# Neural Network Based Fast Optical Simulation Method in ProtoDUNE-VD

Minisymposium: Neutrino Science with the DUNE Experiment

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DPF-PHENO 2024, Pittsburgh

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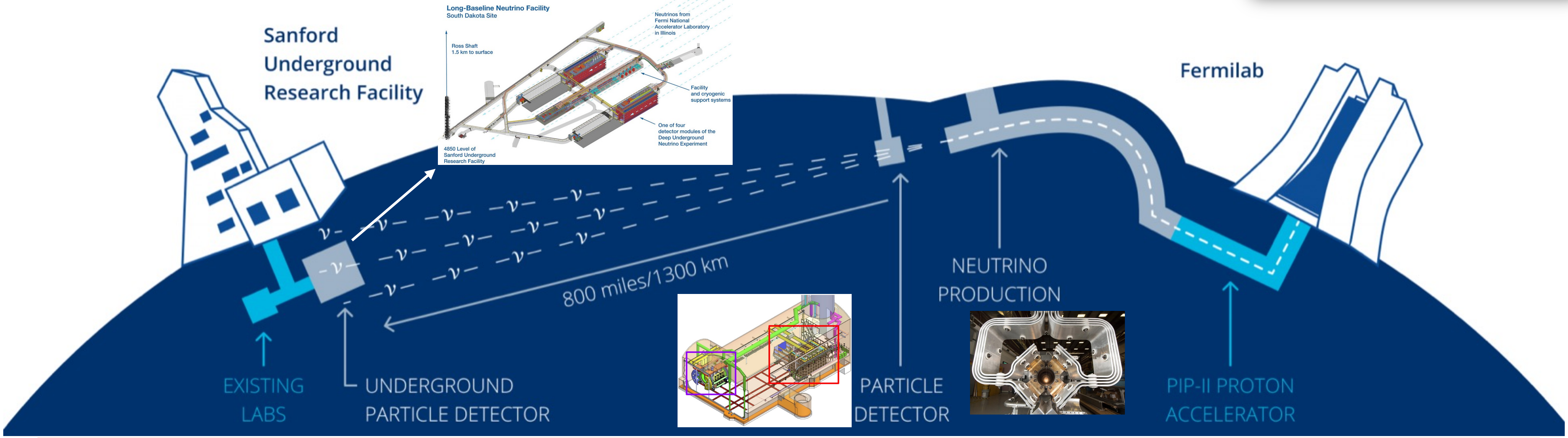
# Contents

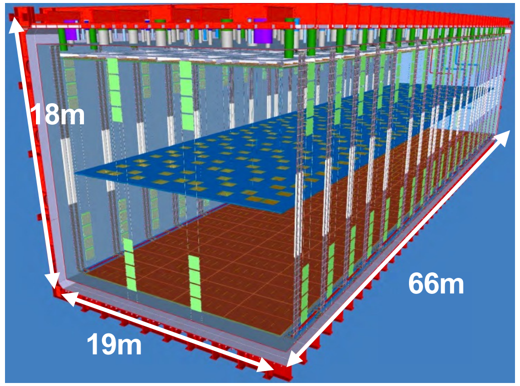
# Sketch of DUNE

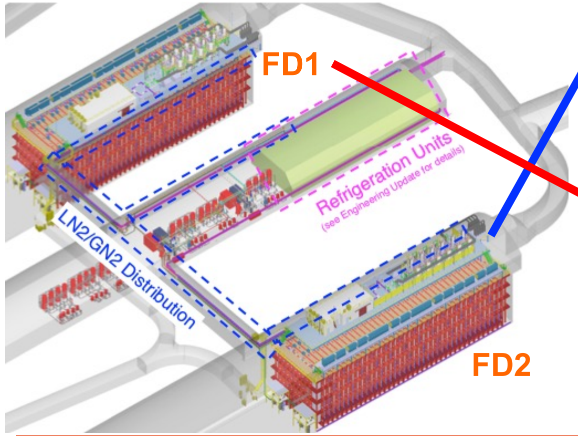
- DUNE: Deep Underground Neutrino Experiment
- Components: Beam (1.2MW, → 2.4MW); Near detectors (SAND, ND-LAr + TMS (PRISM)); Far detectors (FD1 & FD2: LArTPC, FD3 & FD4: Opportunities)
- Timetable: $\sim 2029$ start of science
- Collaborations: $> \mathbf{35}$ countries, $> \mathbf{200}$ institutions, $> \mathbf{1,400}$ collaborators

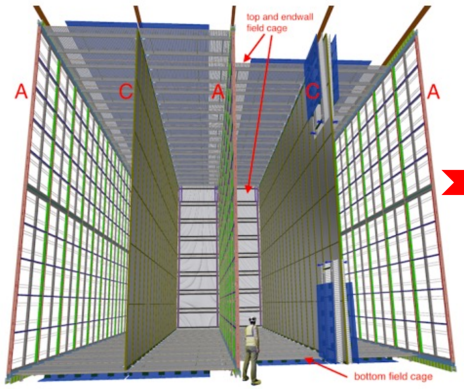



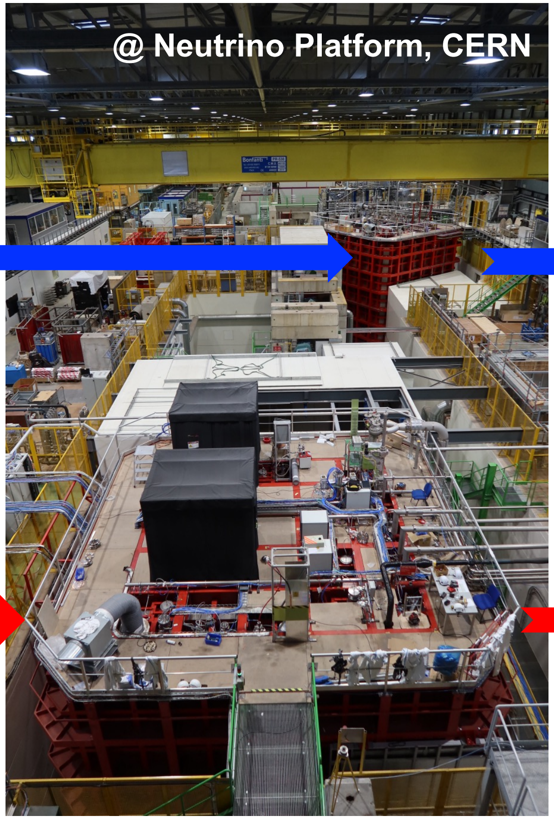
# DUNE Far Detectors & New ProtoDUNEs

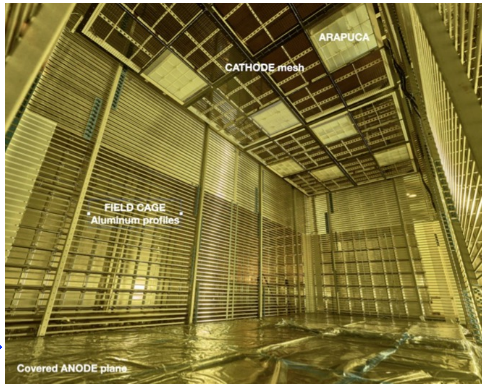
- FD1 & FD2: Cavern finished @ Feb 1, 2024! Construction underway
- FD1 / FD2 ⟶ protoDUNE- HD / VD: horizontal / vertical -drift LArTPC
- ProtoDUNE-HD: running NOW; ProtoDUNE-VD: run @ spring 2025

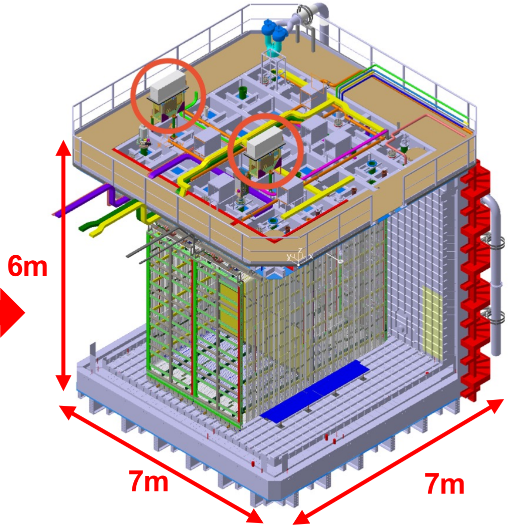



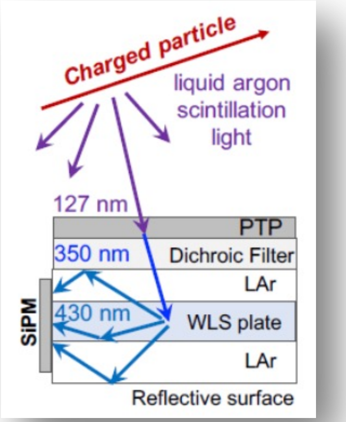



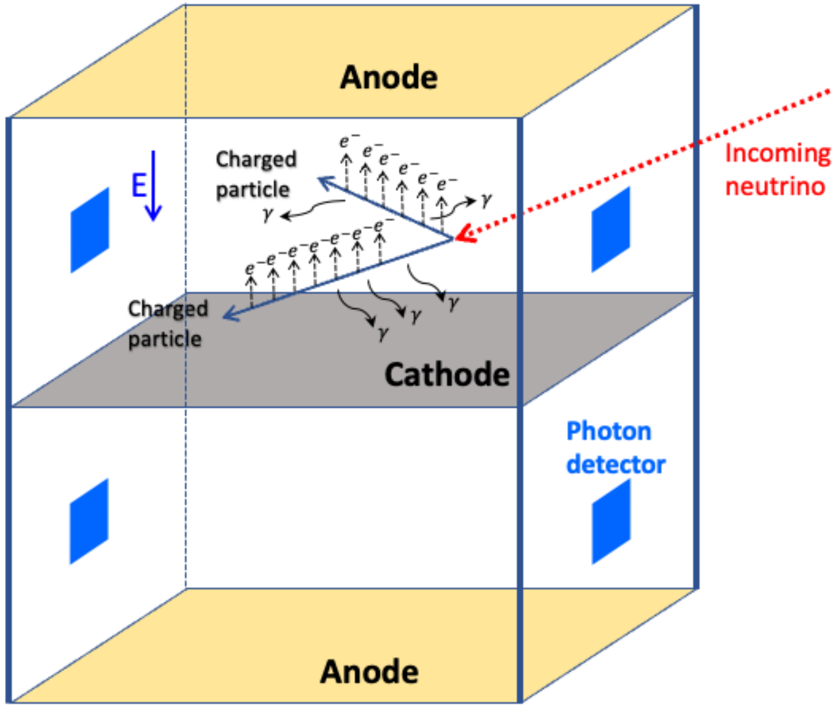



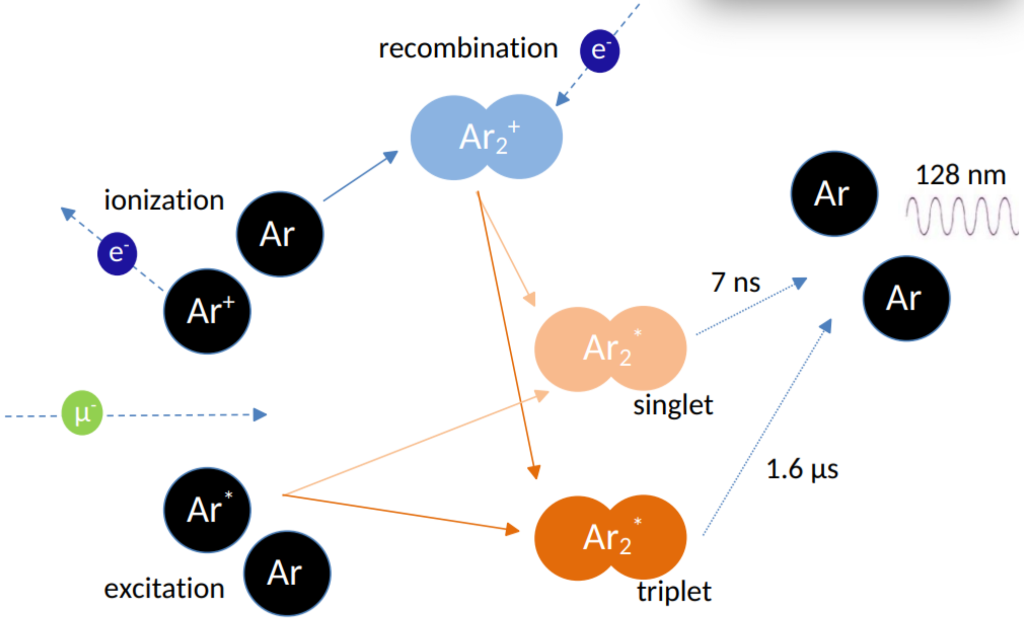
# LArTPC & Scintillation Light

- LArTPC: Liquid Argon Time Projection Chamber
- Scintillation light yield: $\sim 24{,}000\ \gamma/MeV$ @$500V/cm$, peaked at $9.7eV$
- Light components: fast component ($7ns$) , slow component ($1{,}600ns$)

Photon Detector of DUNE: X-Arapuca



# PDS of ProtoDUNE-VD

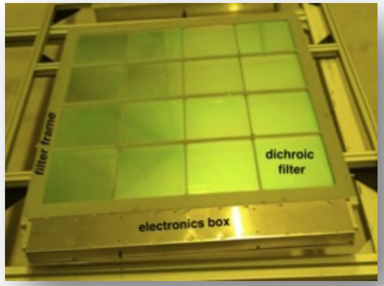
- Optical channels: **40**

  (**16** X-Arapucas + **18** PEN PMTs + **6** TPB PMTs)

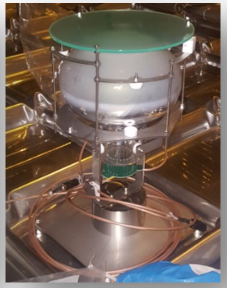
- Photon detection efficiency:

  X-Arapuca: ~3%,

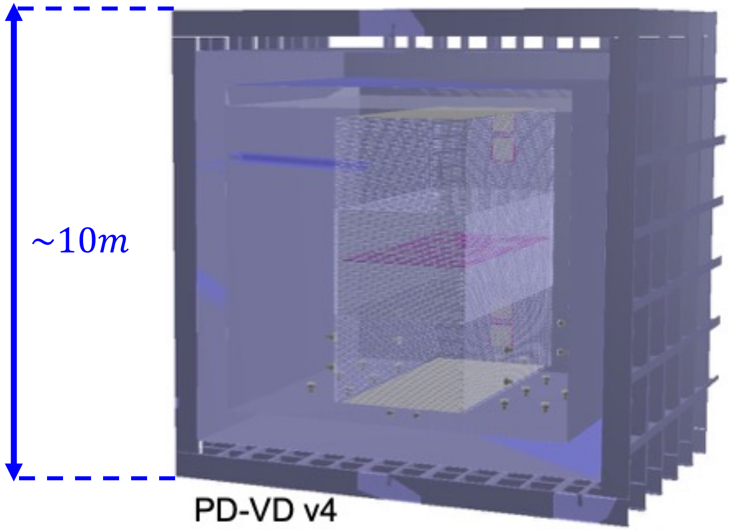
  PMT (PEN, TPB): ~20%



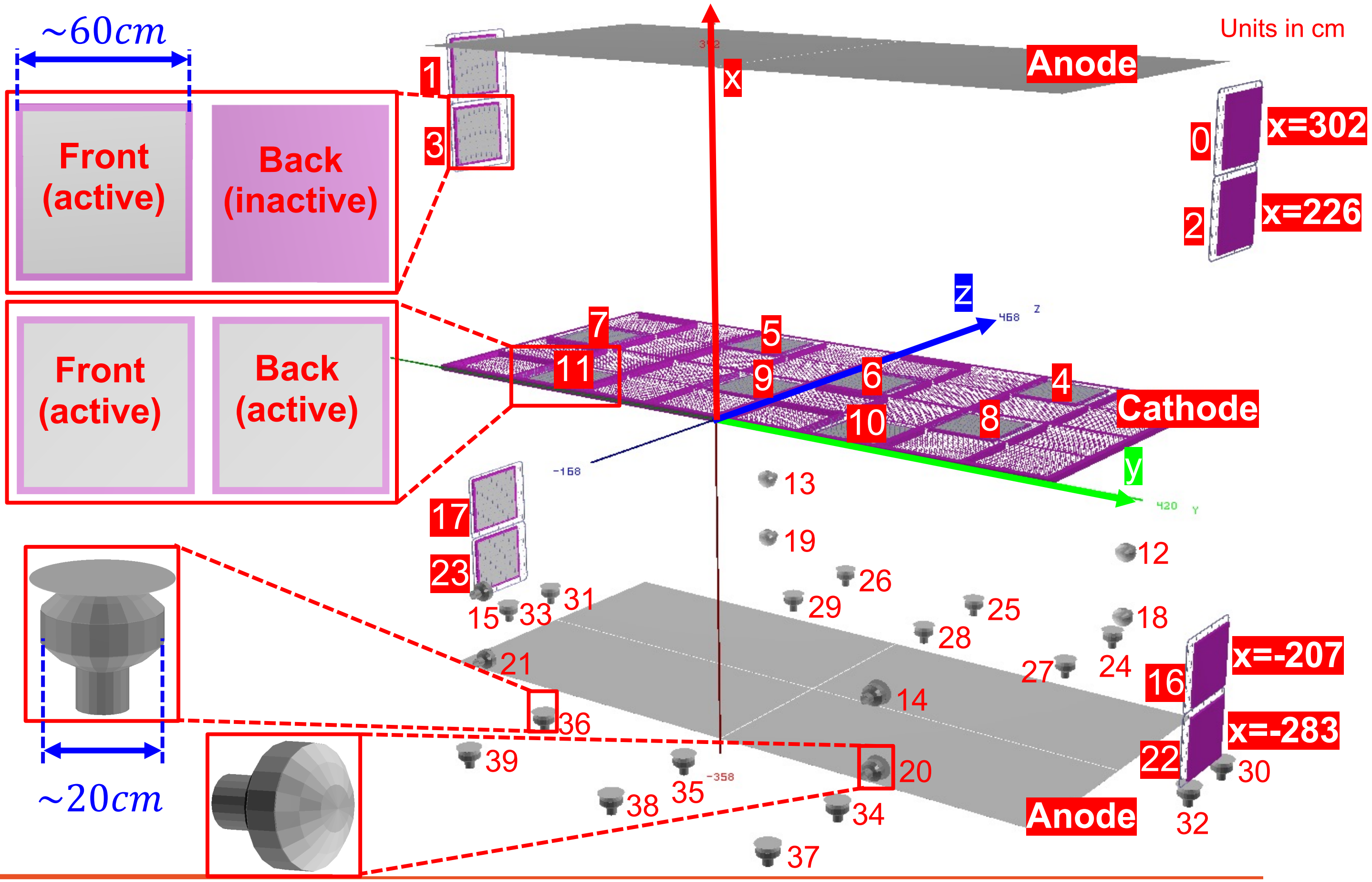
X-Arapuca


PEN PMT


TPB PMT

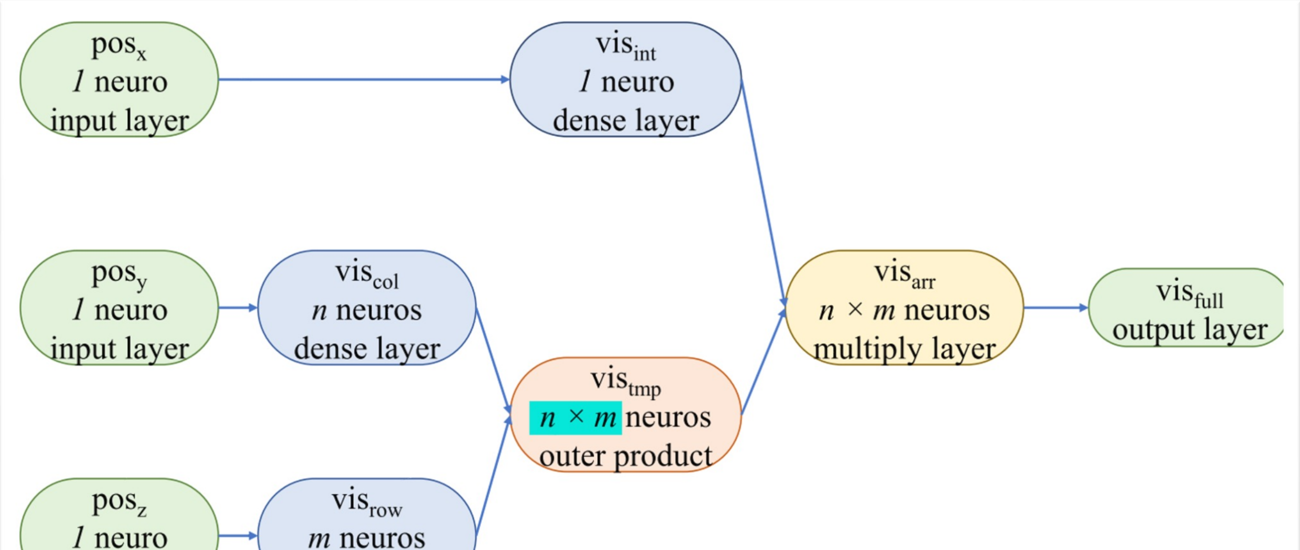


PD-VD v4



# Why Neural Network Method

- Traditional full light simulation (GEANT4): track every photon; Challenge for kT-scale LAr detector & GeV-scale energy deposition; **Giant** computational cost, very **slow**
- Network Based method (comp graph module): Given photon emission vertex, output visibilities of every optical channel directly; **Small** computational cost, $20 \sim 50$ times **faster**



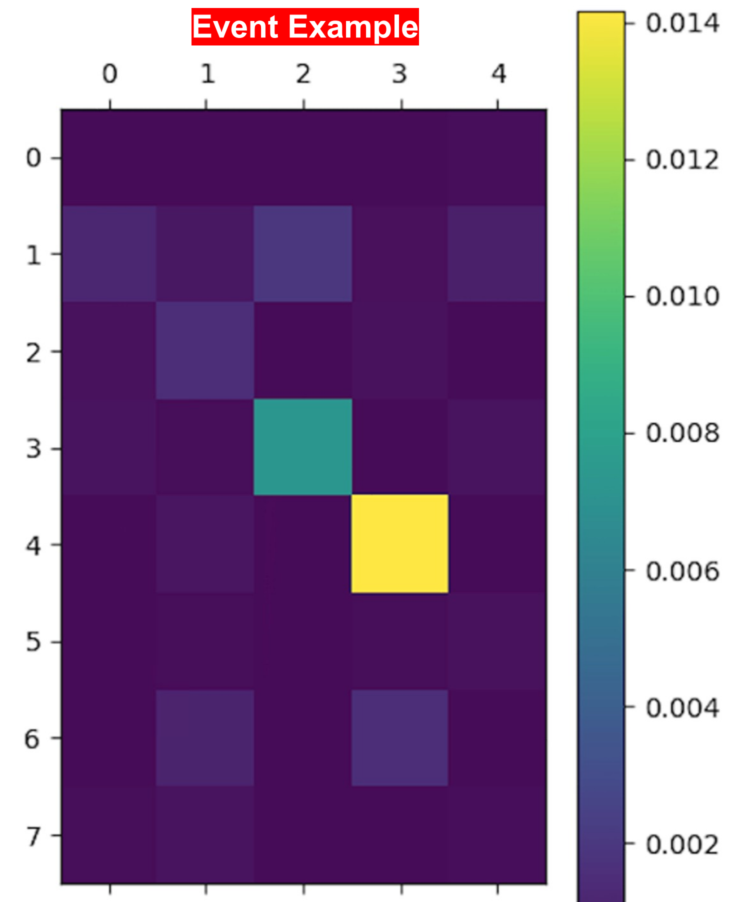

Credit to Alex Himmel & Mu Wei (Fermilab)

https://iopscience.iop.org/article/10.1088/2632-2153/ac58e2

# Training Sample Generation

- Based on LArSoft (GEANT4): track every photon, record photon emission vertex & responses of all 40 optical channels

| Space distribution of events | Uniform |
|---|---|
| Boundaries | $x \in [-375,\ 415]cm$, $y \in [-427.4,\ 427.4]cm$, $z \in [-277.75\ , 577.05]cm$ |
| Events # (training set, validation set, test set) | 1,700,000; 10,000; 10,000 |
| Events average Interval (training set) | $\sim \frac{800cm}{\sqrt[3]{1700000}} = 6.7cm$ |
| $\gamma$ emission vertex / event | # = $10^6$ , isotropic |
| Energy distribution of $\gamma$ | Gaussian with $(\mu, \sigma) = (9.69, 0.25)eV$ |
| Rayleigh scattering length (RSL) | $99.9cm$ @ $9.69eV$ |
| Absorption length (Abs) | $20m$ @ $9.69eV$ |
| Reflectivity considered | [ “STEEL_STAINLESS_Fe7Cr2Ni”, “Copper_Beryllium_alloy25", “G10”, “vm2000", “ALUMINUM_Al” ] |




- Each cube is one optical channel
- Color bar stands for $\gamma_{received}/10^6$

# Network & Training Details

- Optical Channels are divided into different groups based on their geometrical layout:

| | | | | |
|---|---|---|---|---|
| 0 ~ 3 | 4~ 11 | 12 ~ 15 | 16 ~ 17 | 18 ~ 21 |
| 22~ 23 | 24~ 29 | 30 ~ 33 | 34 ~ 39 | |

- Training parameters of network:

```
Total params: 162,922
Trainable params: 156,348
Non-trainable params: 6,574
```

- Training command & hyper-parameters:

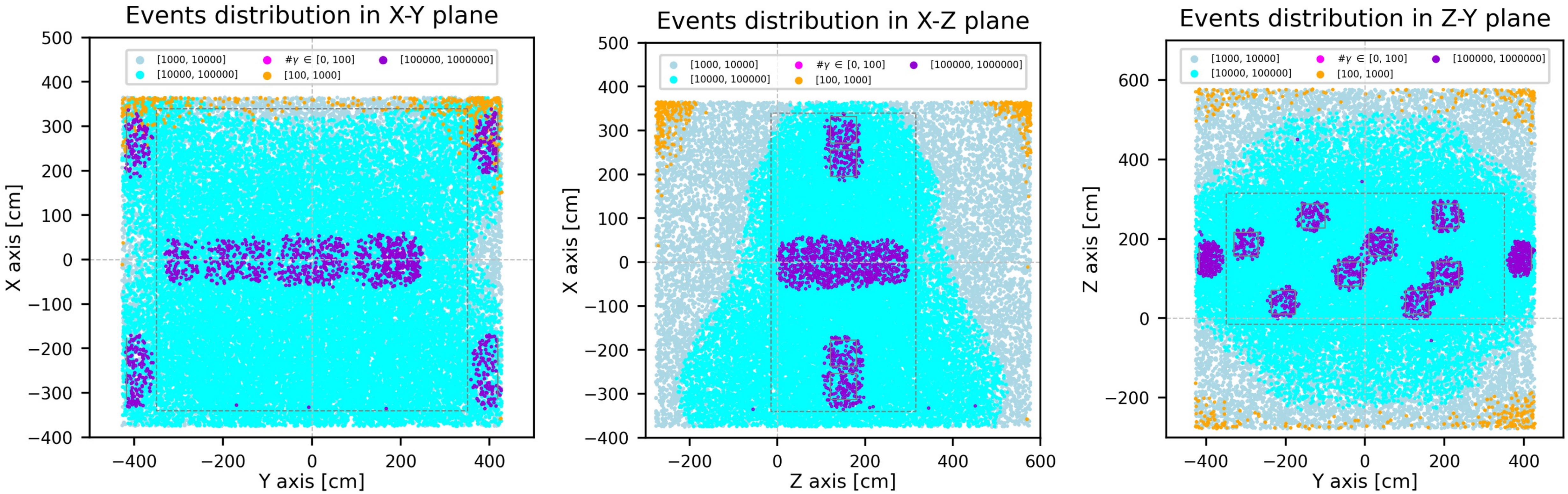
```
(tf_env) initial_train_3 ➤ python3 gnn_Muve/gnn.py -i ./dataSet/
train_18149Files -o output_2048b_10000e -t 0 -b 2048 -e 10000 -n
 18149 -d 40 --train > train_2048b_10000e.log
```

Network snippets

```
def model_protodunevd_v4(dim_pdr):#dim_pdr: num of opchannels
    pos_x       = Input(shape=(1,), name='pos_x')
    pos_y       = Input(shape=(1,), name='pos_y')
    pos_z       = Input(shape=(1,), name='pos_z')
    input_layer = [pos_x, pos_y, pos_z]

...
...

    #combine the nine blocks---
    feat_con = concatenate([feat_cov_1, feat_cov_2,
feat_cov_3, feat_cov_4, feat_cov_5, feat_cov_6, feat_cov_7,
feat_cov_8, feat_cov_9])
    feat_con = Dense(dim_pdr)(feat_con)
    feat_con = BatchNormalization(momentum=0.9)(feat_con)
    feat_con = ReLU()(feat_con)

    pdr     = Dense(dim_pdr, activation='sigmoid',
name='vis_full')(feat_con)
    model   = Model(inputs=input_layer, outputs=pdr,
name='protodunevd_v4_model')

    model.summary()
    return model
```

# Results & Evaluation (I)

- Events from validation set (#events = 93,190)
- For every event, photon numbers received by all optical channels are summed
- Results from Neural Network Module (**comp graph module**)





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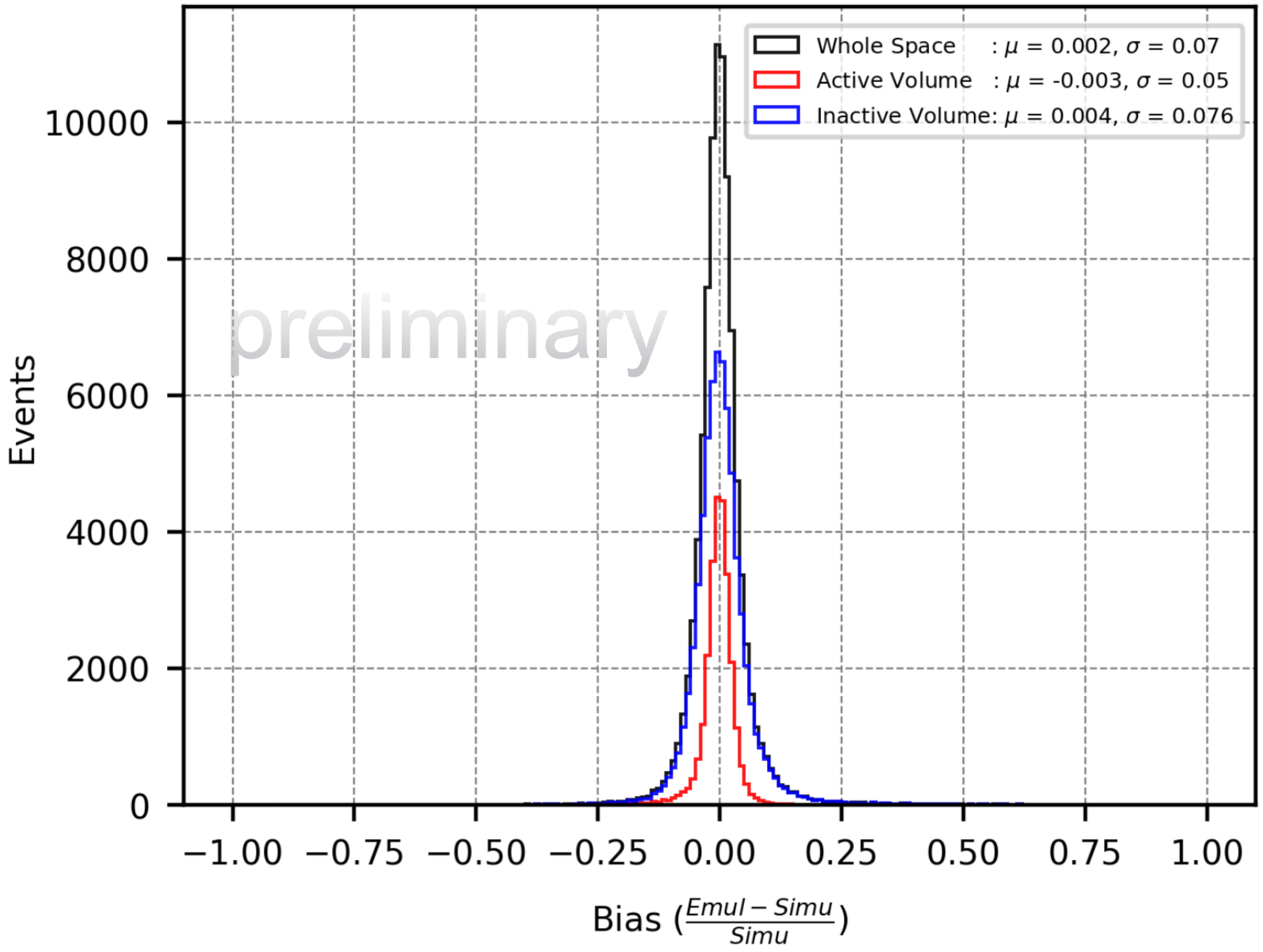
# Results & Evaluation (II)

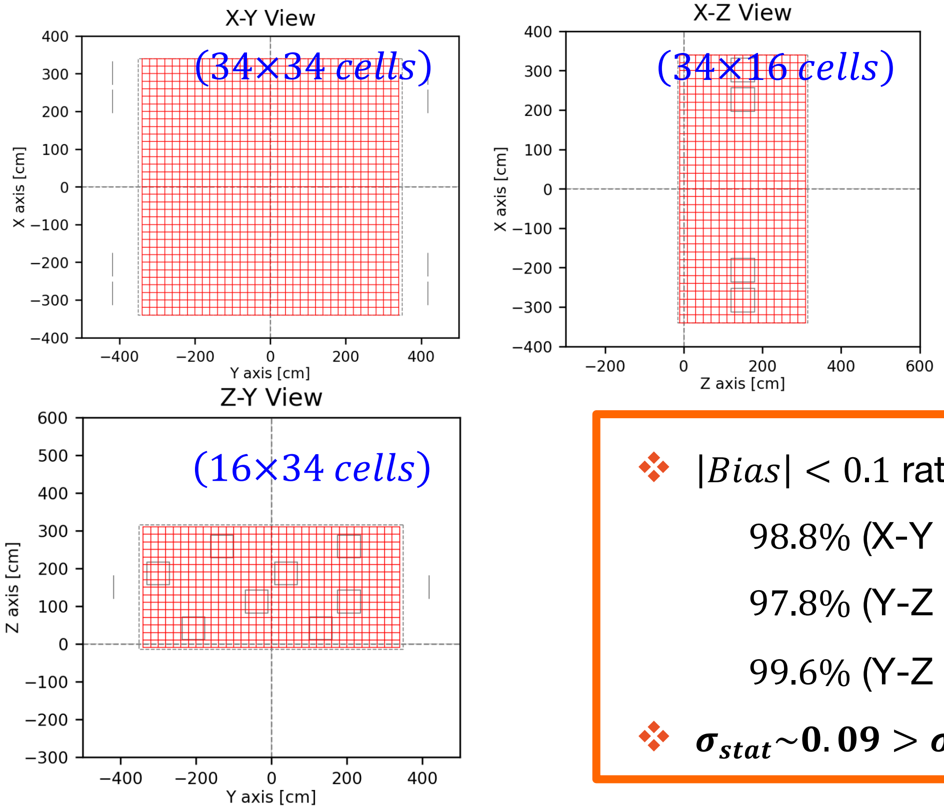


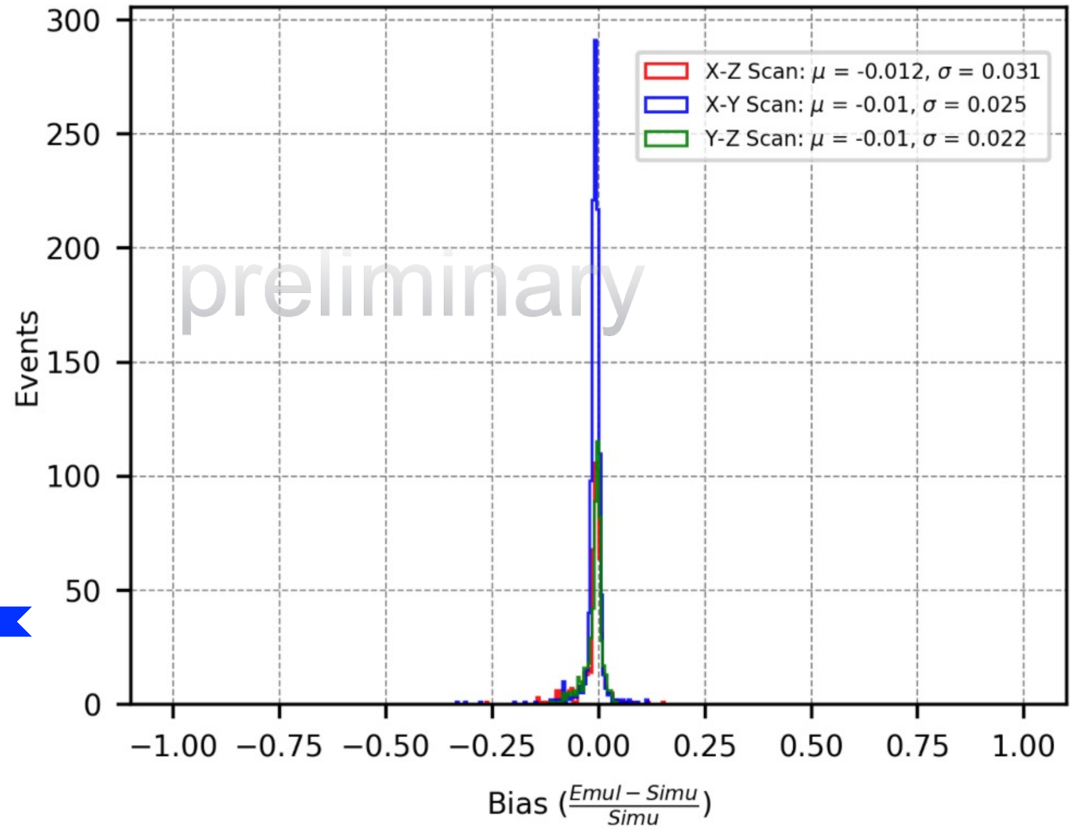

- Collective performance of all optical channels
- Emul: comp graph module; Simu: GEANT4
- Data point: sum up photon counts received by all opChs, then evaluate their difference
- Events distribution:

| | Whole Space | Active Volume | Inactive Volume |
|---|---|---|---|
| Total events num | 93,190 | 26,230 | 66,960 |
| Events with $\lvert Bias \rvert \leq 1$ | 93,045 (99.8%) | 26,210 (99.9%) | 66,835 (99.8%) |
| Events with $\lvert Bias \rvert \leq 0.1$ | 87,225 (93.6%) | 25,474 (97.1%) | 61,751 (92.2%) |

# Results & Evaluation (III)

- Optical channels need NOT to be sensitive to every point (vertex) in space
- “Track-like” evaluation: along certain axis (x, y, z), $\sigma = 20cm \times 20cm$, going trough whole cryostat
- Vertex num per event (cell): $305$




- $|Bias| < 0.1$ rate:
  - 98.8% (X-Y view)
  - 97.8% (Y-Z view)
  - 99.6% (Y-Z view)
- $\boldsymbol{\sigma_{stat} \sim 0.09 > \sigma_{Scan}}$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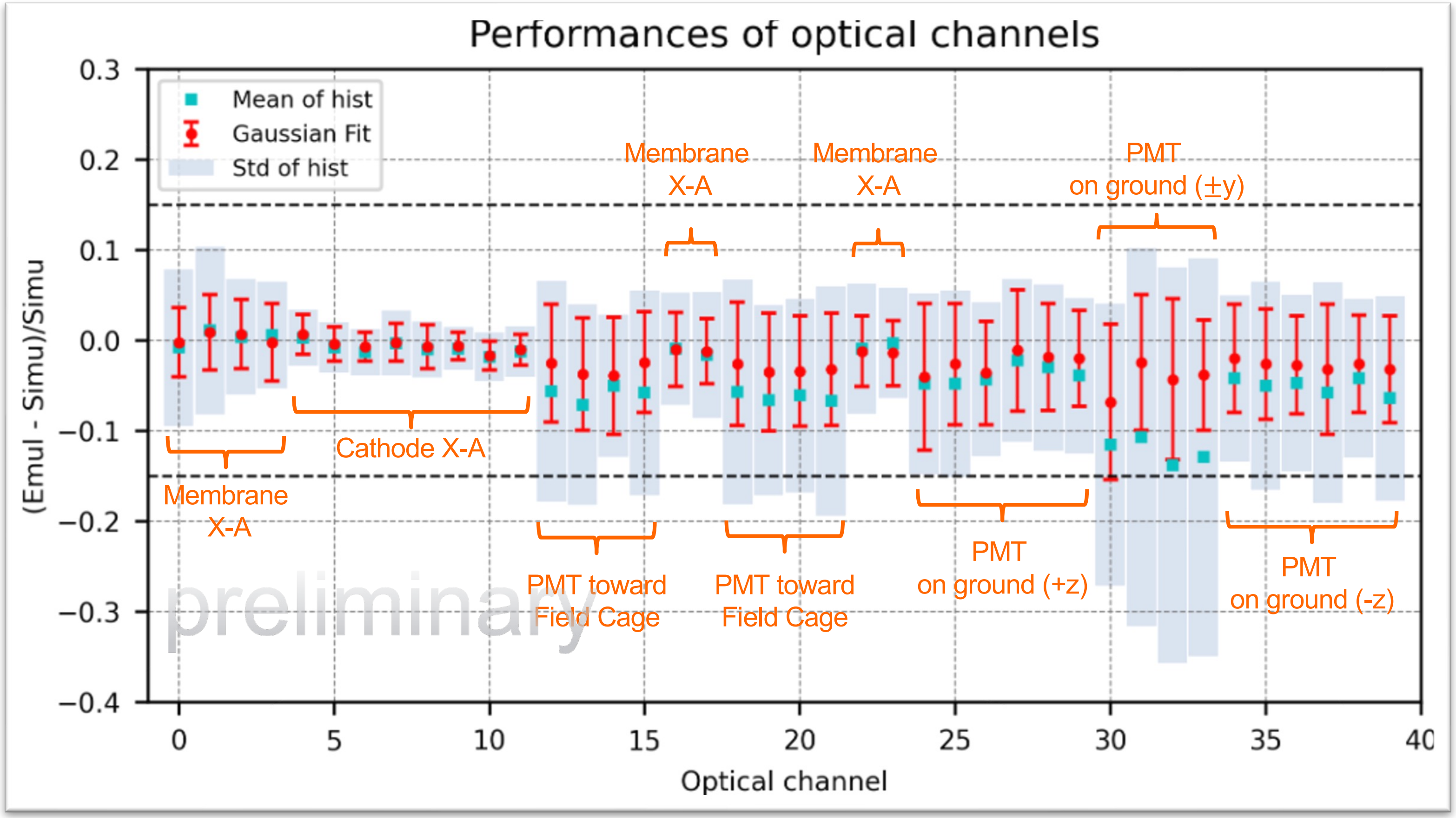
# Results & Evaluation (IV)

- Performances of most optical channels better than statistical fluctuation (expect: **15%**)
- Poor performances of opch30, 31, 32 & 33: Bad layout, higher stat fluctuation expected





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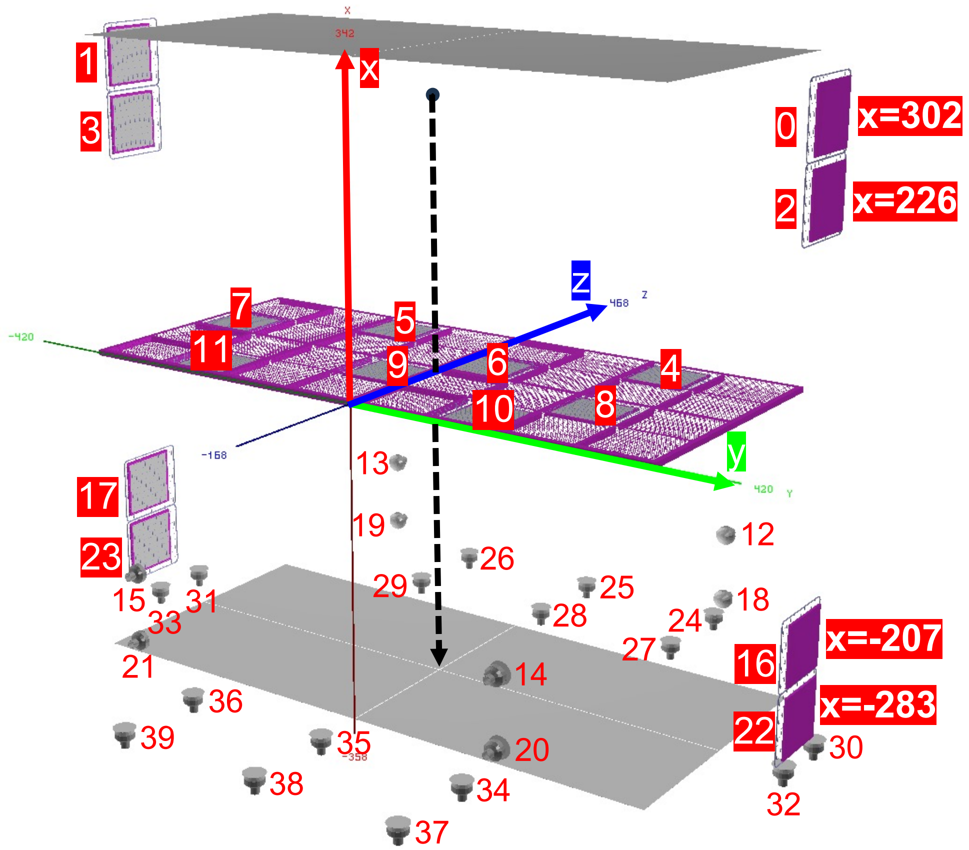
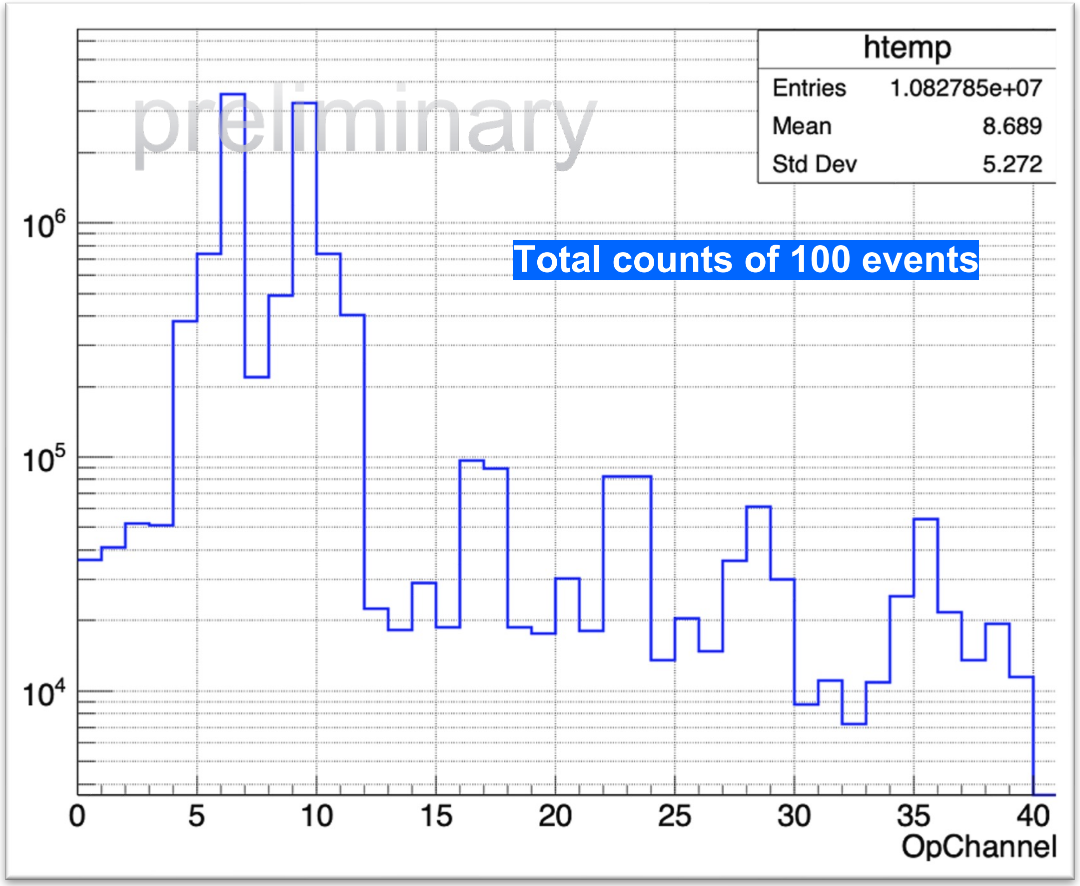
# Performance of Comp Graph Module

- 7GeV, $\mu^-$, $\# = 100$; starting at $(300, 0, 150)cm$, downward
- Simulation time: $\sim\mathbf{1}\boldsymbol{h}$



# Summaries

- Proper structure of neural network developed
- Collective performance of optical channels excellent @ point & track-like evaluation
- Most single optical channels perform well, uncertainty lower than statistical fluctuation
- Quick and reasonable optical simulation based on comp graph module observed
- Merged into DUNE LArSoft; now collaboration-wide available
- Further Steps:
    1. Develop Xe light fast optical simulation module based on this LAr light experience
    2. Make similar module for protoDUNE-HD
    3. Work on specific topic (ex: Rayleigh scattering length)

*Thank you!*

# Backups

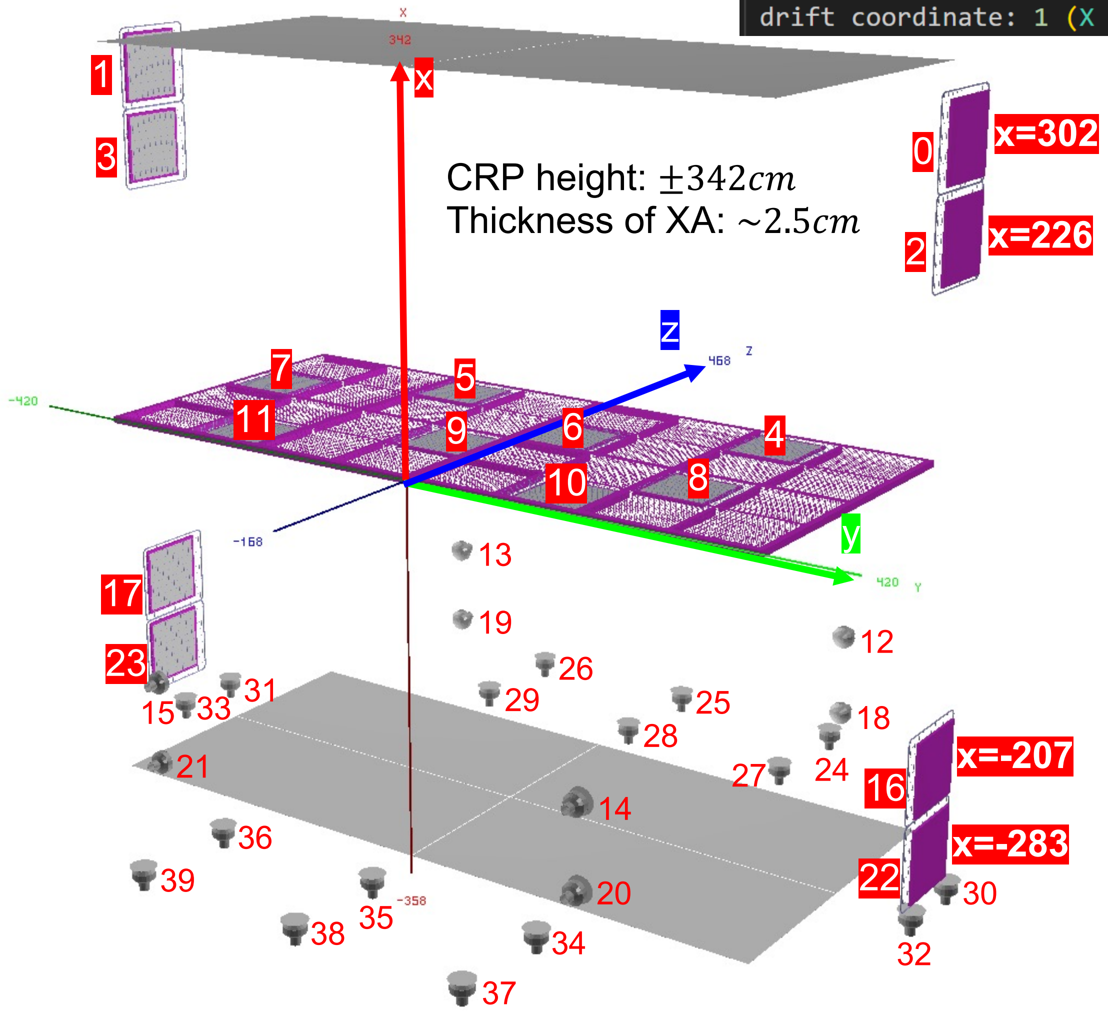
# OpCh Labels in v4 Geometry

Optical Channels positions: 40

| | | | |
|---|---|---|---|
| 0 | 302.18 | 417.61 | 149.65 |
| 1 | 302.18 | -417.61 | 149.65 |
| 2 | 226.38 | 417.61 | 149.65 |
| 3 | 226.38 | -417.61 | 149.65 |
| 4 | 0 | 205.65 | 258.525 |
| 5 | 0 | -131.35 | 258.525 |
| 6 | 0 | 39.15 | 187.275 |
| 7 | 0 | -297.85 | 187.275 |
| 8 | 0 | 205.65 | 112.025 |
| 9 | 0 | -39.15 | 112.025 |
| 10 | 0 | 131.35 | 40.775 |
| 11 | 0 | -205.65 | 40.775 |
| 12 | -205.9 | 221 | 380.988 |
| 13 | -205.9 | -221 | 380.988 |
| 14 | -205.9 | 221 | -68.1242 |
| 15 | -205.9 | -221 | -81.6884 |
| 16 | -207.23 | 417.61 | 149.65 |
| 17 | -207.23 | -417.61 | 149.65 |
| 18 | -281.7 | 221 | 380.988 |
| 19 | -281.7 | -221 | 380.988 |
| 20 | -281.7 | 221 | -68.1242 |

Beam enter point: $\sim(210, 150, 0)$

```
Cryo Boundaries
Xmin: -375 Xmax: 415 Ymin: -427.4 Ymax: 427.4 Zmin: -277.75 Zmax: 577.05
 drift coordinate: 1 (X direction)
```




| | | | |
|---|---|---|---|
| 21 | -281.7 | -221 | -81.6884 |
| 22 | -283.03 | 417.61 | 149.65 |
| 23 | -283.03 | -417.61 | 149.65 |
| 24 | -336.474 | 170 | 455.65 |
| 25 | -336.474 | 1.13687e-13 | 455.65 |
| 26 | -336.474 | -170 | 455.65 |
| 27 | -336.474 | 170 | 353.65 |
| 28 | -336.474 | 1.13687e-13 | 353.65 |
| 29 | -336.474 | -170 | 353.65 |
| 30 | -336.474 | 405.3 | 217.75 |
| 31 | -336.474 | -405.3 | 217.75 |
| 32 | -336.474 | 405.3 | 149.65 |
| 33 | -336.474 | -405.3 | 149.65 |
| 34 | -336.474 | 170 | -54.35 |
| 35 | -336.474 | 1.13687e-13 | -54.35 |
| 36 | -336.474 | -170 | -54.35 |
| 37 | -336.474 | 170 | -156.35 |
| 38 | -336.474 | 1.13687e-13 | -156.35 |
| 39 | -336.474 | -170 | -156.35 |

# RSL, Abs & Reflectivity

Rayleigh scattering length:

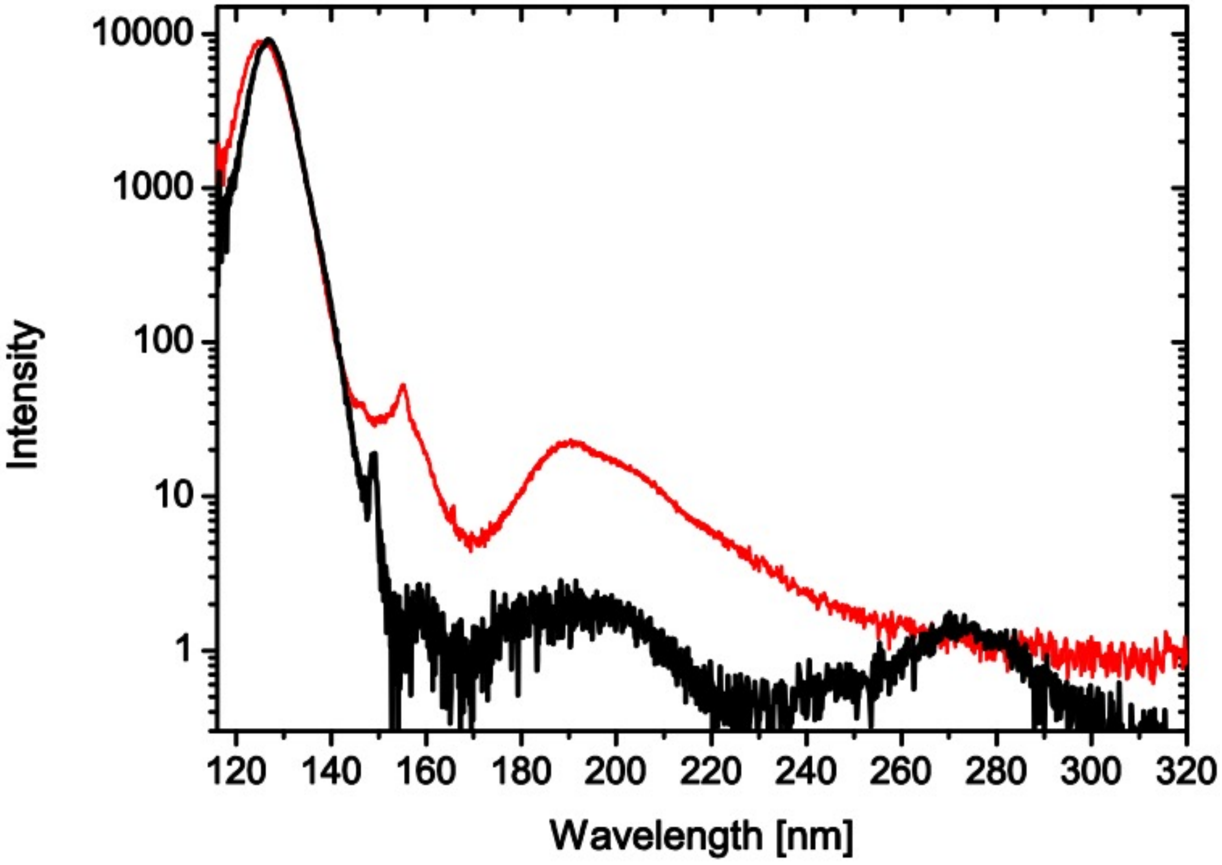
```
services.LArPropertiesService.RayleighEnergies: [1.18626, 1.68626, 2.18626, 2.68626, 3.18626, 3.68626, 4.18626, 4.68626, 5.18626, 5.68626, 6.18626, 6.68626, 7.18626, 7.68626, 8.18626, 8.68626, 9.18626, 9.68626, 10.1863, 10.6863, 11.1863]
services.LArPropertiesService.RayleighSpectrum: [1200800, 390747,  128633,  54969.1, 27191.8, 14853.7, 8716.9,  5397.42, 3481.37, 2316.51, 1577.63, 1092.02, 763.045, 534.232, 371.335, 252.942, 165.38,  99.9003, 51.2653, 17.495,  0.964341]
```

Absorption length:

```
services.LArPropertiesService.AbsLengthEnergies: [4,5,6,6.5,7,7.5,8,9,10,11]
services.LArPropertiesService.AbsLengthSpectrum: [2000,2000,2000,8000,8000,8000,2000,2000,2000,2000]
```

For more details, refer to photonFull_module0_sim.fcl @ https://drive.google.com/drive/u/1/folders/1x9Ux9kvIIA5VsE8mRrrKuzye1tel5owl

# Photon Spectrum of LAr




- Black: LAr, Red: GAr
- LAr: Peak @ **126.8**nm, FWHM: 7.8nm [122.9, 130.7]nm
  Energy: Peak @ 9.78eV, FWHM: 0.602eV

- Assuming Gaussian distribution (Not true…):
  $(\mu, \sigma) = (9.78, 0.256)eV$

**Normal distribution** [ edit ]

*See also: Gaussian beam § Beam waist*

If the considered function is the density of a normal distribution of the form

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$$

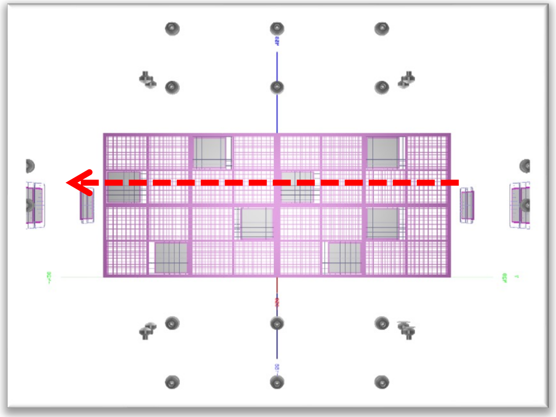
where $\sigma$ is the standard deviation and $x_0$ is the expected value, then the relationship between FWHM and the standard deviation is[1]

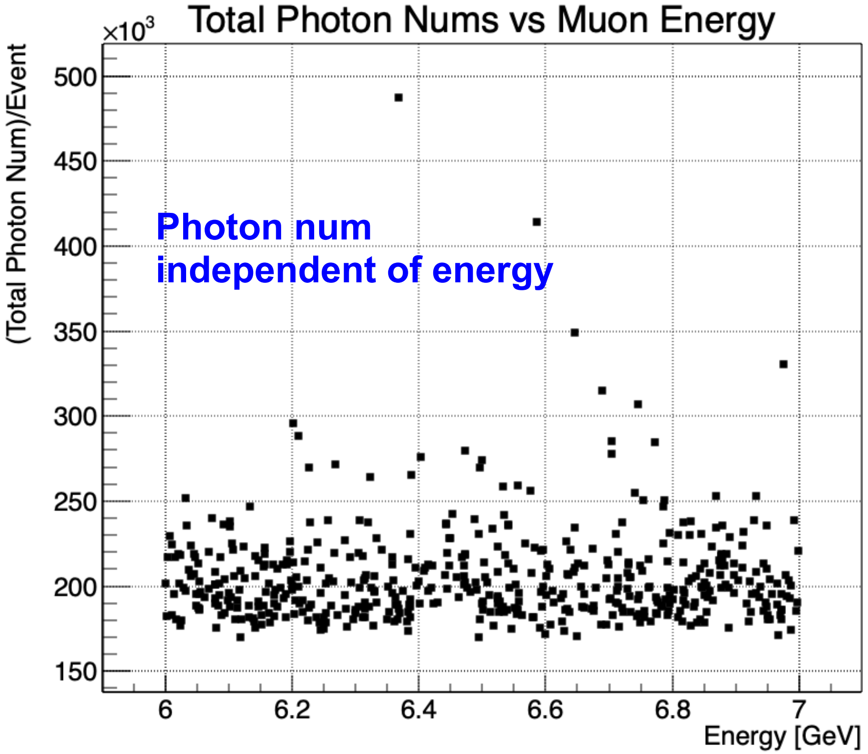
$$\mathrm{FWHM} = 2\sqrt{2\ln 2}\,\sigma \approx 2.355\,\sigma.$$

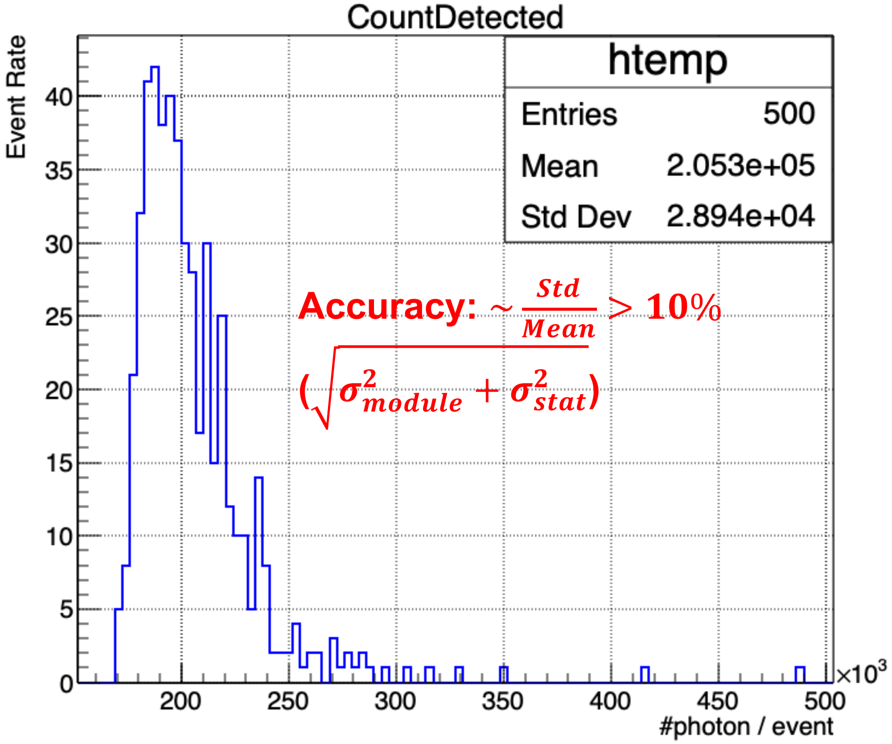
https://arxiv.org/ftp/arxiv/papers/1511/1511.07718.pdf
https://iopscience.iop.org/article/10.1088/1748-0221/15/09/P09009/pdf

# Statistical Fluctuation Estimation (I)

- Simulation details: $\mu^-$; $500$ nums; $[6,7]GeV$ uniformly distributed; detection efficiency: $3\%$
- Track: Starting point: $(x,y,z) = (50,350,187)$ ; toward $-y$ direction; $\delta x \times \delta z = 1cm \times 1cm$
- Computational graph module applied; Rayleigh scattering length: $99.9cm$; Absorption length: $20m$
- Fluctuation: higher than Poisson distribution, due to complicated processes (i.e. reflectivity, $\delta$ electron)






Accuracy: $\sim \frac{Std}{Mean} > 10\%$

$(\sqrt{\sigma^2_{module} + \sigma^2_{stat}})$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# Statistical Fluctuation Estimation (II)

- Performance of OpCh09: X-Arapuca on the cathode

$$\sigma_{total} \sim \frac{Std}{Mean} \sim \frac{4126}{21670} \sim 19\%$$

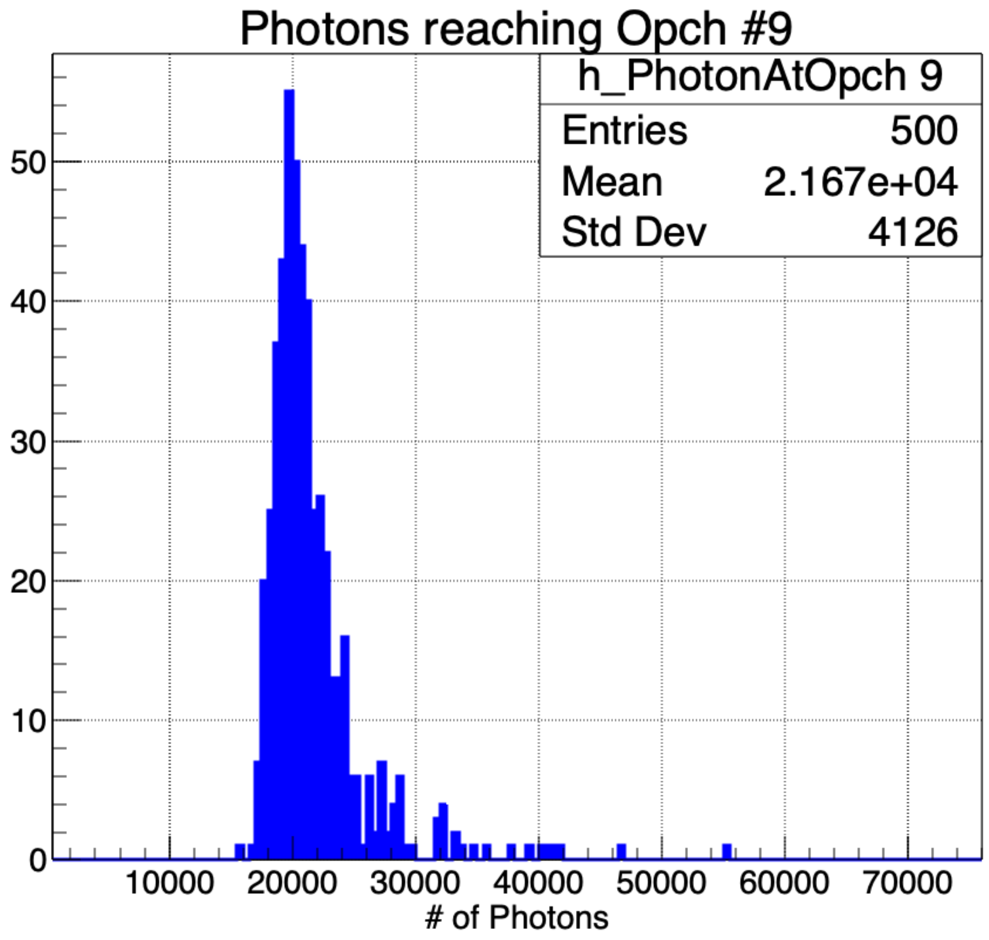
- Due to received photon numbers, and module fluctuation $\sigma_{mod}(C\ XA) < \sigma_{mod}(M\ XA) < \sigma_{mod}(PMT)$:

$$\sigma_{total}(PMT) > \sigma_{total}(Membrane\ XA) > \sigma_{total}(Cathode\ XA)$$

- Underestimation of Membrane X-Arapuca $\sigma_{stat}(M\ XA)$:

$$\sigma_{stat}(M\ XA) \sim \sqrt{\sigma^2_{total}(C\ XA) - \sigma^2_{module}(M\ XA)} \sim 15\%$$

- We can conclude $\sigma_{mod}(M\ XA) < \sigma_{stat}(M\ XA)$





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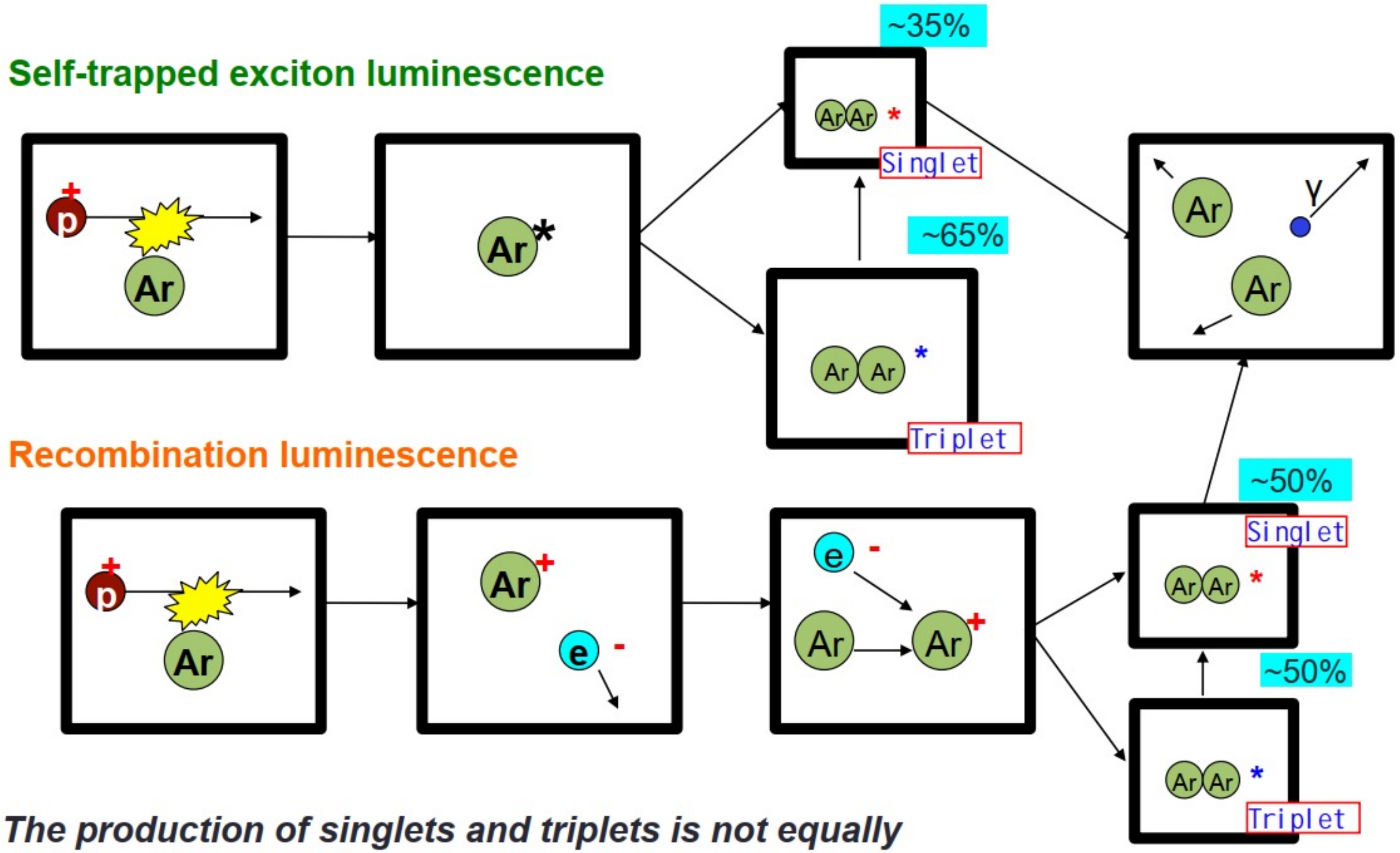
# LAr Scintillation Light Mechanism

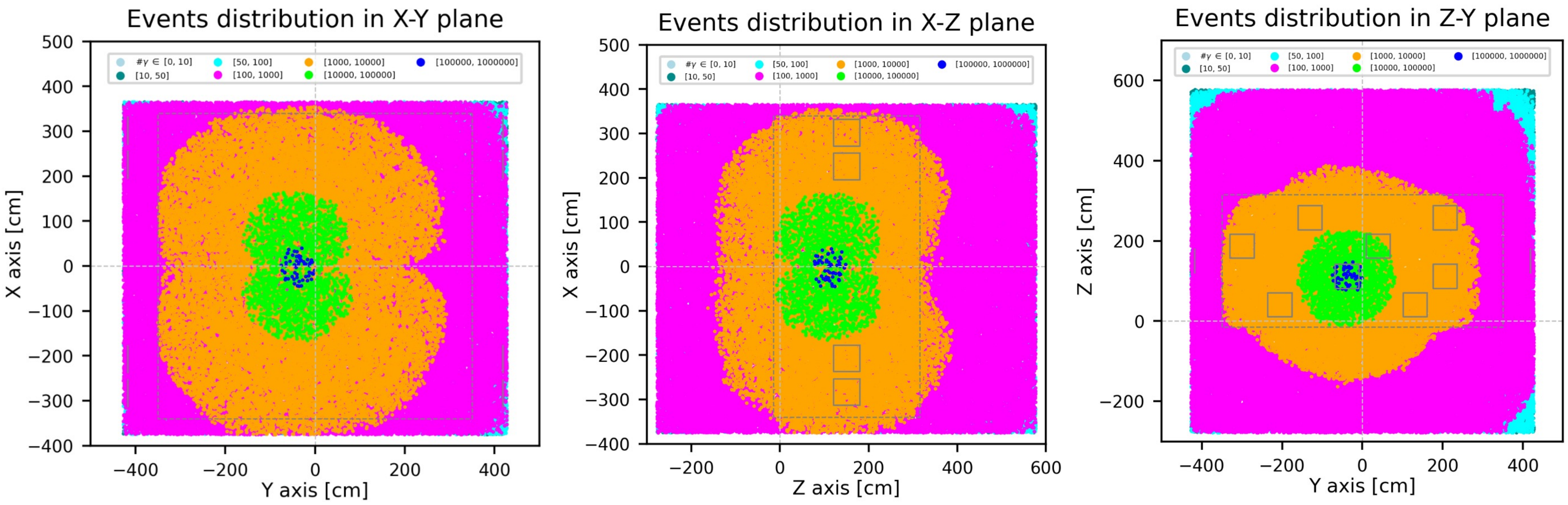



*The production of singlets and triplets is not equally weighted between the two processes* Can be used to PID!

From Ben Jones, MIT

# Photon Coverage of Single OpCh

- $10^6$ photons emitted per event / point.
- Response of optical channel 9, the X-Arapuca located at cathode





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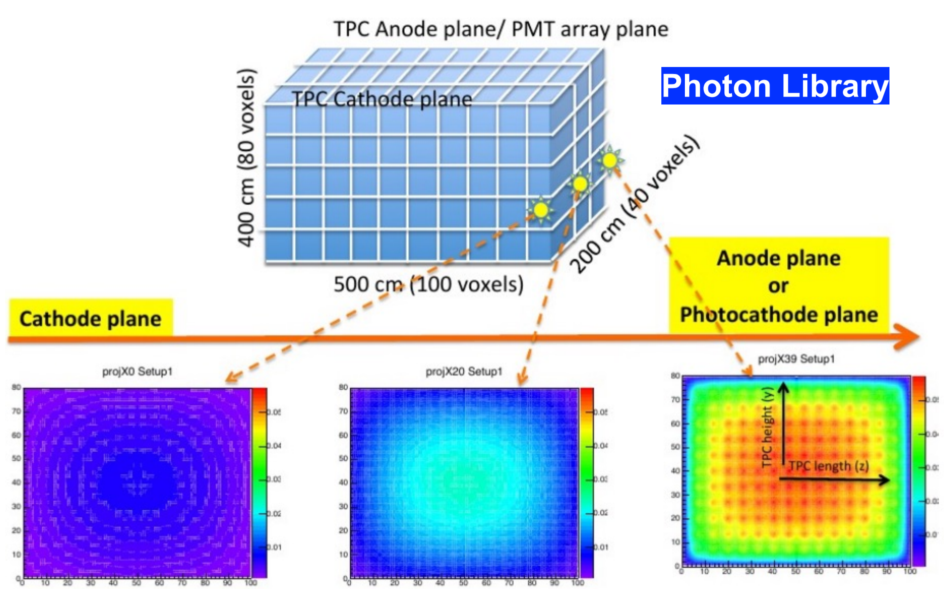
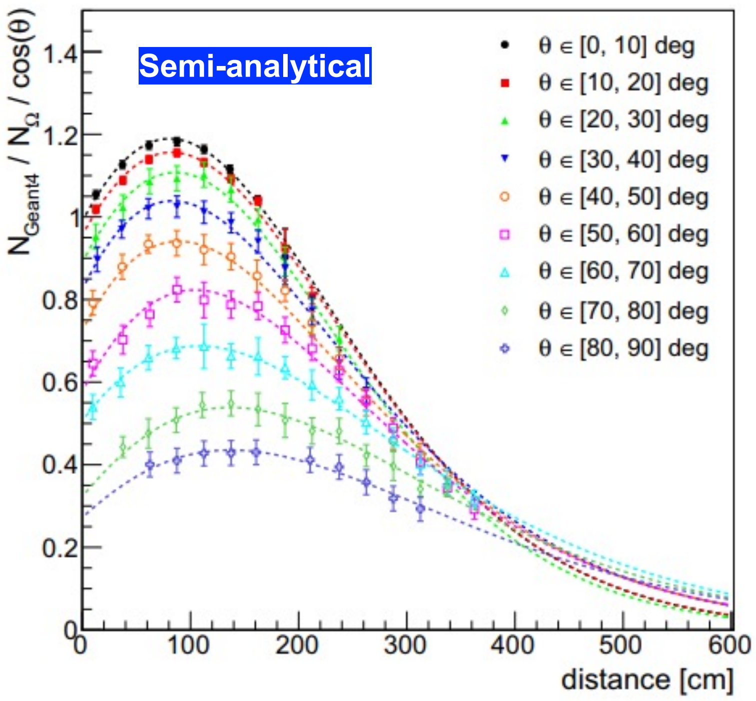
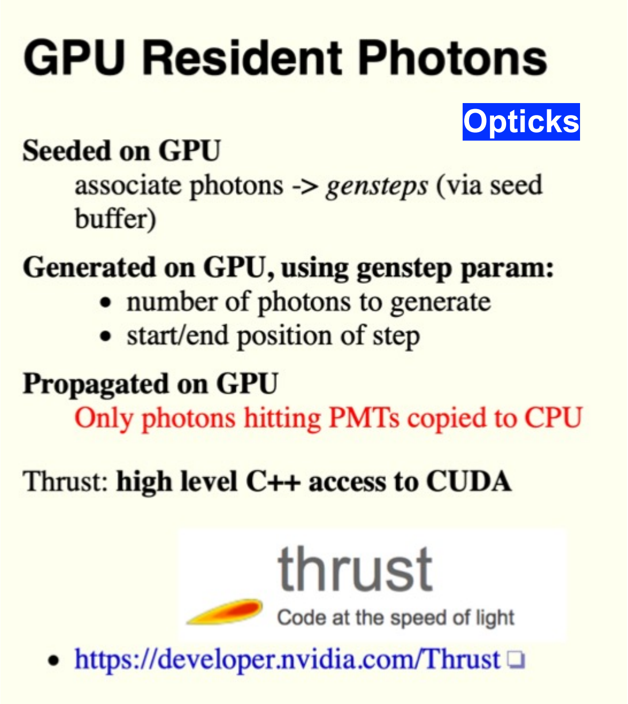
# Other Fast Optical Simulation Methods

- Photon library: https://wiki.dunescience.org/wiki/Fast_light_simulation_options
- Semi-analytical method: https://epjc.epj.org/articles/epjc/abs/2021/04/10052_2021_Article_9119/10052_2021_Article_9119.html
- GPU-based Opticks: https://indico.cern.ch/event/942142/contributions/4016049/attachments/2102768/3535523/Opticksnew3.pdf



# X