PIONEER LXe Calo Optical Simulations: Status & Next Steps

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TRIUMF

2024 PIONEER Collaboration Meeting

June 19, 2024

PIONEER LXe calorimeter simulators @ TRIUMF

- Working team:
  - LXe Calo prototype (Emma, Aleksey)
  - Complete LXe calo (Ben)
    - Jesùs (co-op student)

- Reminders:
  - Calo simulation meeting biweekly – Tuesdays @ 10 am PST: https://pioneer.npl.washington.edu/do/view/Internal/CaloSimMeetings
  - Ben and Emma wrote (and continue to update) a manual for the rootfile output of the MonteCarlo repository “sim” tree

LXe Calorimeter Simulation

- Overview:
  - complete simulation of the LXe calorimeter with ***optical photons***

- Goals

This talk
  - Understand how light is distributed in the calo
    - Effects from detector geometry, materials, fiducial volume?
    - What light do we see and where? Where do we need photosensors?
    - Align optics between LXe prototype (see Emma's talk tomorrow) and full calorimeter (detector talks tomorrow by Toshiyuki, Chloé)

Software workshop
  - Full calorimeter detector response and reconstruction
  - Identify pileup events with the calo, minimize their negative impact

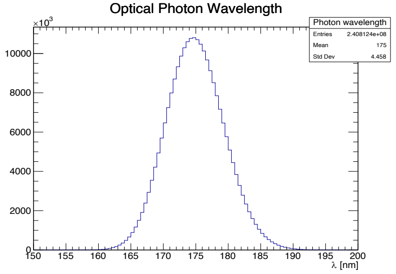
Liquid Xenon Optics

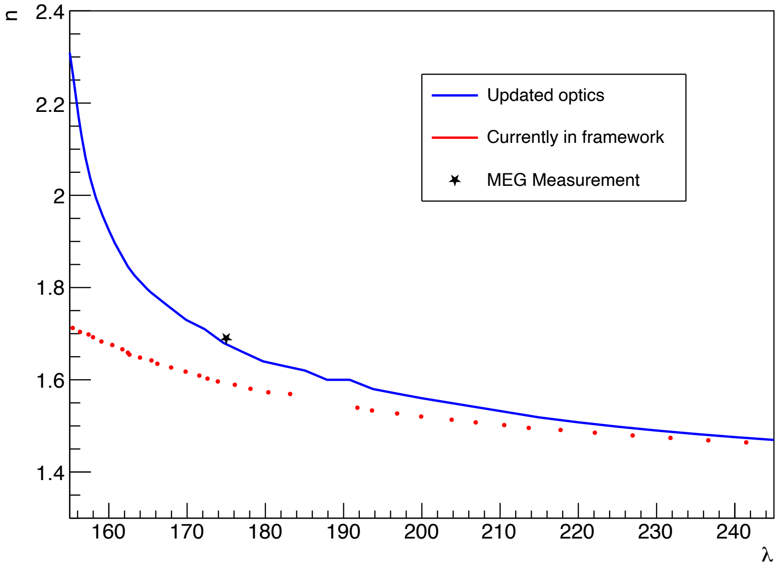
- Lit review by Ben & Emma
  - studies from MEG collaborators, theory, others: summarized in an Overleaf
- Optical parameters updated in simulation framework; some still need improvement
- Physics list: QGSP_BERT_EM4
- Updated:
  - refractive index vs wavelength (see plot)
  - light yield: 45,000 photons / MeV
  - scattering length (Rayleigh scattering)
  - also quartz optical properties
- Revisit:
  - absorption length - 1.5 m
    - Assume purity is better than 1 ppb of oxygen
  - fast & slow decay constants – 45 ns

Kobayashi, 2022 (MEG PhD thesis)

Table 2.10: Standard configuration of simulation for the LXe detector.

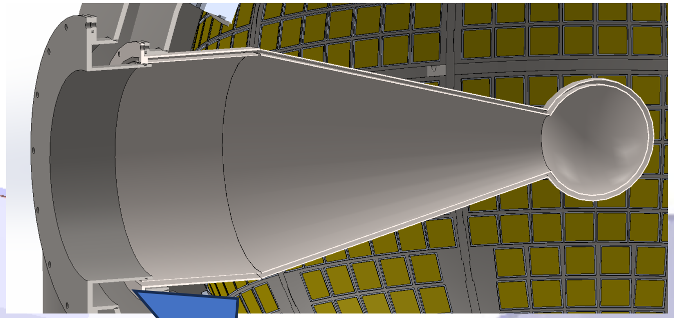
gem4	
Geant4 version	4.10.06.p03
Physics list	G4EmStandardPhysics
W-value for electron [eV]	21.6
W-value for α-particle [eV]	19.6
Scintillation Wavelength (mean) [nm]	175
Rayleigh scattering length [cm]	45
Absorption length [cm]	500
Refractive index of LXe	1.69
Reflectivity of PMT holder	0.5
PDE (MPPC / PMT)	0.12/0.16
Scintillation time constant [ns]	22 (fast) / 45 (slow)

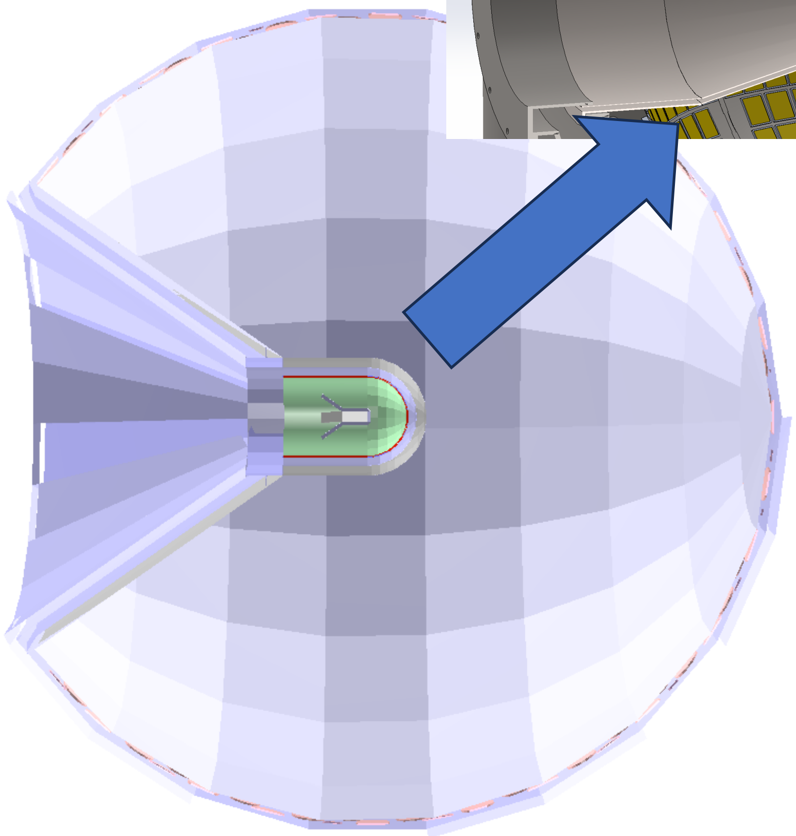




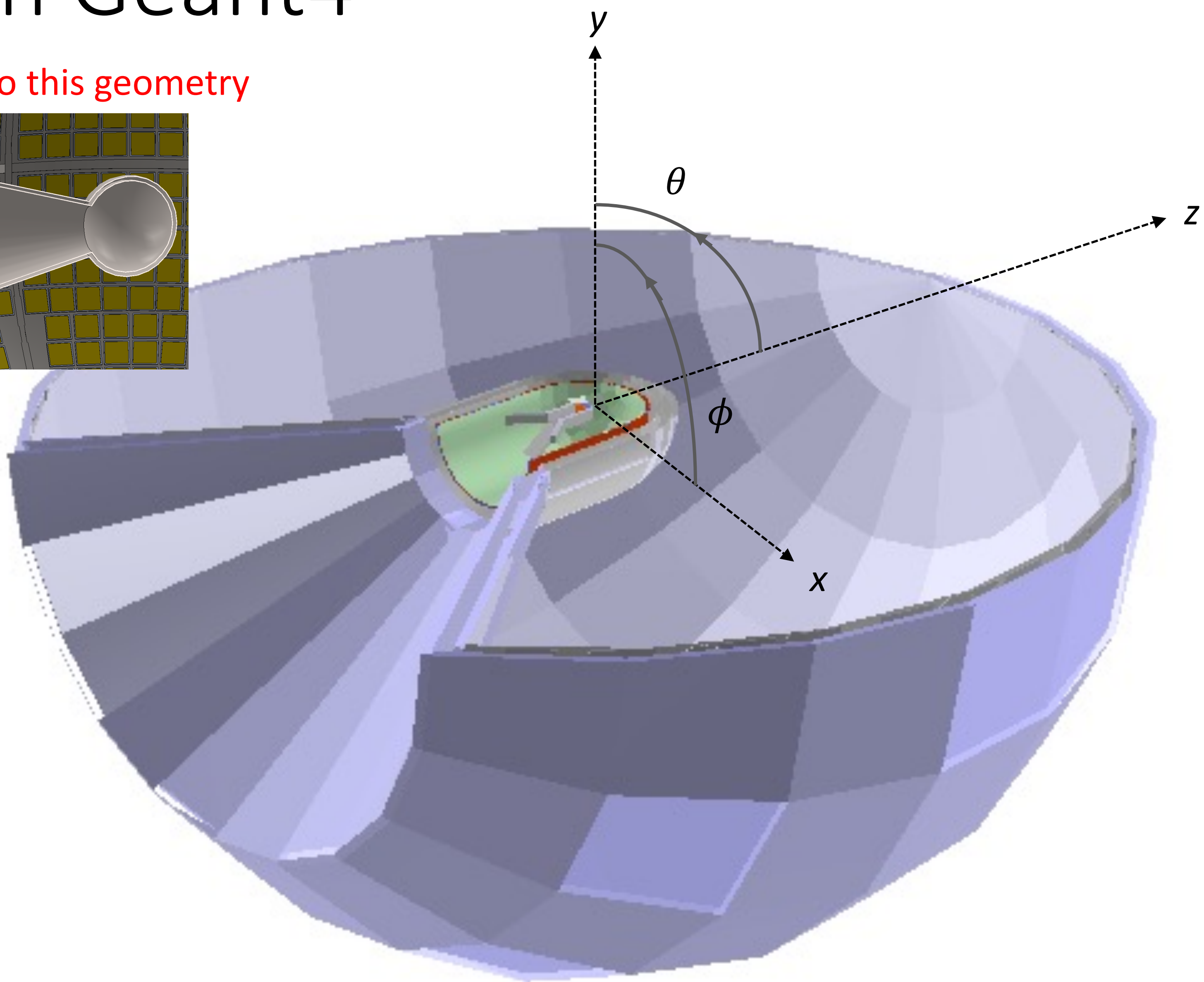
LXe Calorimeter in Geant4

"keyhole" – will move to this geometry





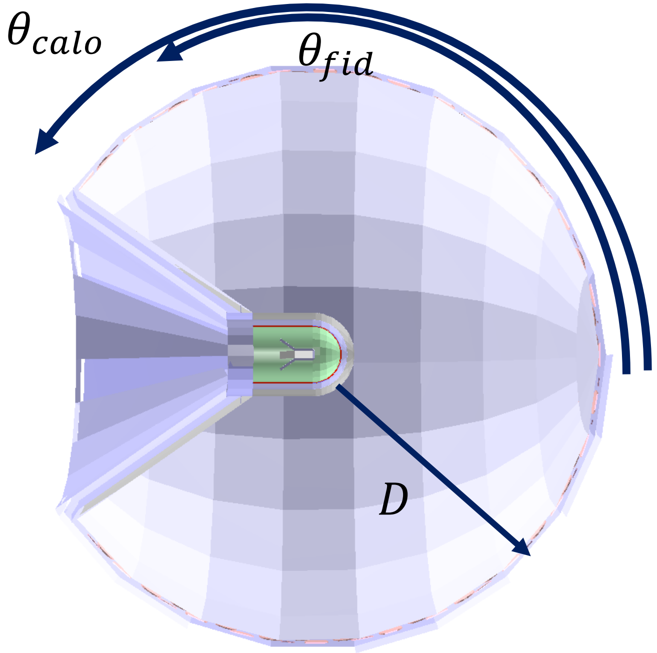
"Pacman" bullet – current geometry

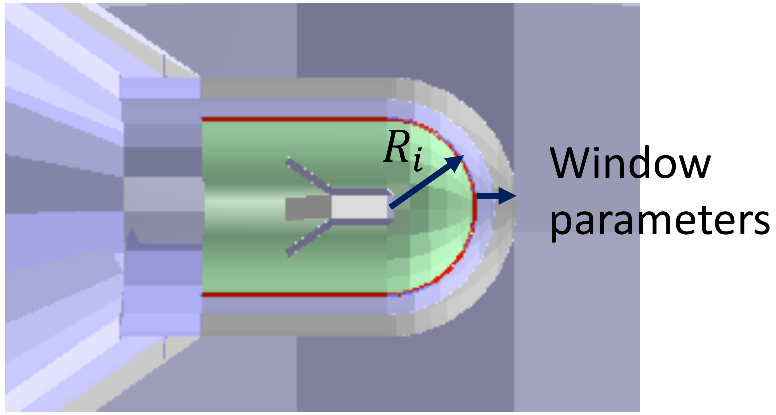


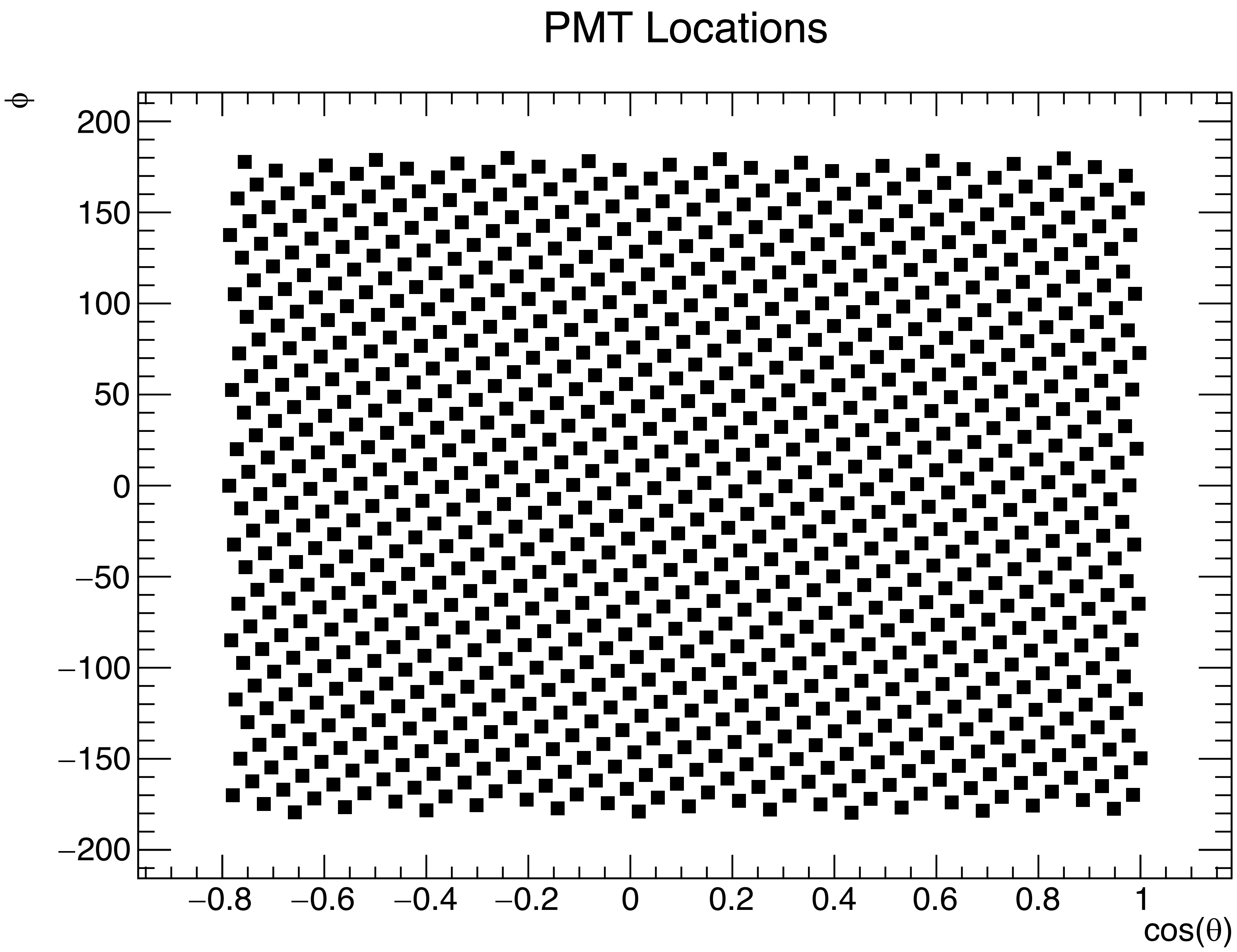
LXe Simulation Geometry – Current setup

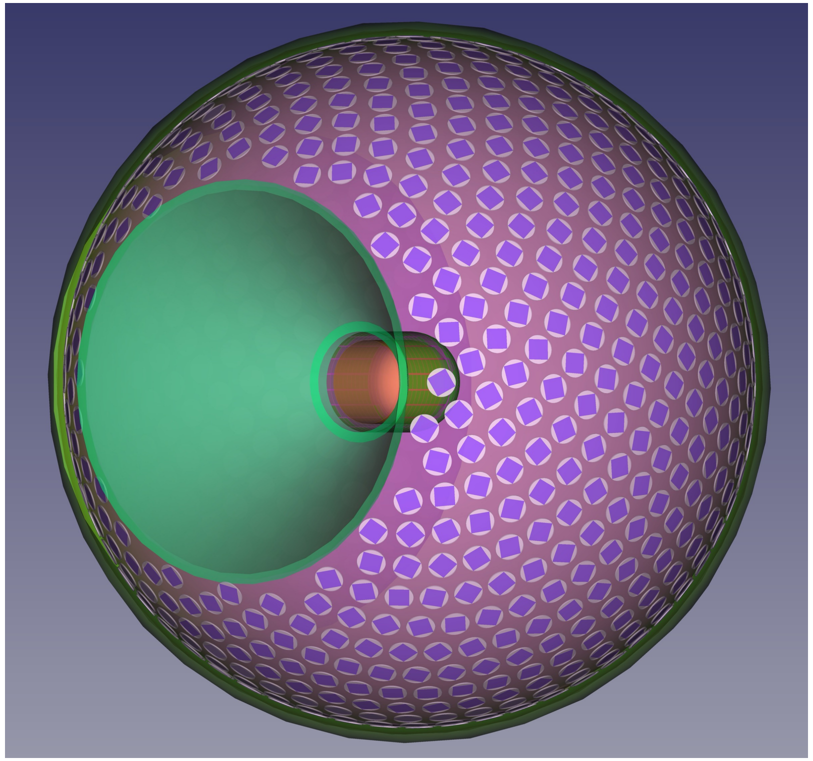
- θ_{calo} = 145°; R_i = 10 cm
- D = 25 radiation lengths (70.24 cm)
- 1000 PMTs uniformly distributed on outer shell
  - Hamamatsu model R12699-406-M4
  - Square: 48.5 mm x 48.5 mm
  - Quartz window with 2.5 mm thickness

- Window:
  - 500 µm Al – 2 cm vacuum - 200 µm Ti-Al alloy
  - (TRIUMF summer student Jesùs working on geometry studies)
- Simulation (calo-only):
  - 100,000 events (ScintScale = 0.2) each of:
  - muons decay from rest at center of calo (Michel)
  - $\pi \rightarrow e\nu$ - forced decay from rest (pienu)





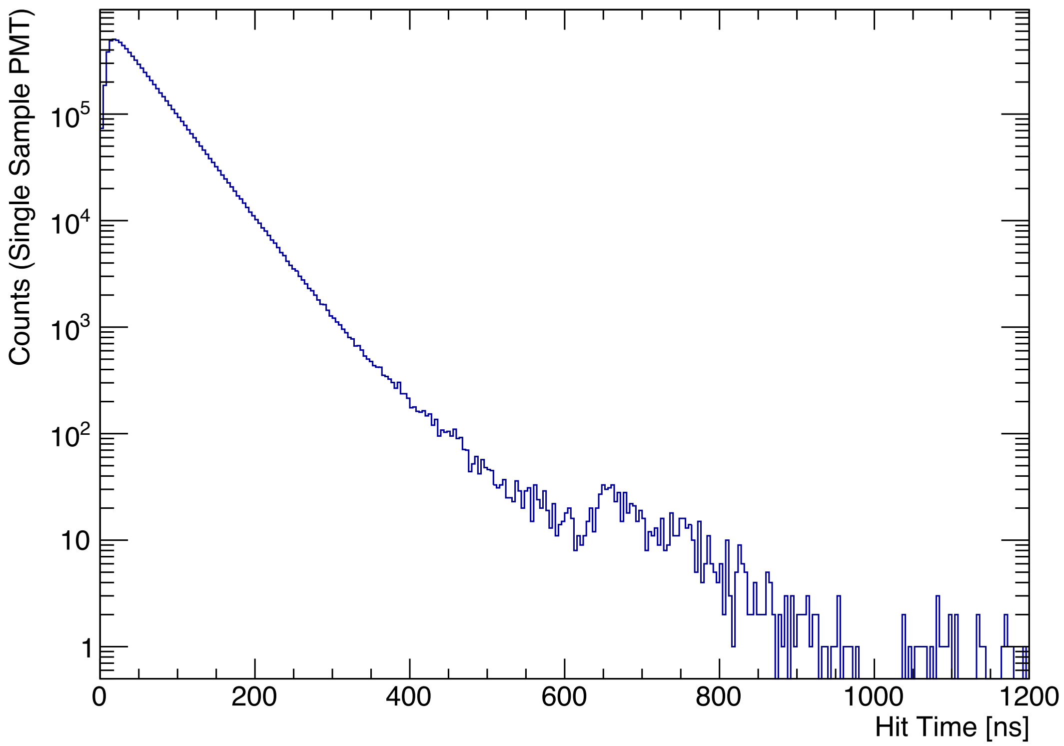




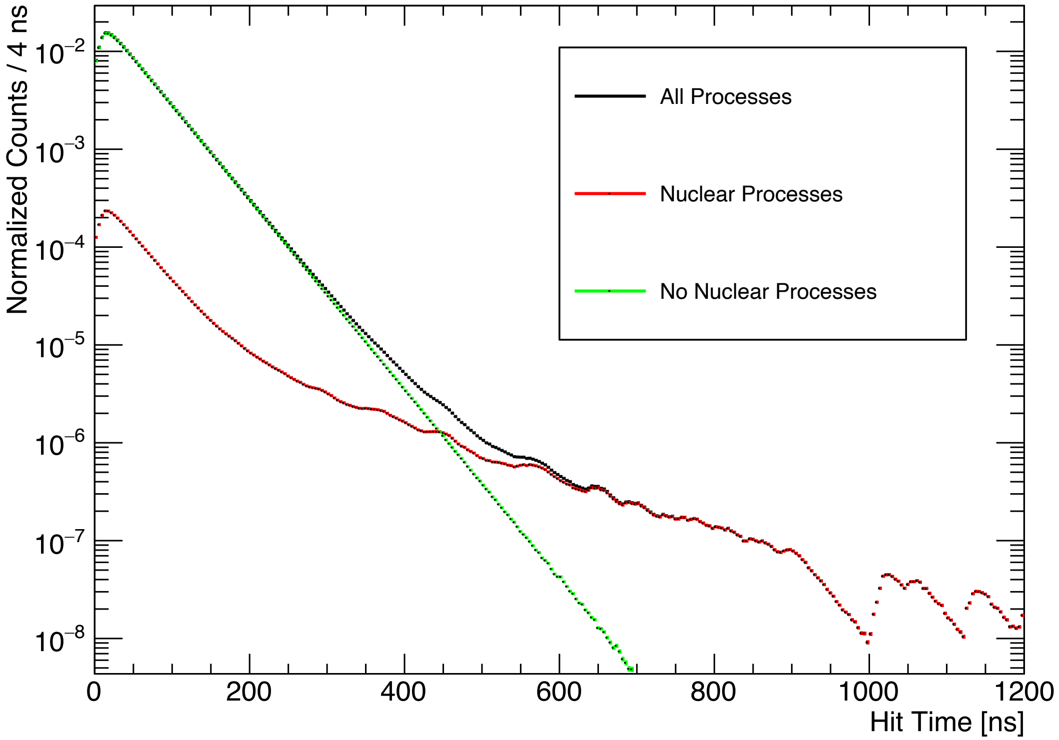
- distribution of 1000 PMTs on the calo outer shell

PMT Hit Times

- Time of photon hitting PMT, relative to time of positron hitting the calorimeter (pienu - $\pi^+ \rightarrow e^+\nu_e$)

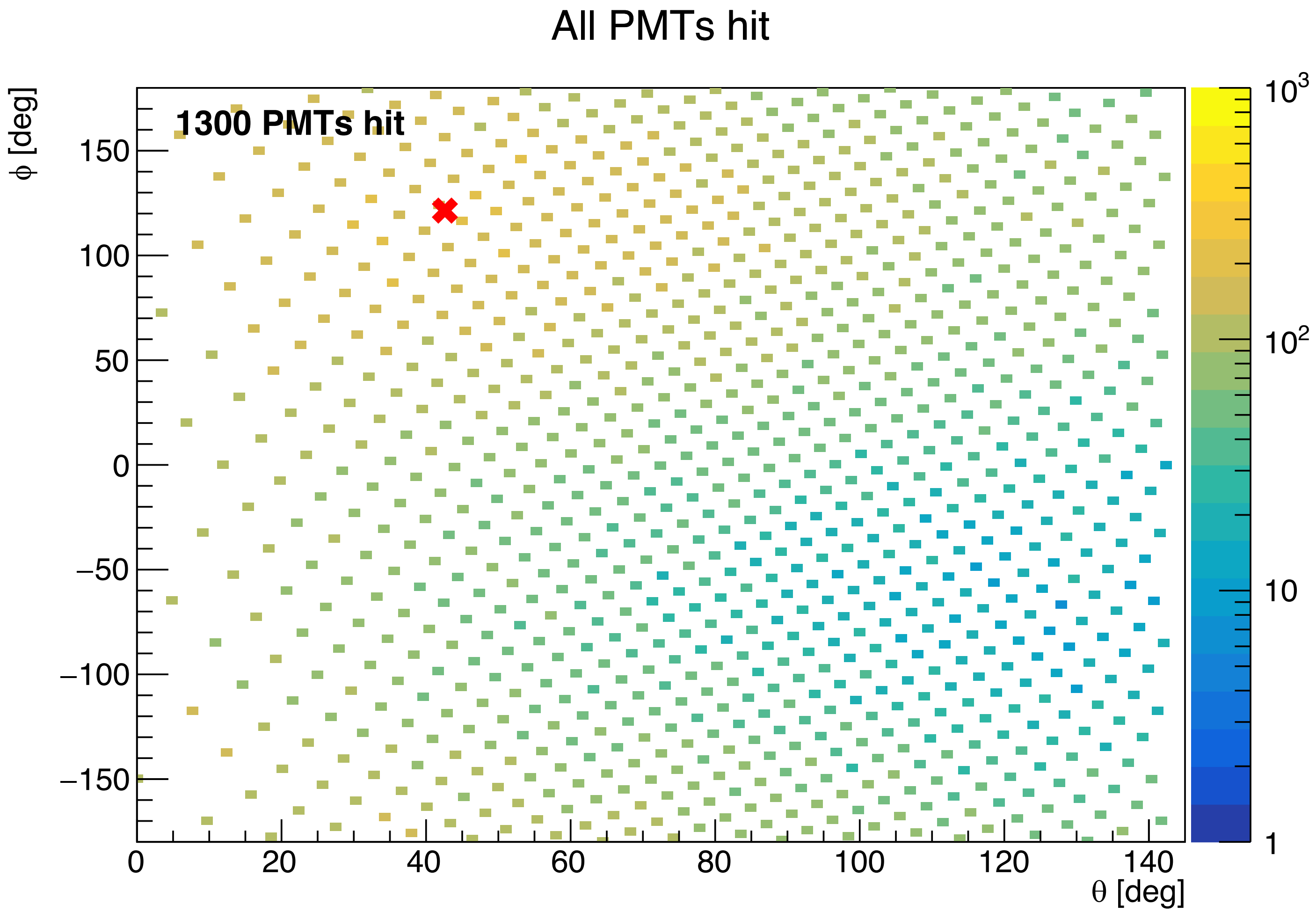


Single PMT, 100,000 events

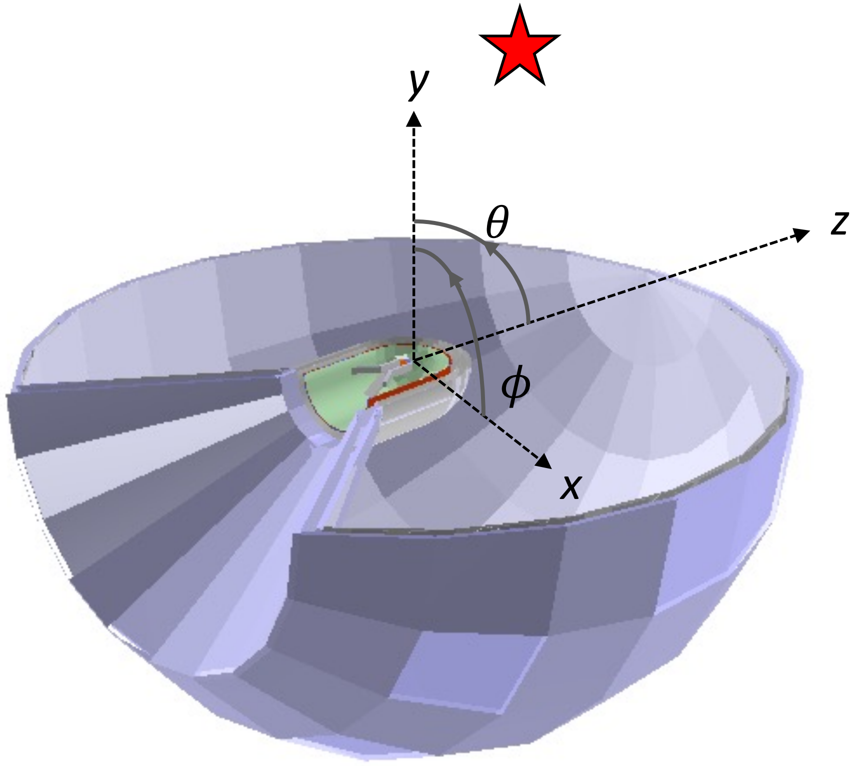


All PMTs, 100,000 events

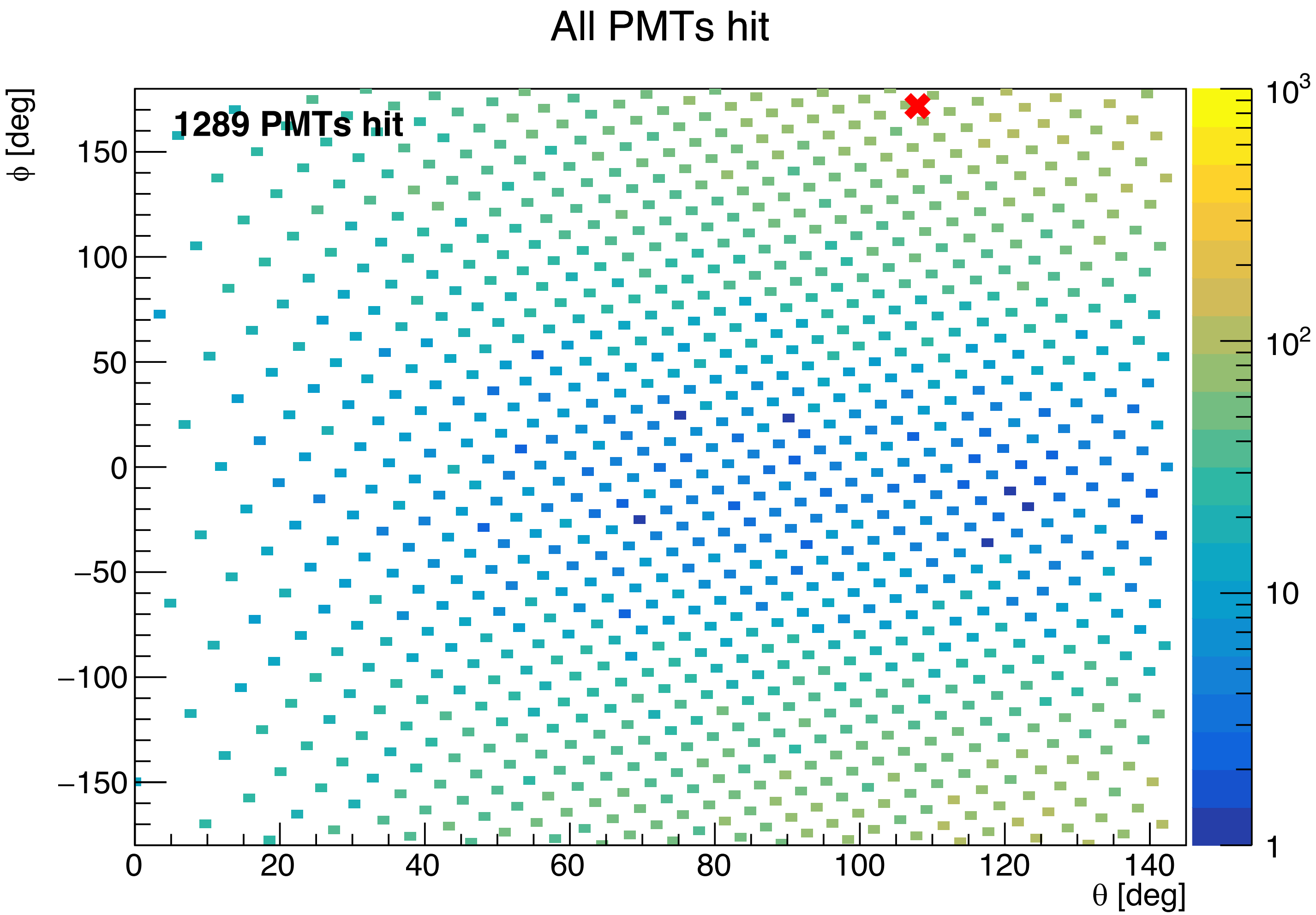
Light Distribution in the LXe Calo



- “random” single pienu event
- z-axis: # of photons hitting the PMT
- red cross (or star): position of e^+ hitting the calo

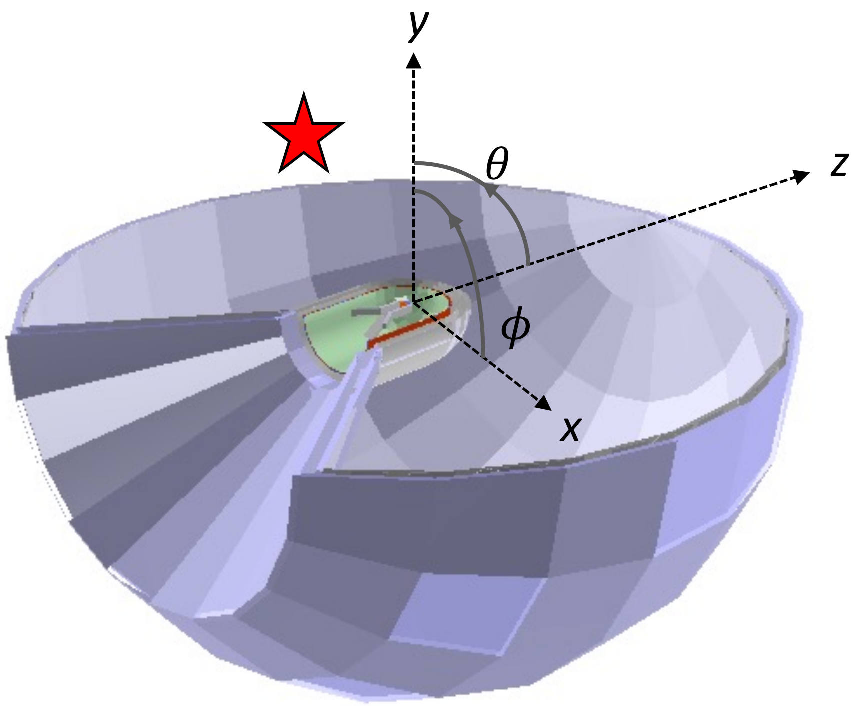


Light Distribution in the LXe Calo



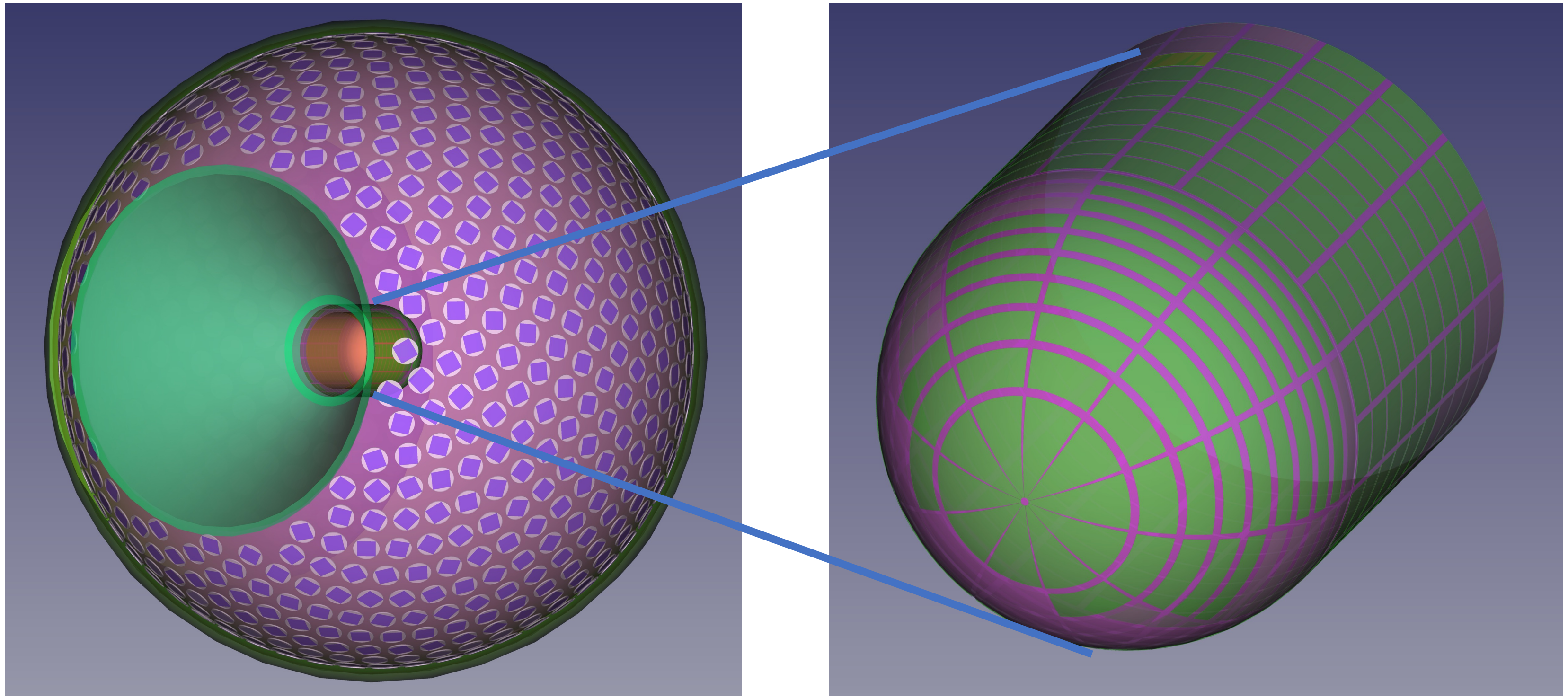
"shadowing" effect from center of calo

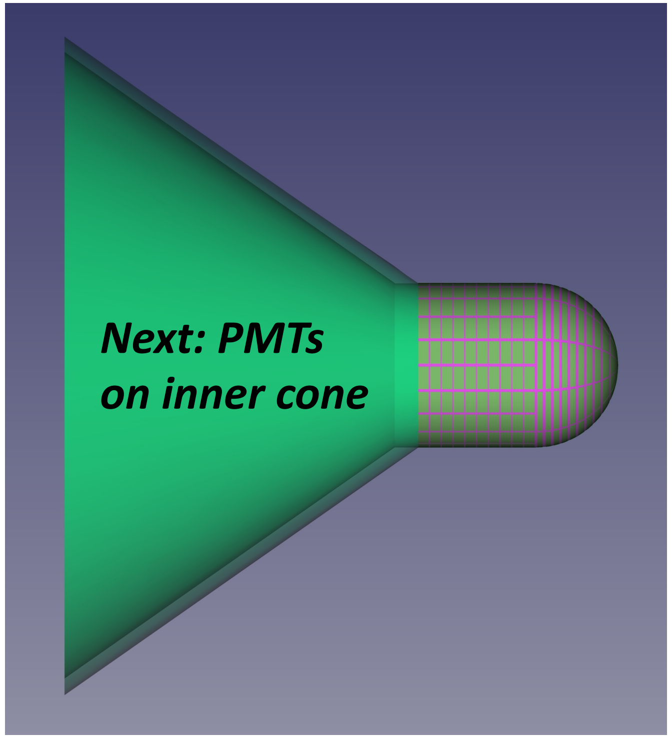
- "random" single Michel event
- z-axis: # of photons hitting the PMT
- red cross (or star): position of e^+ hitting the calo



Photosensors on inner calo window surface

- 300 small photosensors added to bullet
  - 100 on hemisphere, 200 on tube
  - currently just testing the optics and understanding results; for real detector, could implement small, flexible silicon photomultipliers on inner surface (see talk from Toshiyuki tomorrow)



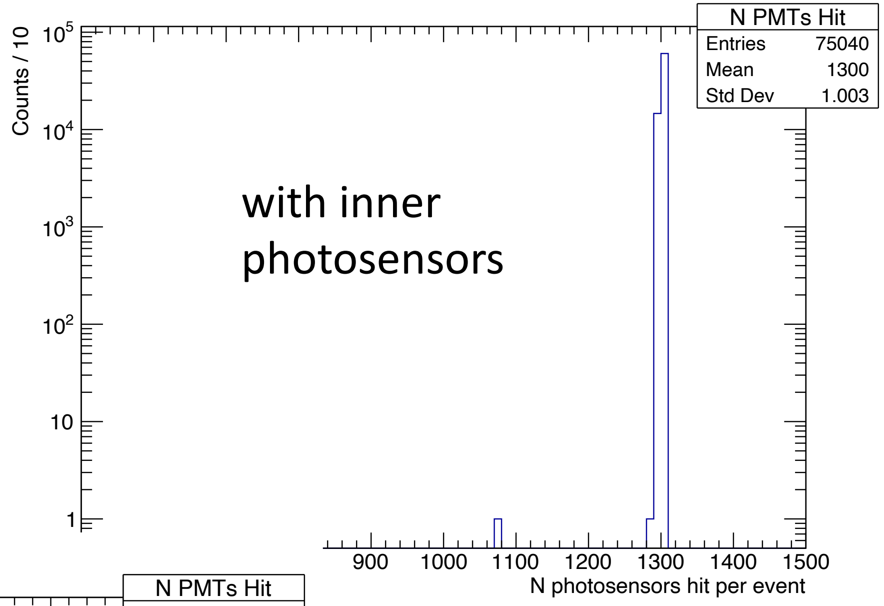


Thanks to Bob for the nice CAD rendering!

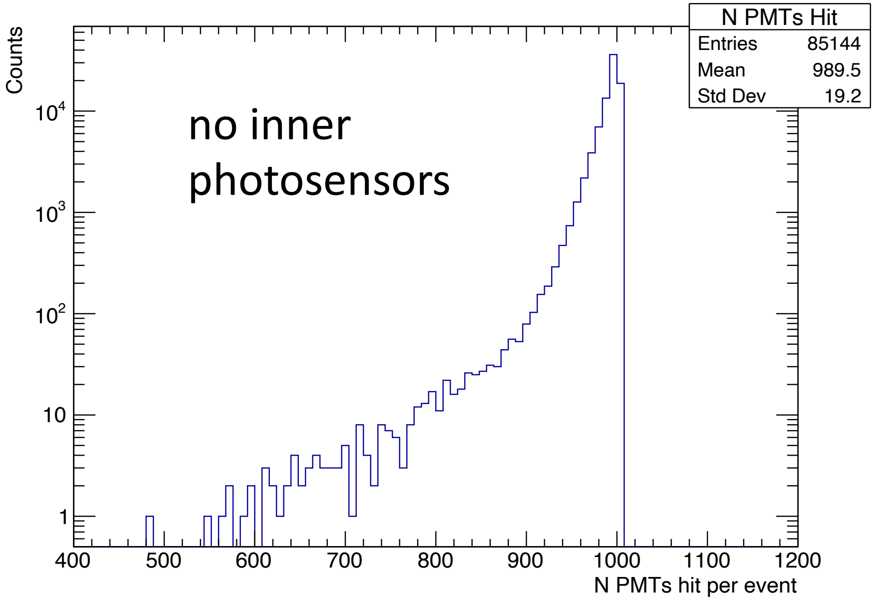
Green = optical surface

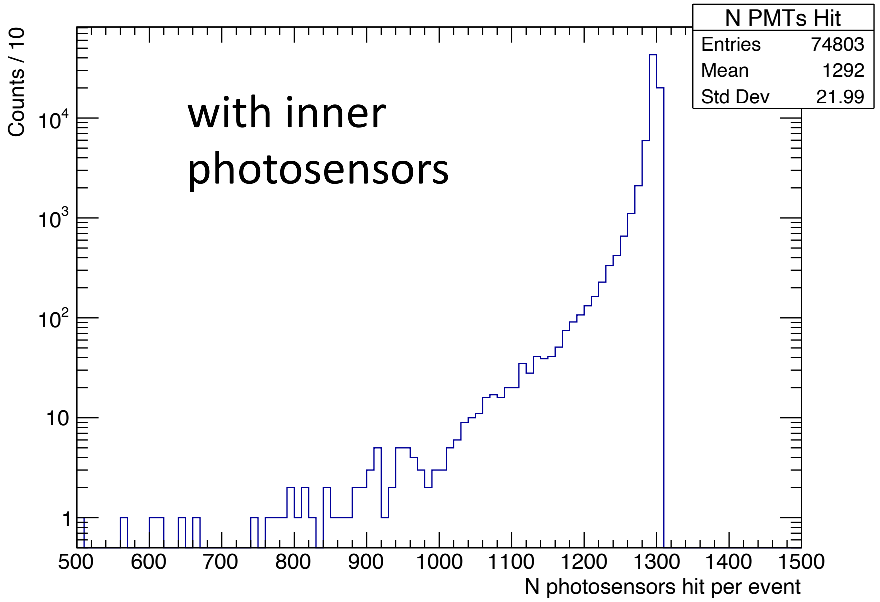
PMTs hit per event

PRELIMINARY: brand new with new photosensors – need to further investigate their effects

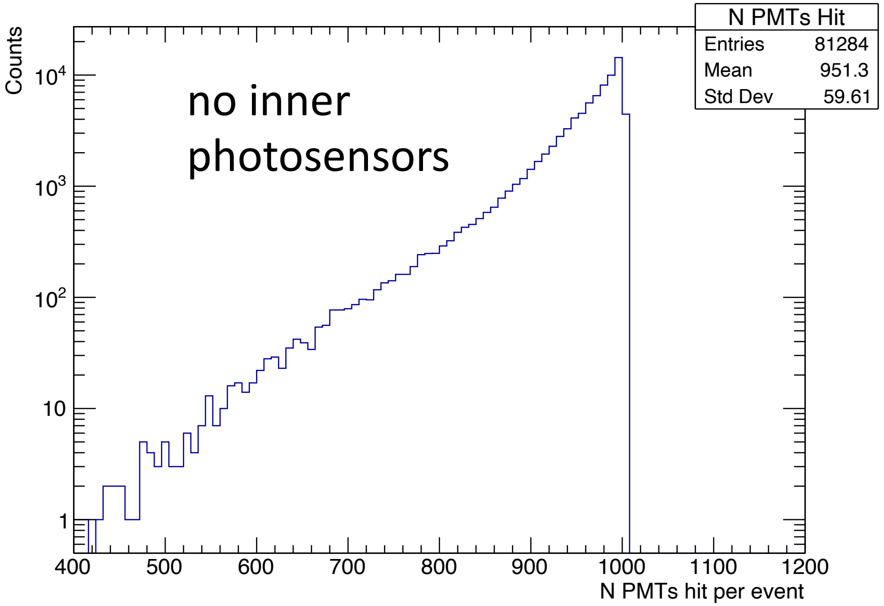


Pienu





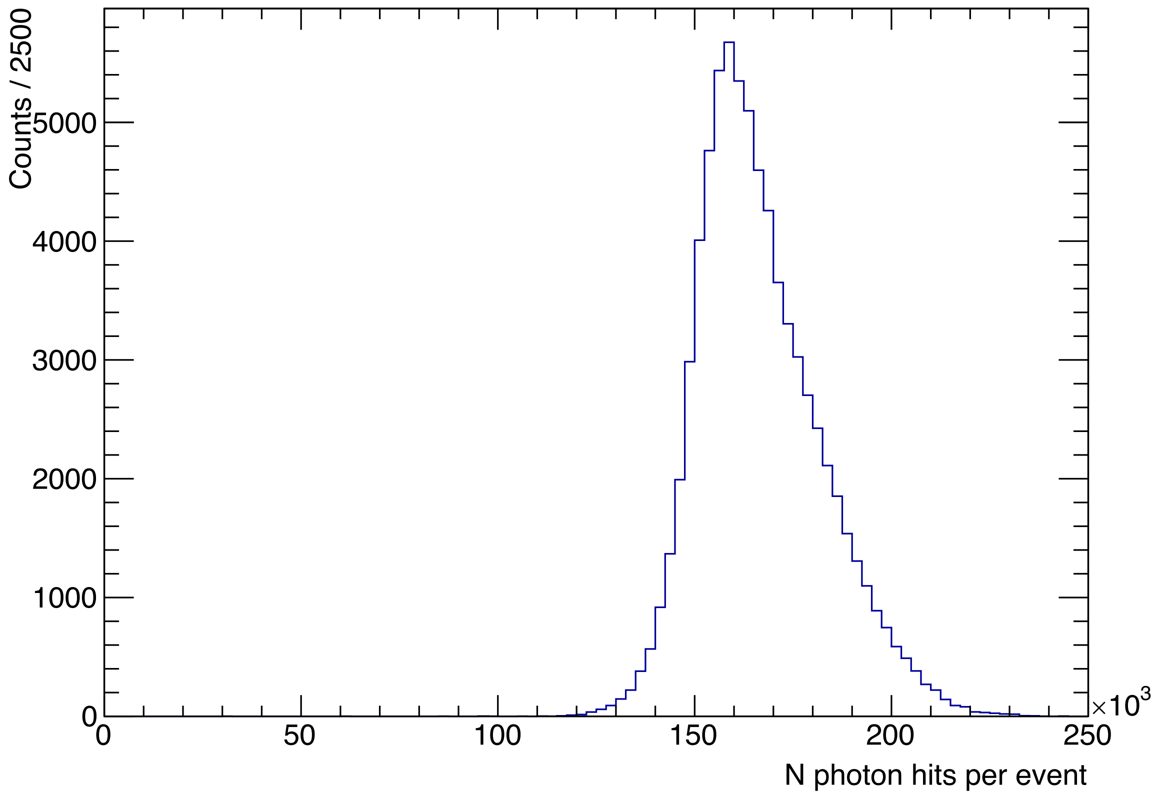
Michel



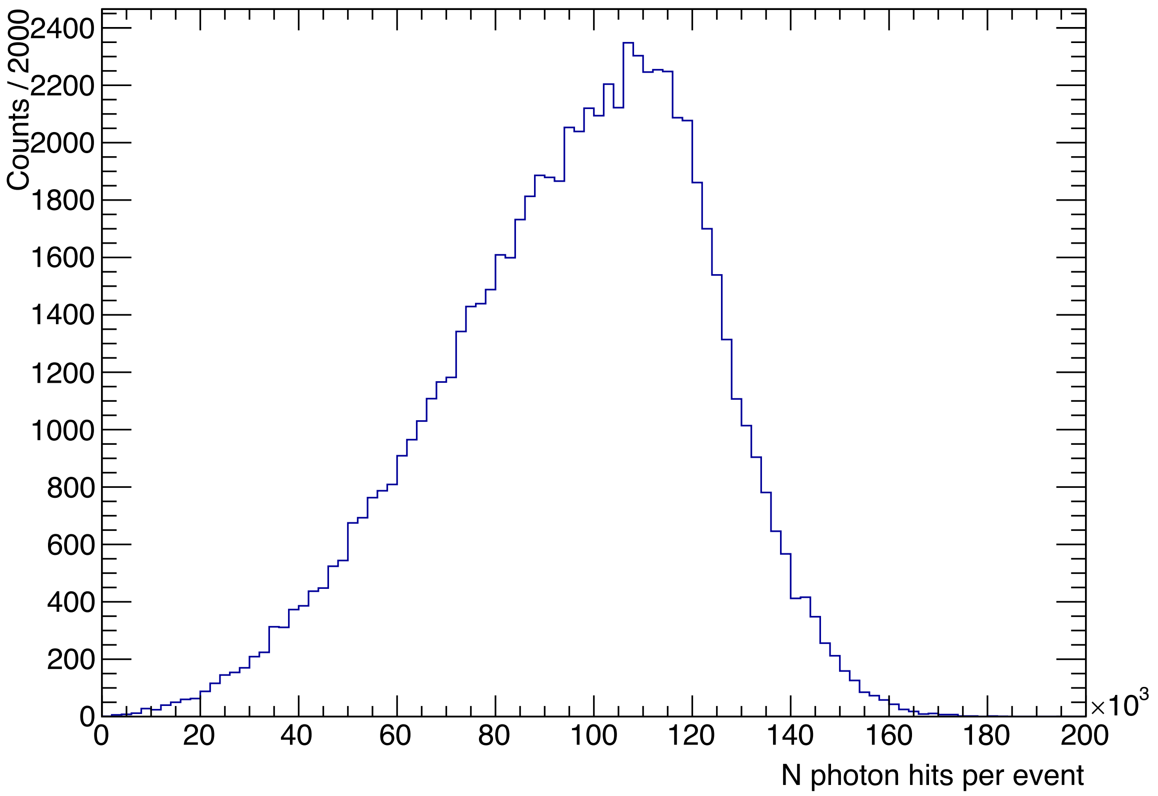
Photons detected per event

PRELIMINARY: need to understand shape before converting to energy

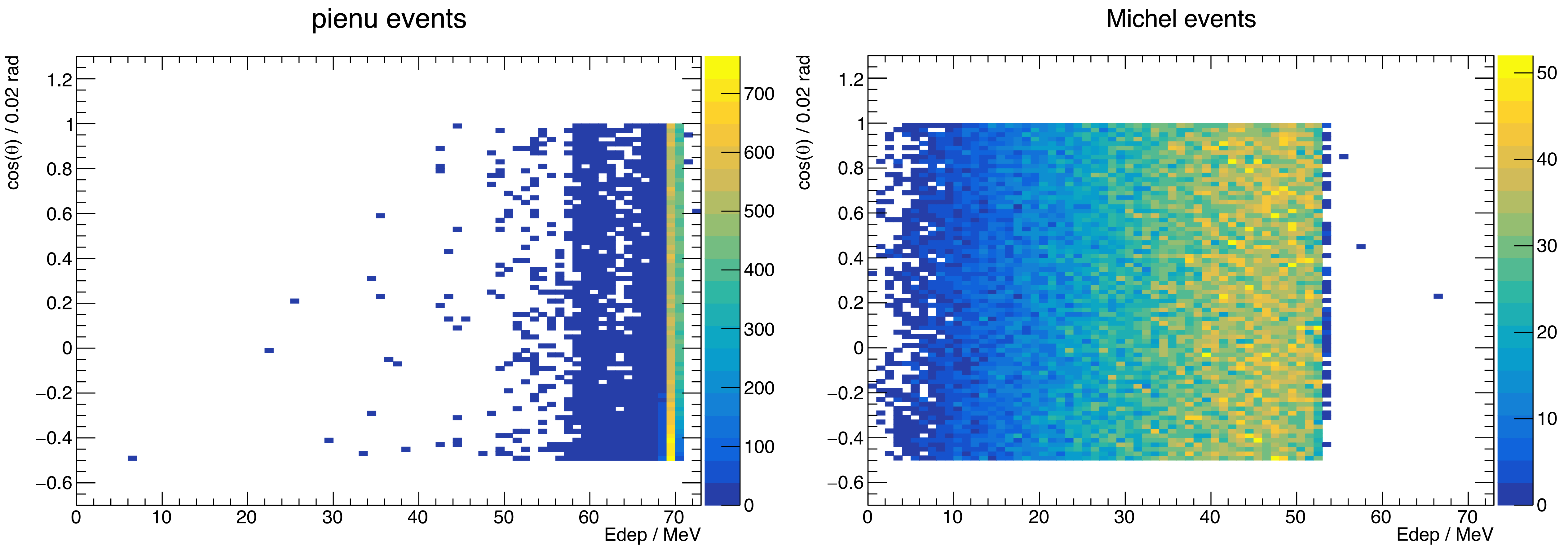
pienu



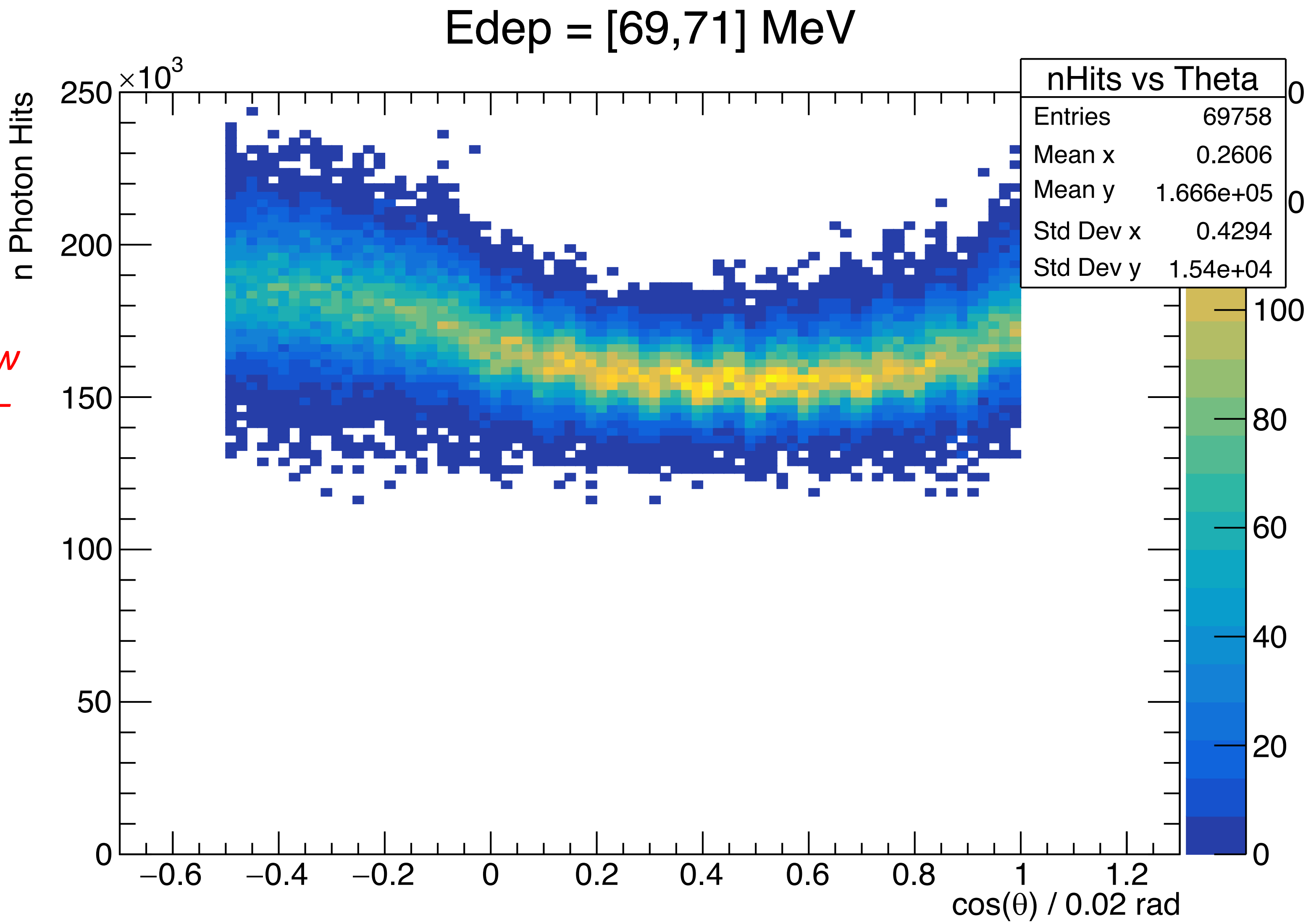
Michel



Energy distribution



Energy and # of photons: pienu



PRELIMINARY: brand new with new photosensors – need to further investigate their effects

Aside: Optical Photons in GEANT4 - Additional Tools/Toolkits Development Work

1. GPUs for improved optical photon simulation:

- GPU acceleration for optical photons (can provide computational advantage)
- Opticks

2. Investigating differences between GEANT4 and NEST:

- Alternative scintillation models: NEST (Noble Element Simulation Technique)
- Does NEST explain MEG discrepancy?

Slides and work by Aleksey Sher

Opticks: GPU
Optical Photon Simulation
via NVIDIA ® Optix ™ 7, CUDA ™

Prospects:

- Promising tool, potential for ~10^2 speed increase
- Aleksey is in contact with developers

Status:

- Implementation underway – developer working through bugs
- Opticks package remains an interesting tool, worth pursuing for TRIUMF Science Technology division

Cedar Cluster CPUs: **338** GPUs: **190**

GPU power is 190*100=19000 CPU equivalent. Which is **x56** more capable cluster.

4 GPUs can replace whole cedar cluster

Link to presentation by Hans Wenzel (G4 integration developer)

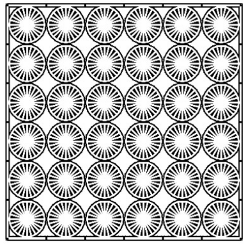
MEG Prototype NEST Testing (Noble Element Simulation Technique)

Simple geometry (taken after MEG prototype):

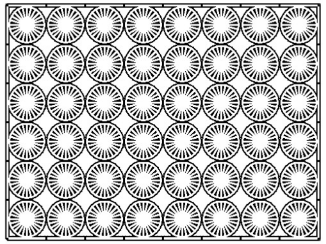
372 x 372 x 495 mm^3 of LXe

57 mm diameter sensitive surfaces placed inside to form a 6x6x8 array

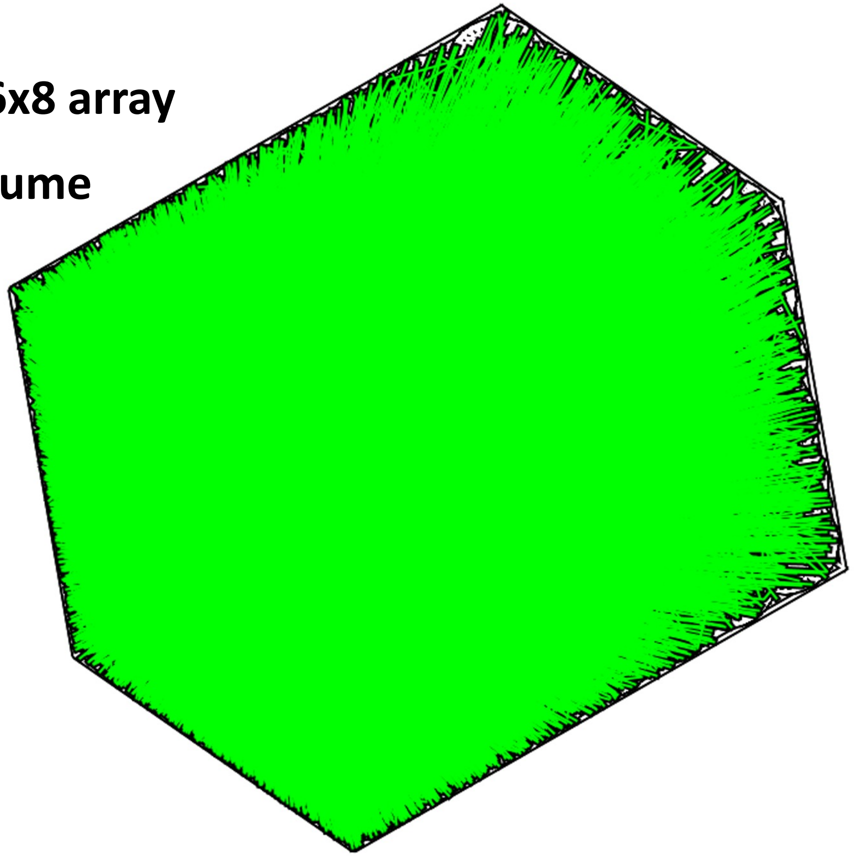
Incoming 10-70 MeV e$^-$ beam shoots into the center of the volume



Front View



Side View

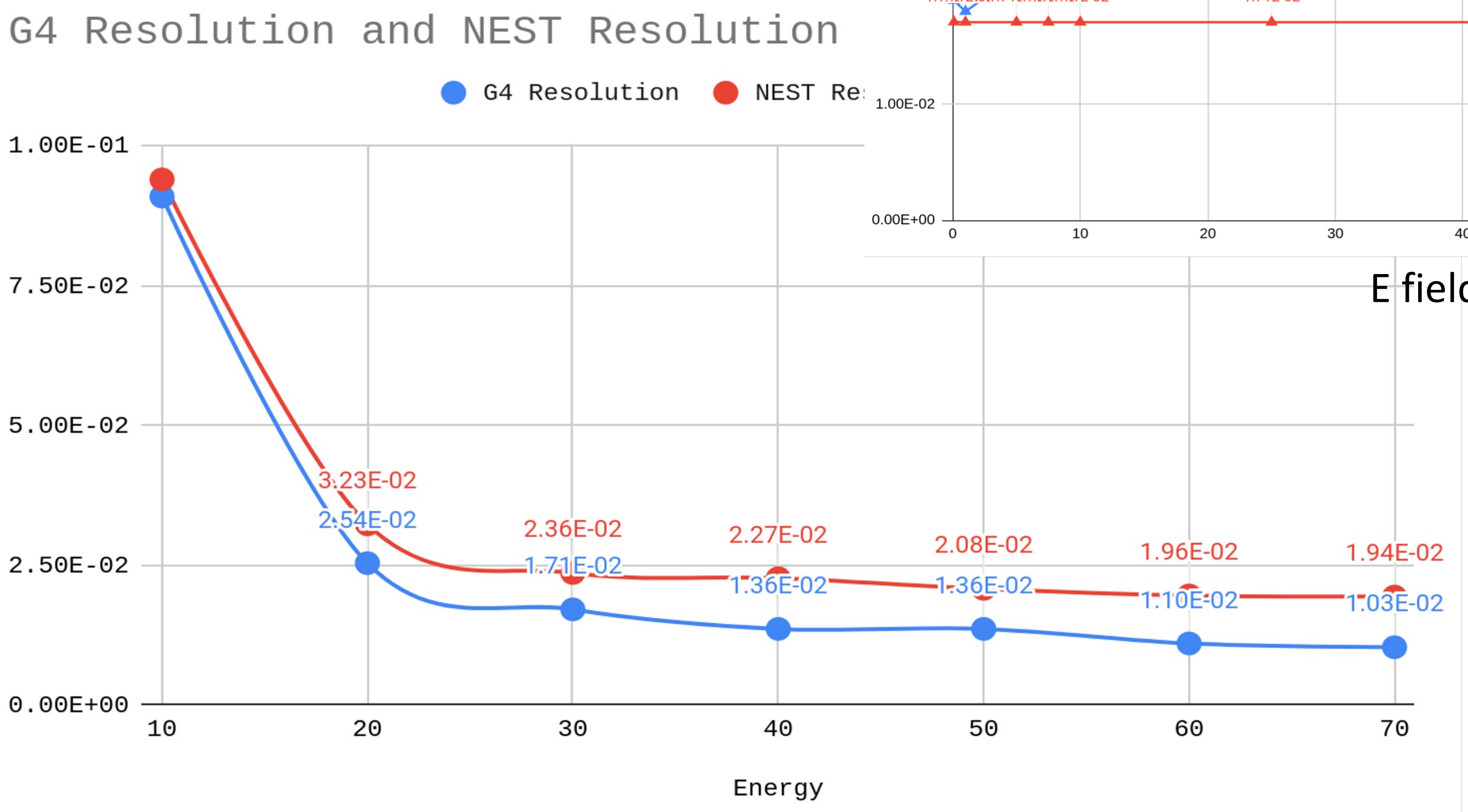


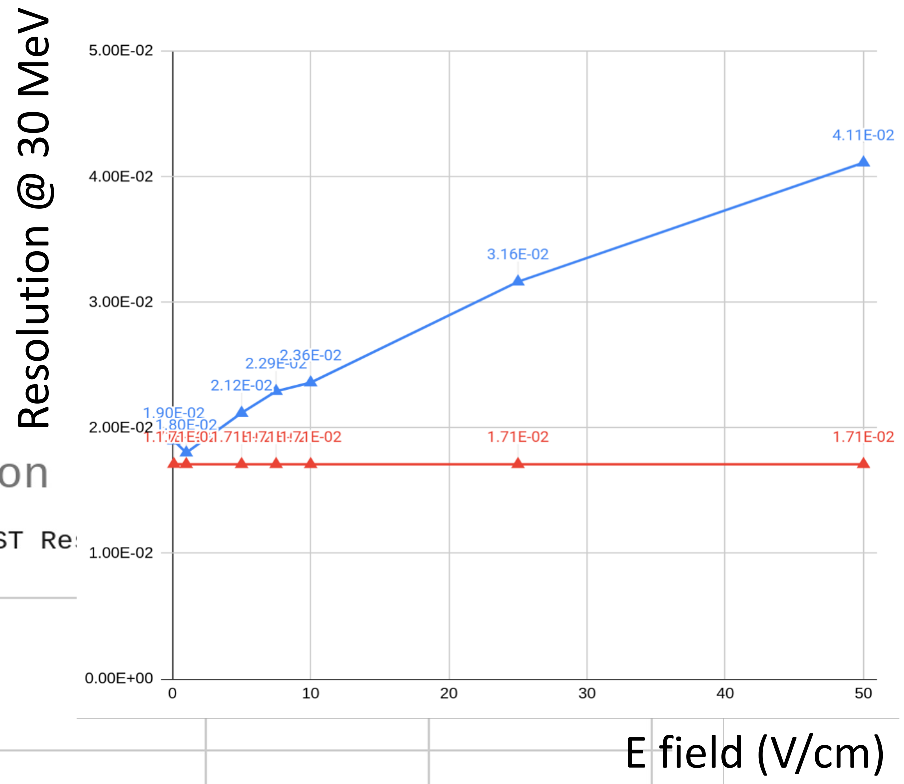
Slides and work by Aleksey Sher

NEST Testing

Difference is clearly observed, however:

- Light yield is different between G4 and NEST
- E field parameter is a tricky one and needs to be better understood

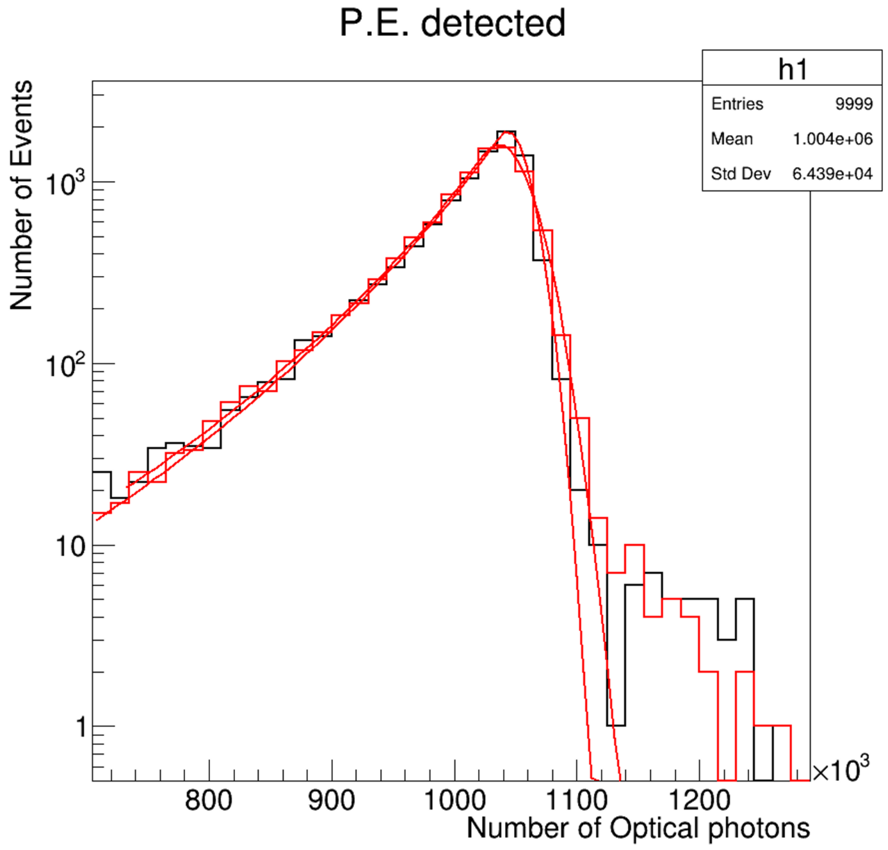




Slides and work by Aleksey Sher

NEST Testing

Equalizing the light yield of G4 and NEST for 30 MeV
*NEST has internally controlled LXe parameters, including light yield.



Beam E (Mev)	G4 σE/E	Nest σE/E	G4 σE/E Light yield normalized to match NEST
30	**1.71E-02**	2.36E-02	**1.62E-02**

NEST Conclusions:

- Results different from G4
- No zero-E-field model in NEST; large effect on energy resolution
- Light yield does not explain the difference
- Has potential for tuning simulation to data, but more work with NEST team required

Summary: LXe Calo Simulation Tasks

- Geometry
  - ✓ optical properties
  - ✓ LXe windows
  - ✓ inner calo radius photosensors
- Optics
  - ✓ light distribution in calo
  - ✓ clustering
  - ✓ NEST investigation
- Energy resolution
  - ✓ window thickness
  - ✓ updated radiation length

- Geometry
  - ❑ inner calo cone photosensors
  - ❑ keyhole calo
  - ❑ corresponding ”realism” i.e. dead material, photosensors
  - ❑ improved optics
- Optics
  - ❑ understand angular energy response
  - ❑ material reflectivity variation
  - ❑ optical segmentation
  - ❑ clustering for pileup ID?
- Energy resolution
  - ❑ albedo
  - ❑ effect of particles exiting fiducial volume
  - ❑ incorporating full detector
- Reconstruction
  - ❑ implement waveforms
  - ❑ event mixing: **Pileup in calo**
  - ❑ Cerenkov vs scintillation light?

Backup

Slides and work by Aleksey Sher

Opticks:GPU
Optical Photon Simulation
via NVIDIA ® Optix ™ 7, CUDA ™

Prospects:

- Promising tool, with a potential of ~10^2 speed up
- Established contact and active communication with developers (Simon Blyth)
- Hans Wenzel (developer on the G4 integration side) is on the task of making the next iteration of workable CaTS/Opticks tandem based on the newer Optix 7.0+
- Simon is very passionate about the project
- Opticks comes as the main recommended tool for GPU accelerated ray tracing by G4 collaboration.
- Other tools either are in the infancy stage, or just at proof-of-concept stage or do not have G4 integration.

Cedar Cluster CPUs: **338** GPUs: **190**

GPU power is 190*100=19000 CPU equivalent. Which is **x56** more capable cluster.

4 GPUs can replace whole cedar cluster

Link to Hans's presentation

Slides and work by Aleksey Sher

Opticks:GPU Optical Photon Simulation via NVIDIA ® Optix ™ 7, CUDA ™

Status:

- Implementation road has been chosen to follow the CaTS G4 example
- Optix 7 transition is claimed to be complete, however difficulties remain. It is done for JUNO experiment, as main developer is a member.
- CaTS example has not been tested/optimized for the Optix 7 and work is ongoing
- As Hans is working out the bugs the work at TRIUMF on this has been paused, leaving it in expert's hands
- Overall, the Opticks package remains to be a very interesting tool worth pursuing for TRIUMF Science Technology division

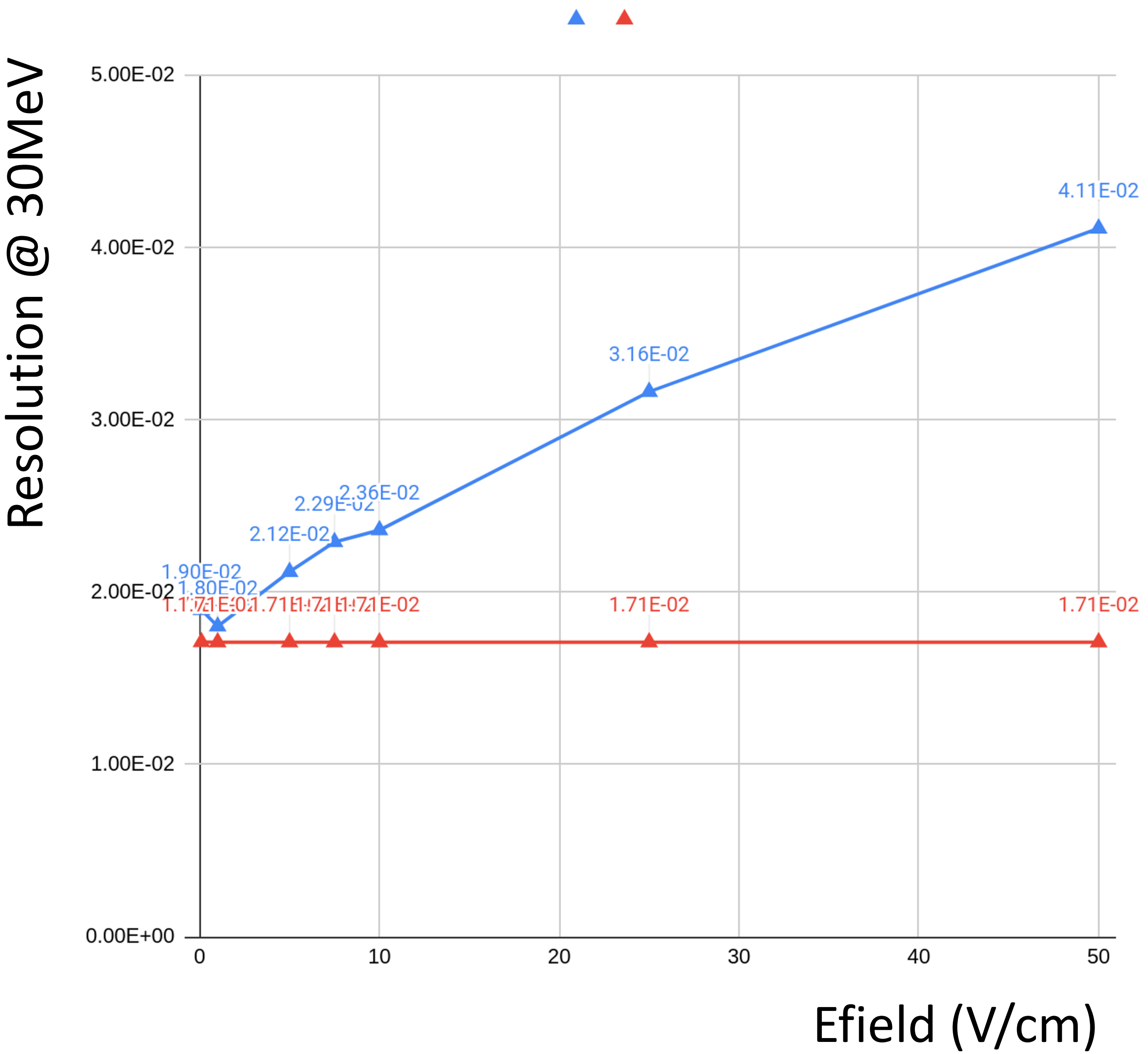
Slides and work by Aleksey Sher

NEST Efield

Looking at 30 MeV and varying the Electric Field within NEST:

- Resolution is highly dependent on the Efield
- https://arxiv.org/pdf/2210.07625.pd
- After contacting Paola Ferrario (*corresponding author for Spanish arxiv paper on LXe low energy measurements*).

In fact, this non-zero value of the electric field is a bit of a problem of using NEST in our applications. For instance, I found relatively large differences in yield and energy resolution varying from 1 V/cm to 10 V/cm. For instance, energy resolution for 511-keV gammas goes from 5.7% to 10.2% FWHM, in my G4-based application using NEST.
I talked to Matthew Szydagis, one of the main NEST developers, about this and he told me that they are aware of this problem and we should include this variation as an error in our results: he suggested I used 10 +- 5 V/cm. However, it seems a too large variation to me, so in the end, I decided to use my Geant4 application without NEST and compare the results with data to see if there is any difference which could be explained by adding the effects simulated by NEST (I haven't definite results yet).

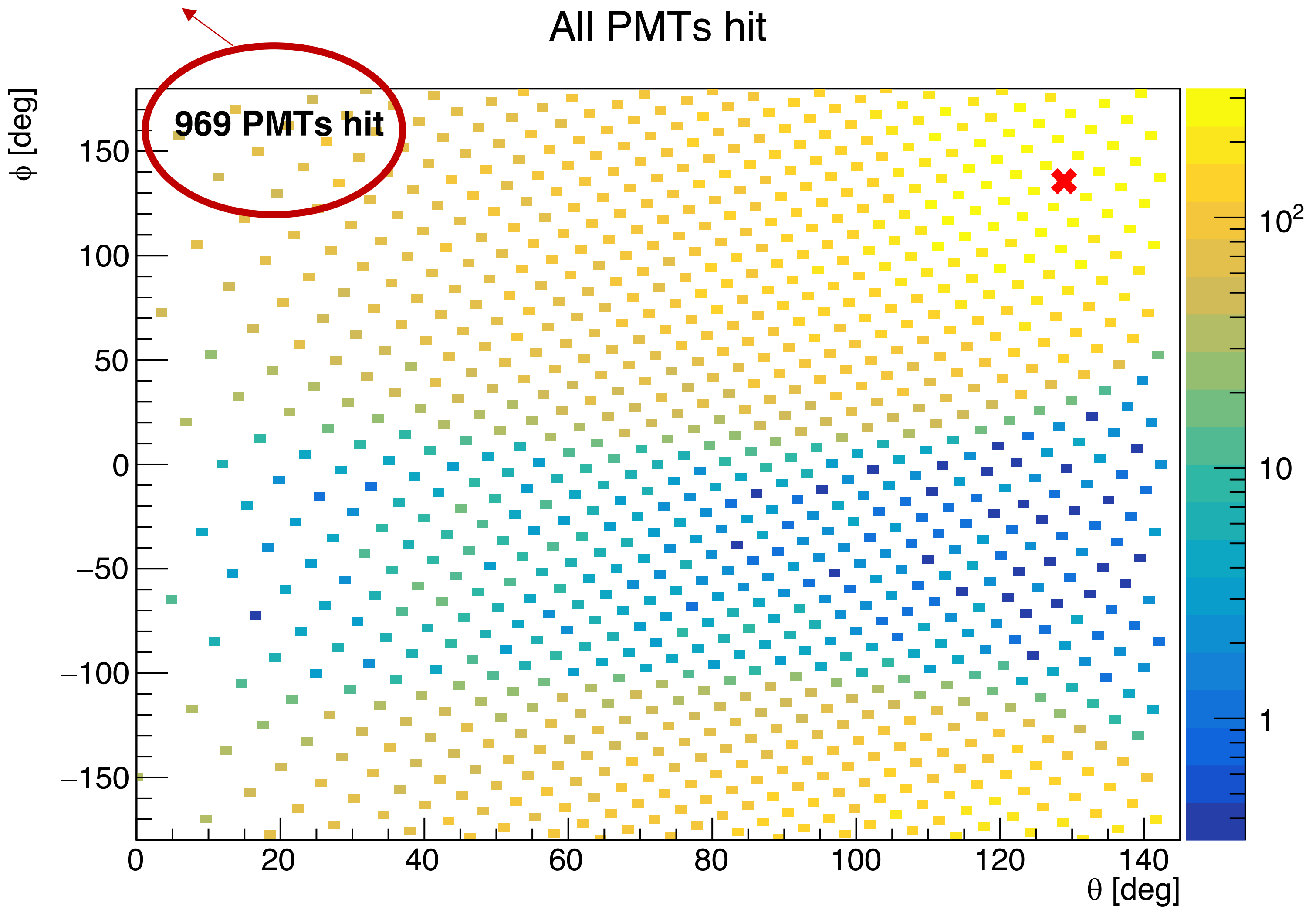


NEST Conclusions

- NEST does produce results different from the proprietary G4
- Efield parameter of the NEST model has a large effect on the deduced energy resolution and there is no zero-field model within NEST
- Average light yield does not explain the difference
- NEST collaboration recognizes problems with near zero field
- NEST has potential for tuning and matching simulation results to data, but reliable data and collaboration with the NEST team is required for this effort to be of value

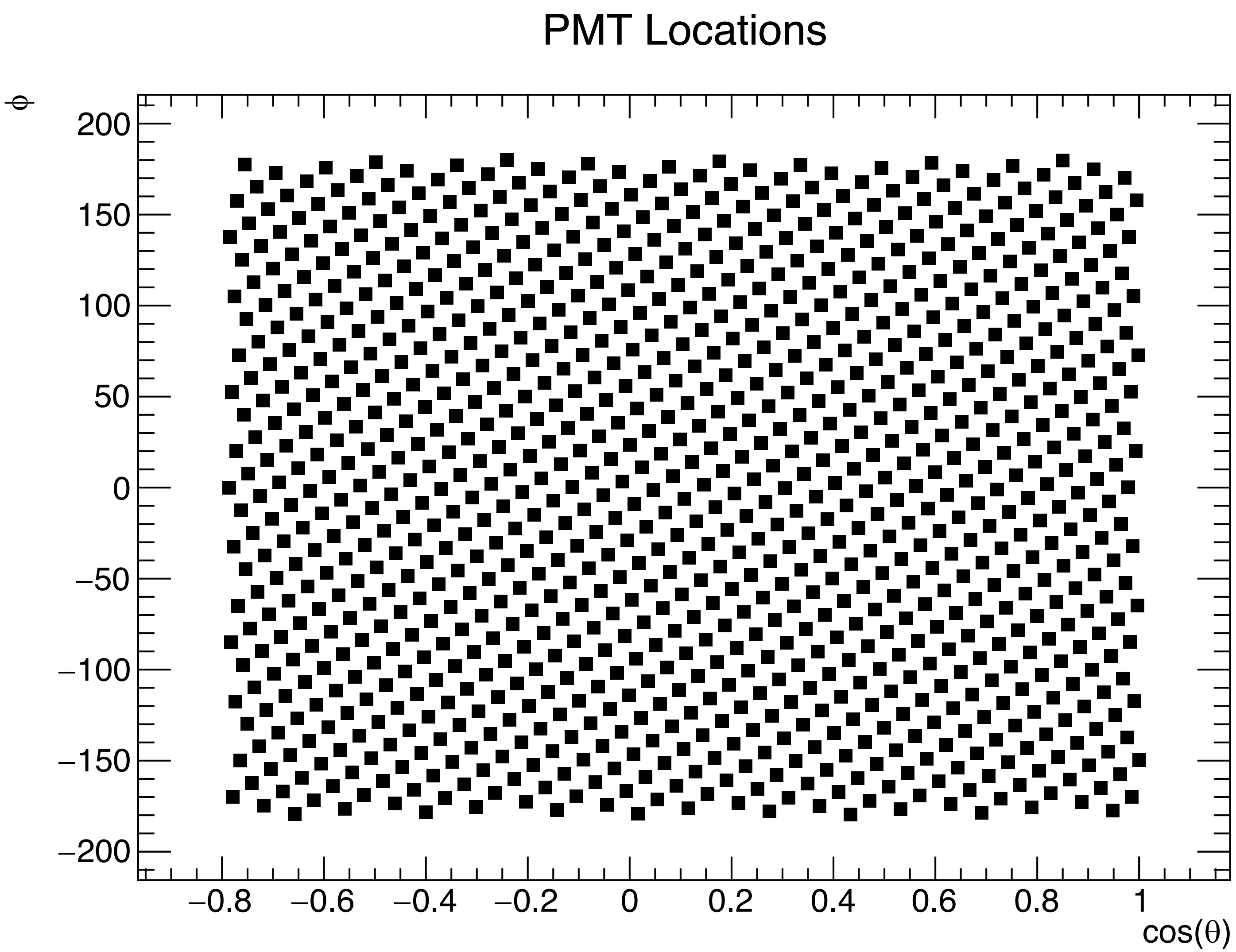
PMT Hit Maps: Single Events

969/1000 PMTs were hit by at least 1 photon



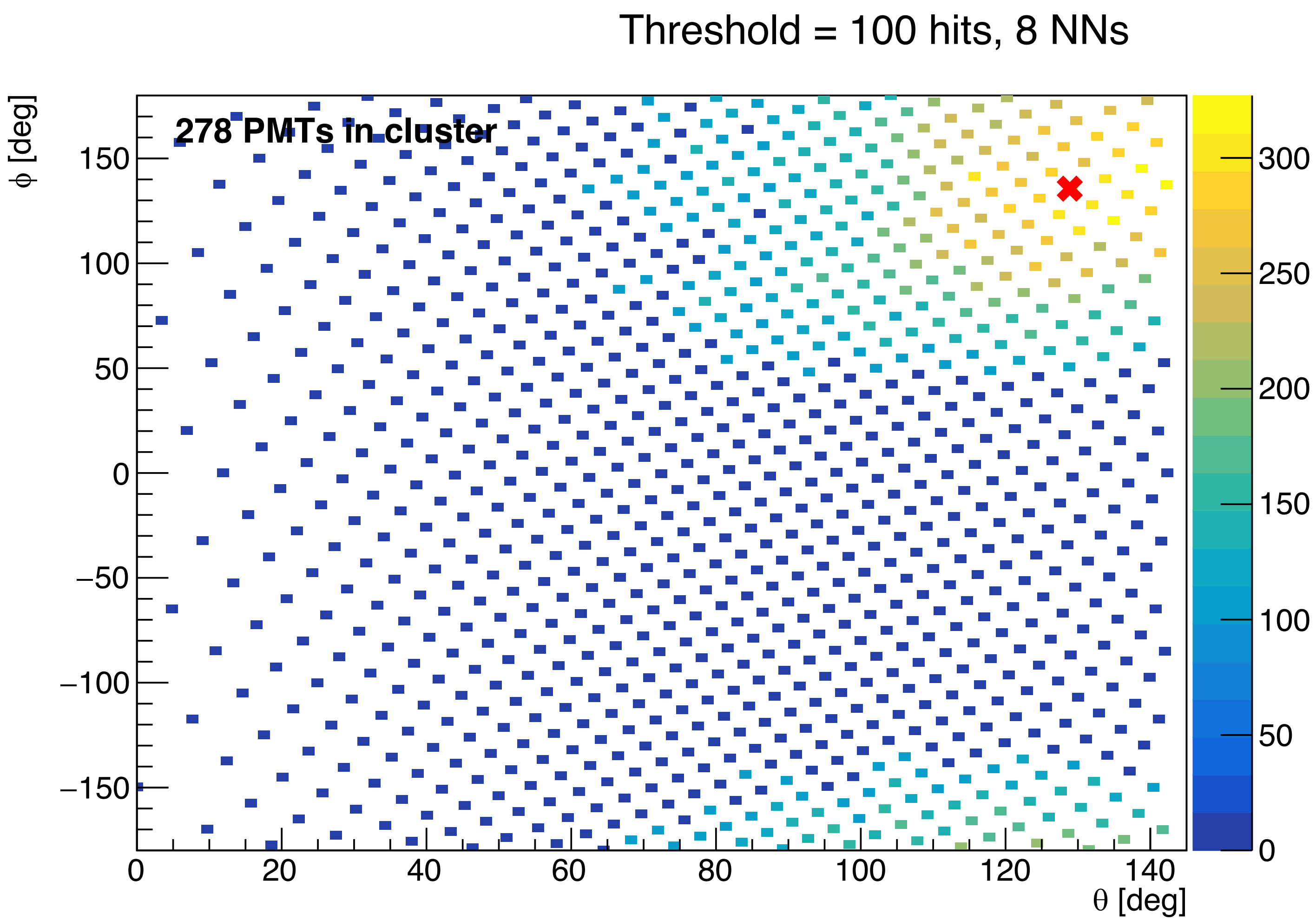
- z-axis: # of photons hitting the PMT
- red cross: position of e^+ hitting the calo

Clustering



- PMT mapping; for every PMT:
  - ID, theta, phi, (nHits), distance to every other PMT
  - Distance ($\Delta\sigma$) calculated using great circle formula:
  - $\Delta\sigma = \cos^{-1}(\sin\theta_1 \sin\theta_2 + \cos\theta_1 \cos\theta_2 \cos\Delta\phi)$
    - $(d = r\Delta\sigma)$
- Sort vector of PMT distances from low to high

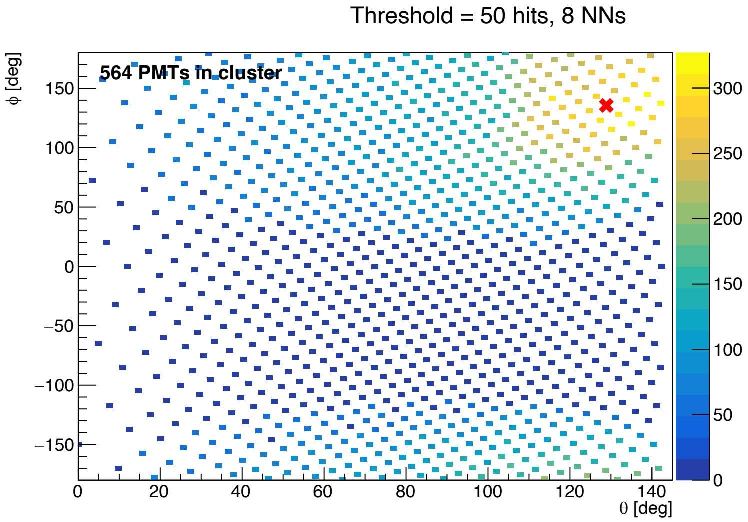
Clustering for pileup identification?

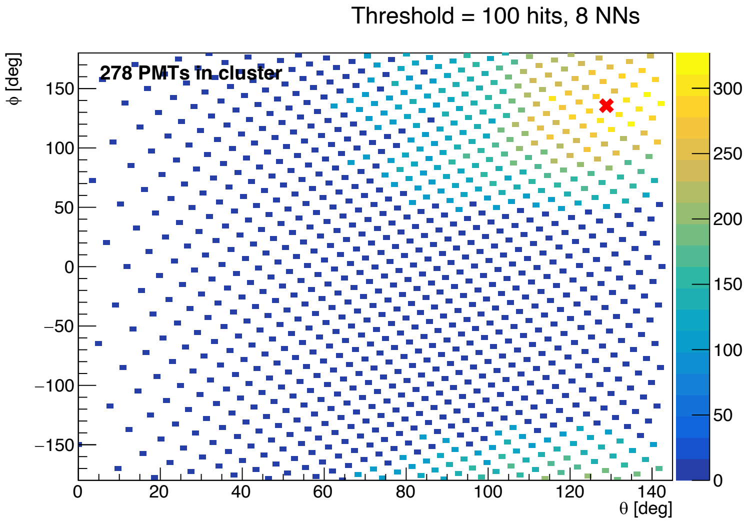


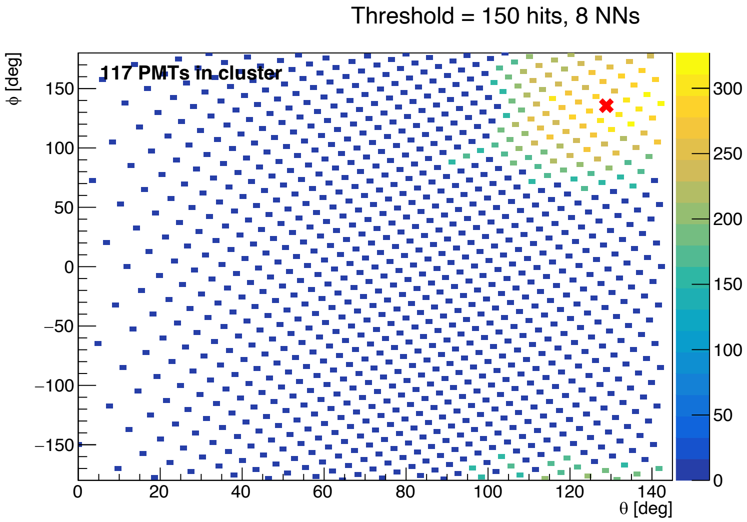
Clustering!

- Seed with max hit in the event
- Select # of nearest neighbours (NNs) to search
- Select PMT hit threshold required for PMT NN to be added to cluster
- If PMT is added to cluster, repeat and check each of its NNs
- Check to make sure no PMTs are double-counted

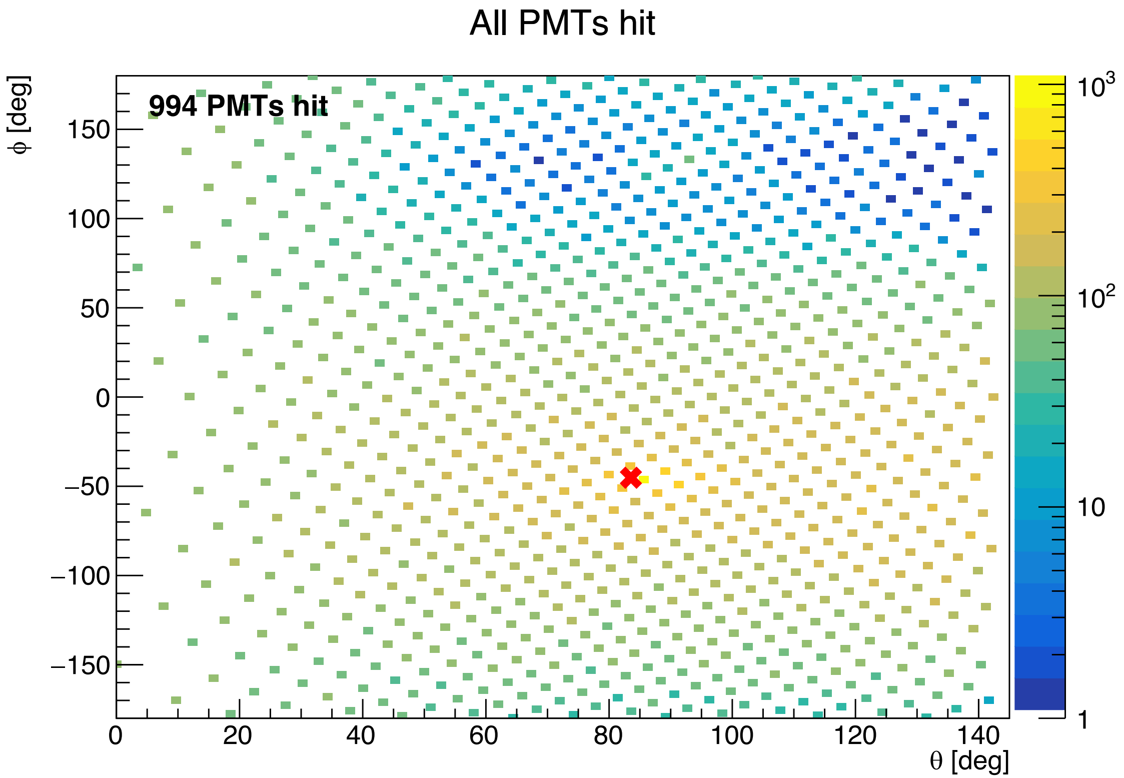
PMT Hit Maps: Single Events

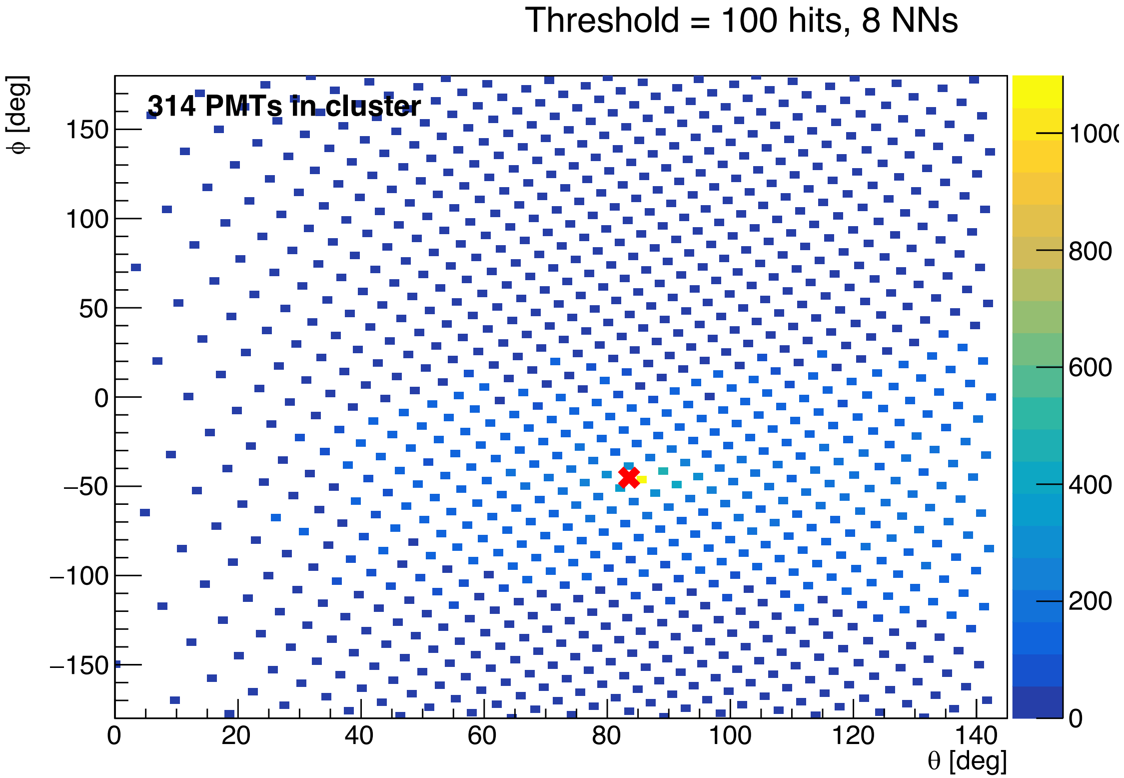






PMT Hit Maps: Single Events



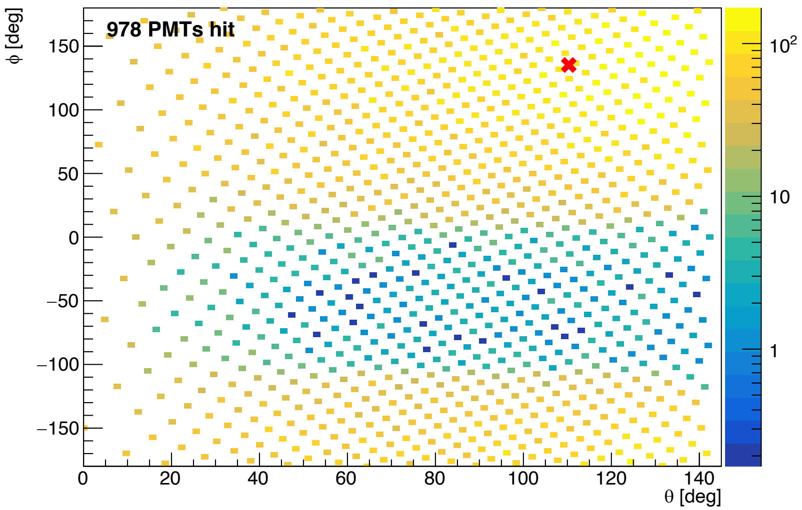


$$\pi \rightarrow e\nu$$

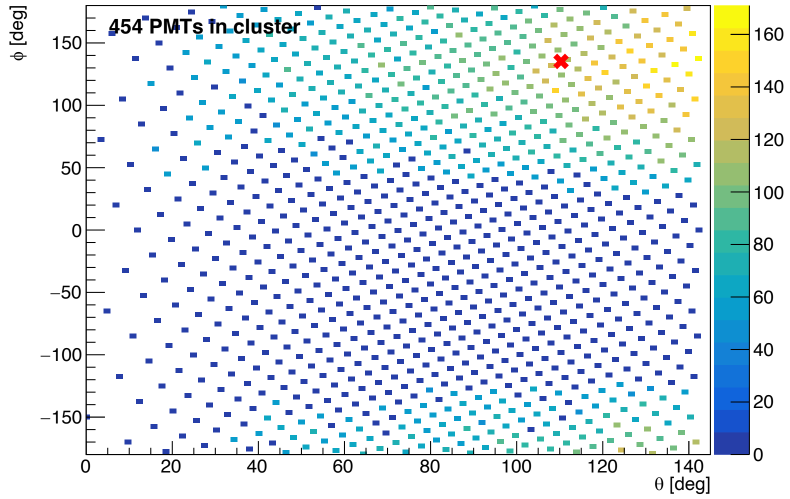
PMT Hit Maps: Single Events

Michel

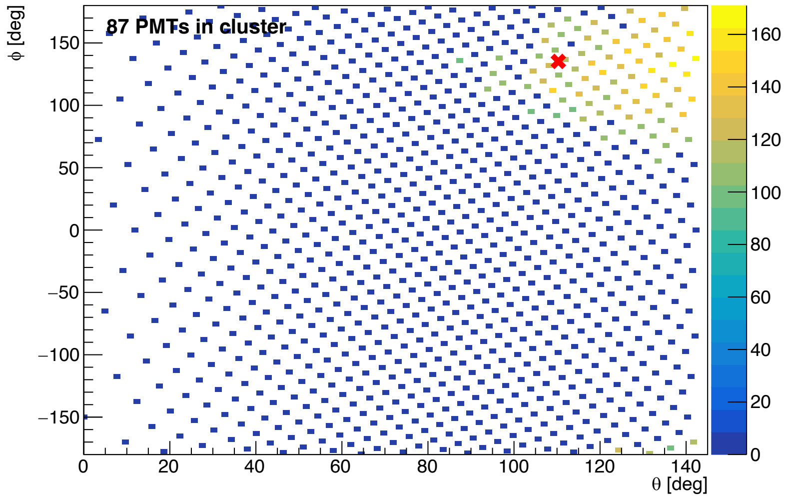
All PMTs hit



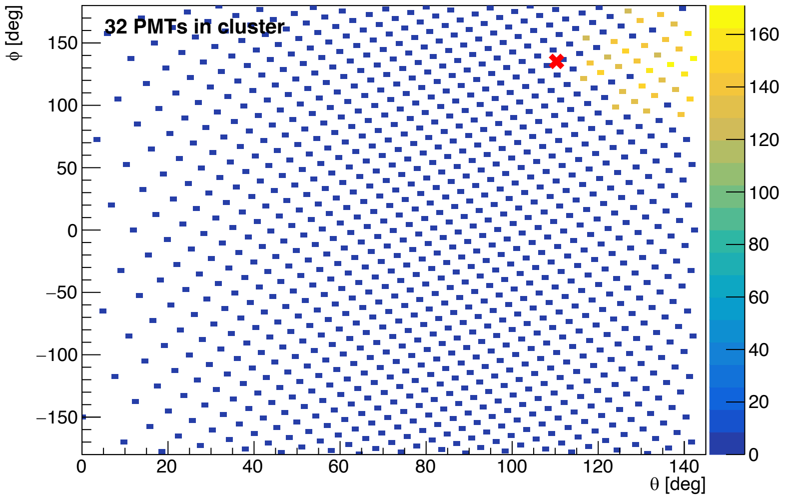
Threshold = 50 hits, 8 NNs



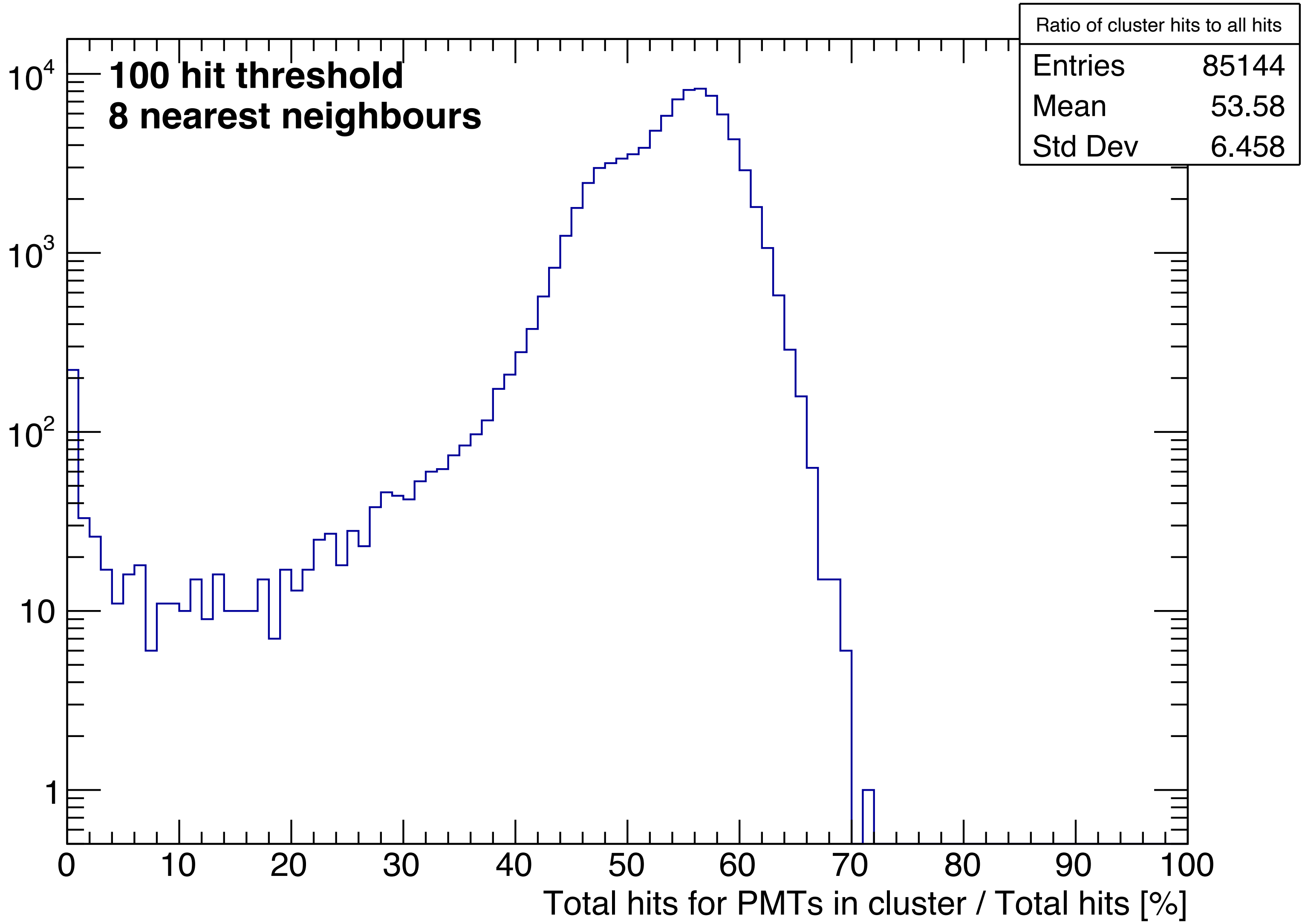
Threshold = 100 hits, 8 NNs



Threshold = 125 hits, 8 NNs

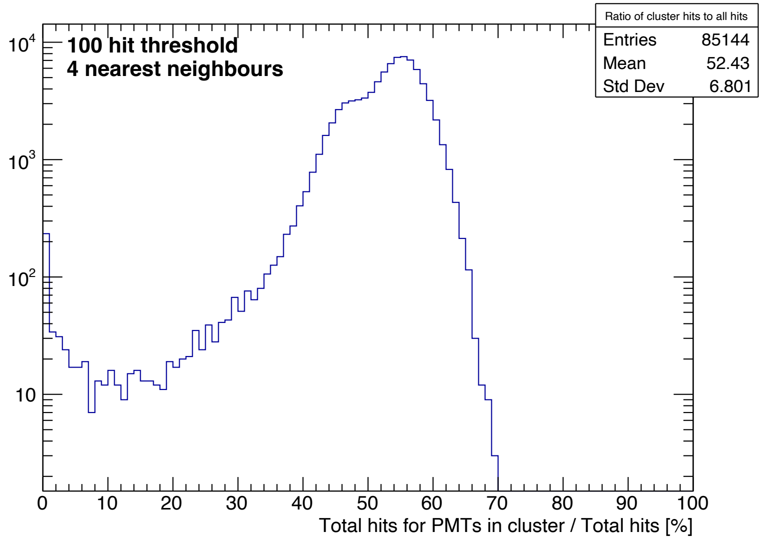


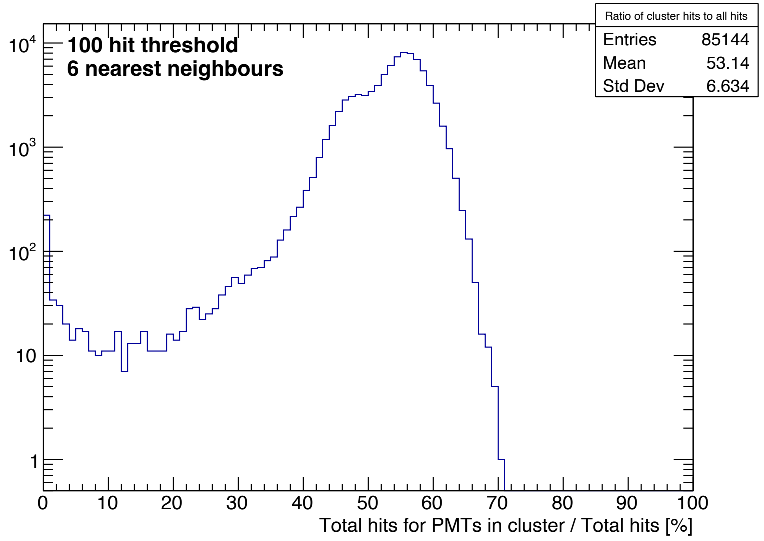
PMT Hit Clustering: Global Information

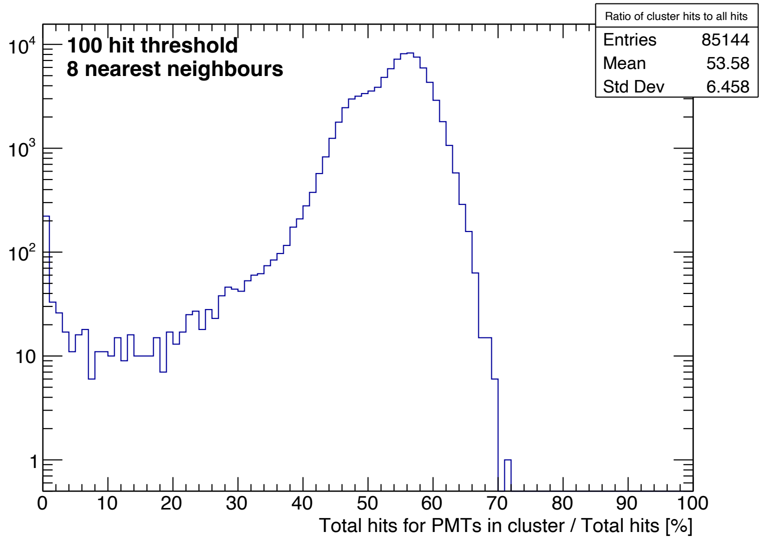


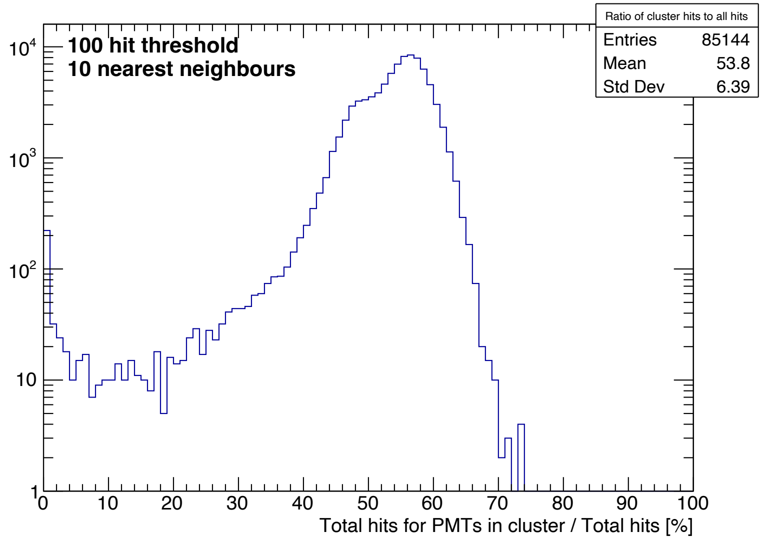
$$\frac{Sum\ of\ hits\ in\ cluster\ PMTs}{Sum\ of\ all\ hits}$$

PMT Hit Clustering: NN effect

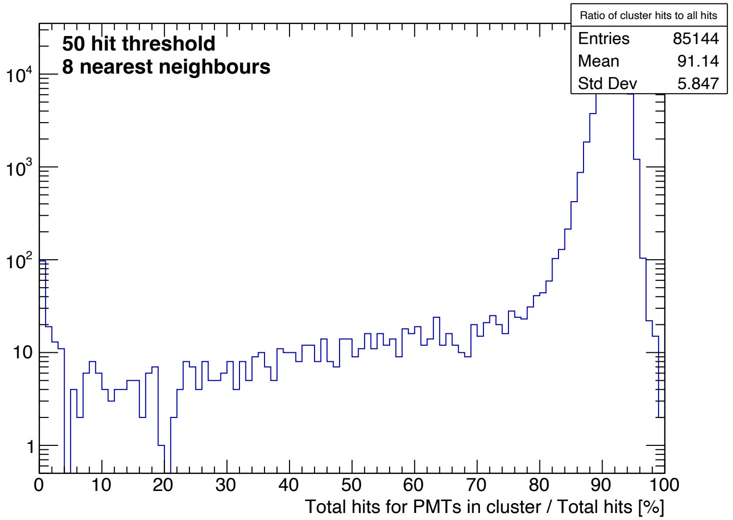


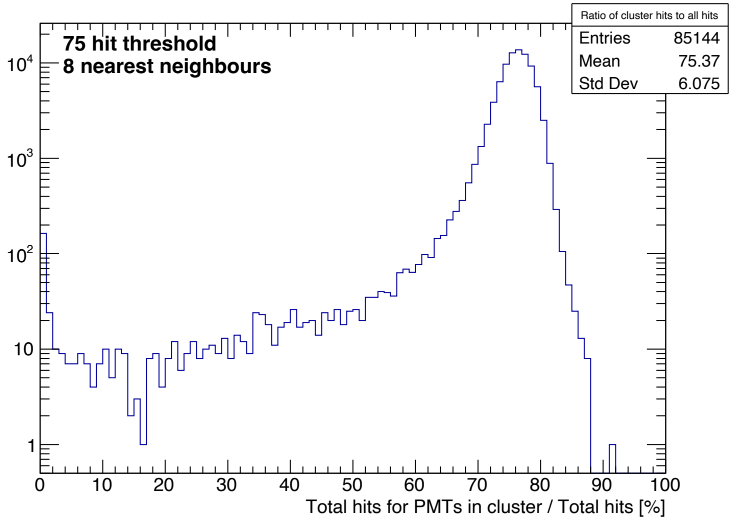


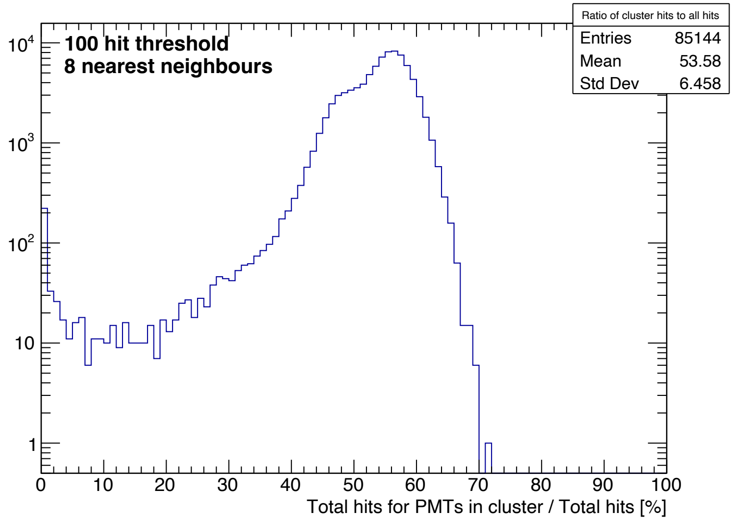


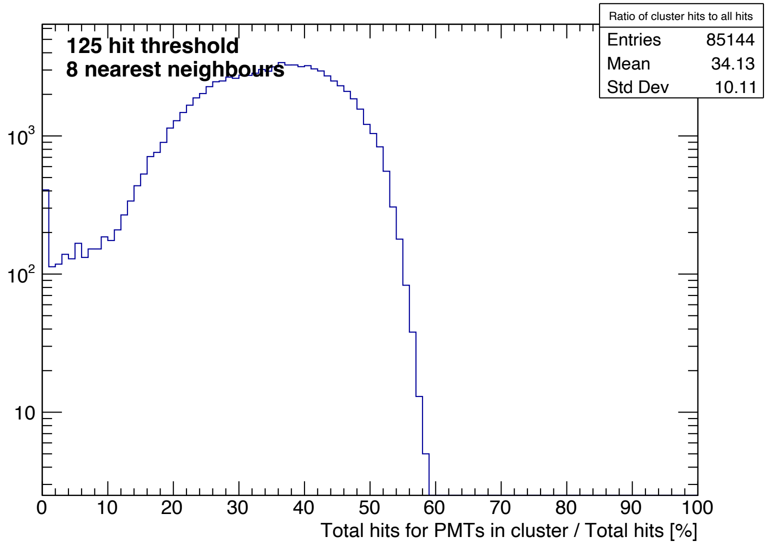


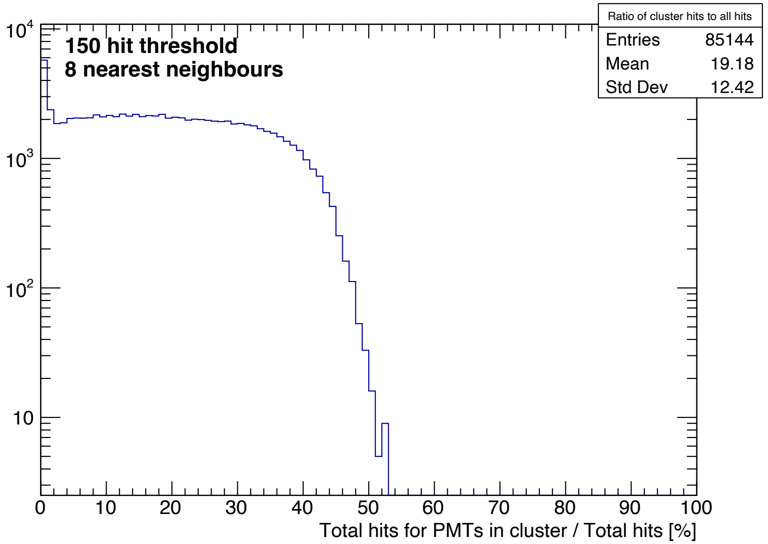
PMT Hit Clustering: Threshold effect



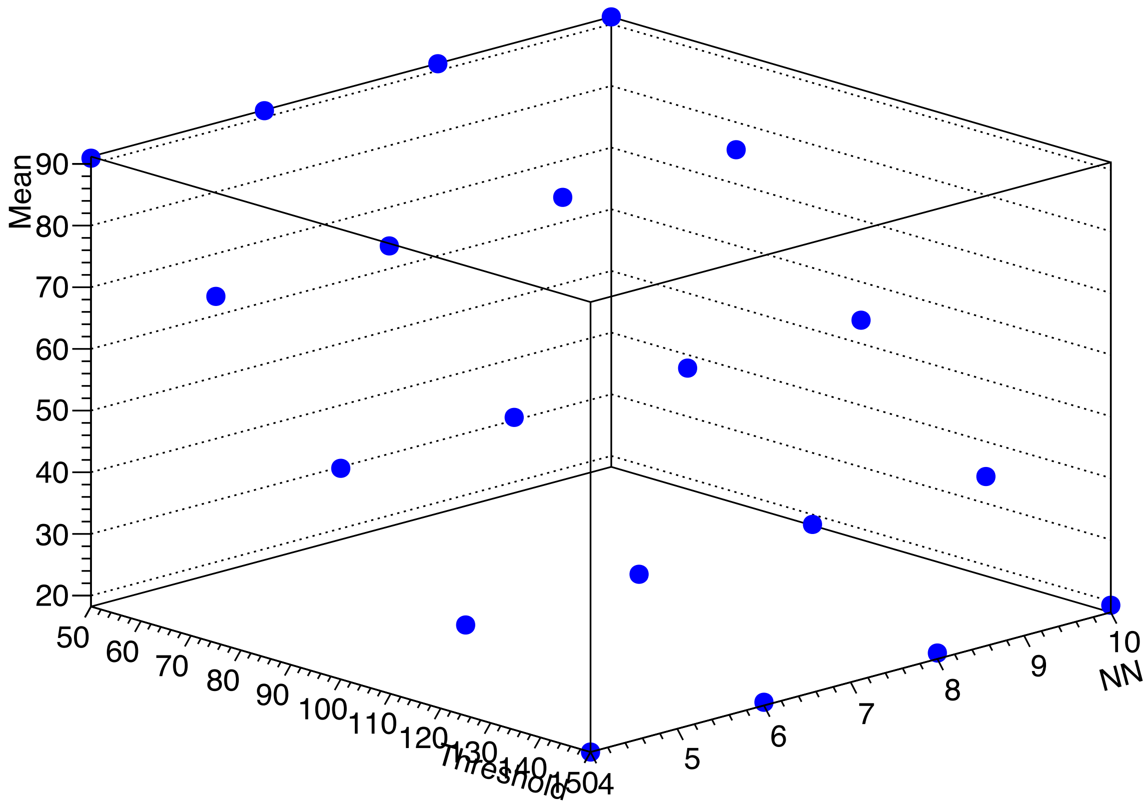


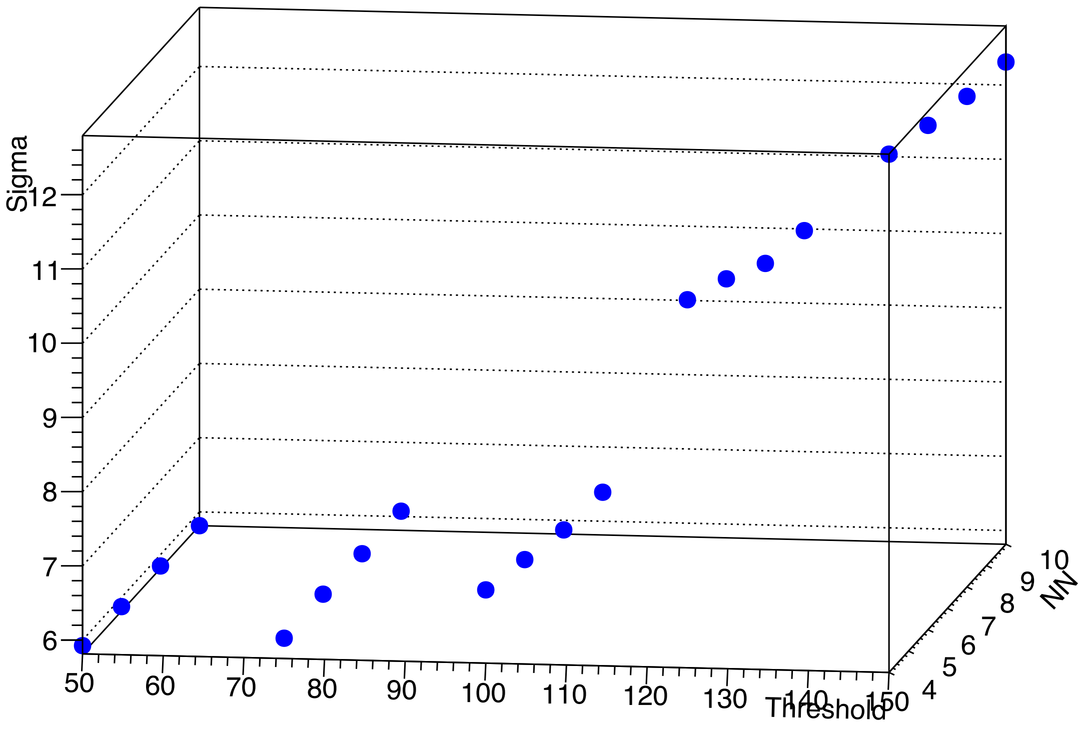






PMT Hit Clustering





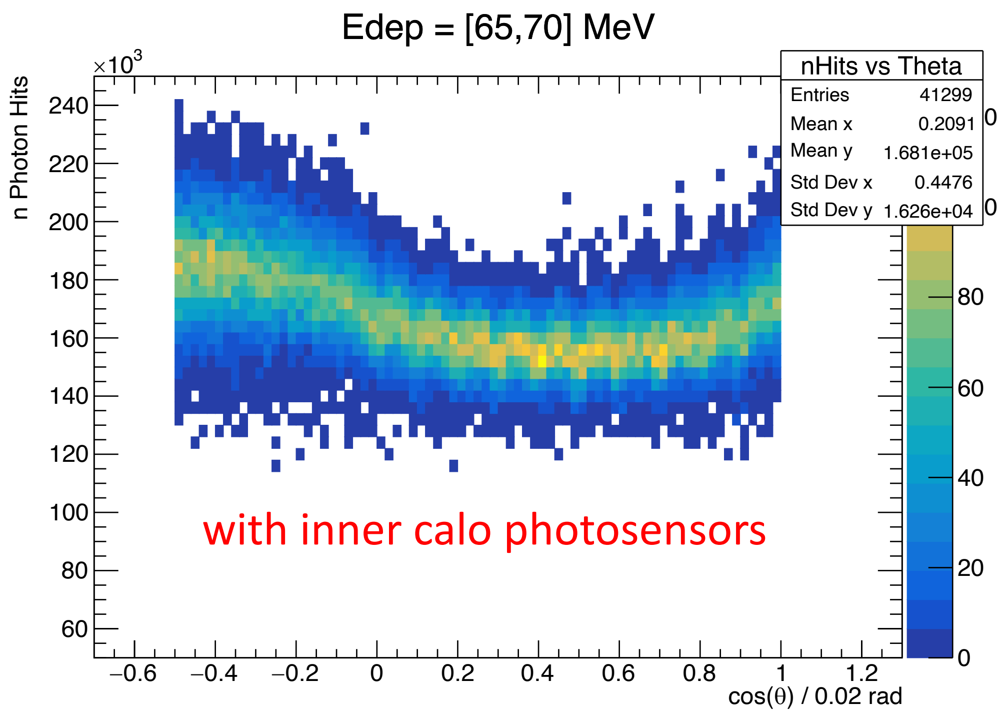
- Change in NN has minor effect – default to 8
- Change in Threshold has large effect – default to 100 hits

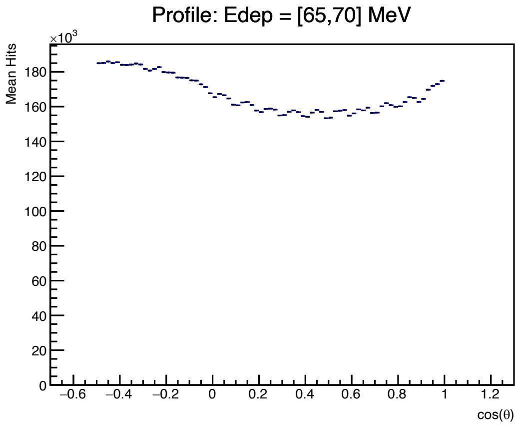
PMT Hit Clustering

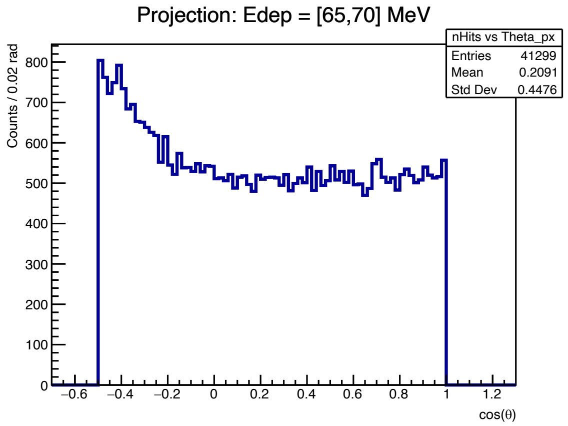
DISCLAIMER:

- PMT clustering interesting and potentially useful, but need to understand how to convert PMT hits to energy deposited and account for lost photons – scale factor will be needed
- Need better understanding of theta energy dependence, Edep in detector, and improved photon counting

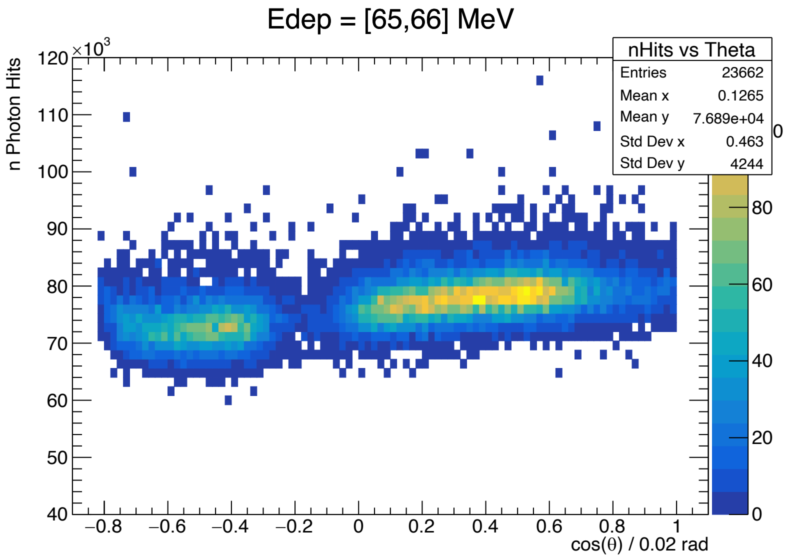
Energy and # of photons: pienu

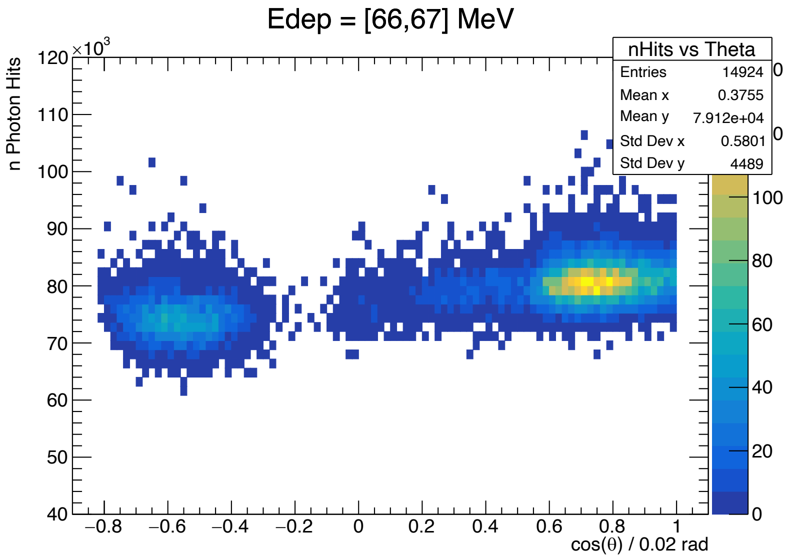






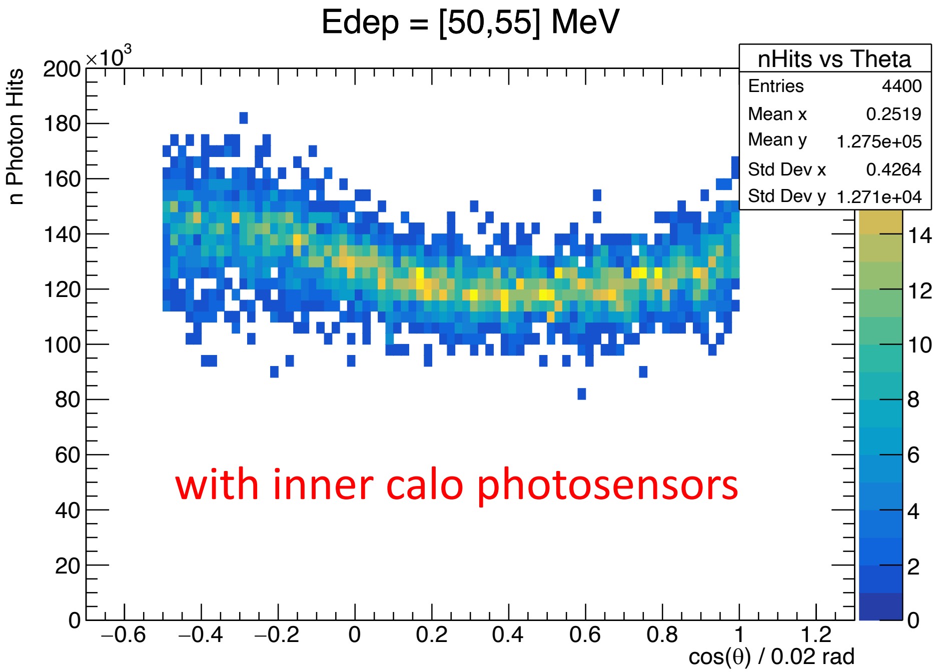
Previous results

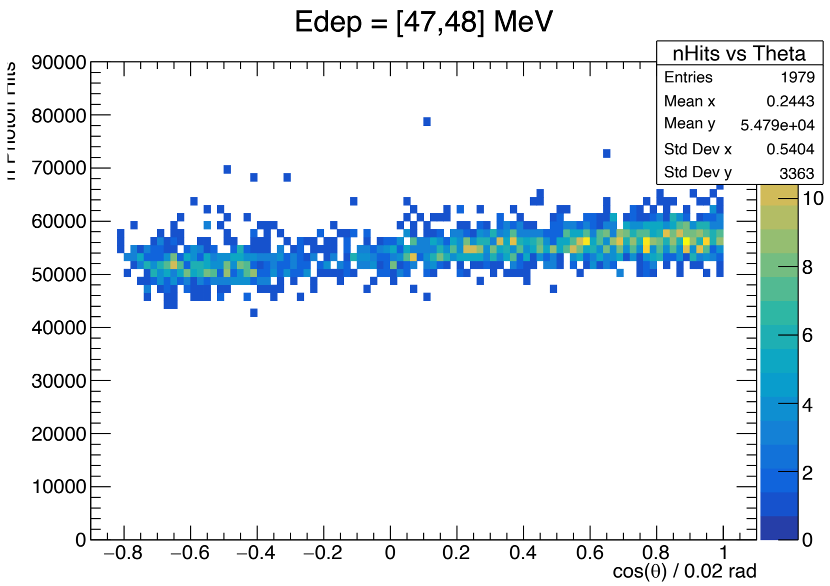


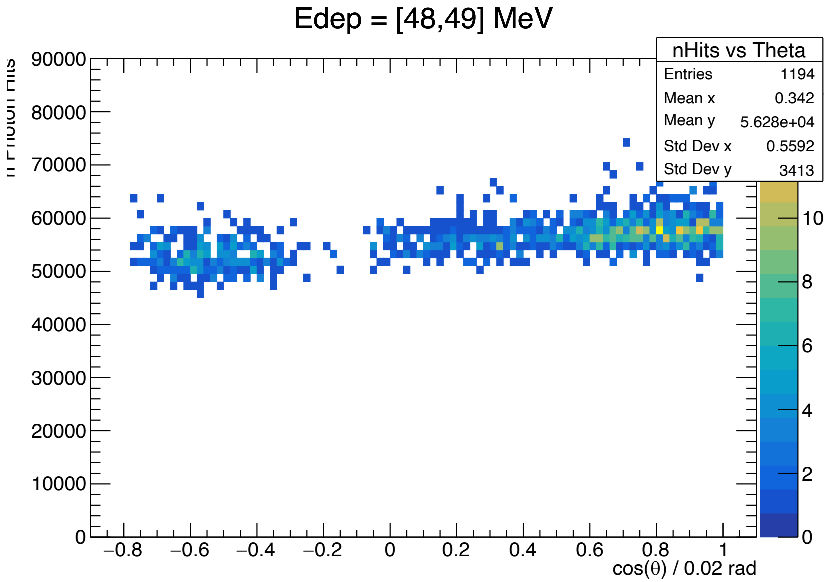


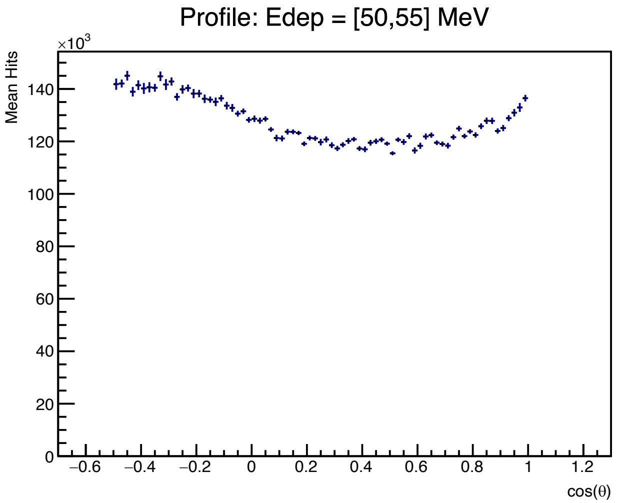
Energy and # of photons: Michel

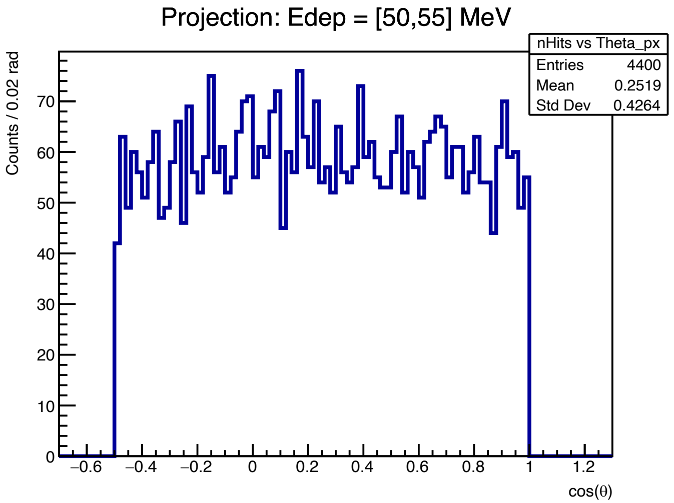
Previous results



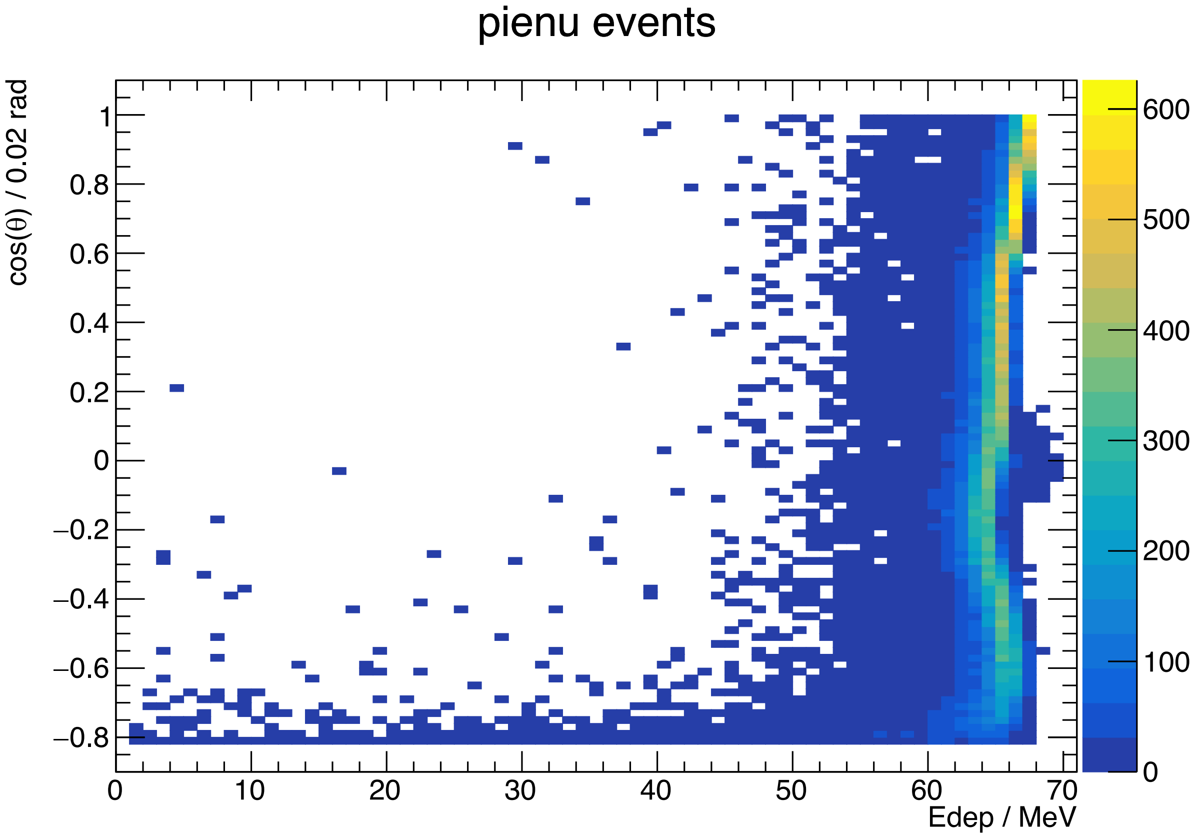


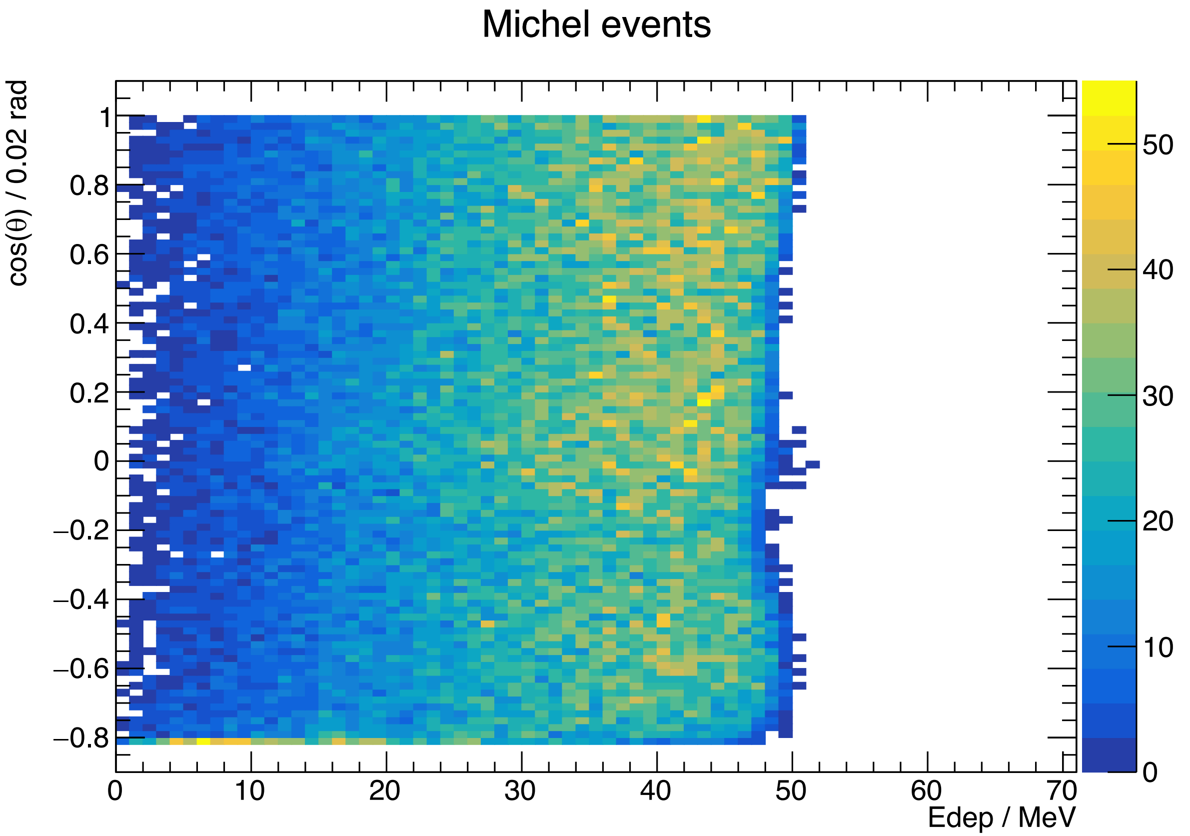




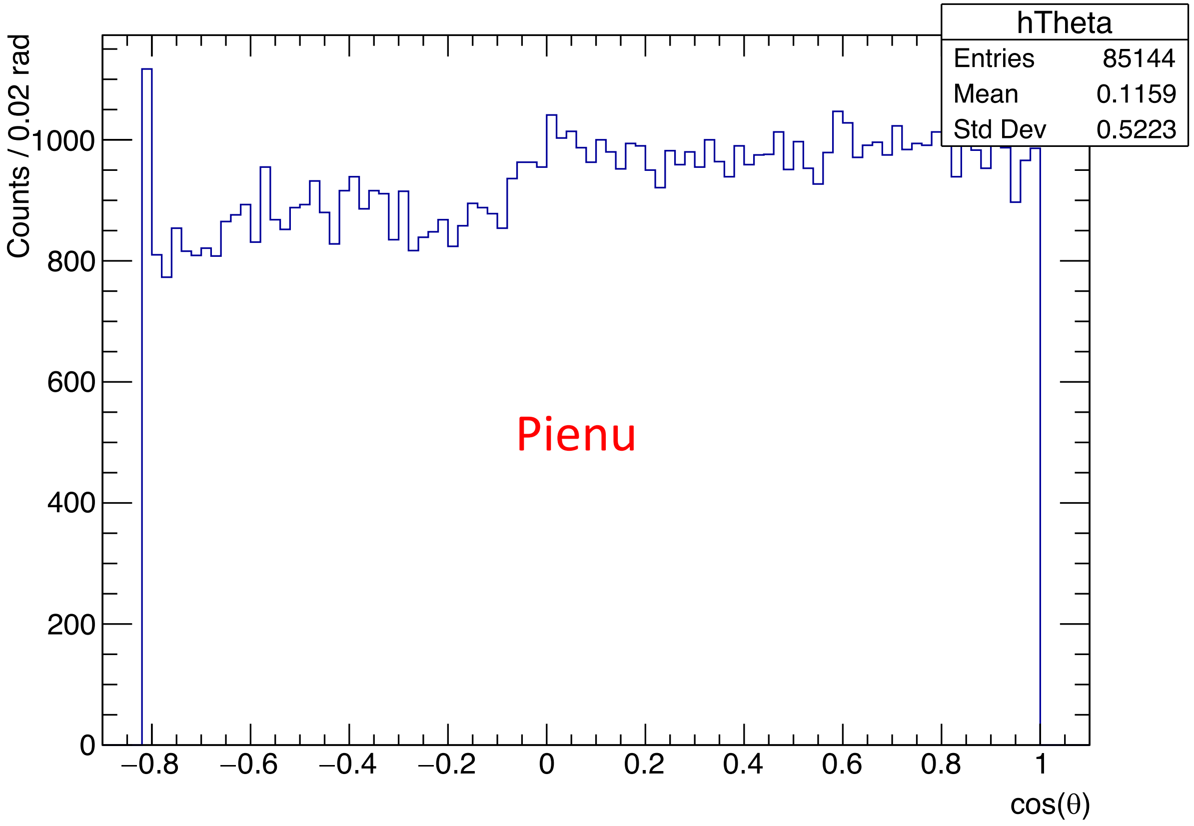


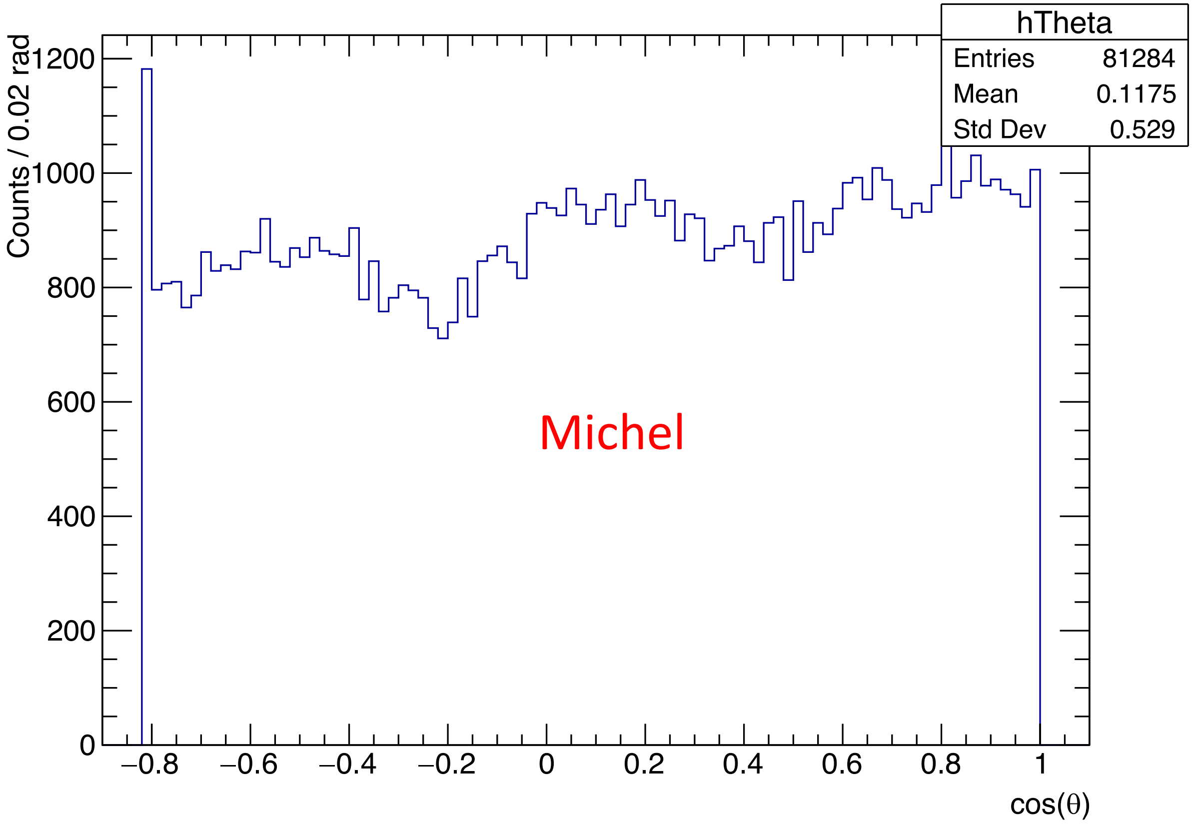
Energy and Angle Dependence (full detector)



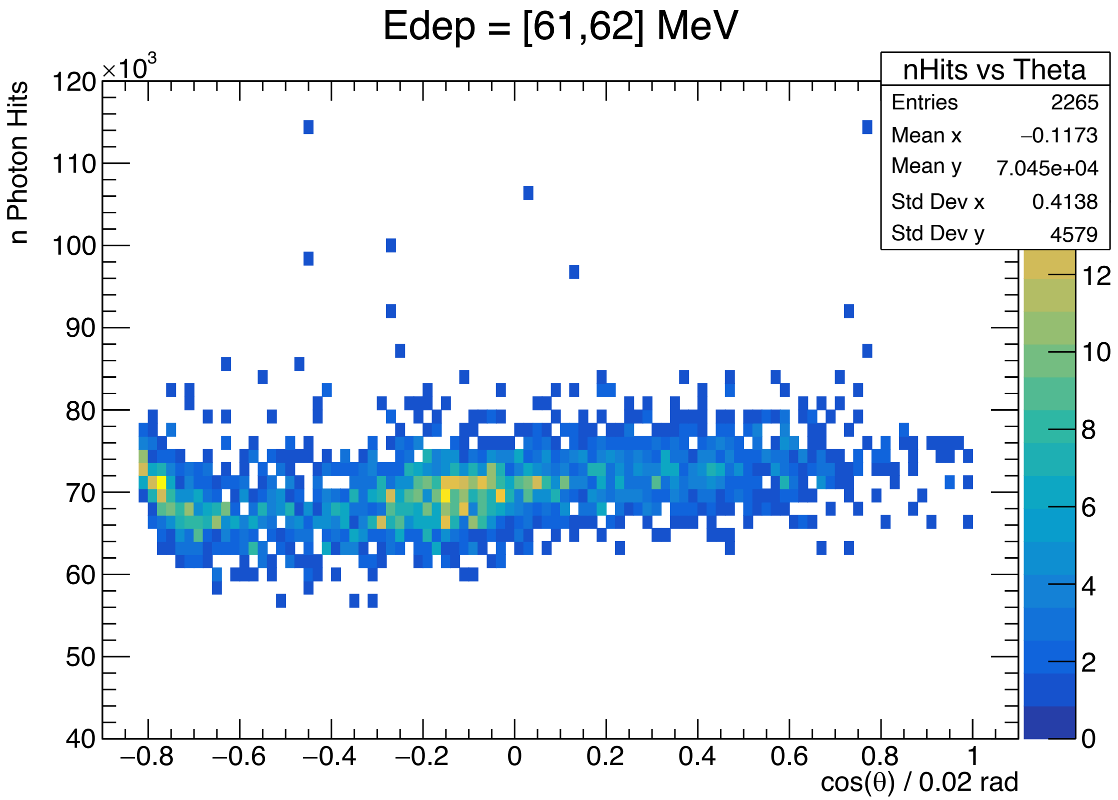


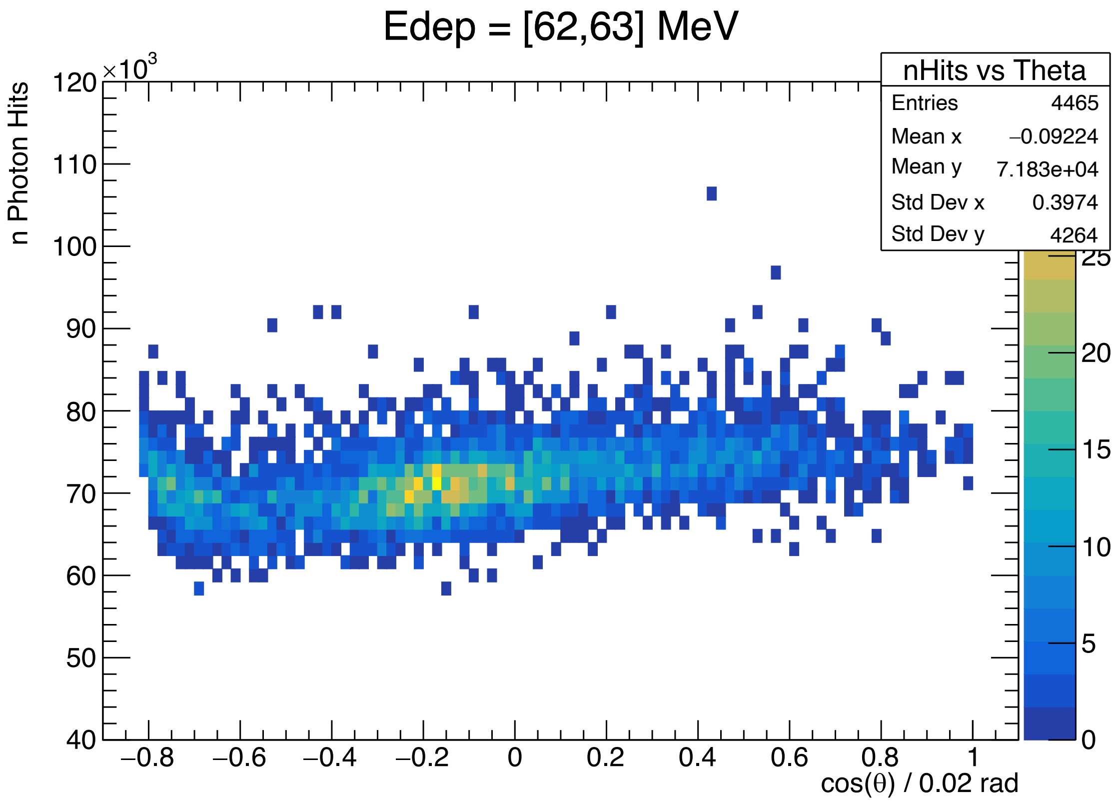
Energy and Angle Dependence (full detector)



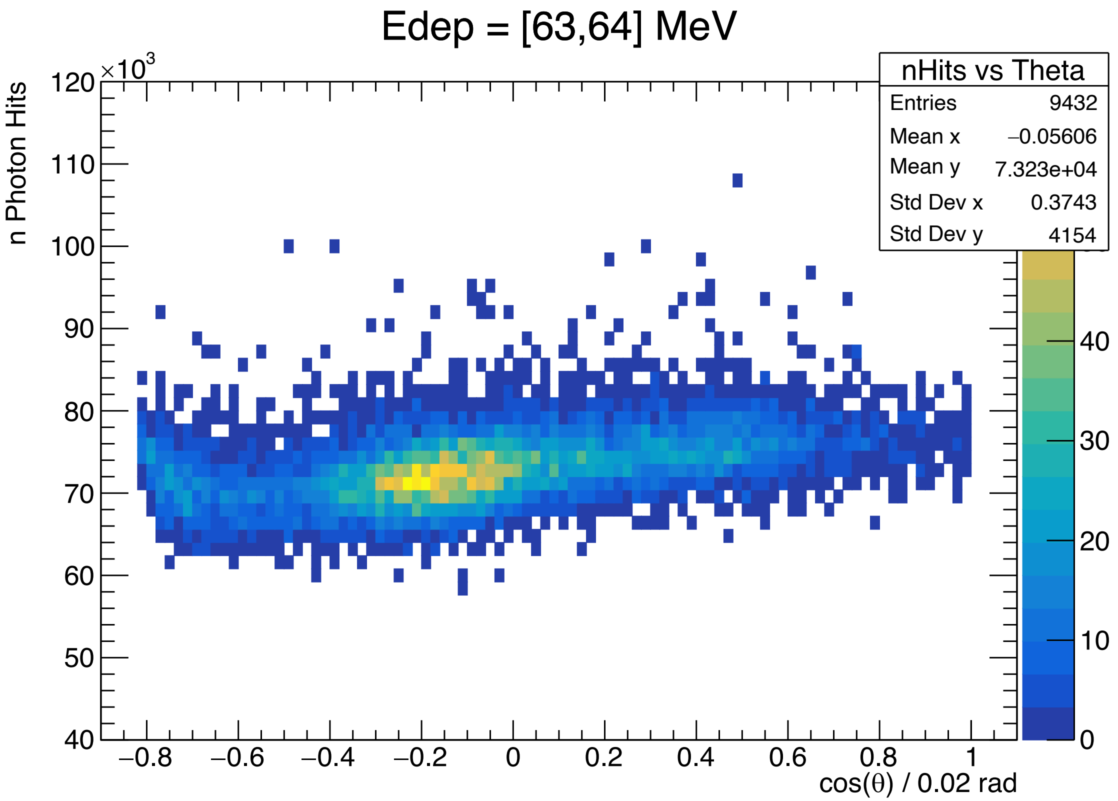


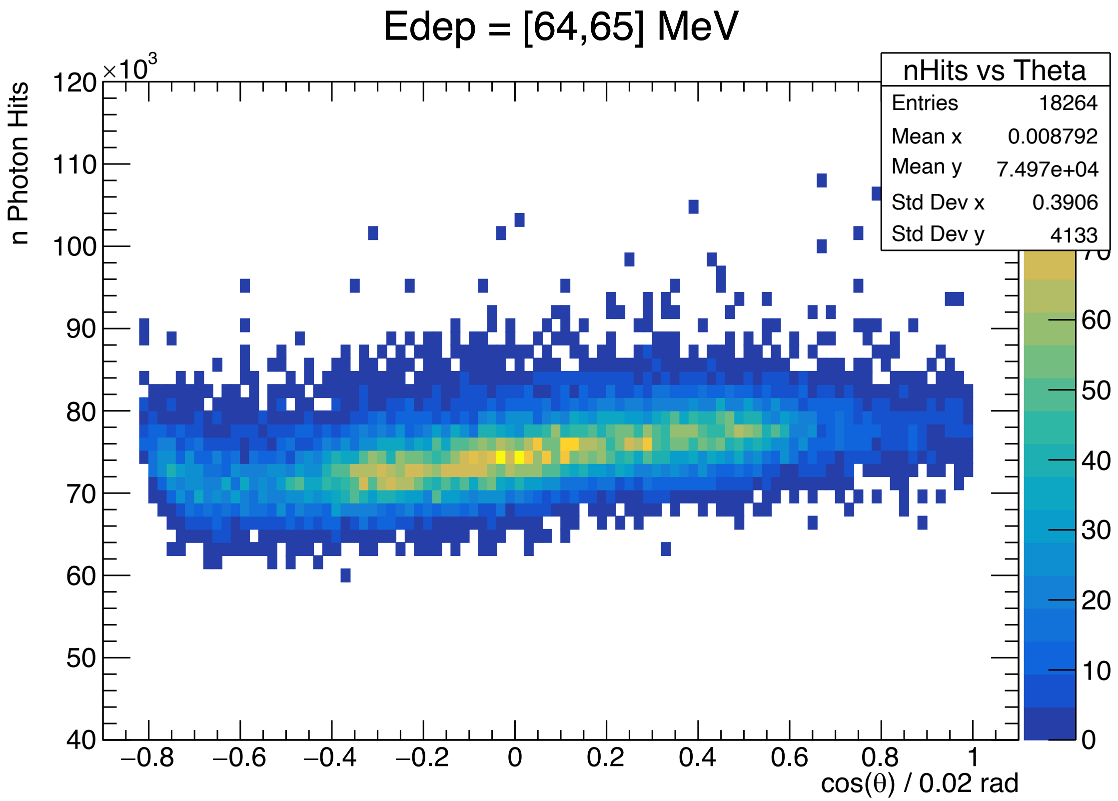
No inner sensors: Pienu Energy and Angle Dependence



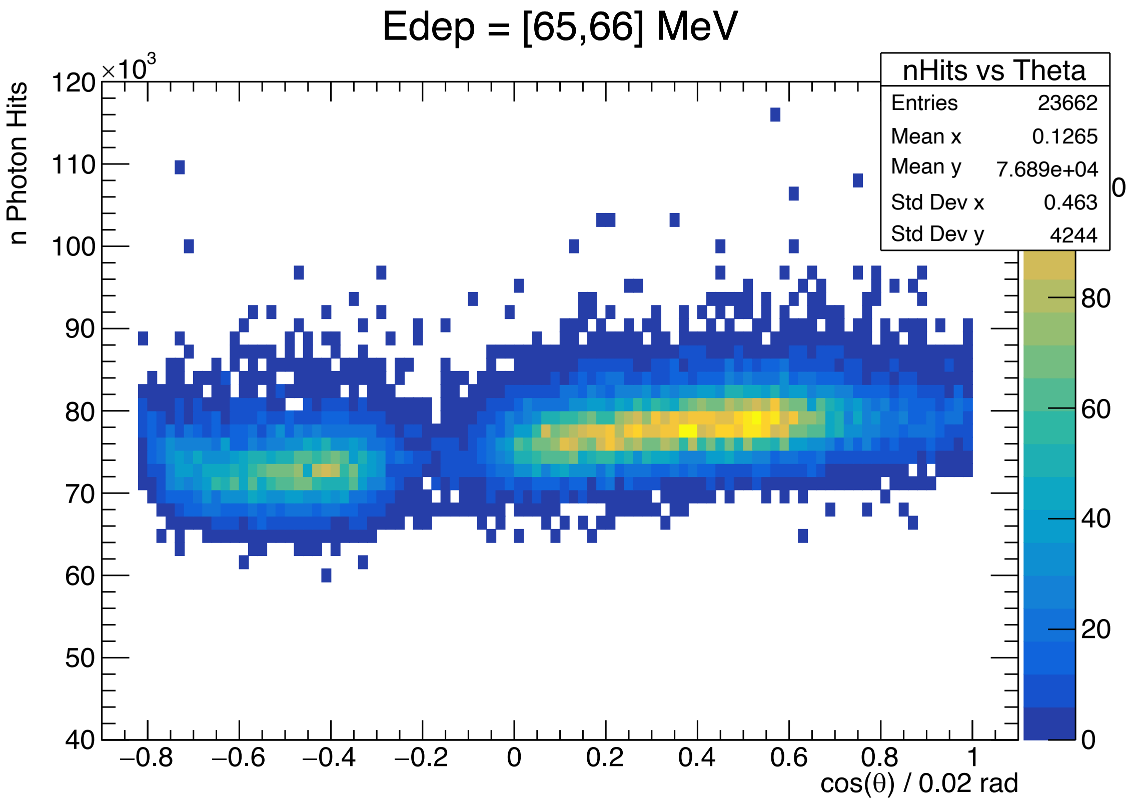


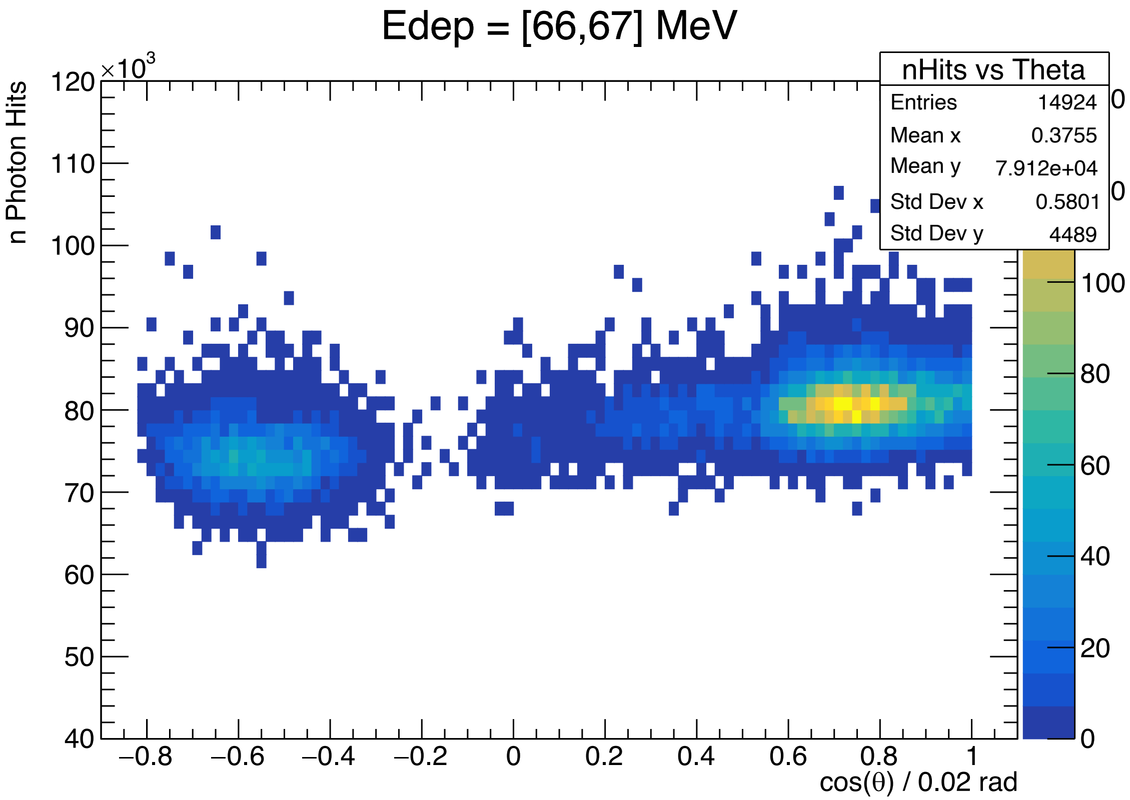
No inner sensors: Pienu Energy and Angle Dependence





No inner sensors: Pienu Energy and Angle Dependence





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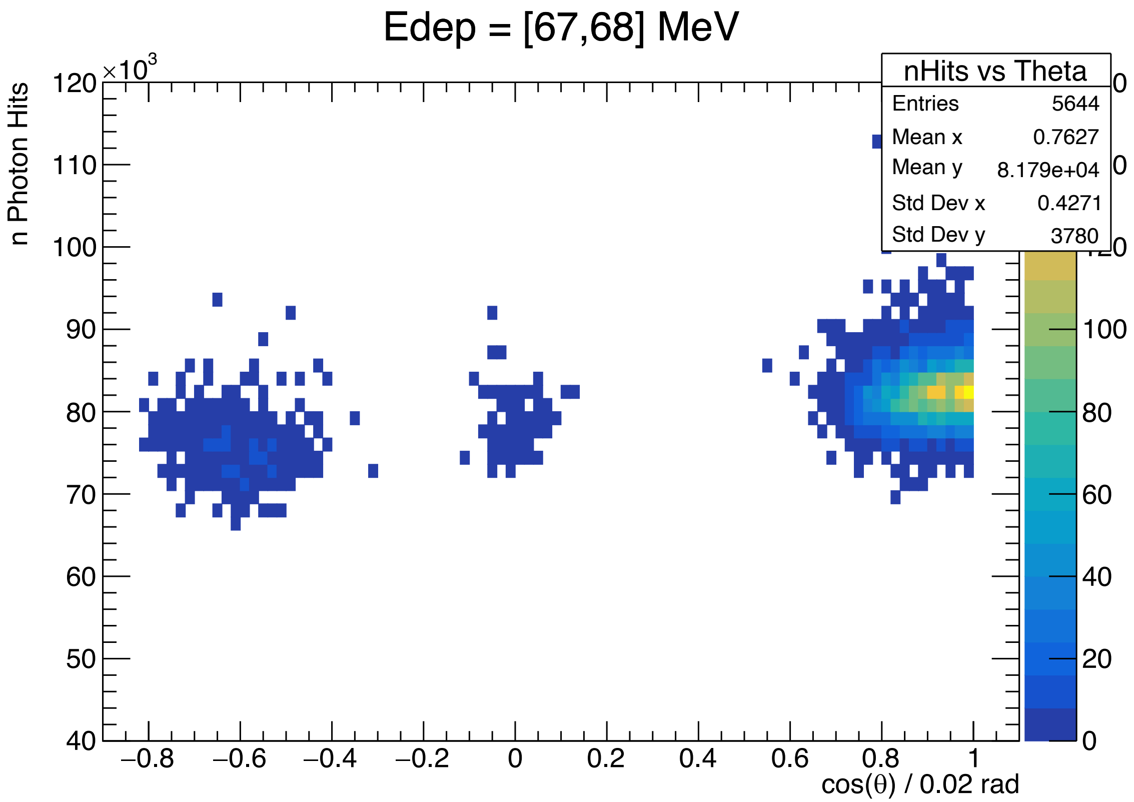

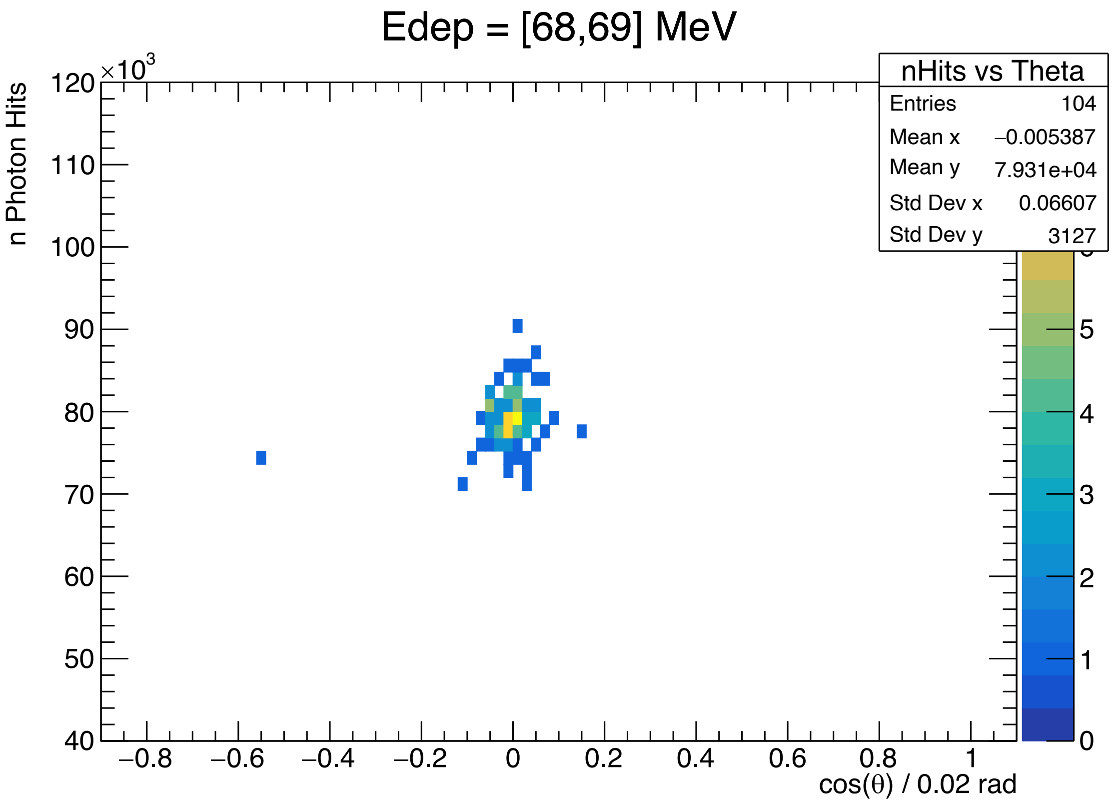

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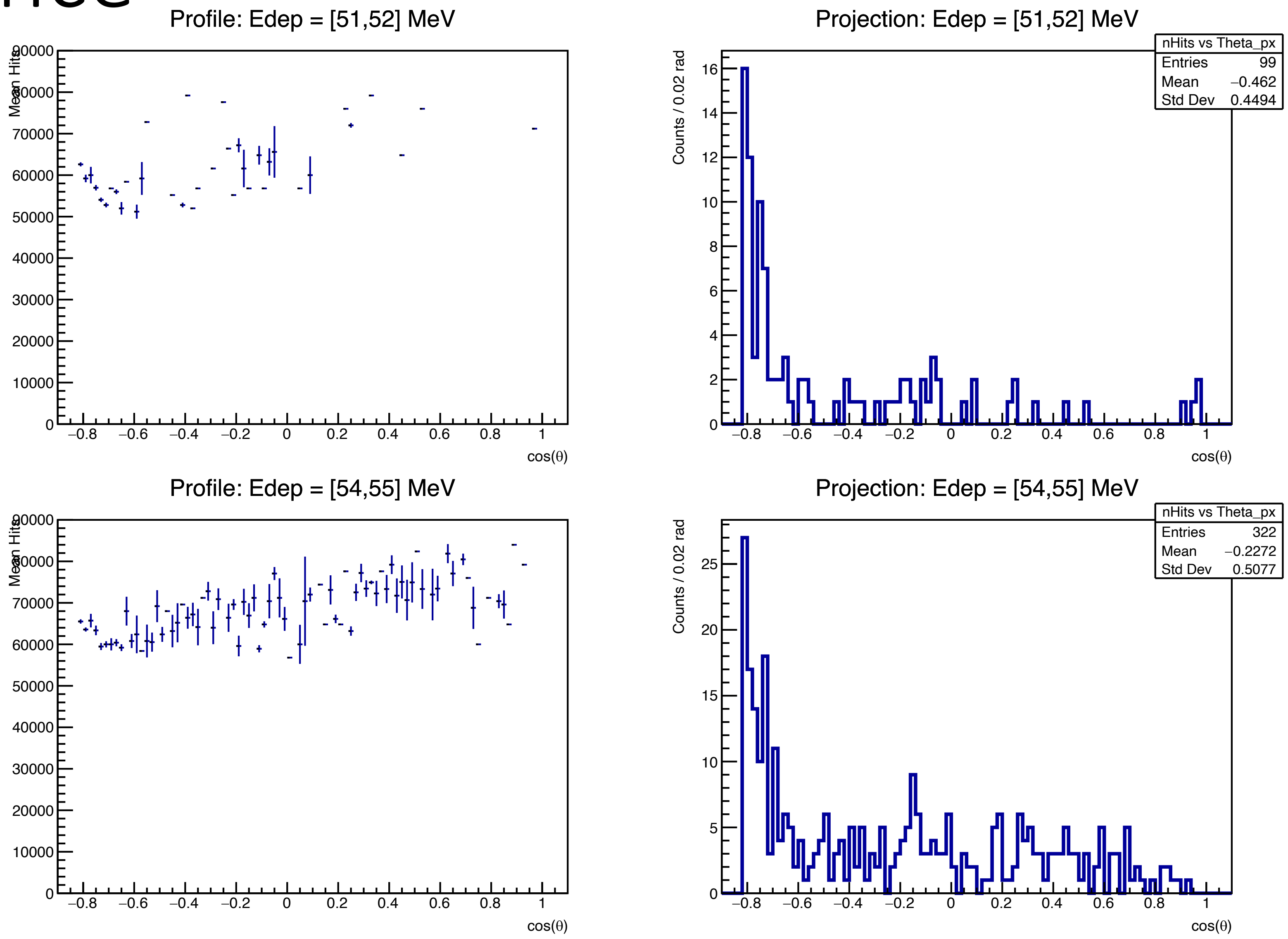

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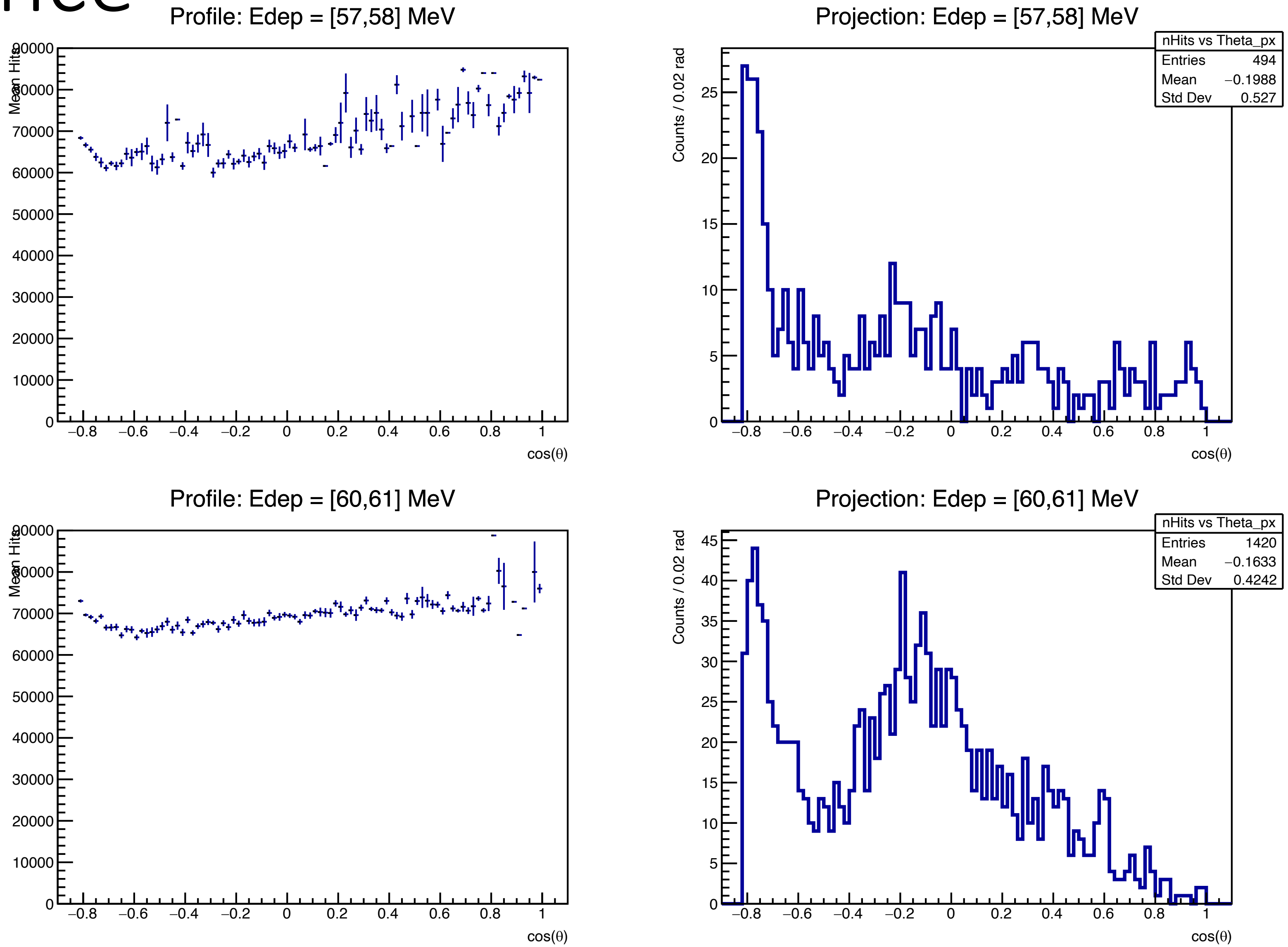
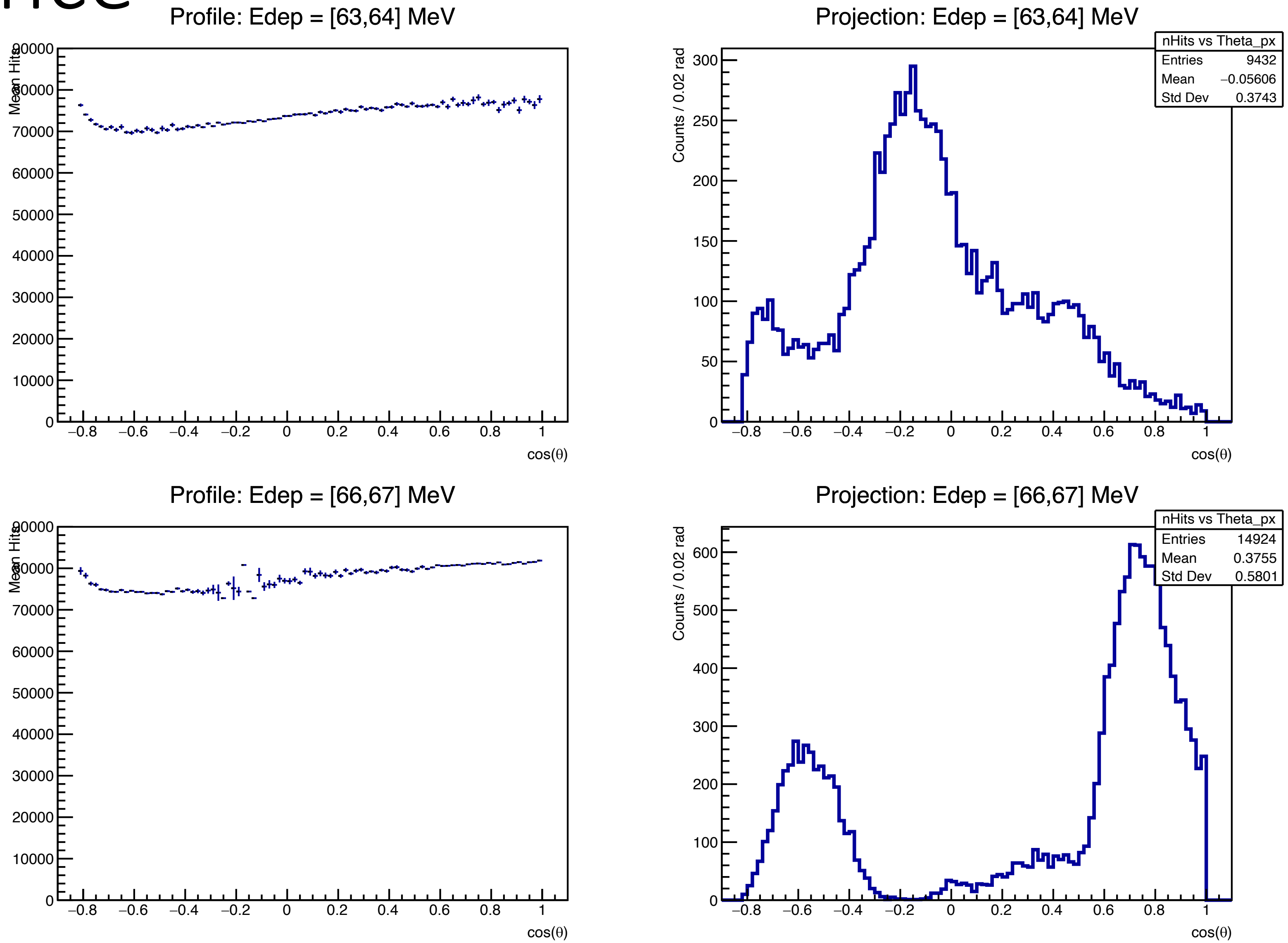


No inner sensors: Pienu Energy and Angle Dependence



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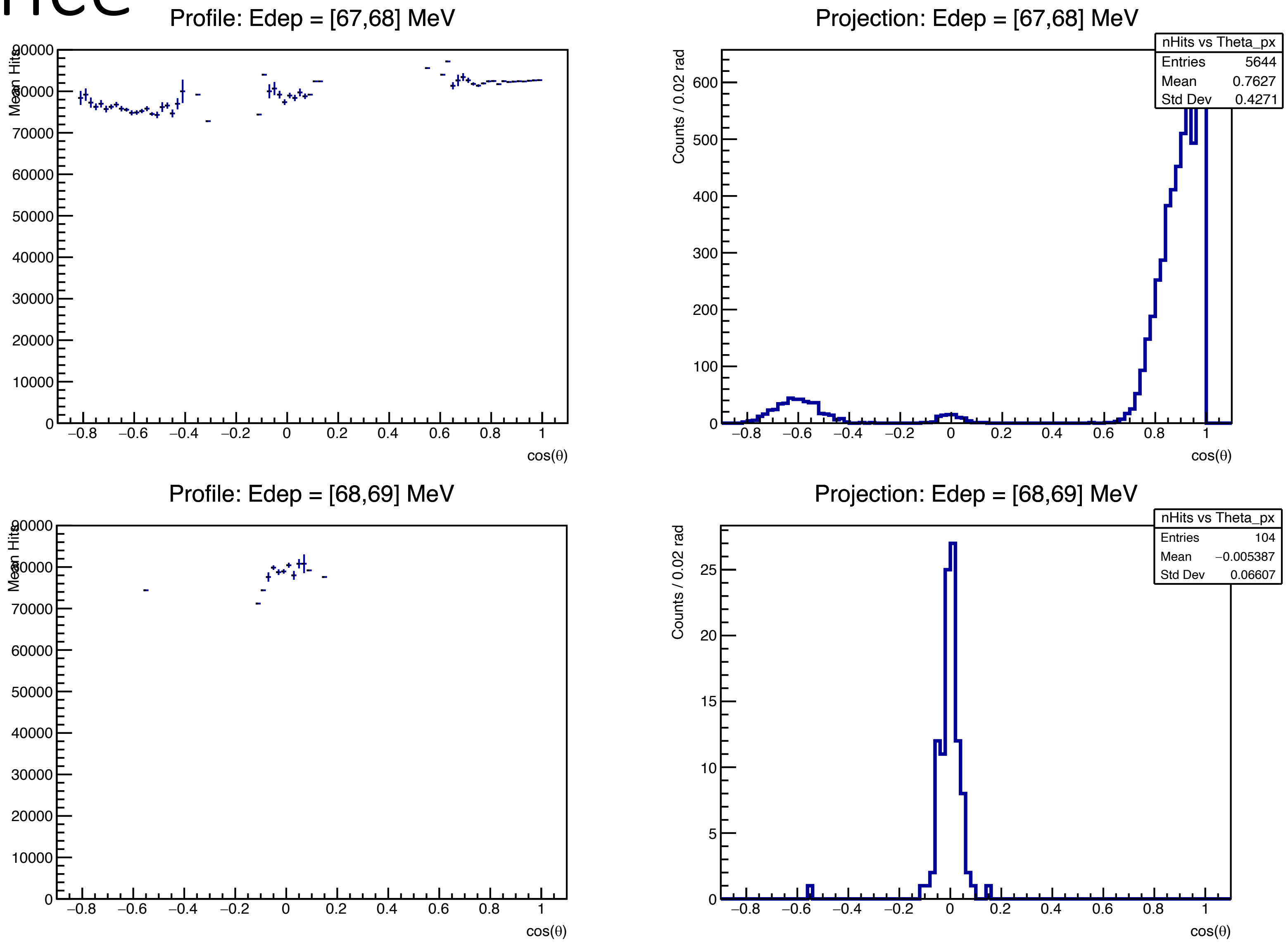
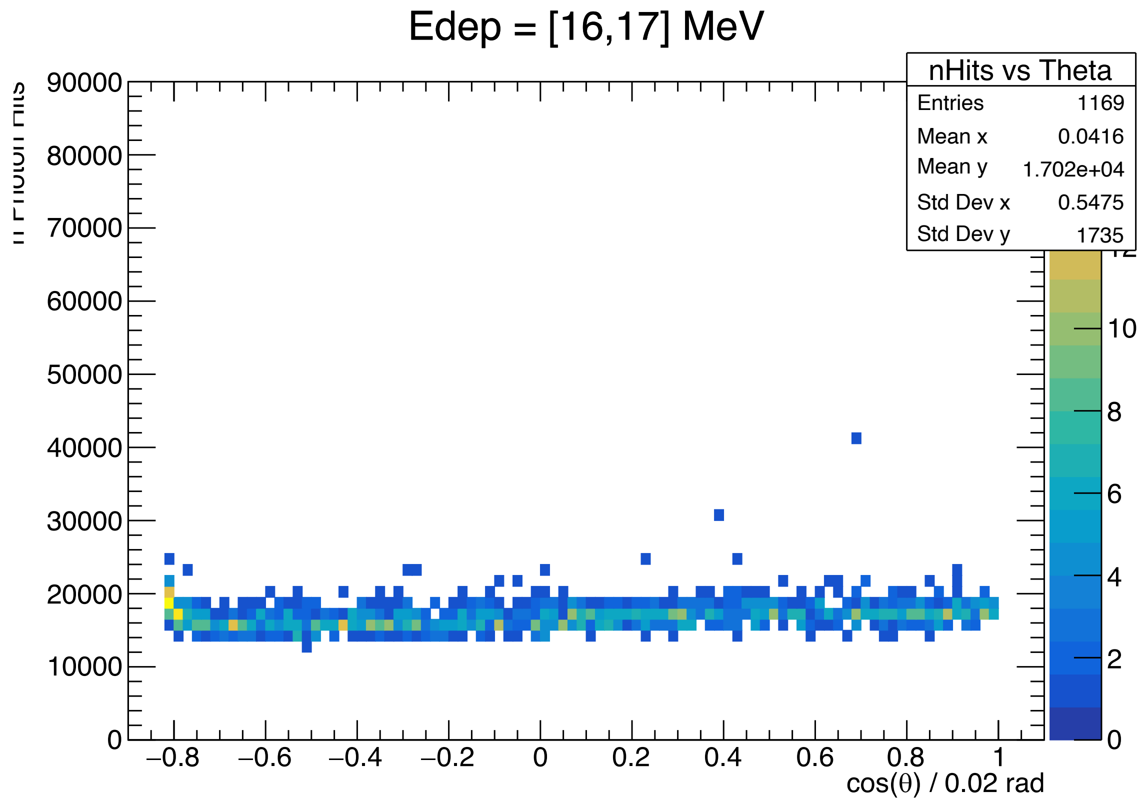
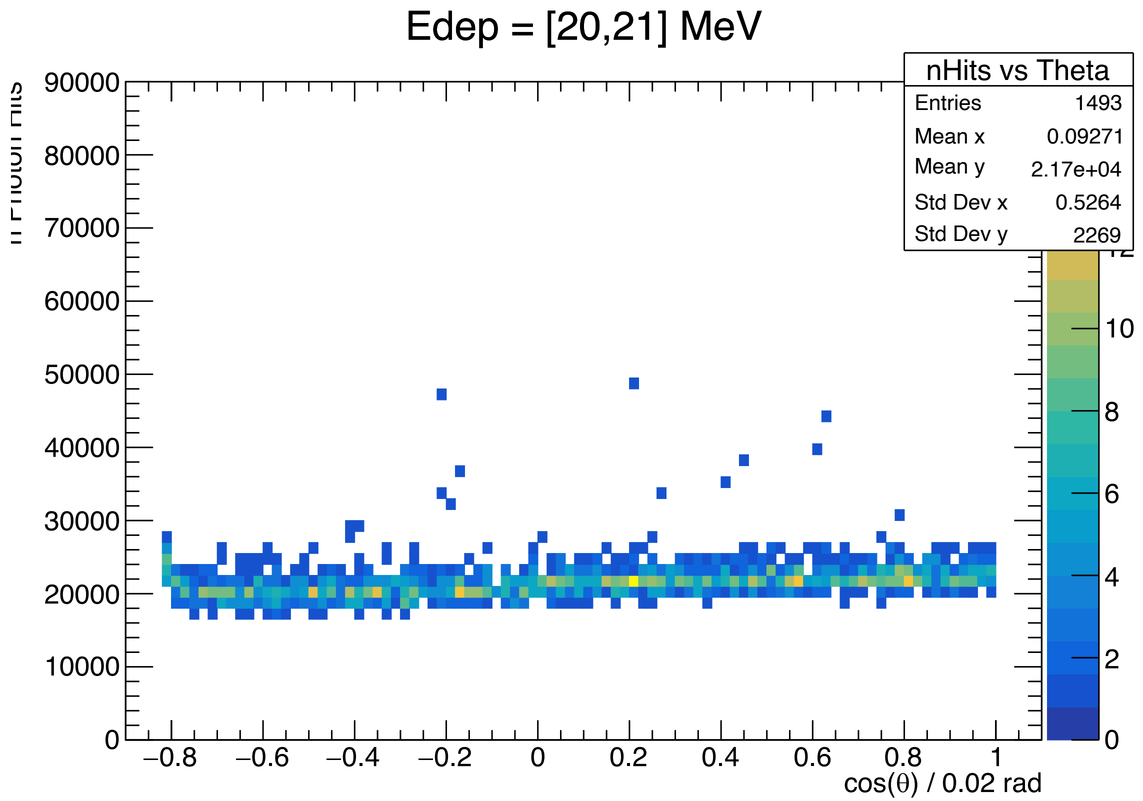
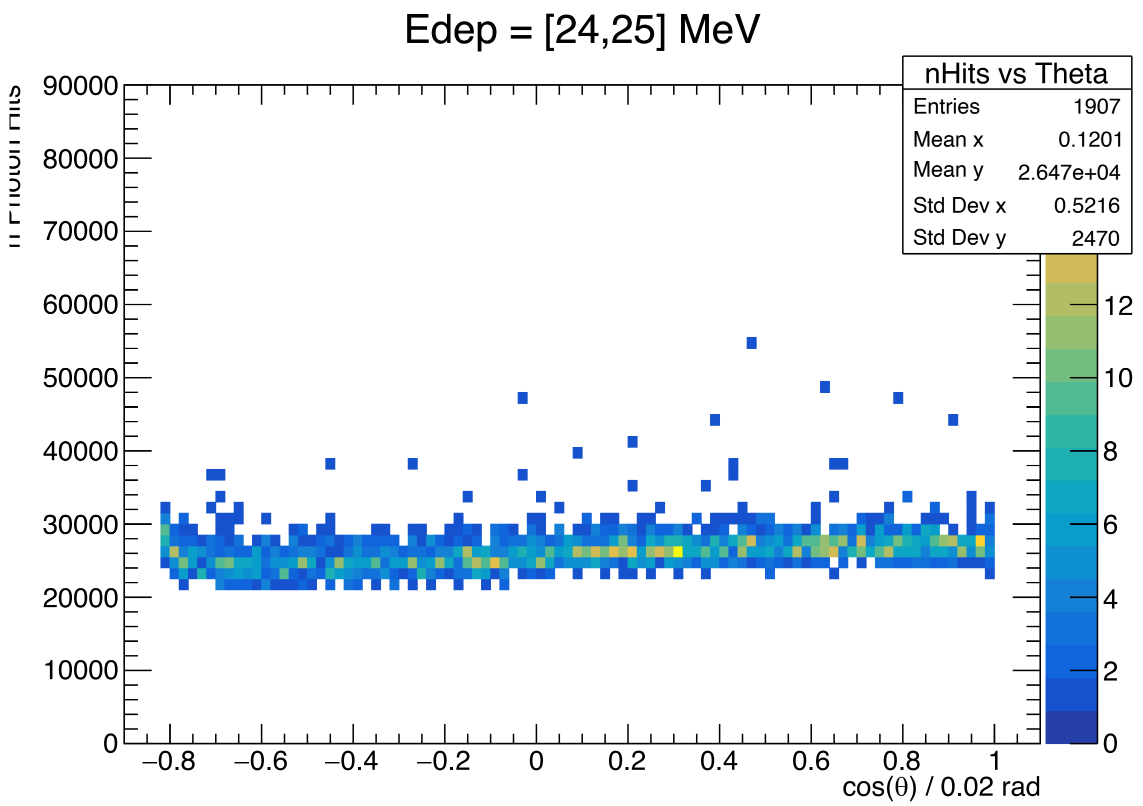


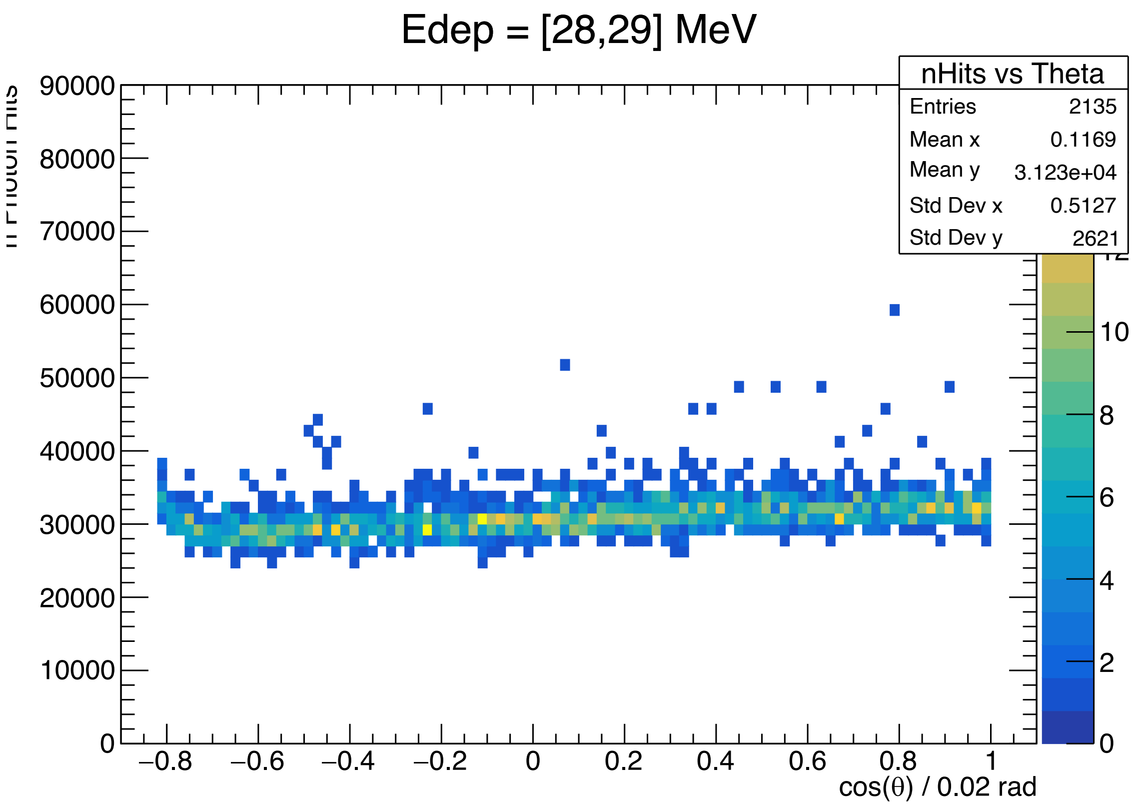
No inner sensors: Michel Energy and Angle Dependence





No inner sensors: Michel Energy and Angle Dependence





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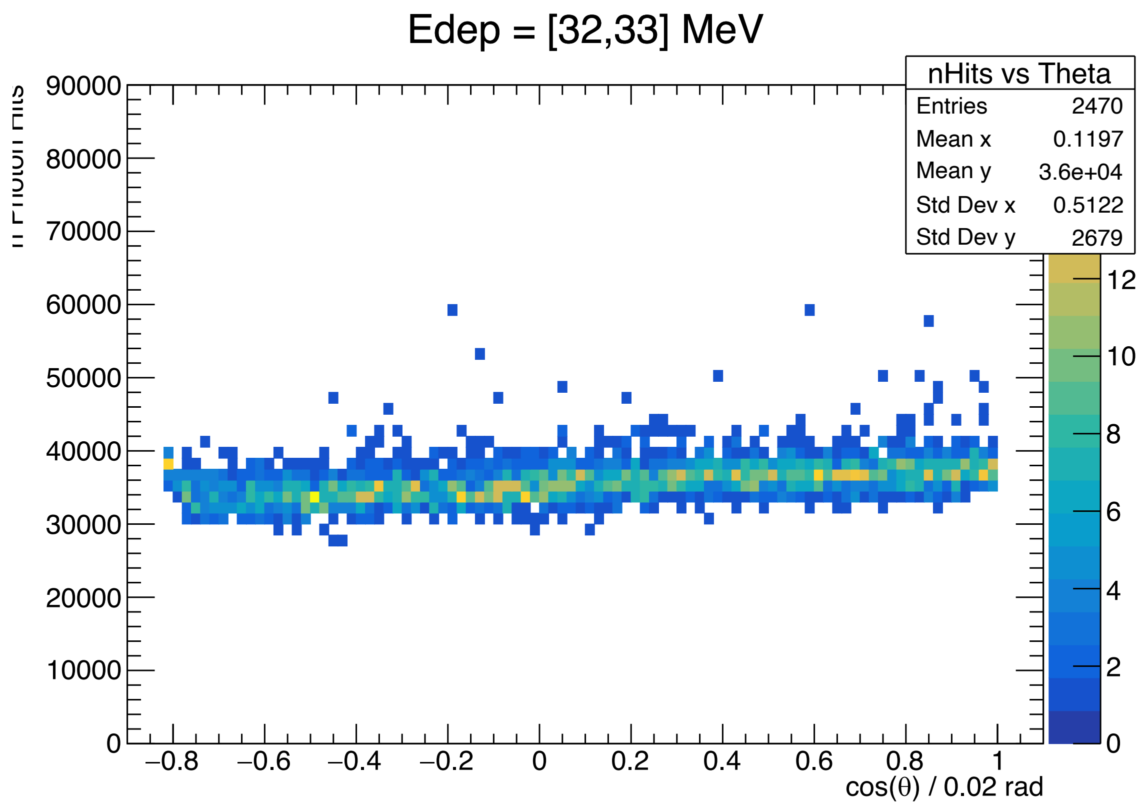
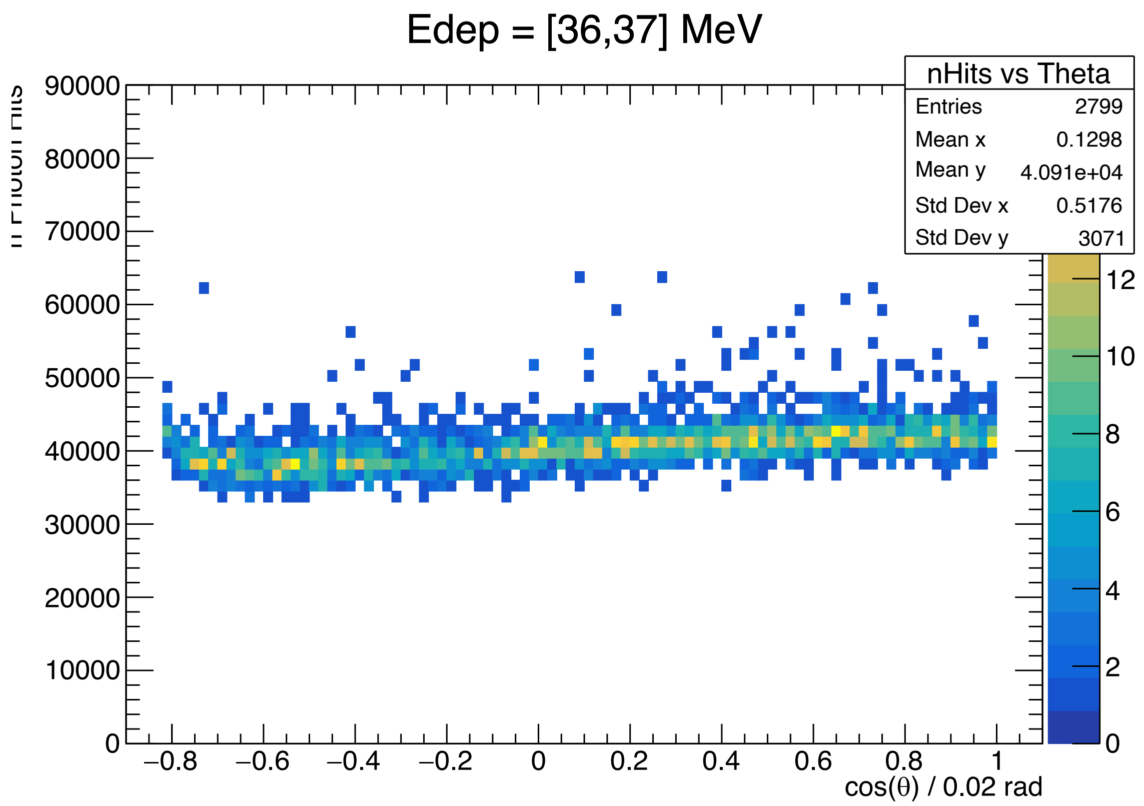
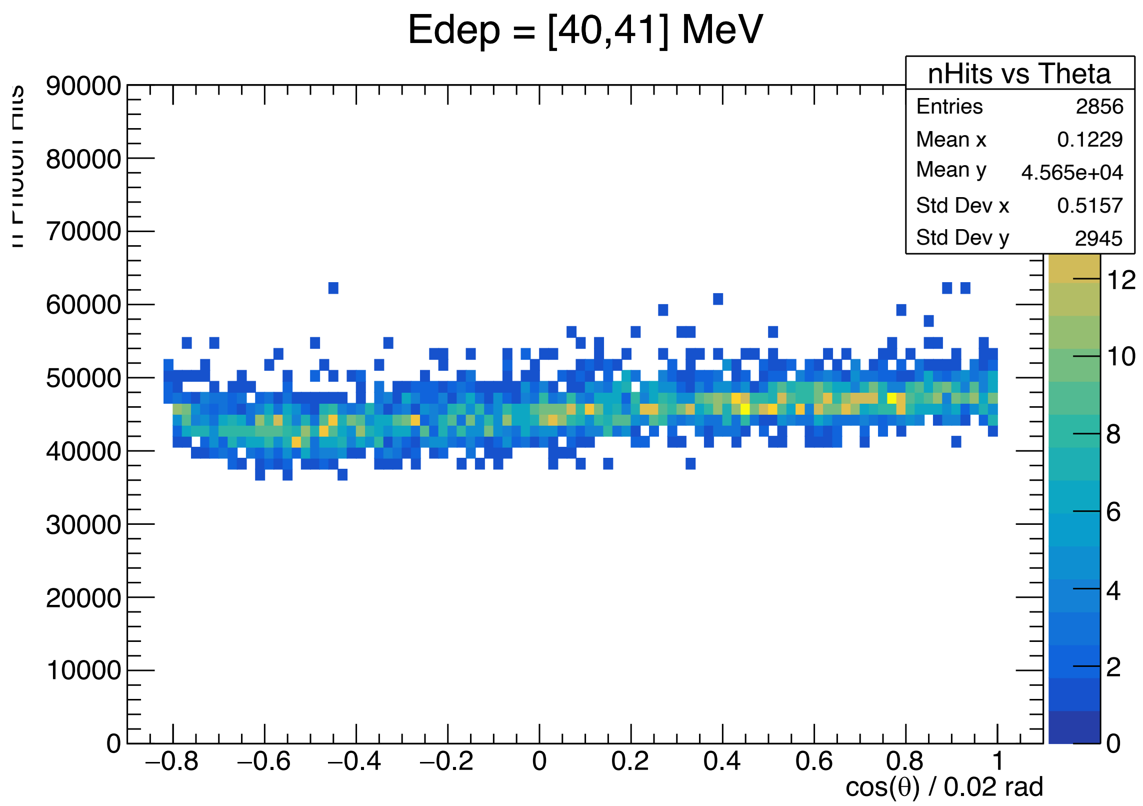
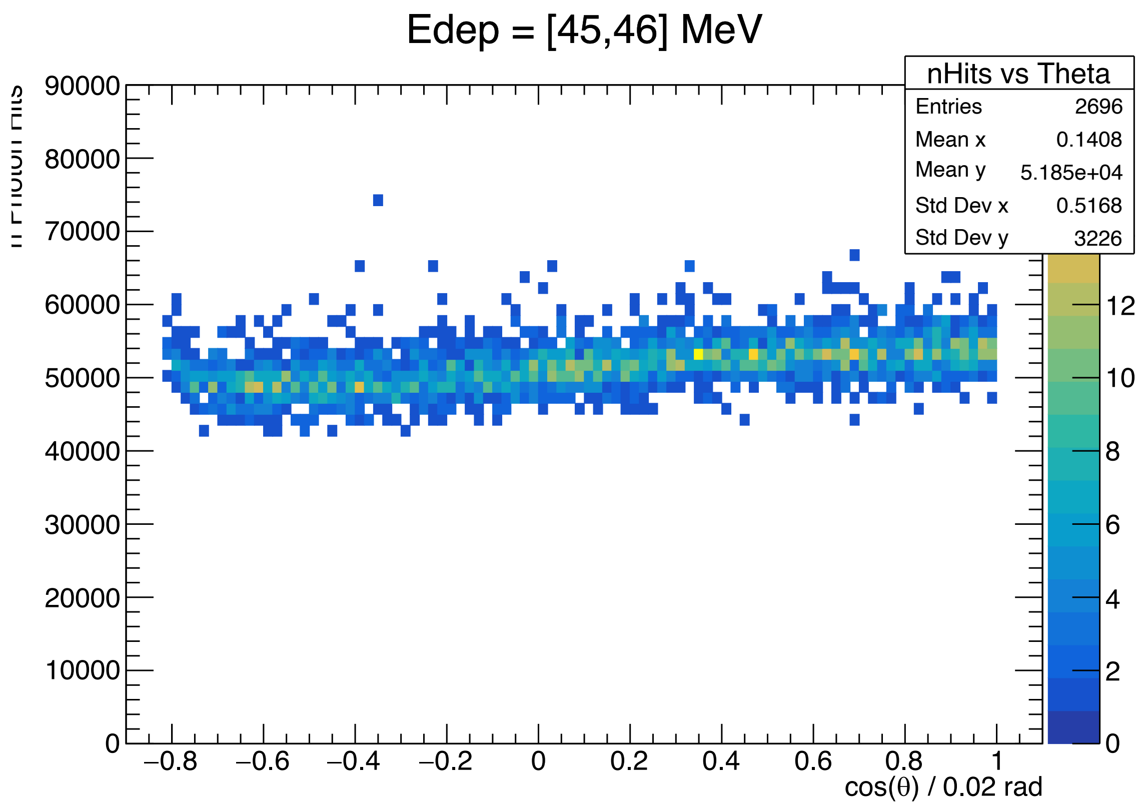


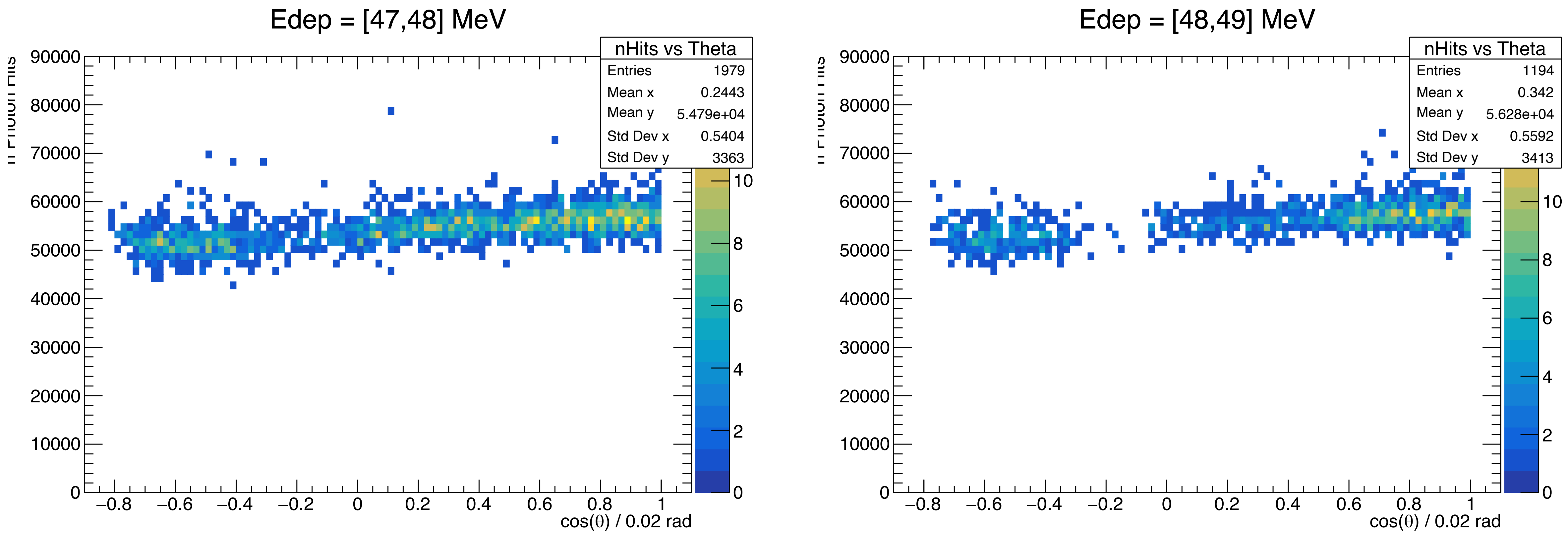


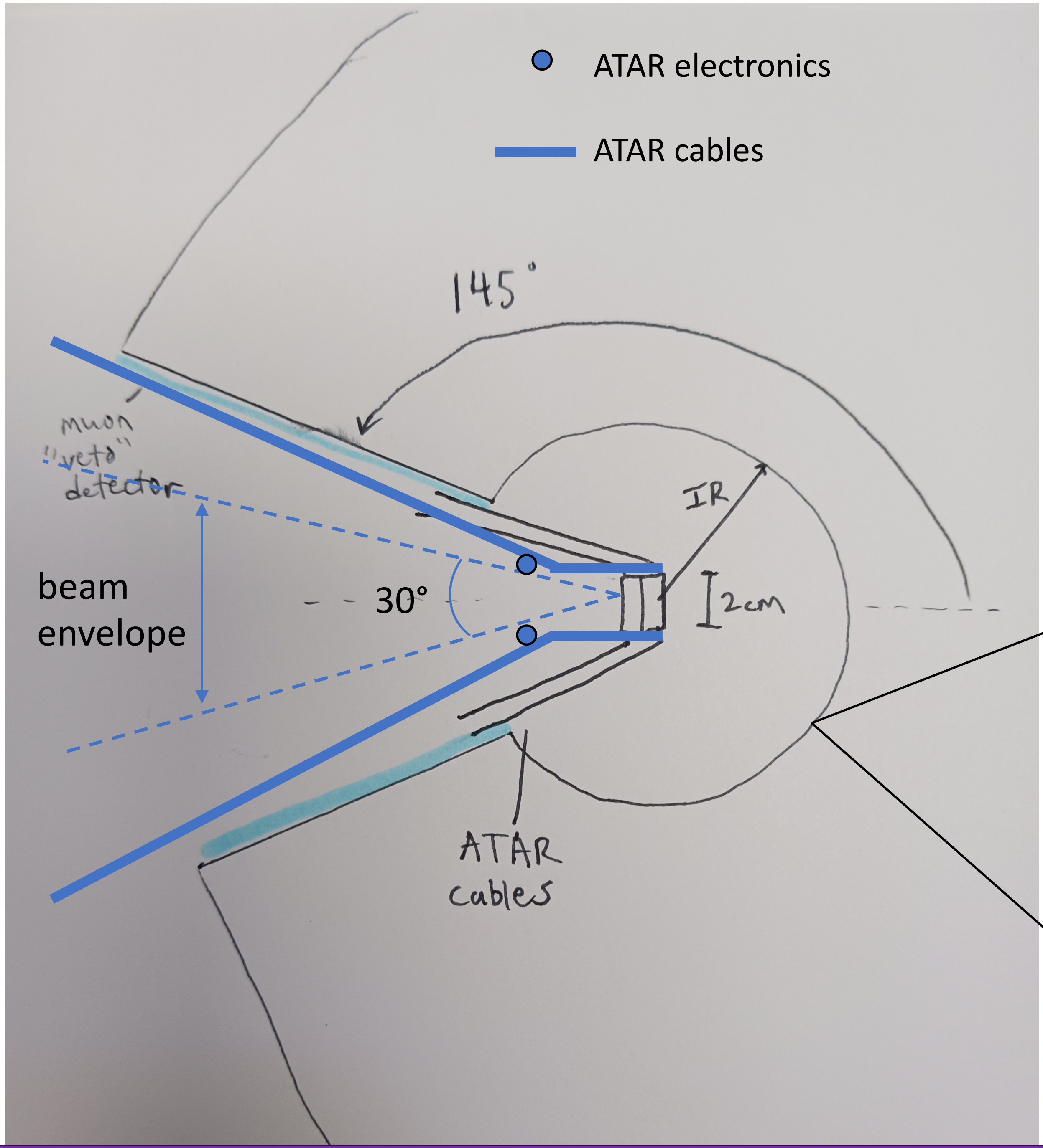
No inner sensors: Michel Energy and Angle Dependence





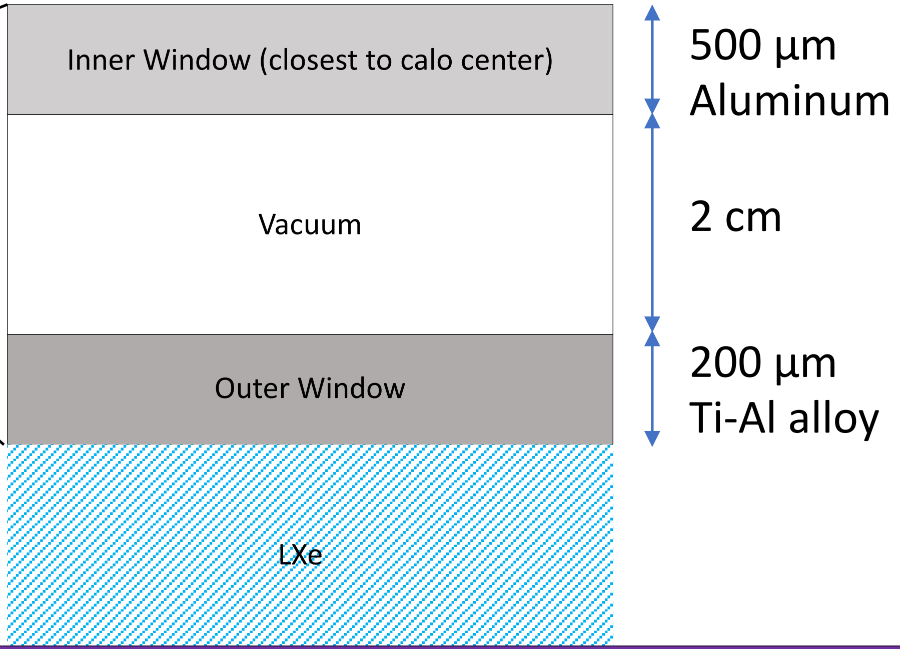
No inner sensors: Michel Energy and Angle Dependence



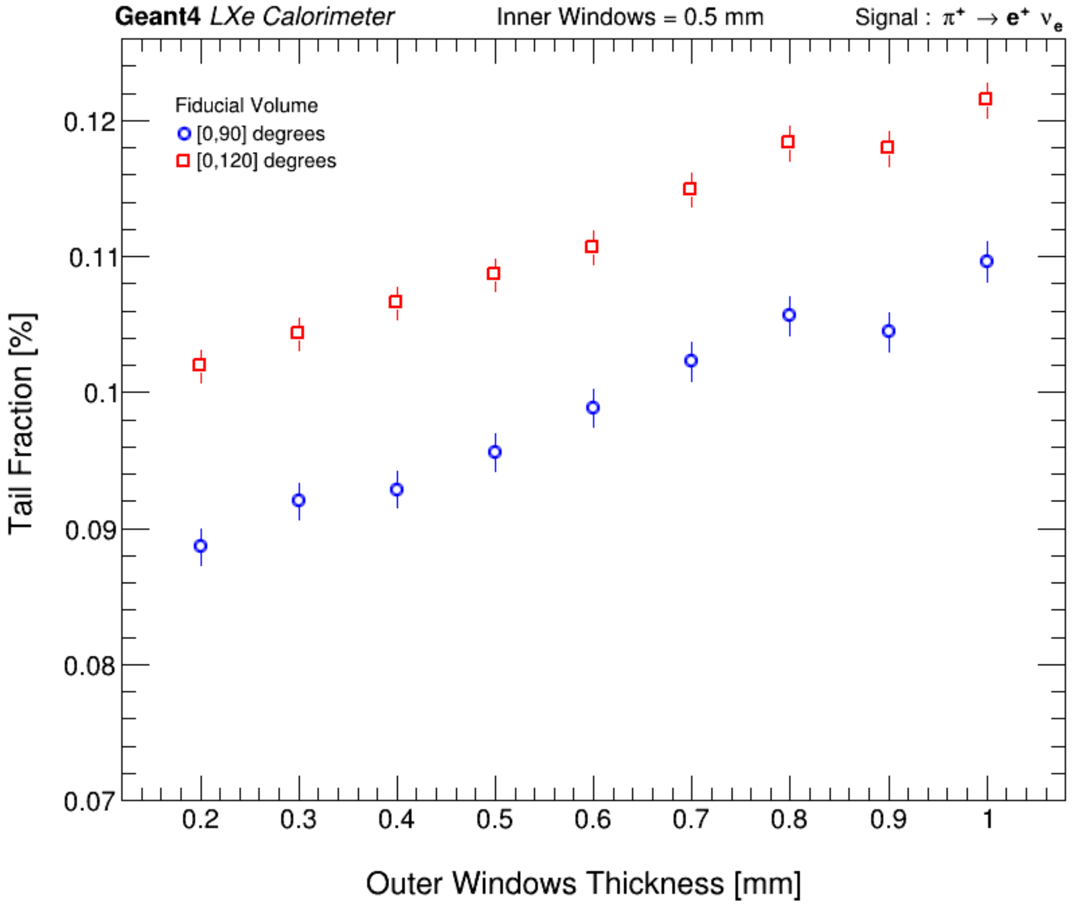


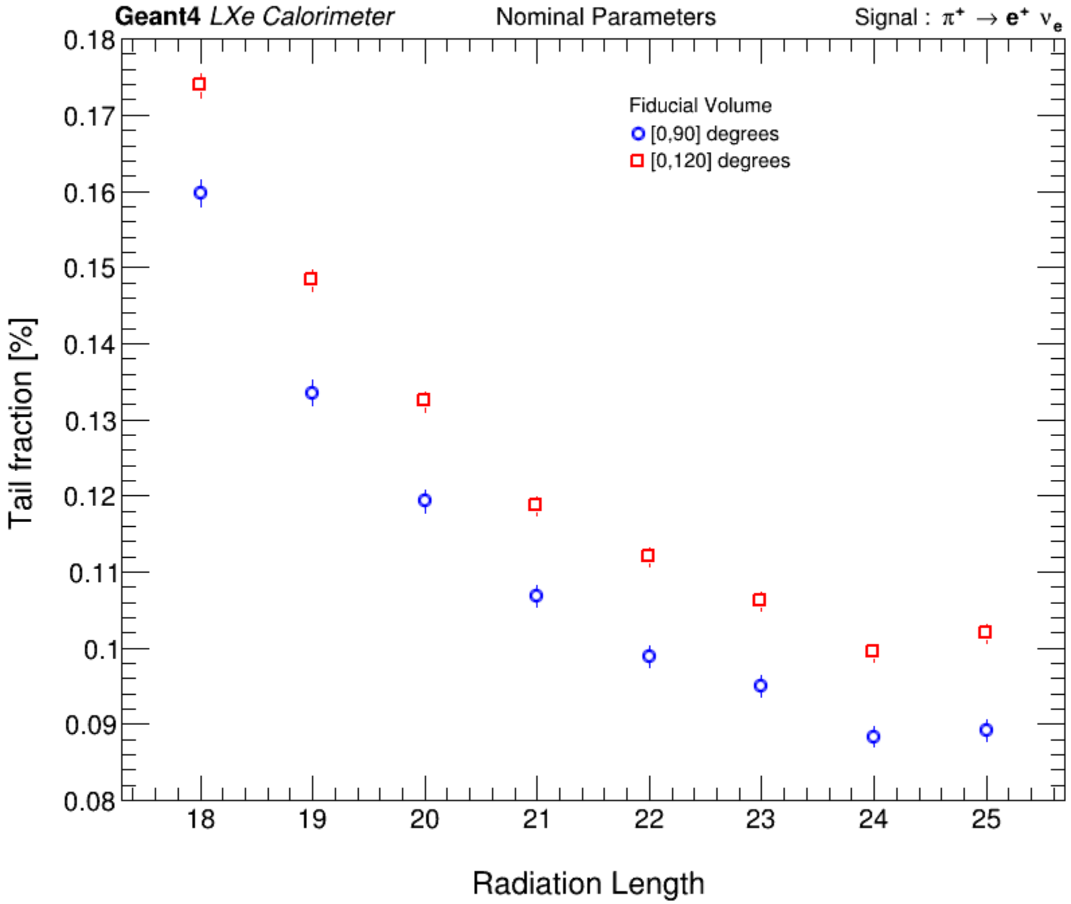
- Opening angle, inner radius, ATAR cables, beam size all must be considered together
- Cables must not intercept the pion beam

Aside: Window geometry



Geometry Studies (co-op - Jesus Corral)





- Tail fraction: relative # of events in low energy (< 53 MeV) bin (Edep in calo)
- Still need to add back Edep in window

MEG position resolution

Kobayashi, 2022 (MEG PhD thesis)

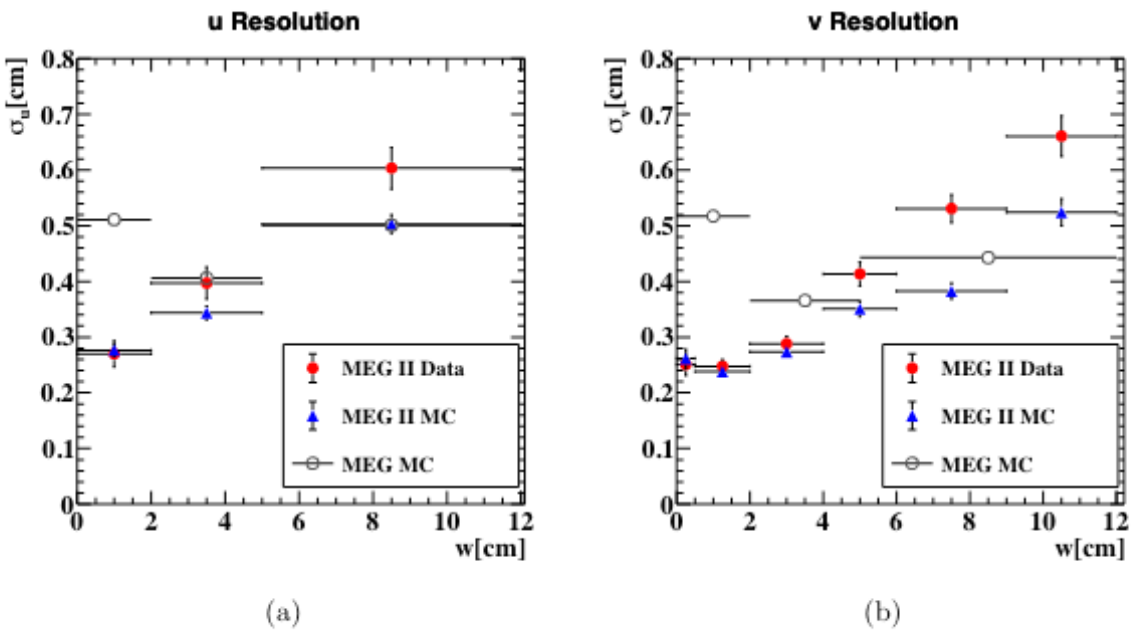


Figure 6.12: The position resolution in the (a) u and (b) v direction as a function of w. The resolutions measured at all four slits are combined. The measured resolution of the MEG II LXe detector (red) is worse than the expected resolution from the simulation (blue), but significantly better than the resolution in the MEG (black).

between the two directions within the statistical uncertainty. The reason for the discrepancy is not understood. If the following situation is different between data and MC simulation, it might explain the worse resolution.

- Scattering or absorption in LXe.
- Reflection at the PMT holder.
- Size of the gamma-ray vertex at the target.

Open Questions / Tasks (May 2024)

- What is the final/nominal calo geometry including acceptance?
  - Inner radius, opening angle, radiation length
  - PMT distribution
- How does light get distributed in the detector?
- What is the effect of the “shadow” from the center of the calo?
- What are the various material effects and how can they be tuned?
  - window thickness and dead material effect
  - reflectivity of inner surface, PMTs
- What will be the full calo detector response and reconstruction?
- ***How can we identify and minimize the negative impact of pileup events?***