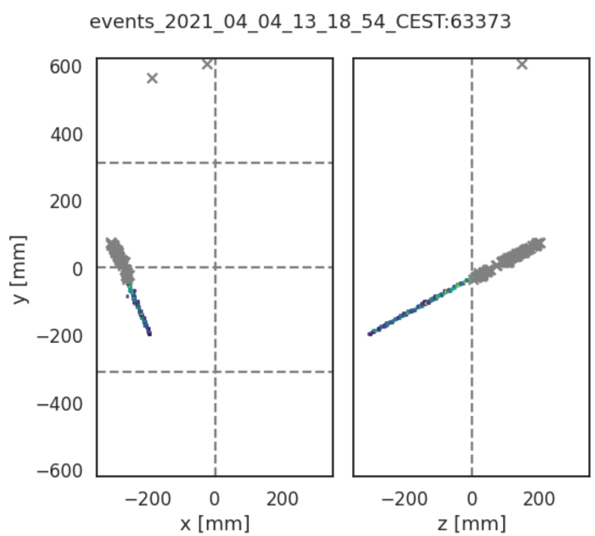
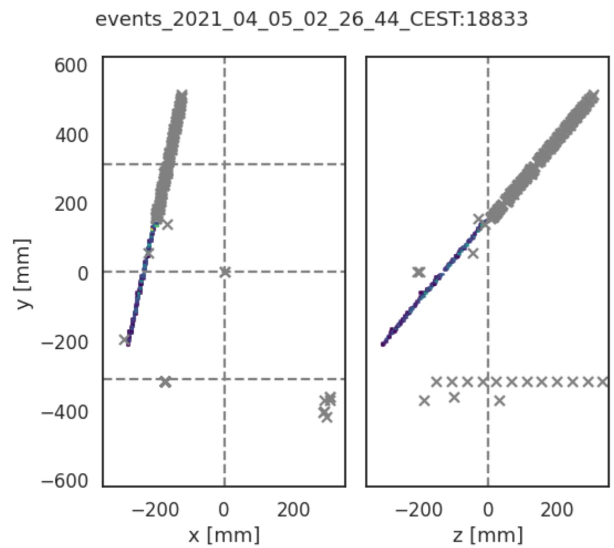
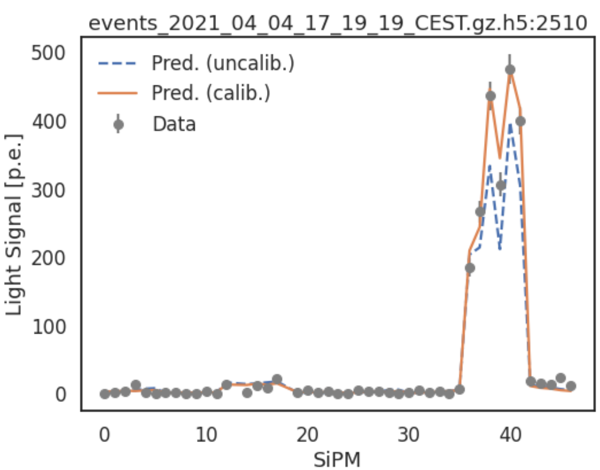
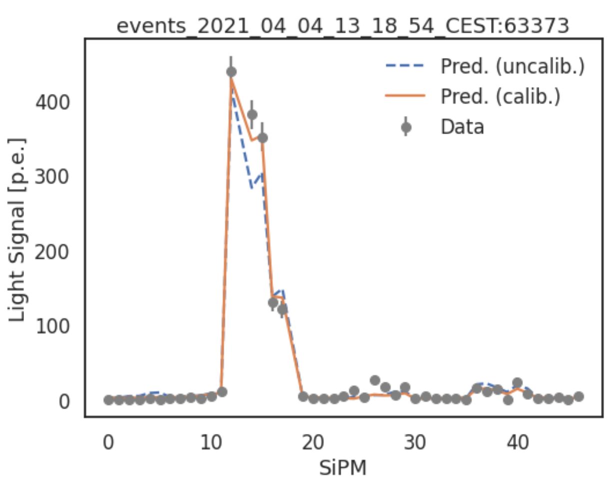
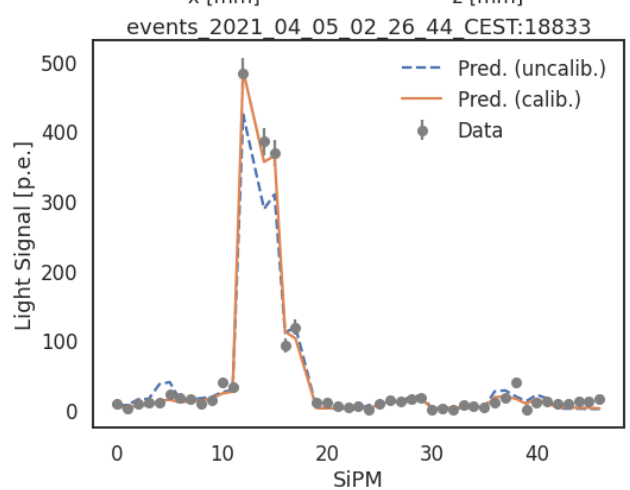






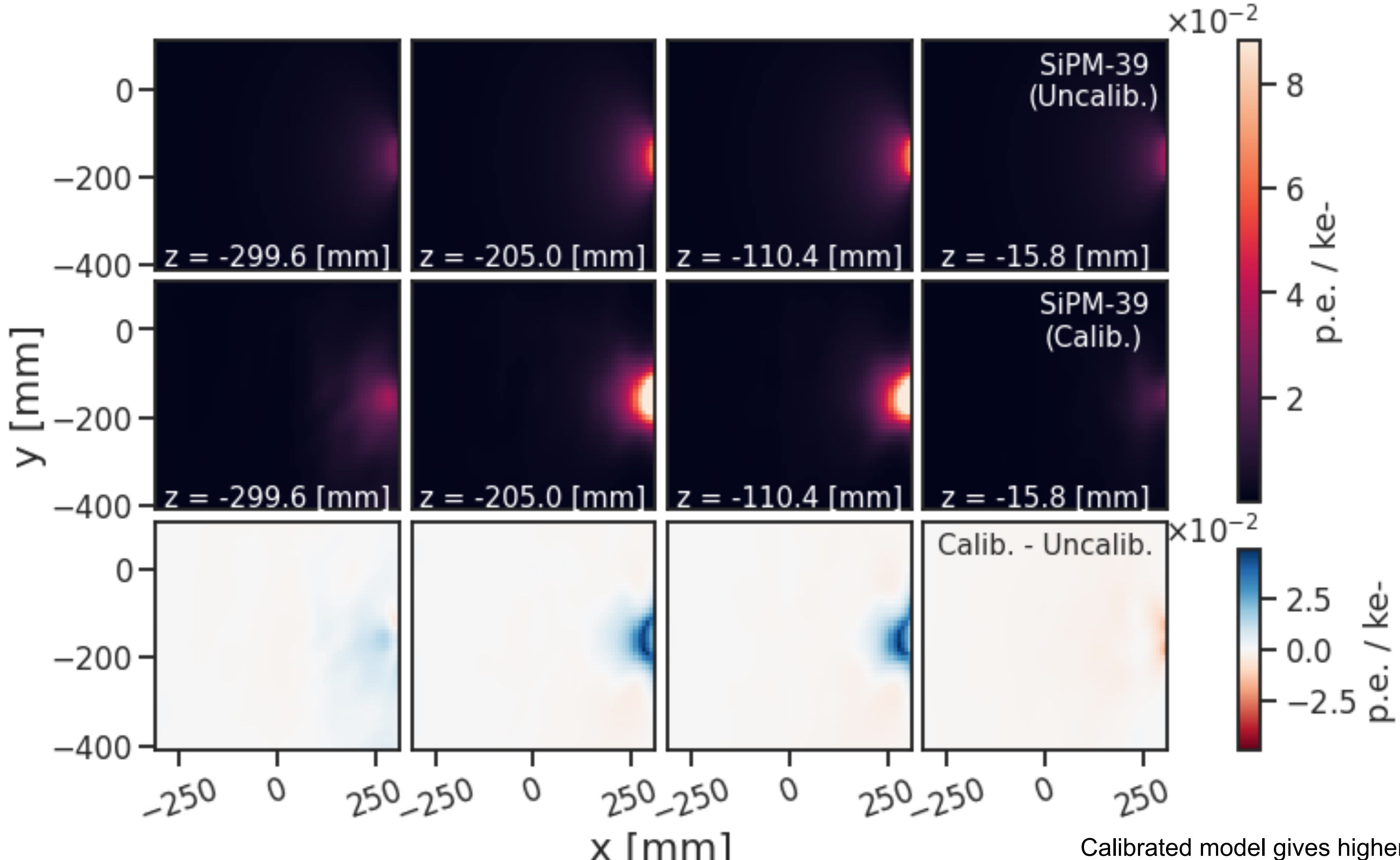






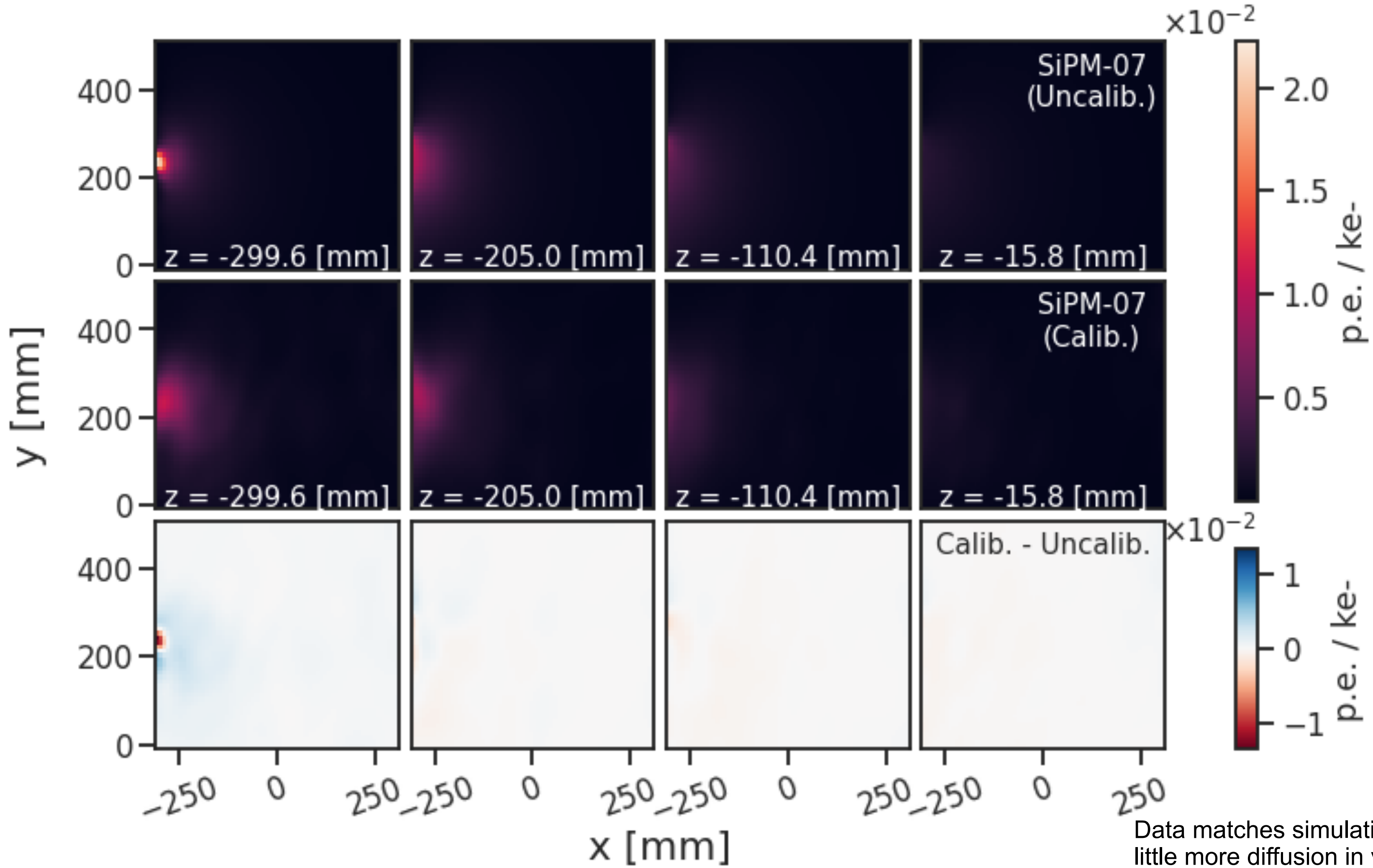
Better agreement after calibration.

Visibility Map (LCM)



Calibrated model gives higher visibility near SiPM.

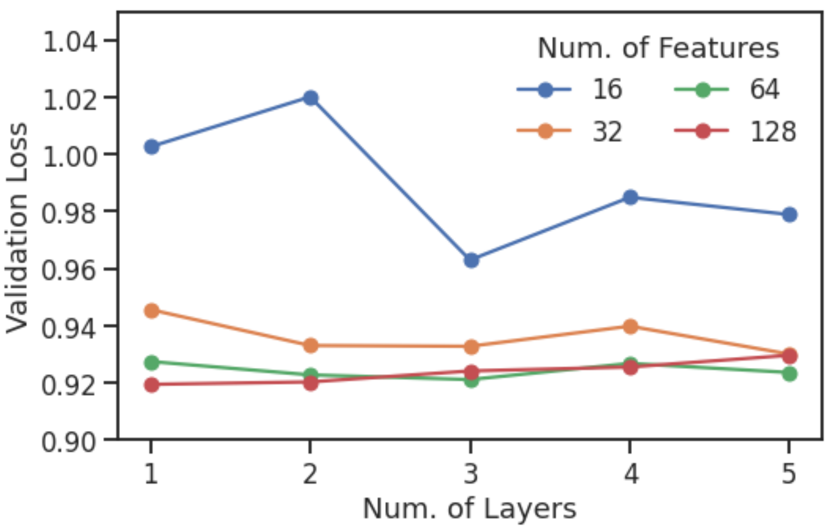
Visibility Map (ArcLight)

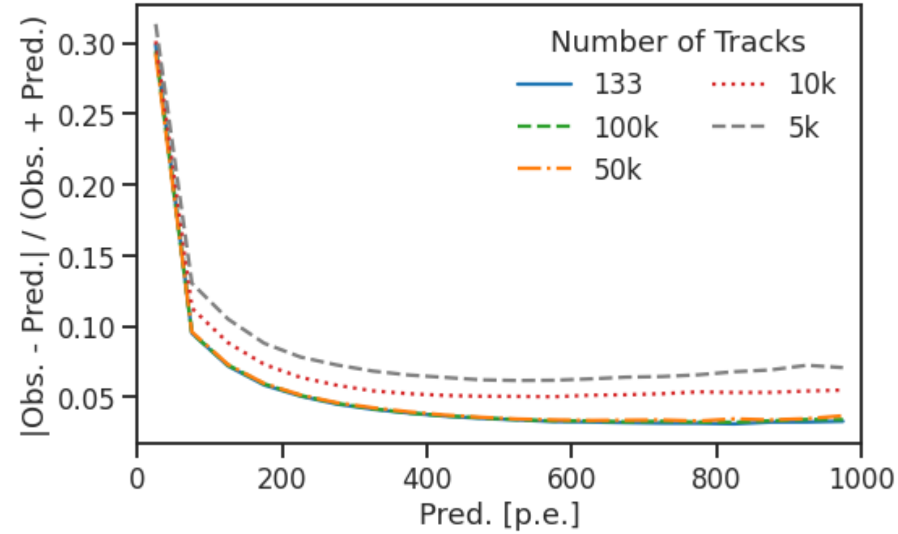


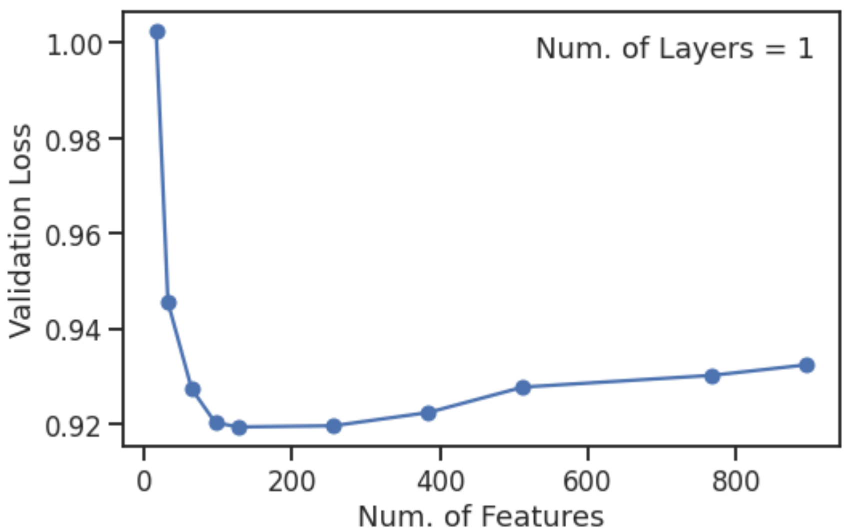
Data matches simulation, with a little more diffusion in visibility.

May provide useful insights for detector R&D.

Hyper-Parameter Optimization w/ Data

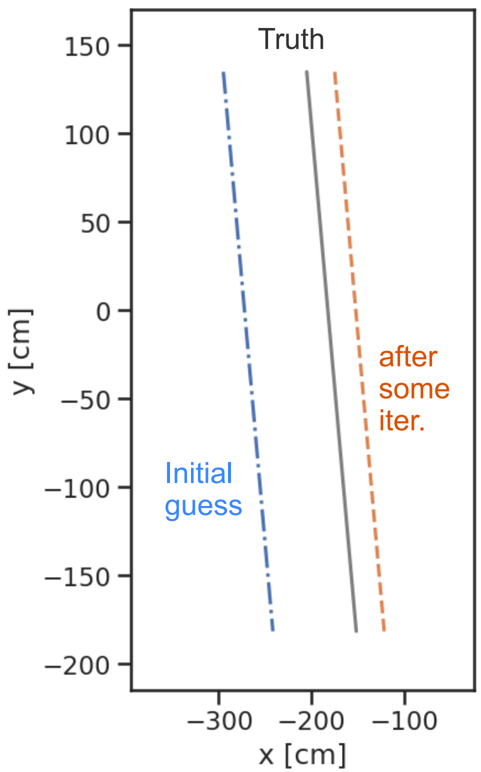


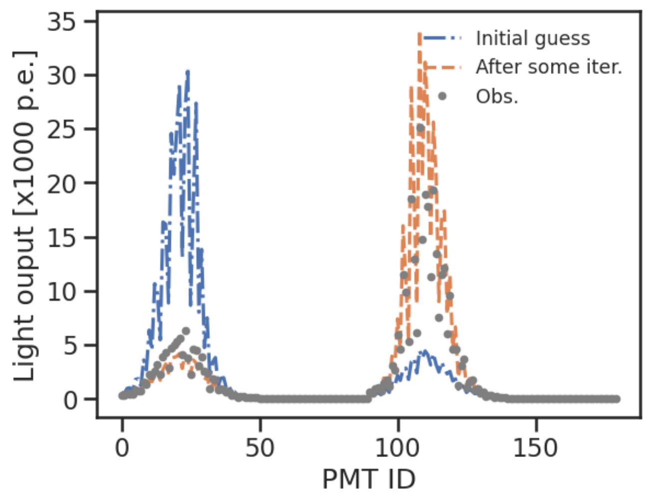


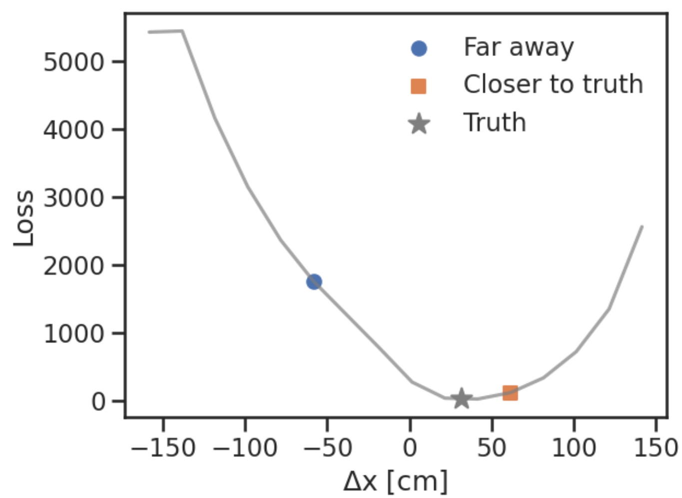


Data driven method to determine the optimal model parameters and minimum sample size.

Application: T0-Finding





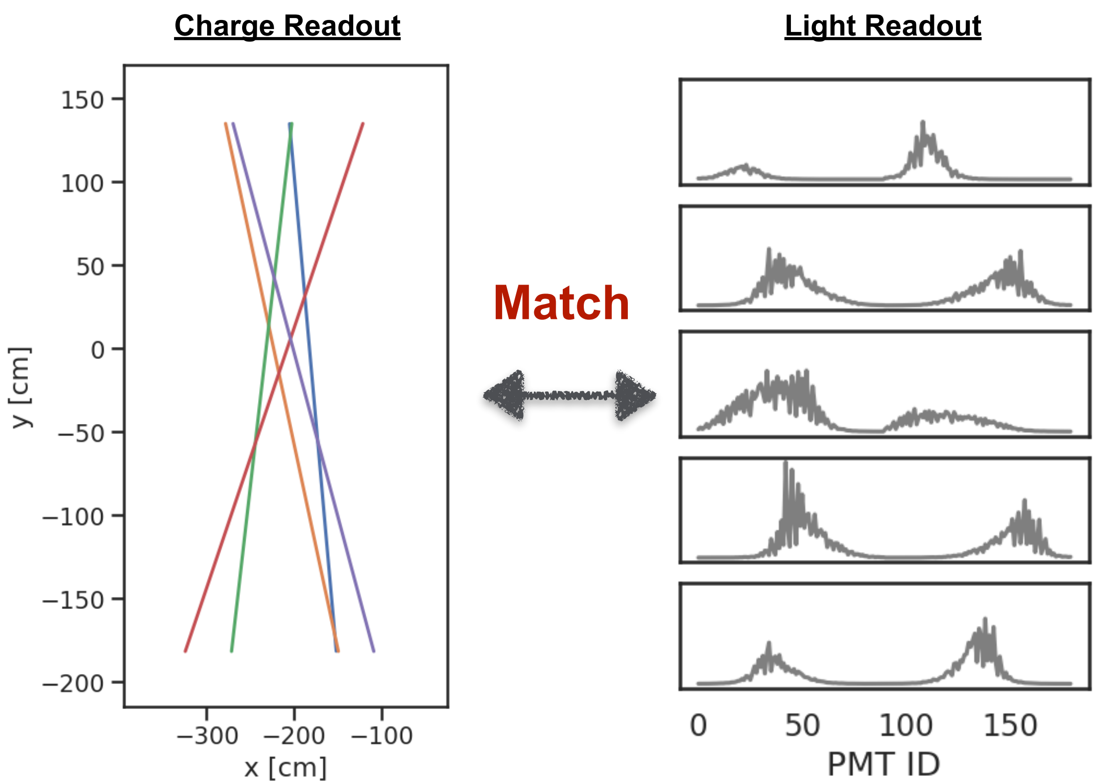


1. Given a charge-light pair, randomly initialize t0 within detector volume
2. Calculate loss w.r.t. observed light output
3. Shift the whole track by Δx and repeat until "best" match is found.

Classical ***gradient descent*** optimization problem.

More advanced examples of multi-parameters optimization in upcoming talk(s).

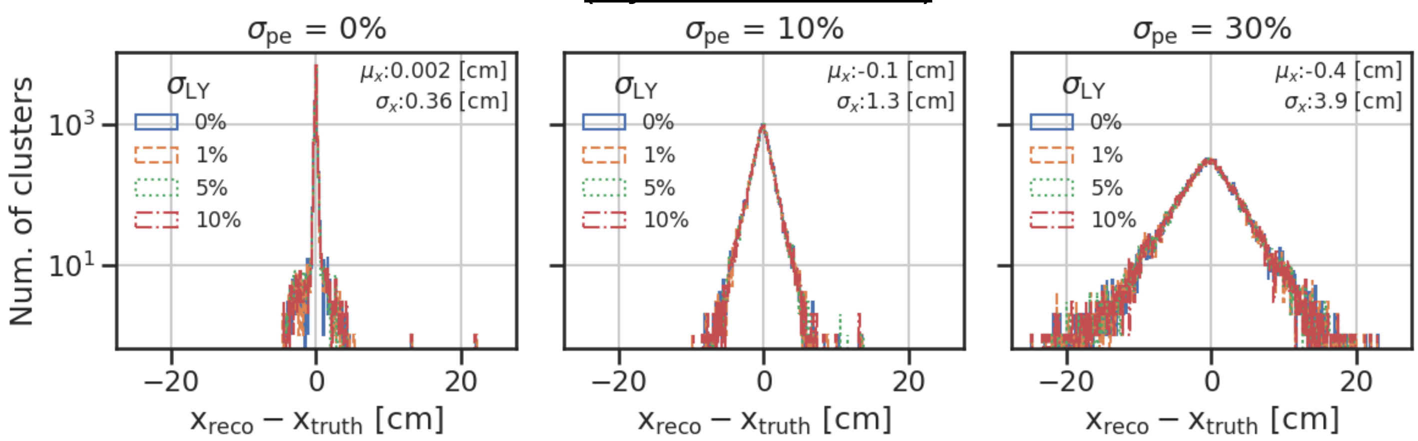
Application: Flash Matching



1. Make a hypothesis of associate *i-th* charge to *j-th* light readouts
2. Minimize pairwise loss L_{ij}
3. Repeat for all pairs (N^2)
4. Bipartite matching - find the optimal pairs to minimize the total loss

Flash Matching (cont.)

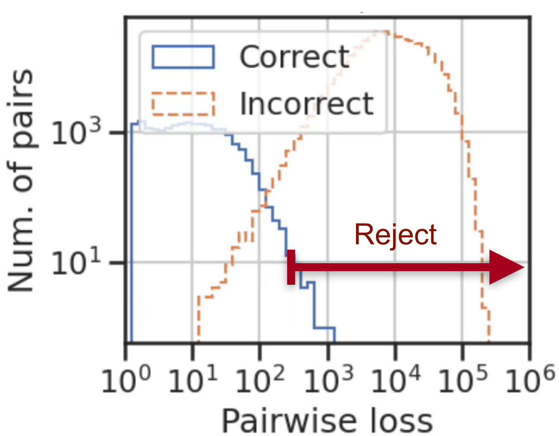
Flash-matching Performance w/ variations in charge and PMT
(Toy ICARUS Simulation)



To Speed Up

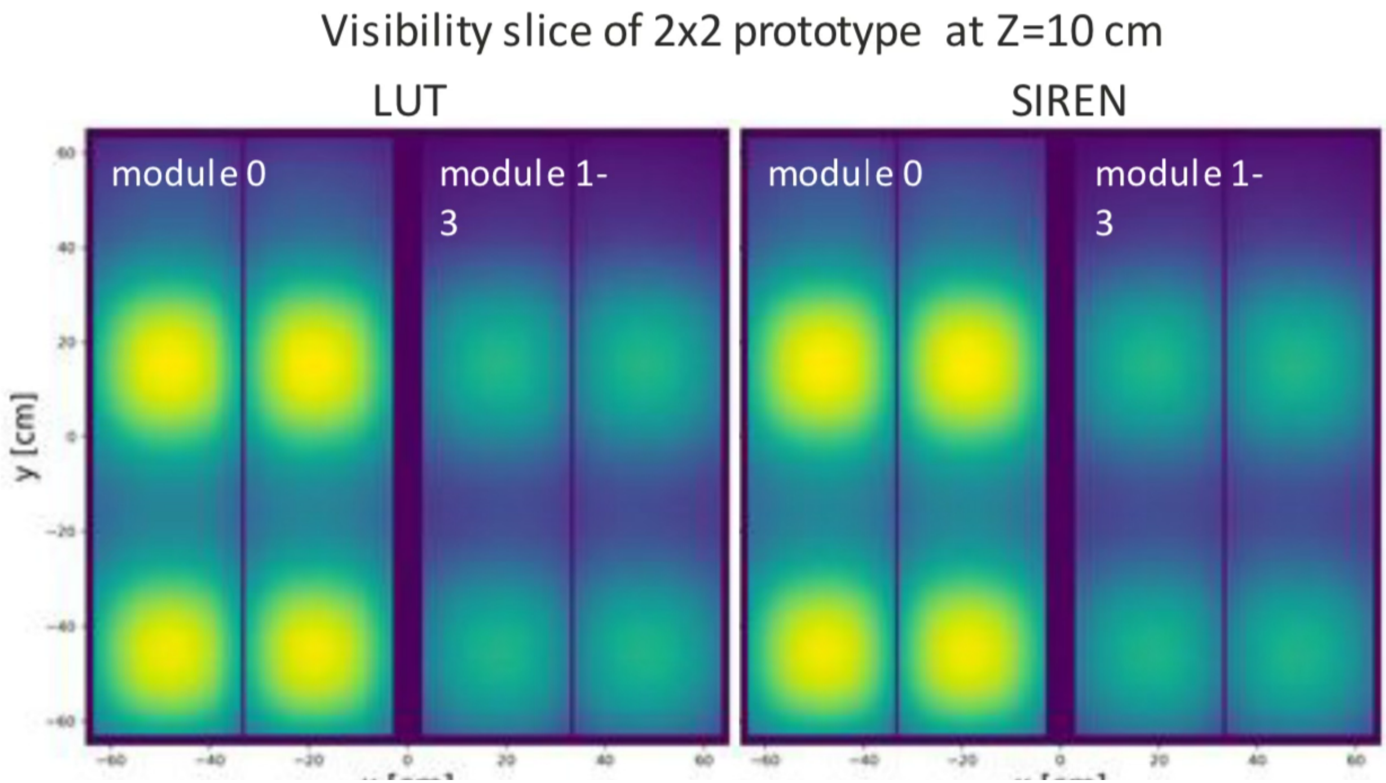
- Scan pairwise loss in a coarse Δx step
  - Reject "obvious" mismatched pairs, or keep only top-k pairs
  - $N^2 \rightarrow O(N)$ pairs
- Optimize in batch
- Benchmark: matching O(10) clusters, ~1s

Pairwise Loss Scan



Real World Application: DUNE 2x2 ND
Oops… No Data!

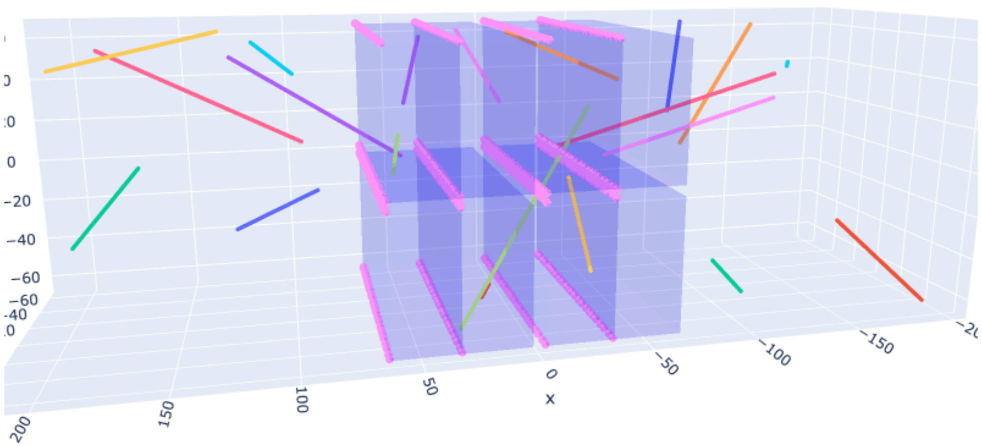
Application for DUNE-ND 2x2



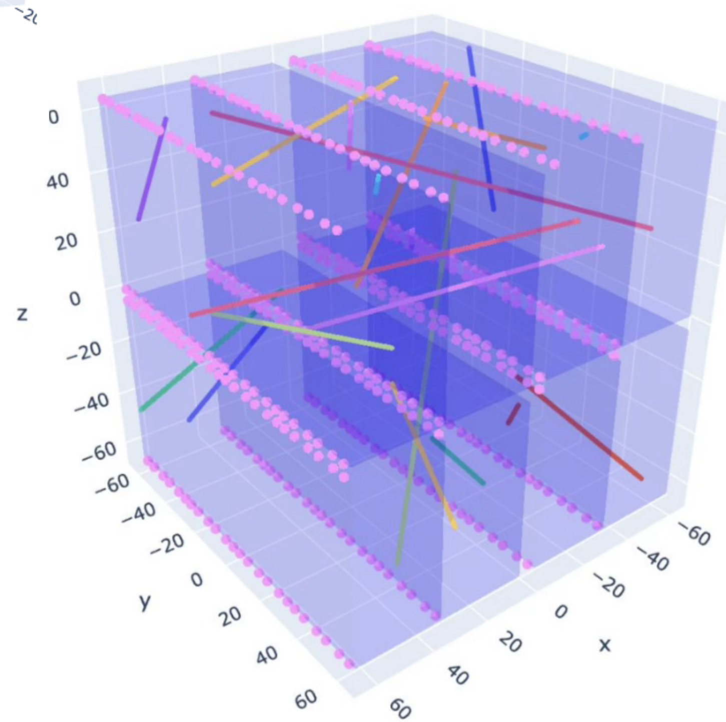
DUNE-ND 2x2 Multi-Module Visibility
Sam Young (Stanford) @APS Apr 2024

Application for DUNE-ND 2x2 (cont.)

Before Matching



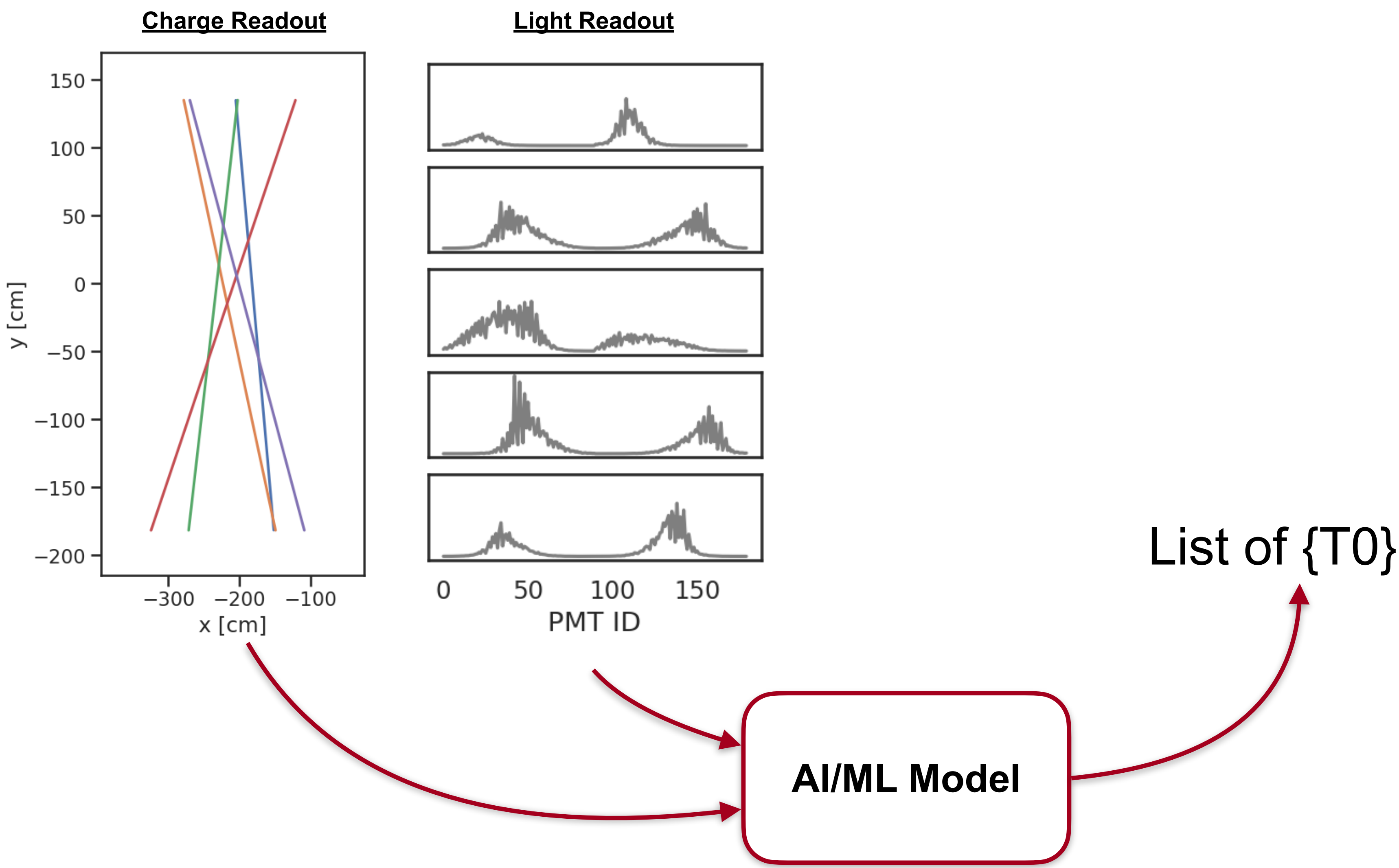
After Matching



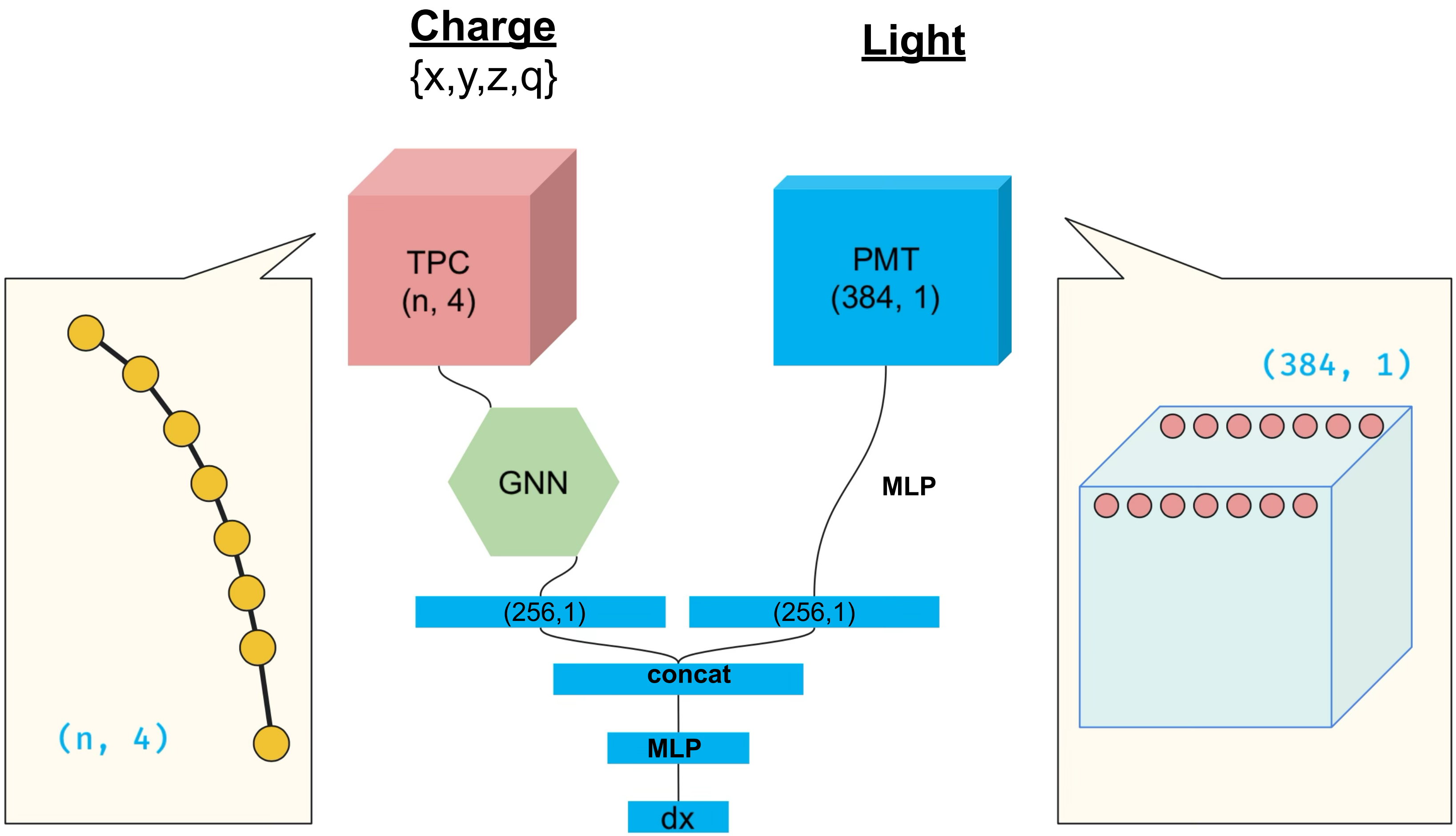
DUNE-ND 2x2 Flash Matching - Toy Simulation

Carolyn Smith (Stanford) @APS Apr 2024

Work in Progress: AI/ML T0 Reconstruction



Proof-of-Concept Model: Single Track

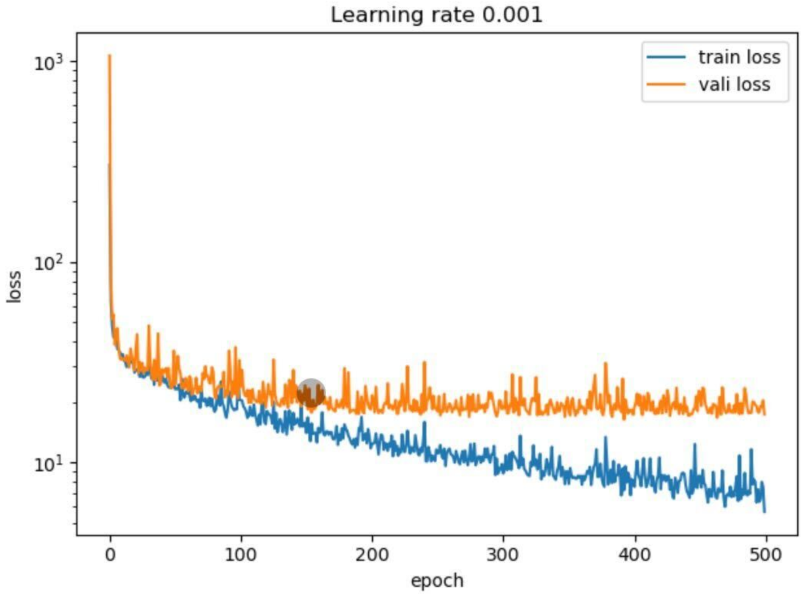


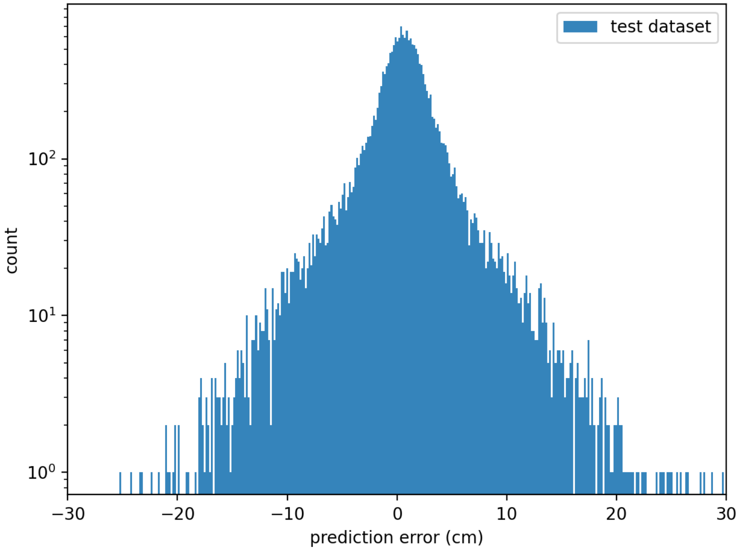
Nodes: Sample n points along the track
Edges: Connect nearest neighbor(s)
GNN: GCNConv w/o edge weights

Zhe Zhang (SLAC)

Preliminary Results on AI/ML T0 Reco.

Zhe Zhang (SLAC)





Training 60k single tracks
batch size 1000

Test sample 20k
RMS = 4.49 cm

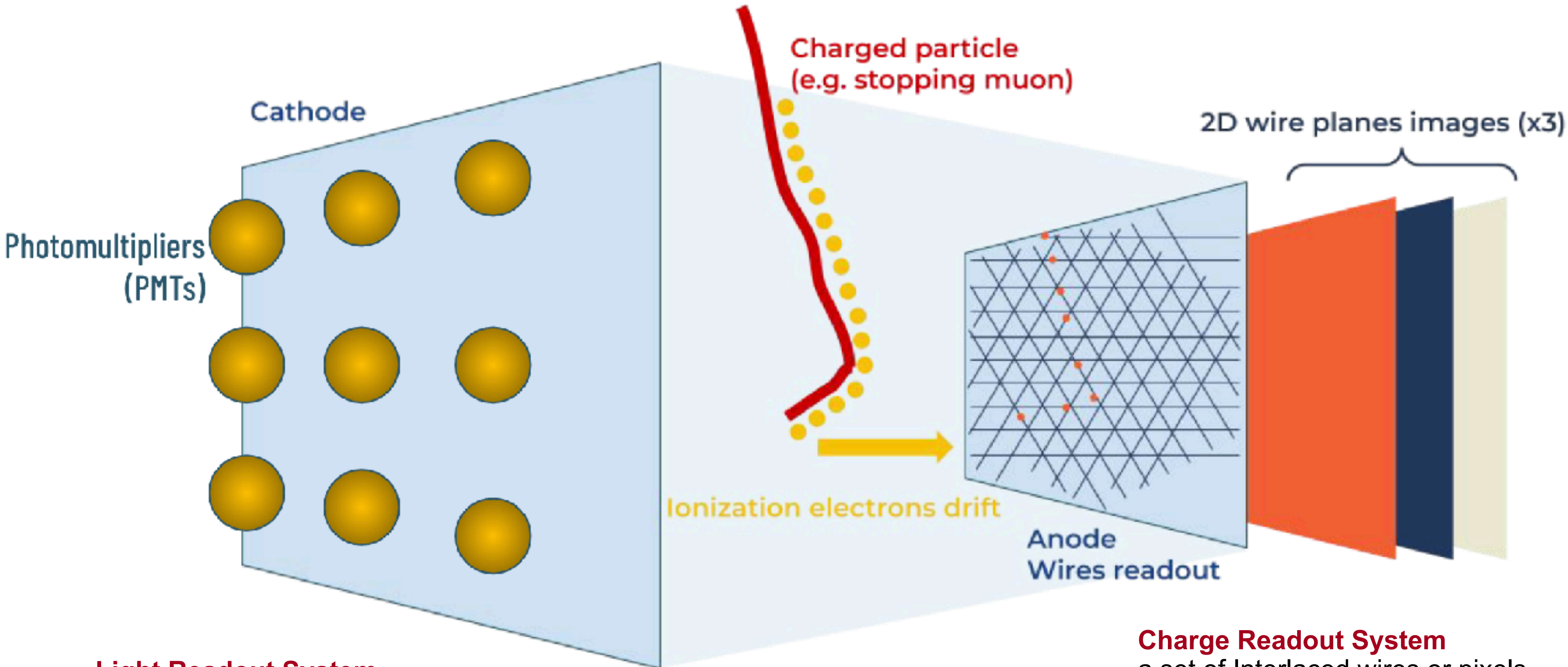
- not bad for an initial attempt
- how to aggregate charge image with multiple objects?
- how to match multiple charge and light clusters?

Conclusions

- propose the use of sinusoidal representation network (SIREN) to model the light propagation for LArTPCs
  - memory efficient => scalable for large detectors
  - optimizable w/ data => calibration
  - smooth gradient surface => further applications
- more use cases of differentiable modeling in the upcoming talks

Backup Slides

Liquid Argon Time Projection Chamber (LArTPC)



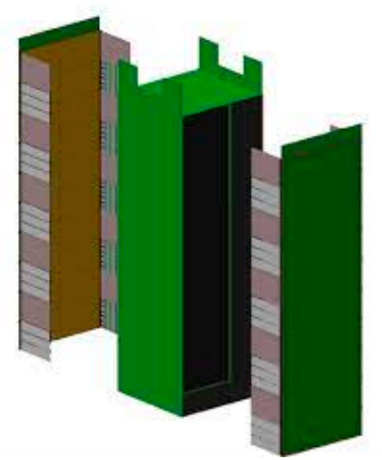
Light Readout System
detection of scintillating photons at O(ns)

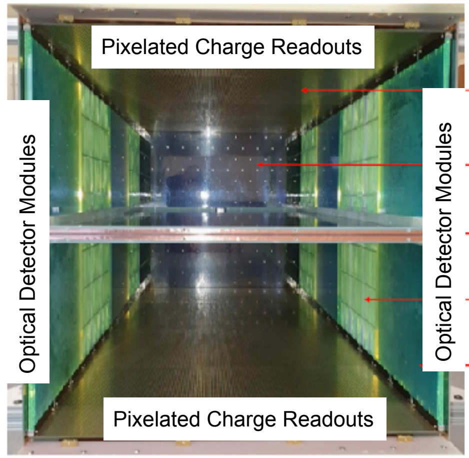
$$e^- + {}^{40}Ar^+ + {}^{40}Ar \rightarrow {}^{40}Ar_2^* \rightarrow 2\,{}^{40}Ar + \gamma.$$

Charge Readout System
a set of Interlaced wires or pixels
drift time O(ms)

$$\boxed{\text{Drift distance = Drift Velocity * } (t - t_0)}$$

Examples of LArTPC Detectors





Module-0 Demonstrator

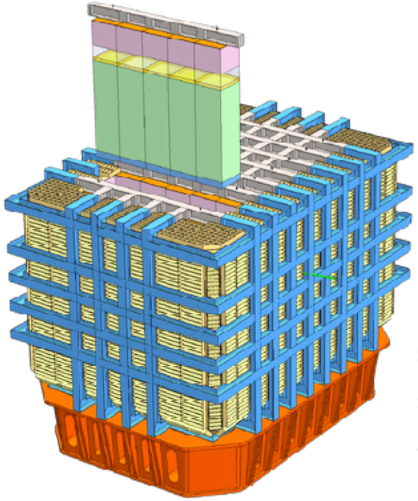
- 1st ton-scale prototype of DUNE* near detector design
- ~0.7 m x 0.7 m x 1.4 m
- divided into 2 TPCs
- pixelated charge readout
- 2 different optical detector prototypes: LCM & ArcLight

ICARUS**

- largest LArTPC in operation with wire readout
- 760 ton LAr in 2 TPCs
- each ~3.6 m x 3.9 m x 19.9 m

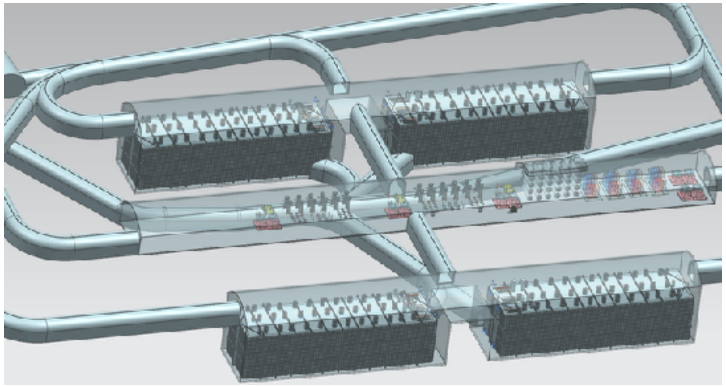
*DUNE: Deep Underground Neutrino Experiment
**ICARUS: Imaging Cosmic And Rare Underground Signals

Proposed LArTPC Detectors



DUNE Near Detector-Liquid Argon (ND-LAr)

- 7x5 array of 1 m x 1m x 3m detector modules (similar design as module-0 demonstrator)
- ~67 ton of LAr

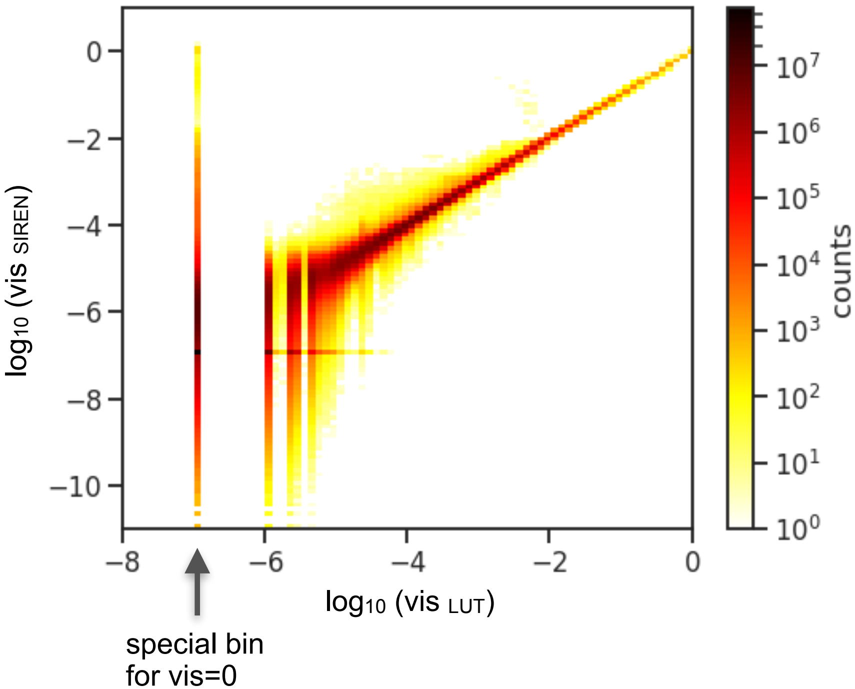


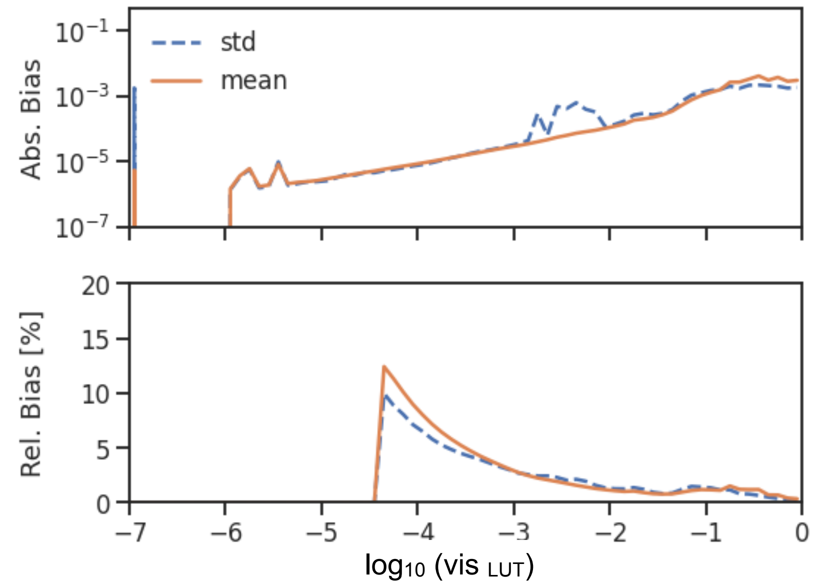
DUNE Far Detector

- 4 x ~17-kton detector modules
- each ~19 m x 18 m x 66 m

Scalability is the key for the future

SIREN Performance





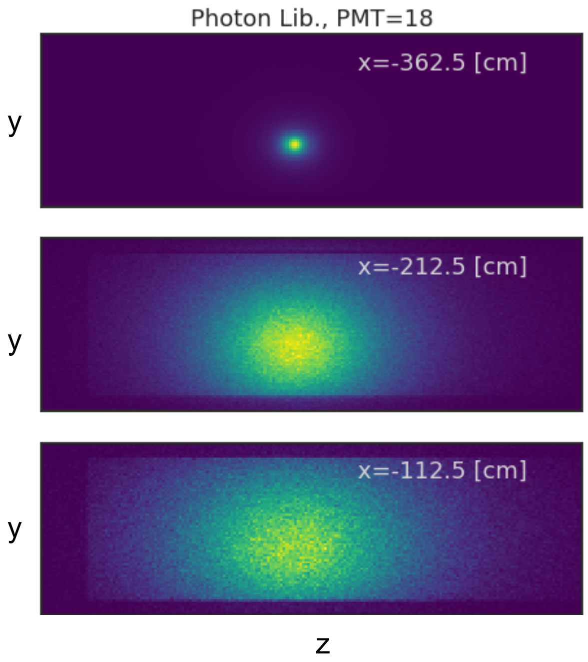
SIREN is able to represent LUT with ~1% in the high visibility region (vis. > 1e-2).

The overall (average) bias is ~7-8%, which is dominated by the *statistical fluctuation* of the LUT at low visibility.

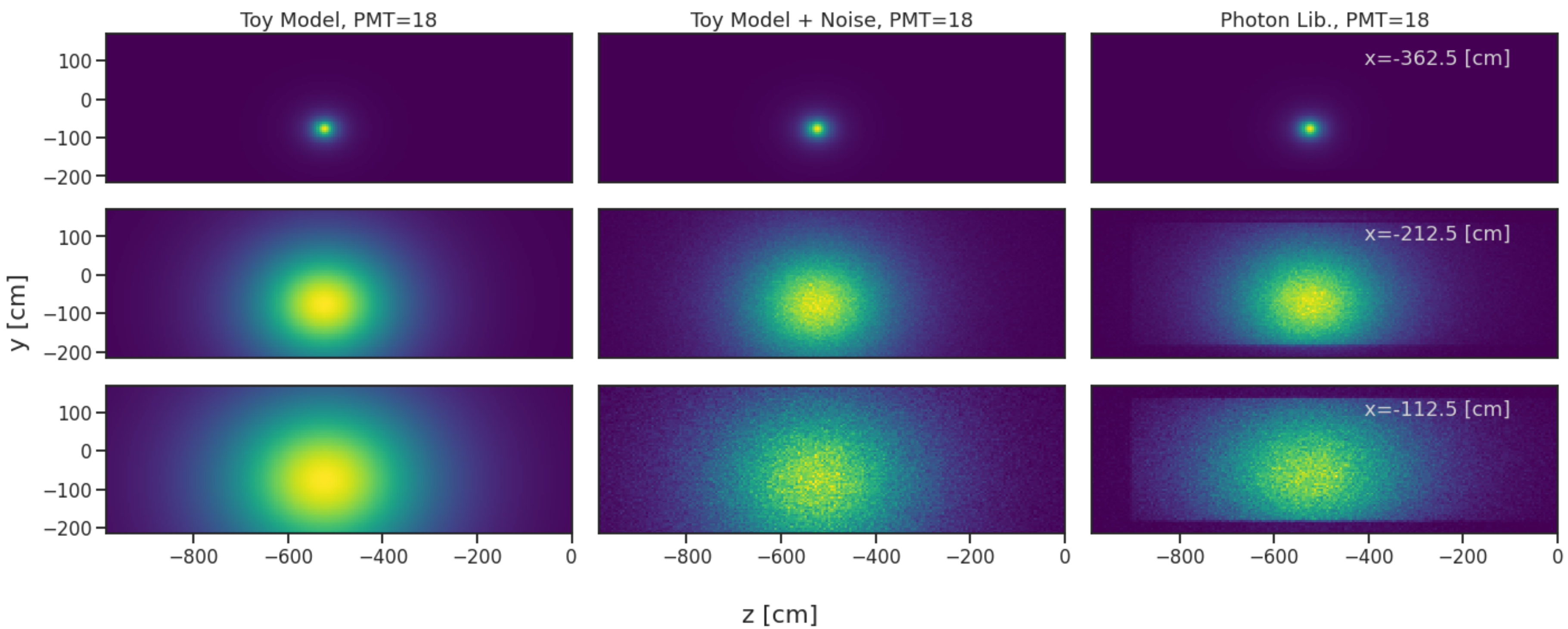
Statistical Uncertainty in LUT

Generation of the photon library is limited by *finite statistics*.

The input data to the SIREN are subjected to *statistical uncertainty* (more prominent for voxels with low visibility).



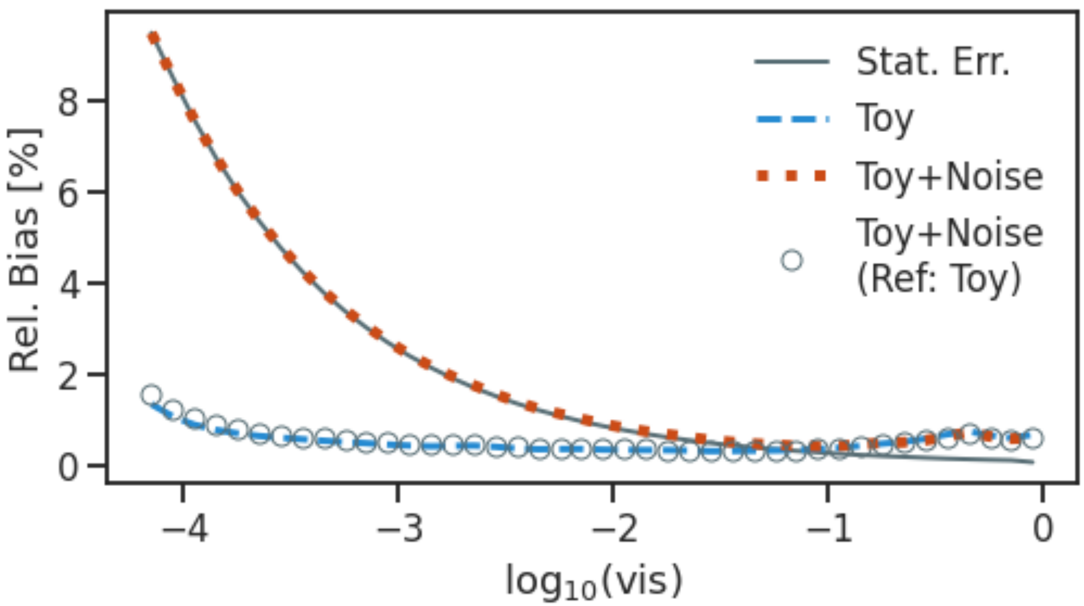
Toy Model: A Study w/ and /o Stat. Err.



Toy Model: analytical (smooth) model that roughly reassemble the features of LUT. No statistical fluctuation.

Toy Model + Noise: sampling from toy model, assuming 1e6 photons per voxel, ~same statistical uncertainty as the LUT.

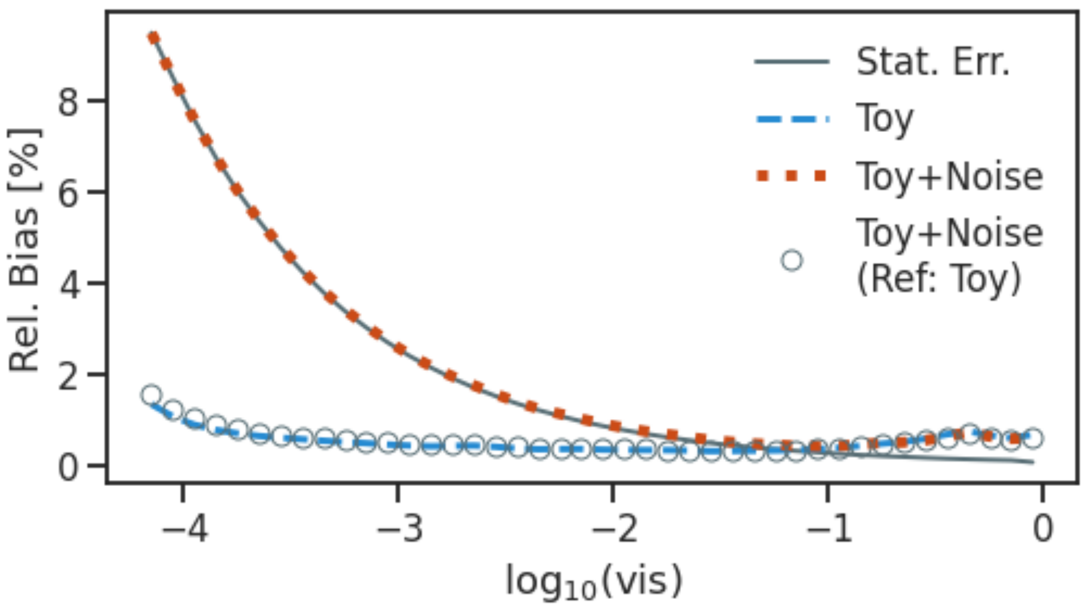
SIREN Performance
w/o Statistical Uncertainty



Toy Model

- train SIREN w/ toy model
    - *NO* stat. fluctuation
- compare SIREN output to the analytical model
- ≤ 1% bias
- *systematic* error for SIREN

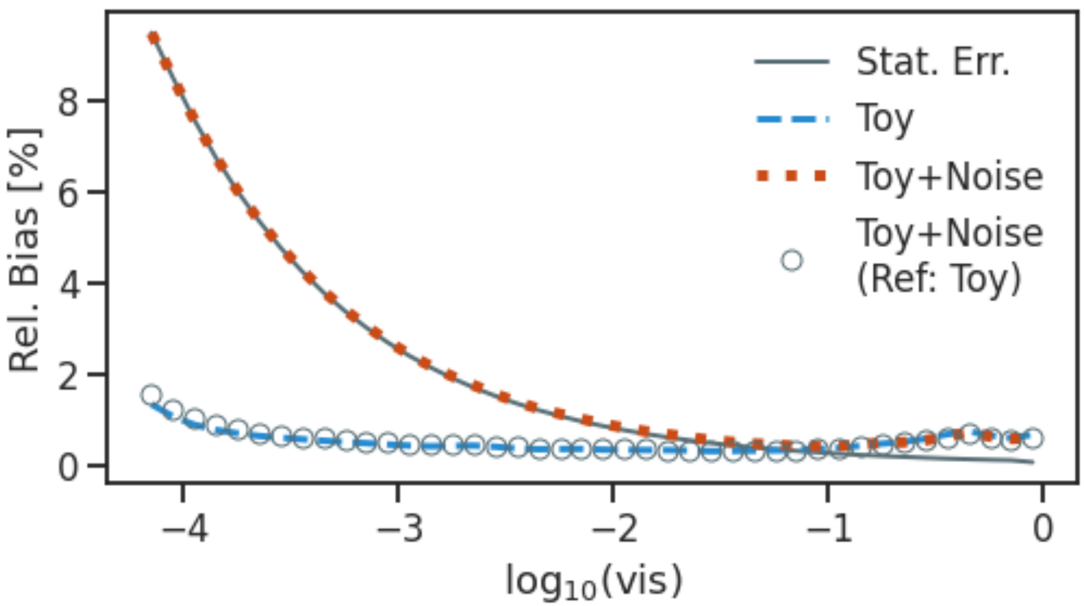
SIREN Performance w/ Statistical Uncertainty



Toy+Noise Model

- train SIREN w/ toy+model
    - input data *with* stat. fluctuation
- compare SIREN output to the *input data*
- ≤ 1% bias at high visibility values
- bias increases gradually for lower visibility
    - comparable to the expected stat. err.
- contributions from both *statistical* and *systematic*

SIREN Performance
Learning the Underlying Distribution

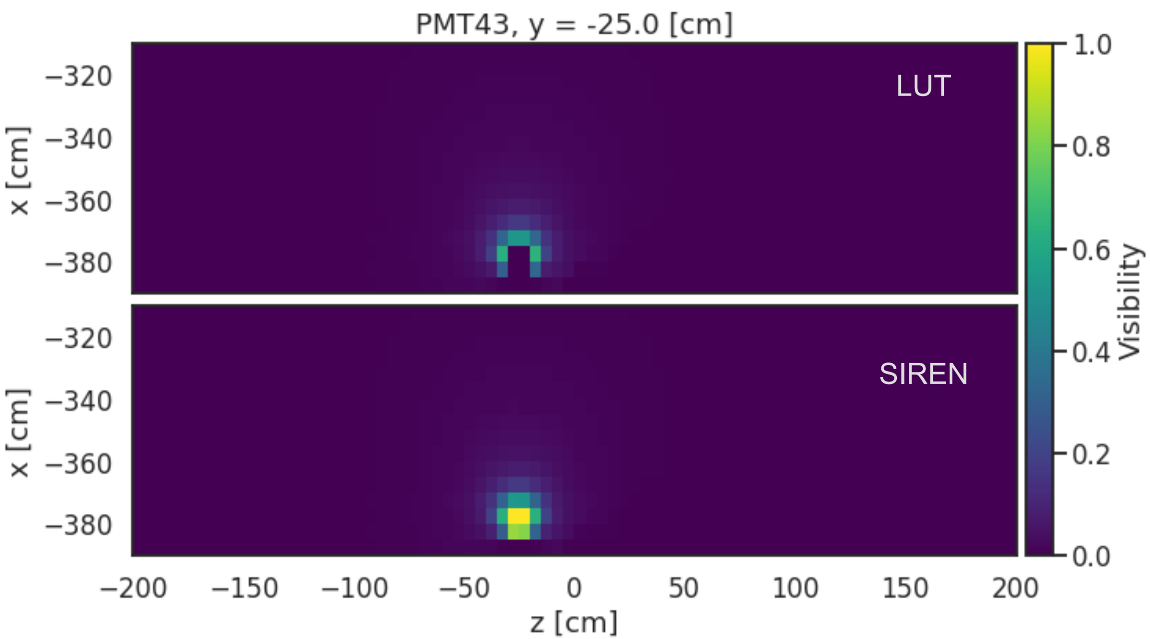


Toy+Noise Model (Ref: Toy)

- train SIREN w/ toy+model
  - input data *with* stat. fluctuation
- compare SIREN output to the *analytical model (i.e. the truth distribution)*
- same bias as trained with Toy Model (i.e. input data w/o stat. uncertainty)
- statistical fluctuations suppressed

SIREN is able to learn the underlying distribution at ≤ 1% level, even with the imperfect input data.

Case 1: LUT == 0, SIREN high vis.

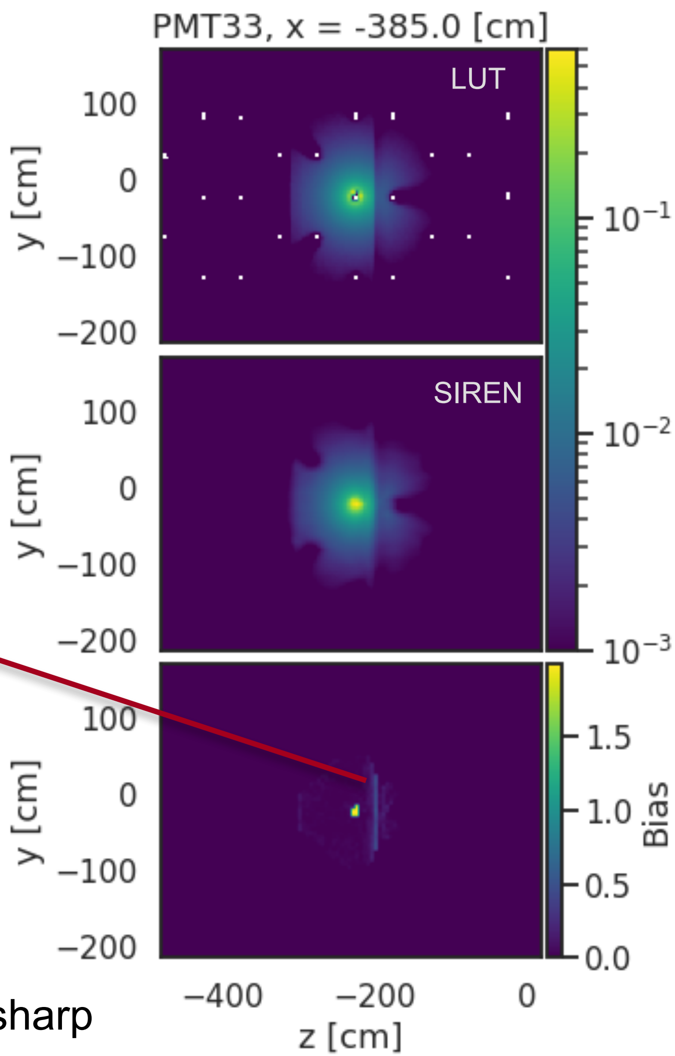


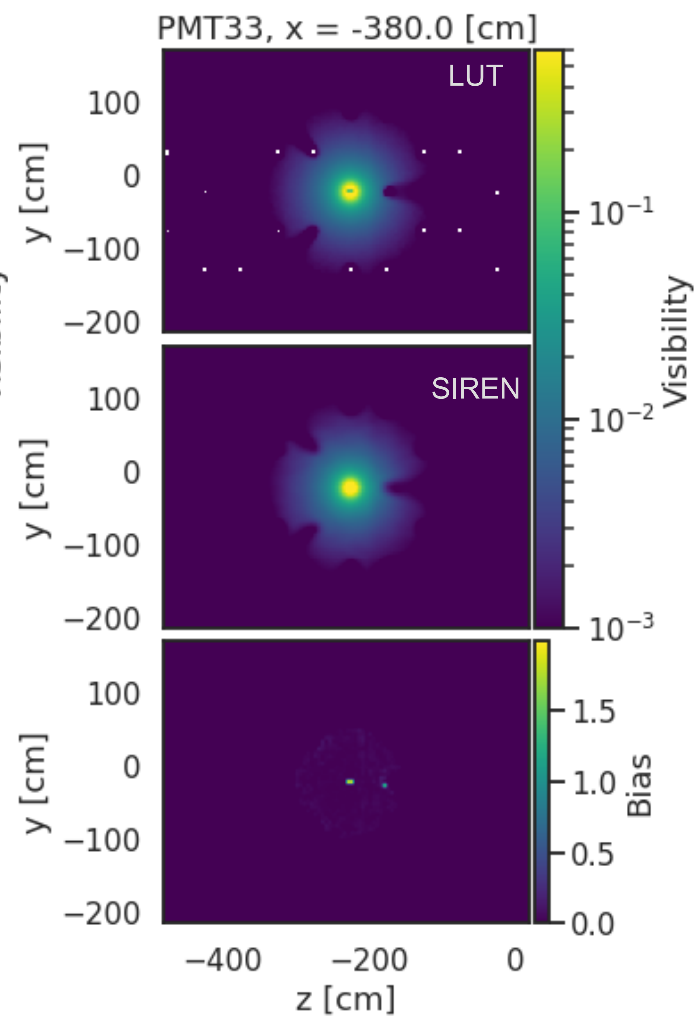
No light at the base / mount of PMT.

SIREN (as a continuous parameterization) tries to map the visibility toward max. visibility = 1.

Negligible impact on physics. It corresponds track hitting directly to the PMT, leaving *NO* ionization charge. Likely there is a fiducial volume in the high level analysis.

Case 2: SIREN Overpredicts Visibility





SIREN's limitation on sharp edge transition.

Module-0 Detector

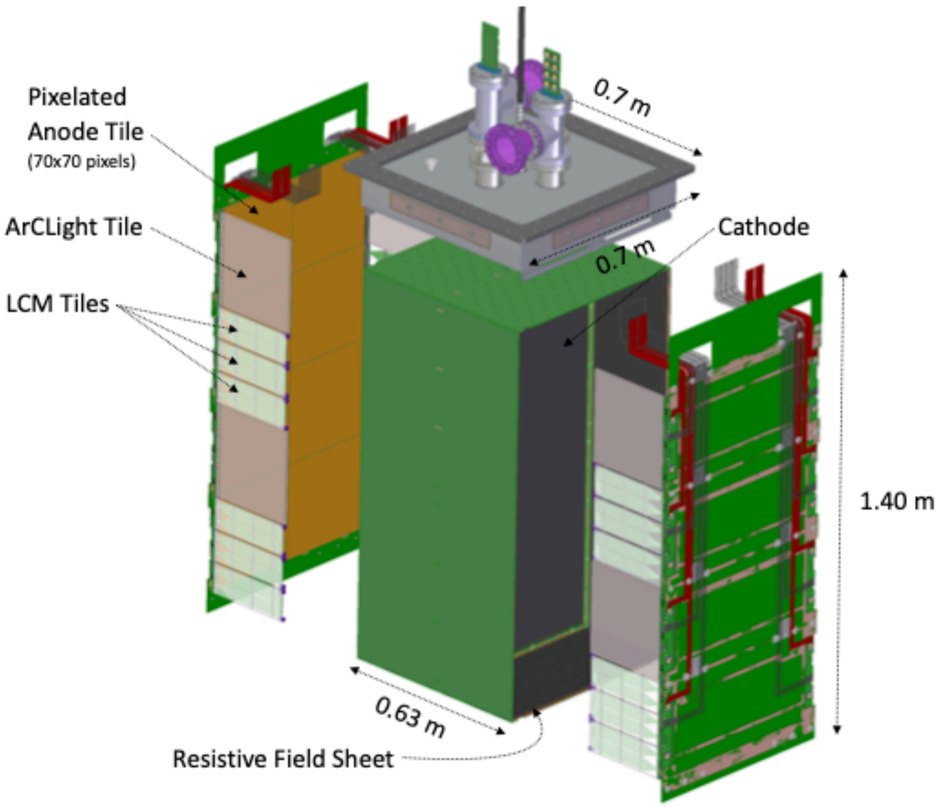


Figure 1. Schematic of the 0.7 m × 0.7 m × 1.4 m Module-0 detector with annotations of the key components.

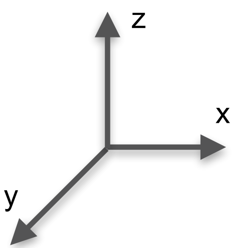
Short term goal

- build a prototype of 2x2 array of detector modules
- test w/ NuMI neutrino beam at Fermilab

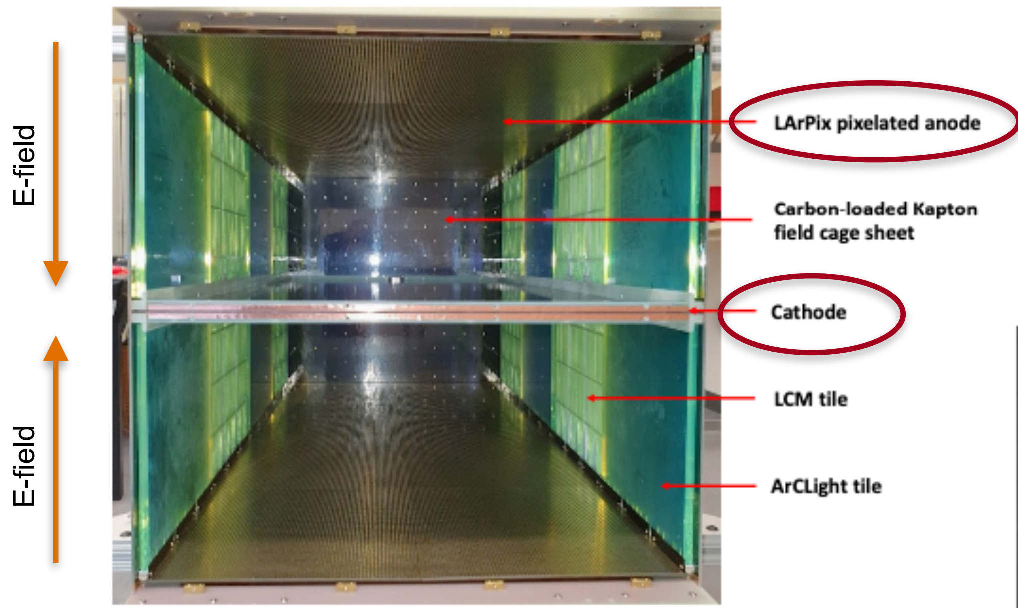
Long term goal

- build a 7x5 array (TBC) for the DUNE Liquid Argon Near Detector

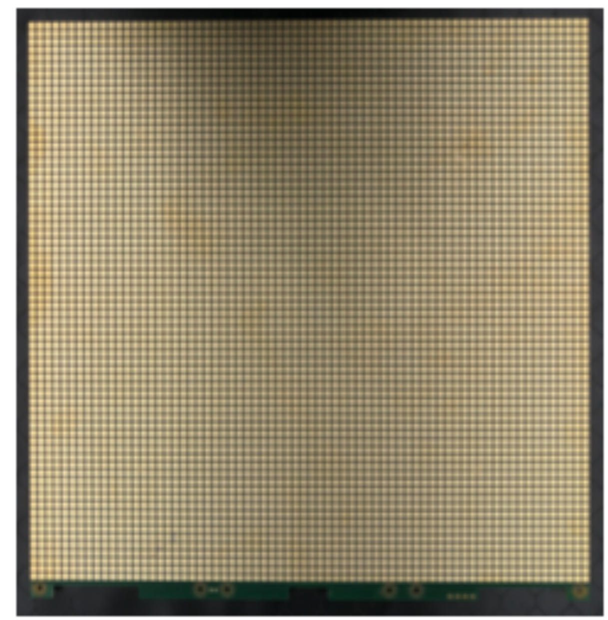
Module-0 Charge Readout System



View from the top of Module-0

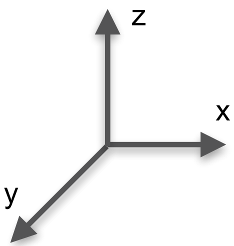


LArPix Tile

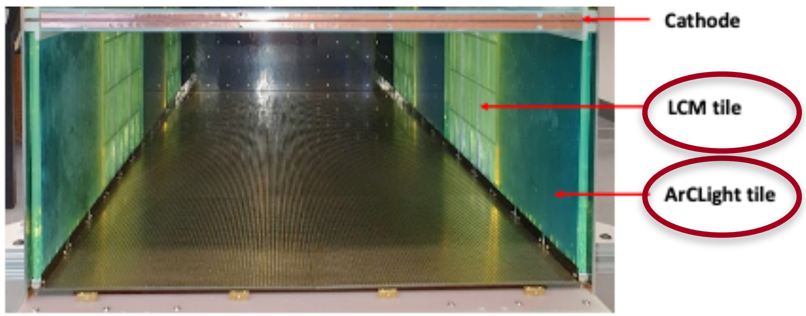


- 2 drift volumes (TPCs)
- separated by a cathode plane
- 4x2 LArPix tiles per anode plane
- 70x70 pixels per tile
- pixel pitch 4.43 mm

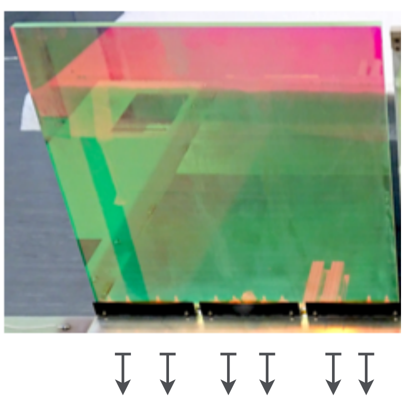
Module-0 Light Readout System



Light Readout System of Module-0

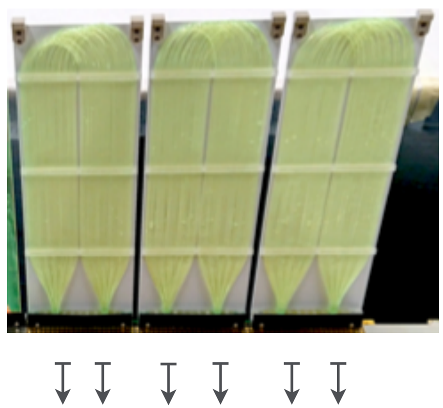


ArCLight tile



6 SiPMs

LCM tile



2 SiPMs 2 SiPMs 2 SiPMs

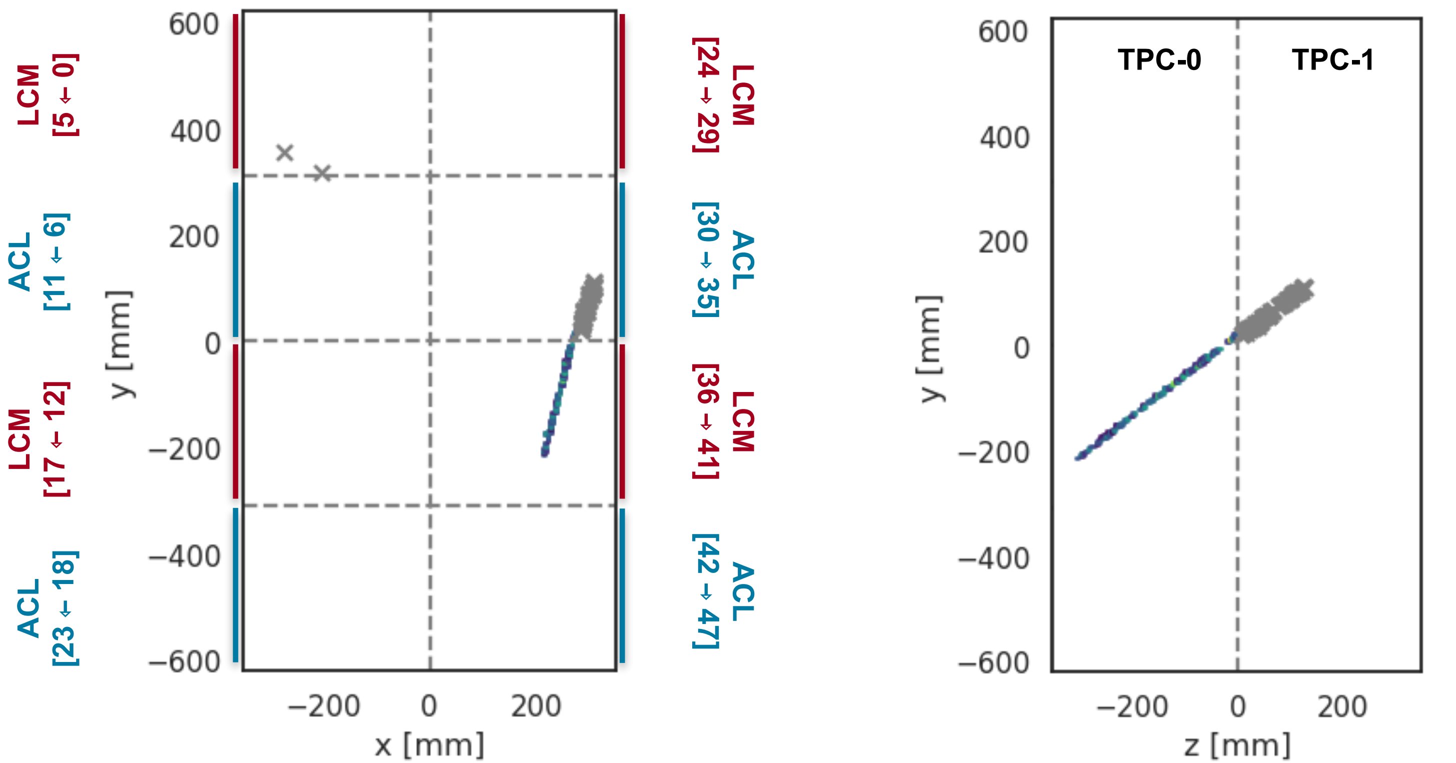
- 4 LCM and 4 ArCLight tiles per TPC
- each tiles ~300 mm x 300 mm x 10 mm
- 6 SiPMs per tile
- total of 48 SiPMs per TPC

Data Selection for Module-0

SLAC

- data collected between 4/4/21 - 4/10/21 at Bern
  - "*default*" settings (0.5 kV/cm, med. threshold ….)
- cathode-anode crossing tracks in TPC-0
  - one clustered object per charge image
  - dbscan eps=25 mm, min_samples=5
- matching charge-light pairs by trigger timestamp
- ~680k tracks selected
  - training/validation/testing samples in 75-15-15 splitting ratio
  - for track statistic study, splitting ratio is 20-80 for training/testing

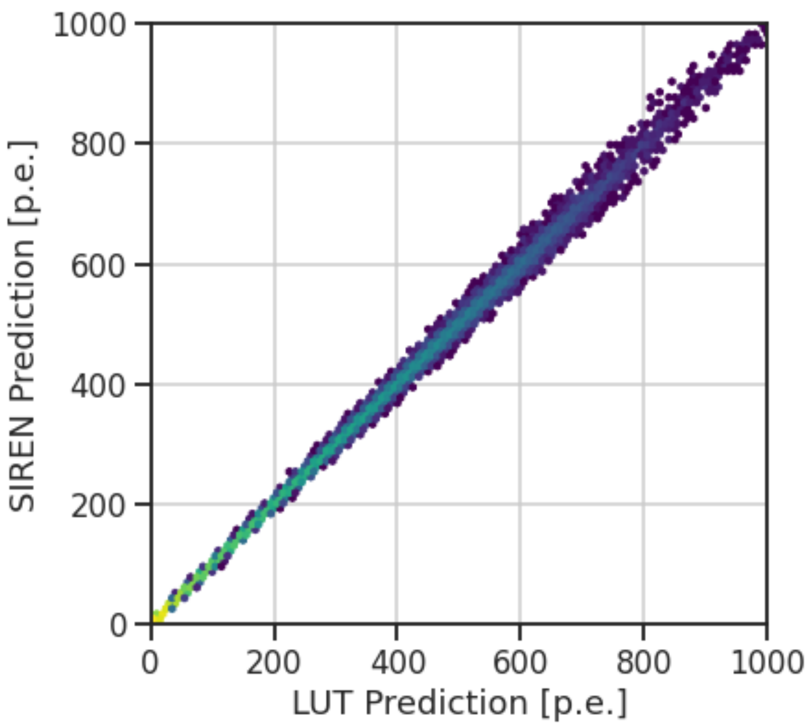
Note on SiPM Indexing



** Grayed out points are excluded from this analysis

- unclustered points, or
- portion of track in TPC-1

Charge-to-Light: SIREN v.s. LUT



- train a SIREN model using simulated data (i.e. LUT)
- point-source input
  - $\{x_i, y_i, z_i\}$ -> $\{vis_i^0, vis_i^1, \ldots, vis_i^{47}\}$
- calculate charge-to-light prediction
  - pred. ~ $\sum Q_i \, vis(r_i)$
- $vis(r_i)$: either from LUT or SIREN
- both methods are practically the same <<1% difference

Calibration of SIREN Model

Calibration => Multi-parameters optimization problem of the SRIEN model

Objective minimize the difference between observation and prediction

"effective light-yield"
for 48 SiPMs (floating)

visibility by SIREN
~7k parameters (floating)

Prediction for SiPM-j $\text{pred}_j = Y_j \times \sum Q_i \, \text{vis}_j(r_i)$

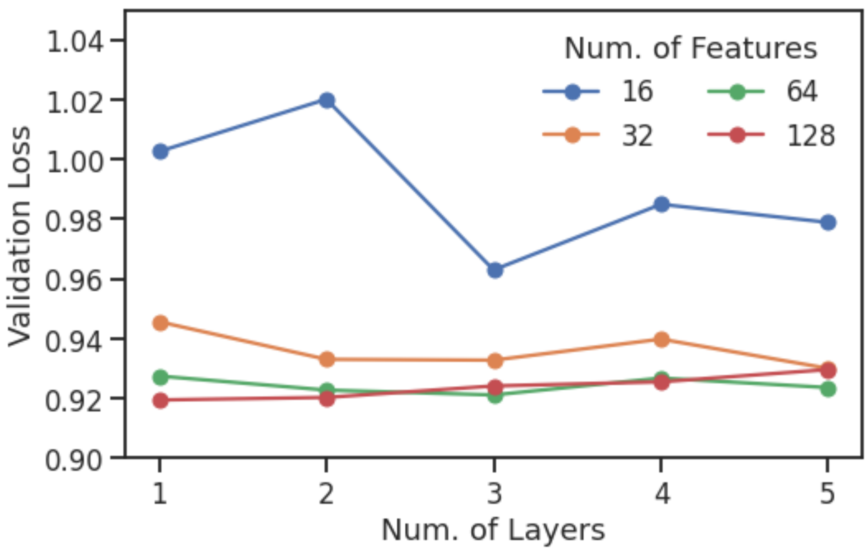
measured charge
of the track (fixed)

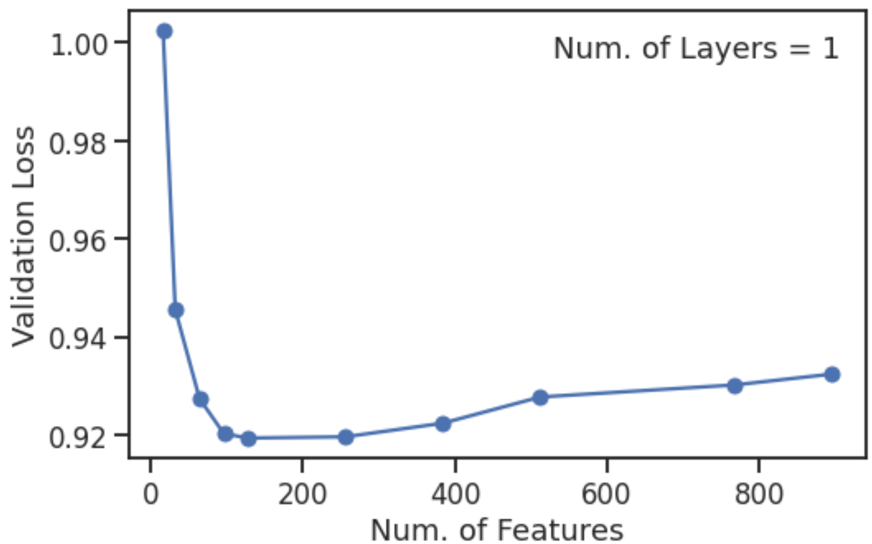
locations of charge
deposition (fixed)

Loss function $\text{chi2} = \sum_j (\text{obs}_j - \text{pred}_j)^2 / (\text{pred}_j + \varepsilon^2)$

ε = 5 p.e.

Hyper-Parameter Optimization w/ Data

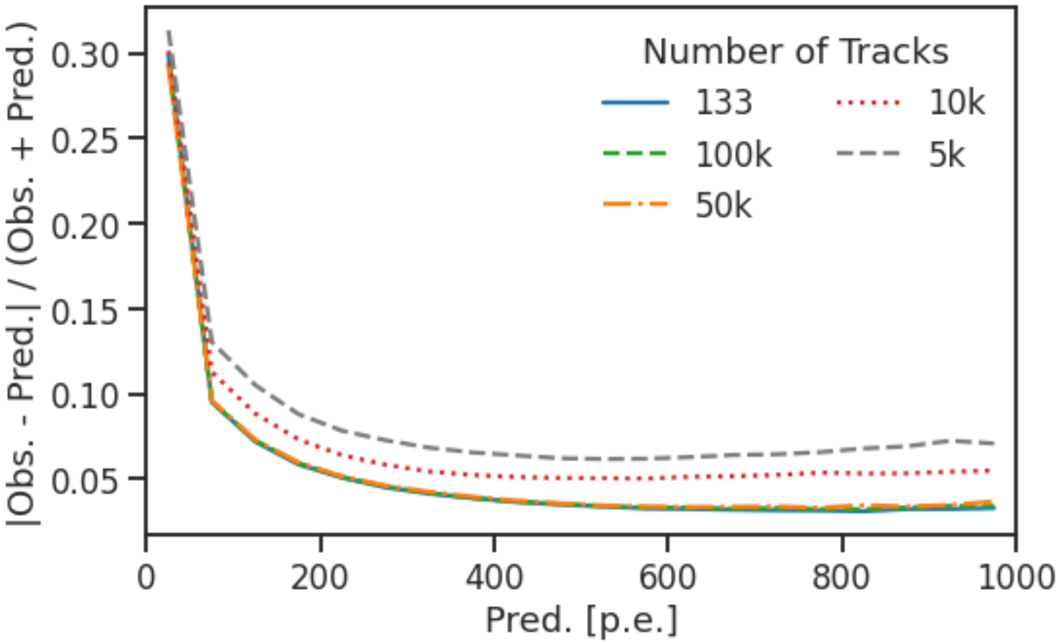




Optimal SIREN model for module-0 demonstrator

- determined by track data
- # of layers = 1
- # of features = 128
- ~23k parameters
- c.f. 12.6M for LUT in ~1 cm voxel size

How Many Tracks Needed?



- performance increase significantly from 5k to 50k tracks
- difference diminishes to ~0.1% from 50k and beyond
- *~100k tracks* are good enough to build a SIREN model for Module-0 demonstrator