

Bug fix for Neutron Transport Simulation

Jingbo Wang

University of California, Davis, Department of Physics



Pulsed Neutron Source
Working Group Meeting
May 13, 2020

Outline

- Bug in previous simulation
- Time of neutron capture: simulation and calculation
- Energy of captured neutron
- Neutron transport in DUNE-size detector
- Summary

Bug in Previous Simulations

- There existed a bug in the previous simulations: both NeutronHP model and G4HadronElasticPhysicsHP model were enabled in the physics list. The neutrons were simulated twice for each step.
- This bug affects the moderator design and the neutron transport in liquid argon TPC
- Capture times increased by up to a factor of two, but neutrons also spread out more

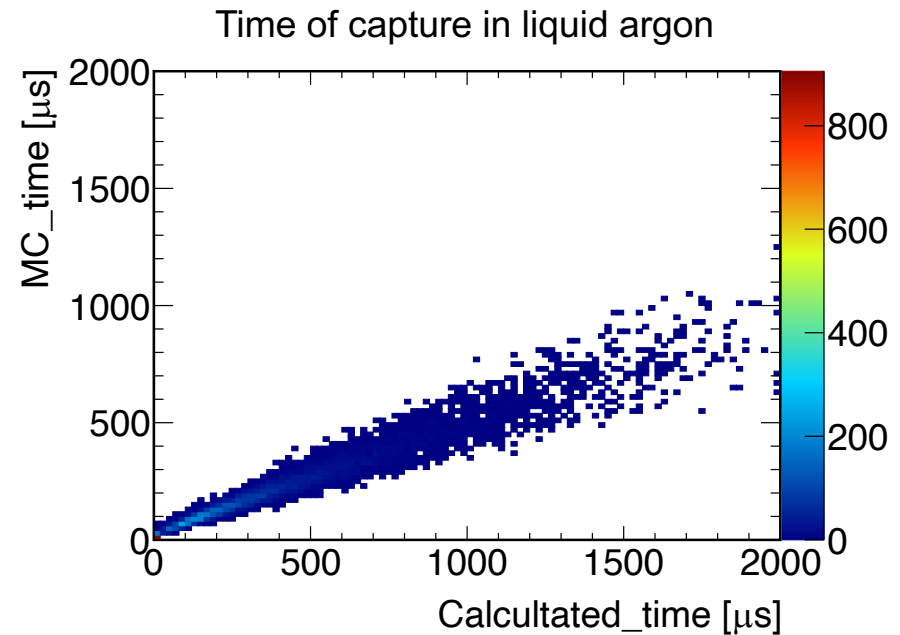
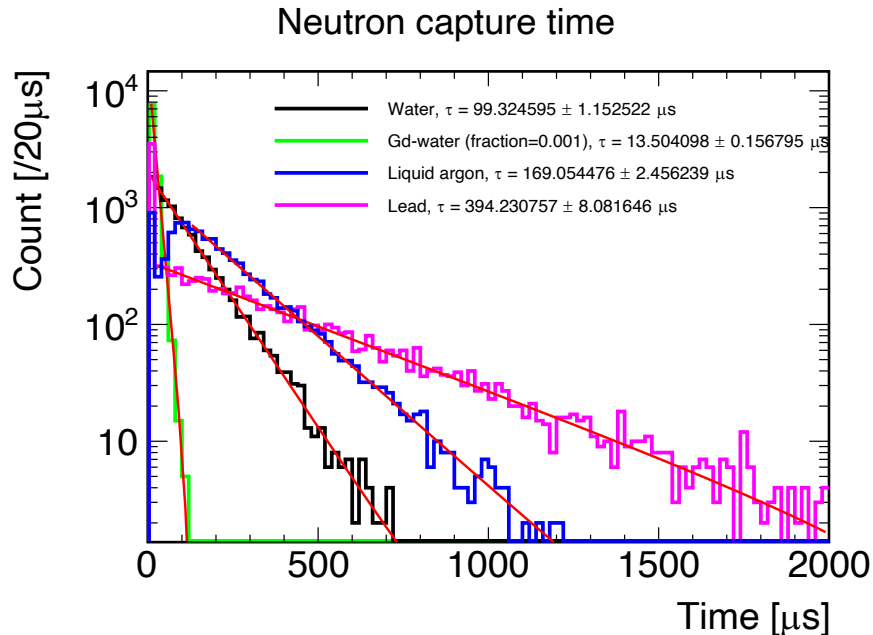
Infinite Volume Simulation

- 2.5 MeV Neutrons are generated inside an effectively infinite volume
- Neutron capture time is saved to data file for analysis
- Neutron capture time is simulated for pure water, 0.1% Gd-doped water, liquid argon, and lead

Define neutron capture time: time between generator and capture processes

Neutron Capture Time in Previous Simulation

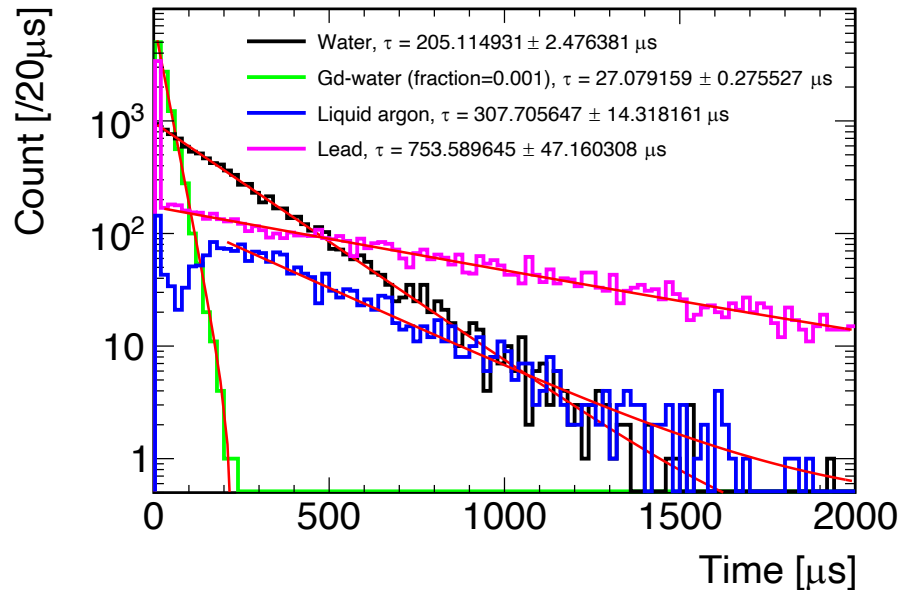
- Effectively infinite volume
- With bug in the physics list
- Confirms that capture time is off by a factor of two



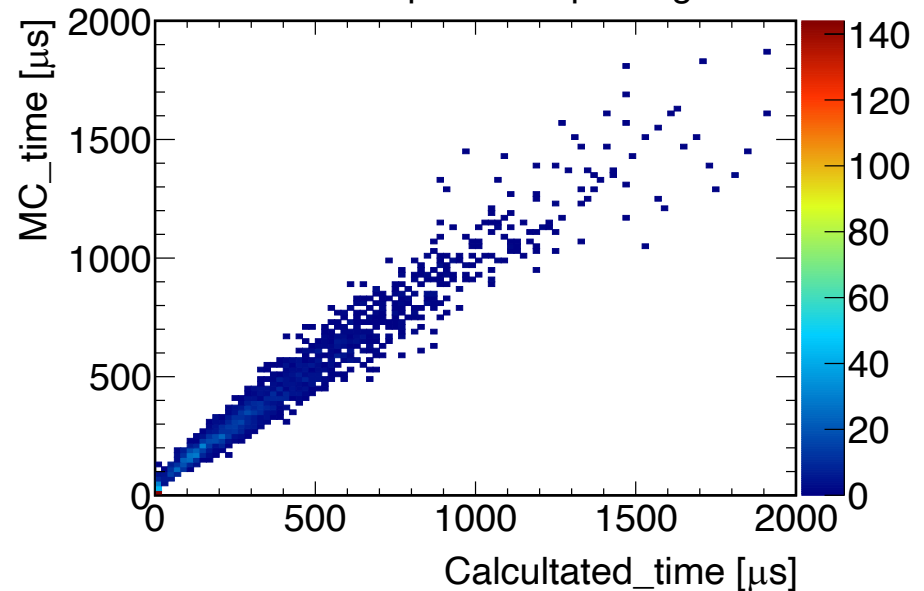
Neutron Capture Time in Current Simulation

- Effectively infinite volume
- Bug **fixed** in the physics list

Time of neutron capture



Time of capture in liquid argon



Time-Energy Correlation

The neutron lethargy u is defined as

$$u = \ln\left(\frac{E_0}{E}\right) \quad \text{so,} \quad du = \frac{-dE}{E}$$

The average change (ξ) in lethargy per collision, assuming elastic scattering

$$\xi = 1 + \frac{\alpha}{1 - \alpha} \ln(\alpha) \quad \text{where,} \quad \alpha = \left(\frac{A - 1}{A + 1}\right)^2$$

For ^{40}Ar , $\xi = 0.049$. For water, $\xi = 1.0$, For lead, $\xi = 0.01$

The slowing-down time can be derived from the general equation

$$du = \xi \Sigma_s v dt \quad \text{where,} \quad v = \sqrt{\frac{2E}{m_n}}$$

Solving the equation, we get:

$$t = \frac{\sqrt{2m_n}}{\xi \Sigma_s} \left(\frac{1}{\sqrt{E}} - \frac{1}{\sqrt{E_0}} \right) = \sqrt{K} \left(\frac{1}{\sqrt{E}} - \frac{1}{\sqrt{E_0}} \right)$$

Ref: Y. Danon, Measurements with a Lead Slowing Down Spectrometer

Slowing-down calculation for LAr

$$\xi = 0.049$$

Assume constant elastic scattering cross-section

$$m_n = 939 \times 10^3 \text{ keV}/c^2$$

$$\Sigma_s = n\sigma_s = \frac{1.4 \text{ g/cm}^3}{40 \text{ g/mol}} \times 6.02 \times 10^{23} / \text{mol} \times 0.9 \times 10^{-24} \text{ cm}^2 = 0.0194 / \text{cm}$$

$$K = \frac{2m_n}{\xi^2 \Sigma_s^2} = \frac{2 \times 939 \times 10^3 \text{ keV}/c^2}{0.049^2 \times (0.0194 / \text{cm})^2} = 2309 \text{ keV} \cdot \mu\text{s}^2$$

If the neutron is slowed down from 2.45 MeV to 0.025 eV

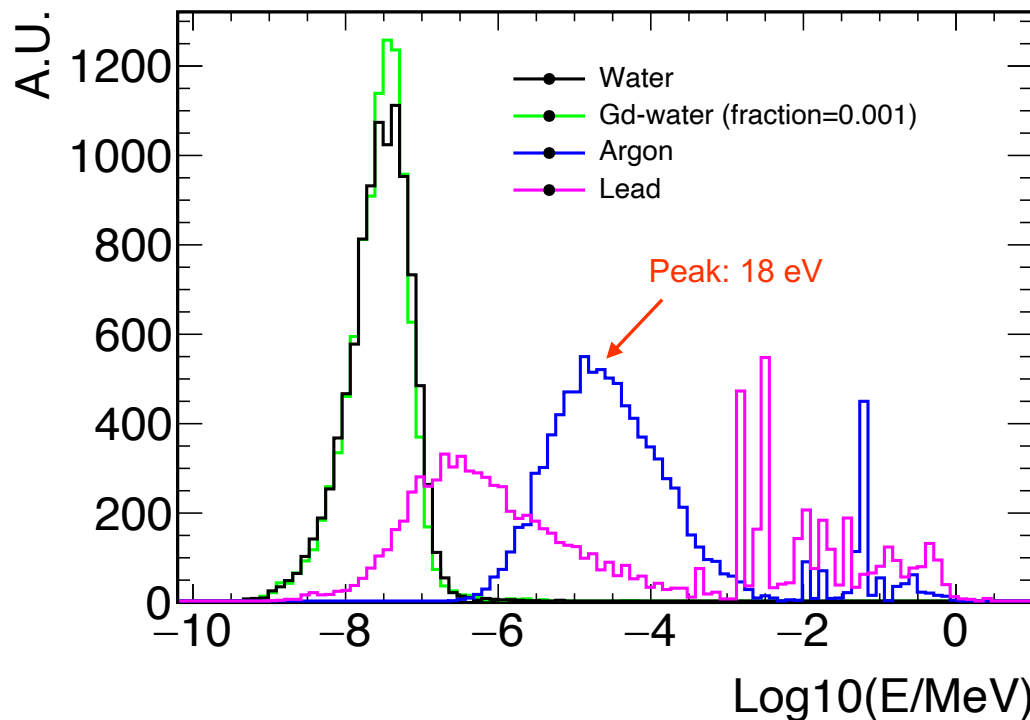
$$t = \sqrt{2309 \text{ keV} \cdot \mu\text{s}^2} \left(\frac{1}{\sqrt{0.025 \times 10^{-3} \text{ keV}}} - \frac{1}{\sqrt{2.45 \times 10^3 \text{ keV}}} \right) = 9609 \mu\text{s}$$

If the neutron is slowed down from 2.45 MeV to 18 eV (for reason in next slide)

$$t = \sqrt{2309 \text{ keV} \cdot \mu\text{s}^2} \left(\frac{1}{\sqrt{18 \times 10^{-3} \text{ keV}}} - \frac{1}{\sqrt{2.45 \times 10^3 \text{ keV}}} \right) = 357 \mu\text{s}$$

Energy of Captured Neutron

- **Problem:** the neutrons in liquid argon is not fully thermalized when they are captured. The average capture energy is **18 eV** (Gaus fit). Is this true?
- This distribution determines the neutron capture time.
- Possible reason: “capture ratio” of argon is higher (slide 11)



Also see Sofia's
simplified
simulation (next
slide)

Separate Toy MC Model

Work done by Sofia Andringa

Moderation & Capture

Simplified cross-sections from ENDF

Elastic scattering: $xs_{el} \sim 0.7$ barn (25 barn in Pb)

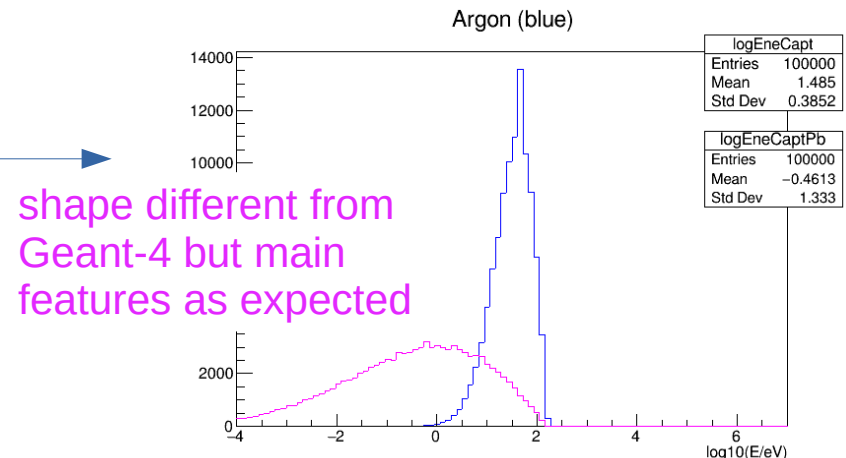
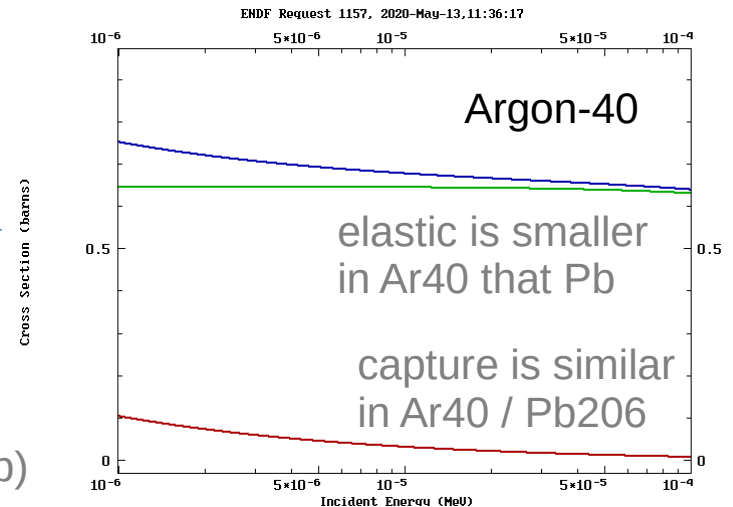
Energy drop to: $E_f / E_o \sim (A-1)/(A+1) \sim 0.95$ (0.99 in Pb)

Capture: $xs_{cap} \sim (0.1 - 0.045 \log_{10} E)$ barn (x 0.5 in Pb)

Start neutron at 150 eV (above $xs_{cap} \sim 0$)

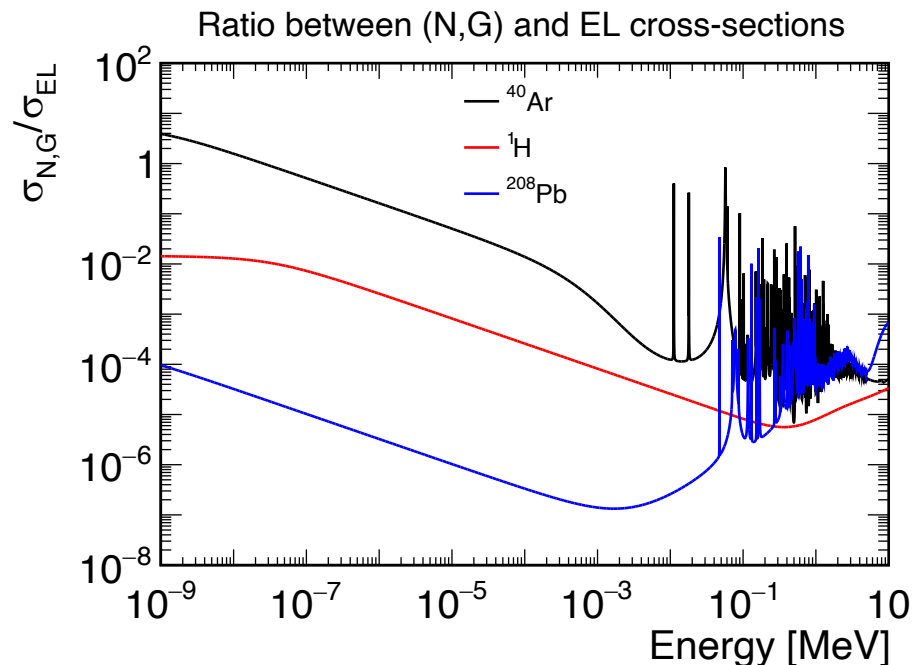
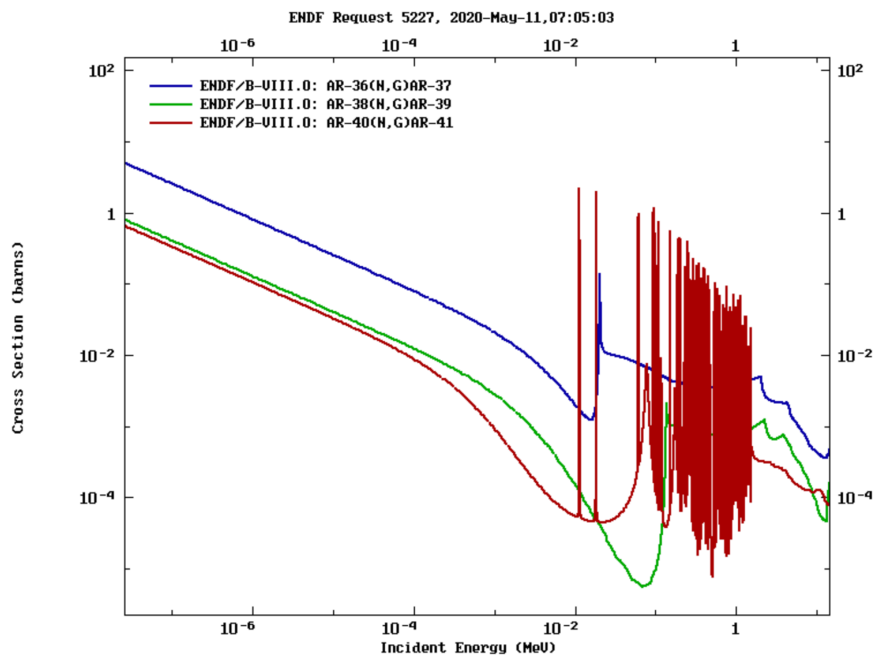
if $xs_{cap} > \text{random} \cdot (xs_{cap} + xs_{el})$
draw capture energy
else
loose energy

Ratio of captures increases almost linearly
by 0.1% in each collision (0.001% in Pb)



Neutron capture cross-section

- Possible reason for 18 eV capture energy: “capture power” of argon is higher
- The “capture power” is defined as the ratio between capture cross-section and elastic scattering cross-section (need more study)

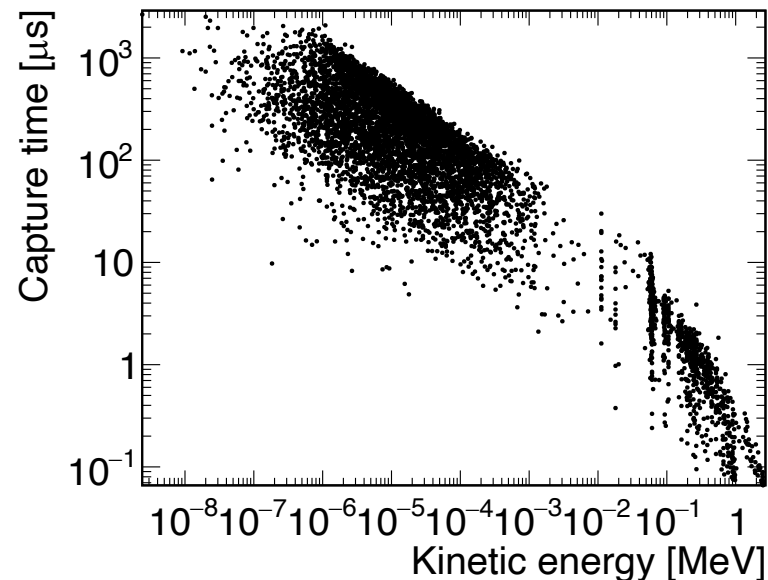
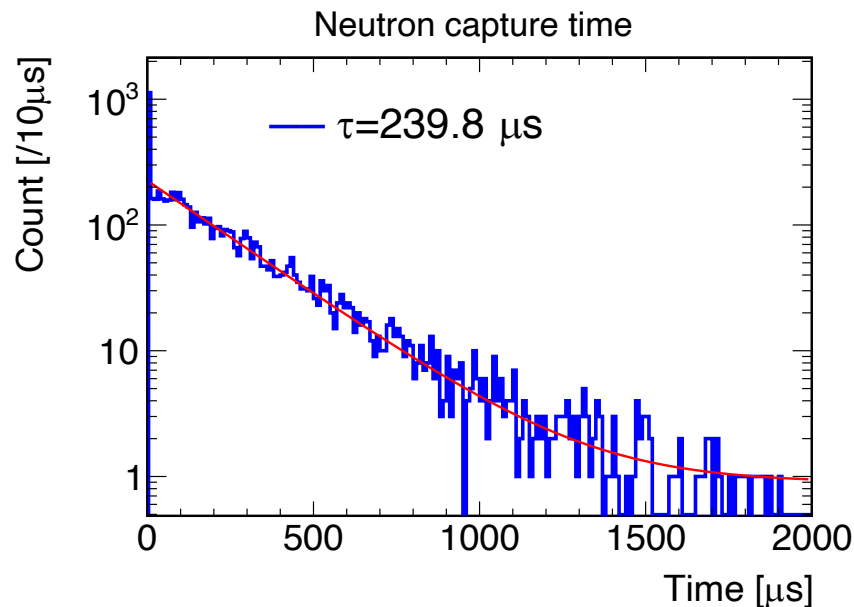


DUNE Far Detector Simulation

- Inject downward neutrons to the DUNE-size liquid argon volume (about 60m x 20m x 20m)
- Save neutron capture position and time

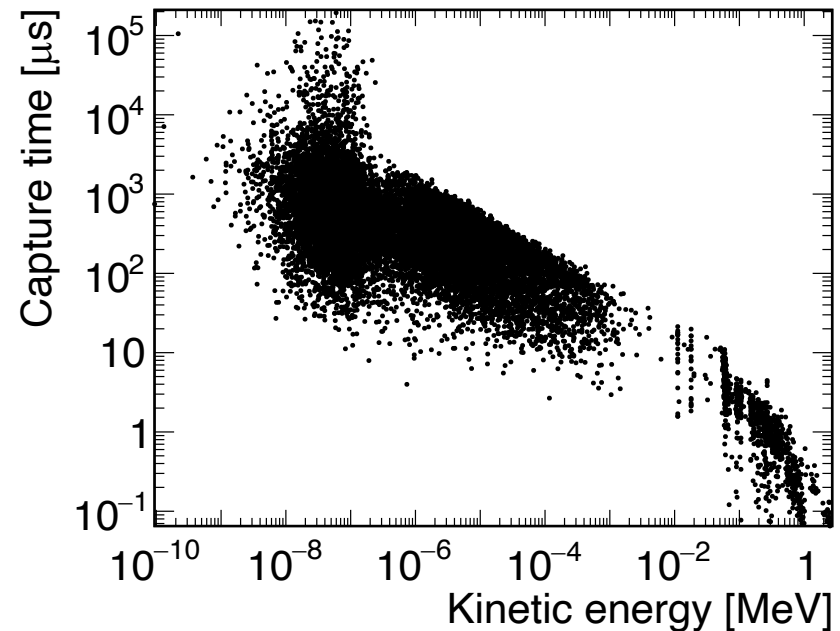
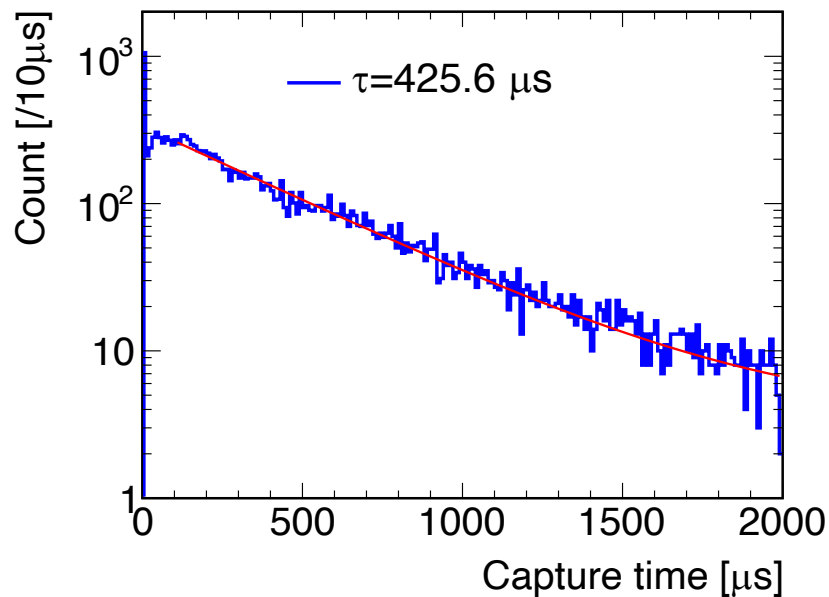
Neutron capture time in PNS Simulation

- **Cryostat Insulator is set to be Li-Polyethylene.** Neutrons hitting the insulator go through inelastic scattering and don't scatter back to liquid argon volume
- 2.5 MeV neutron capture time in the PNS simulation (bug fixed) is shorter than that in the infinite-volume simulation
- The peak near zero is due to resonance capture at 0.1 – 2.5 MeV

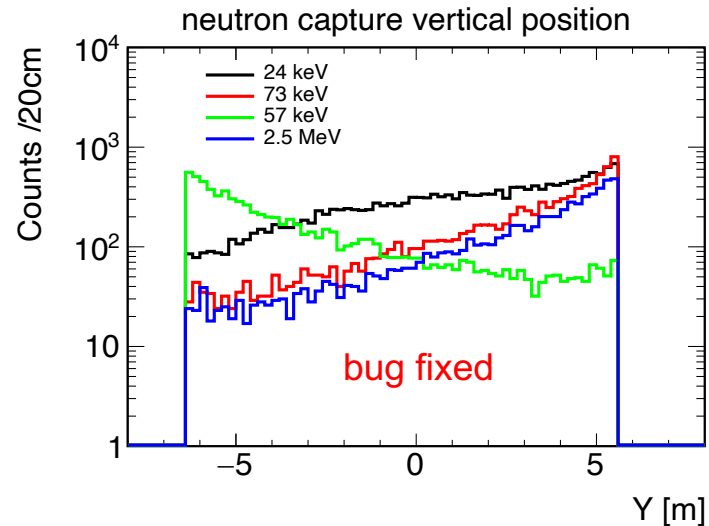
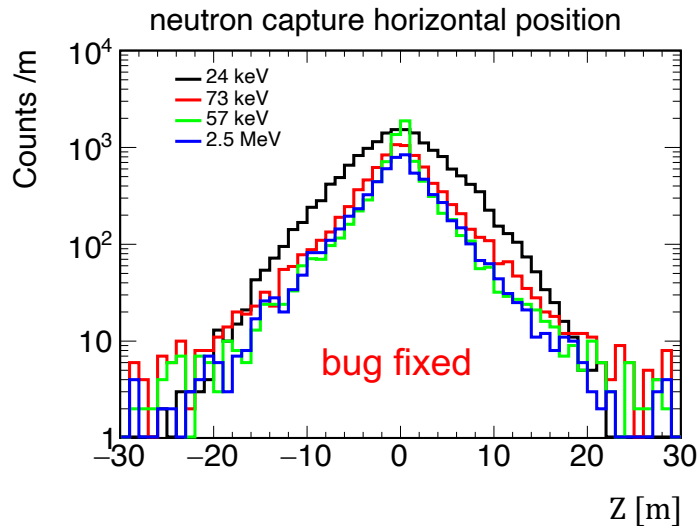
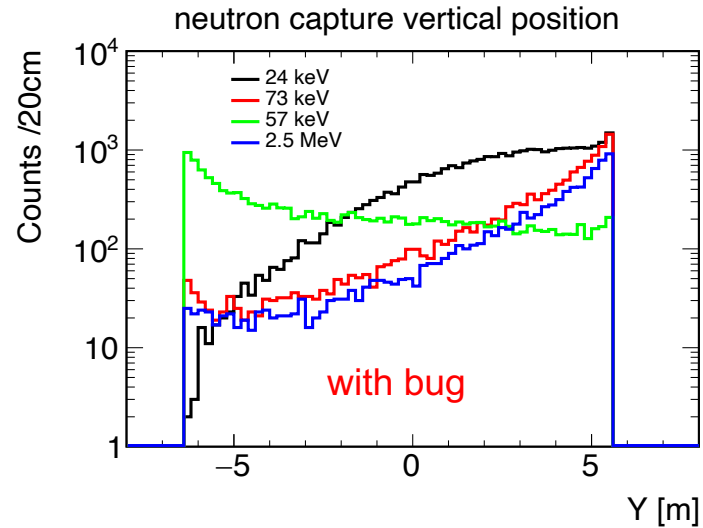
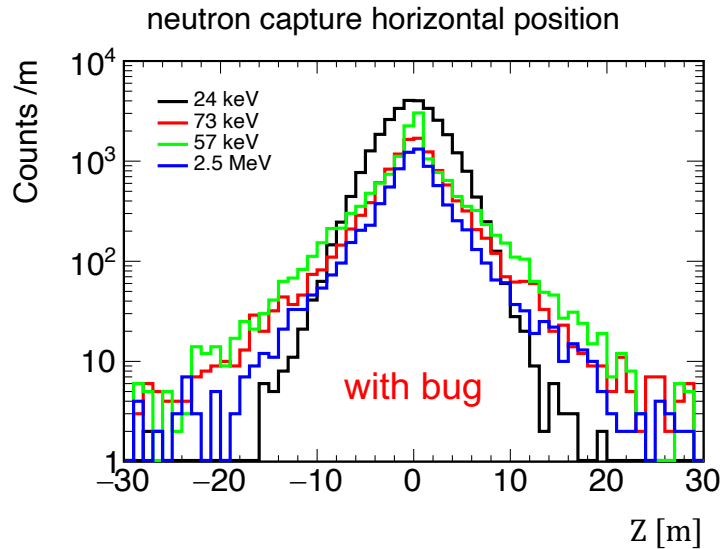


Neutron capture time in PNS Simulation

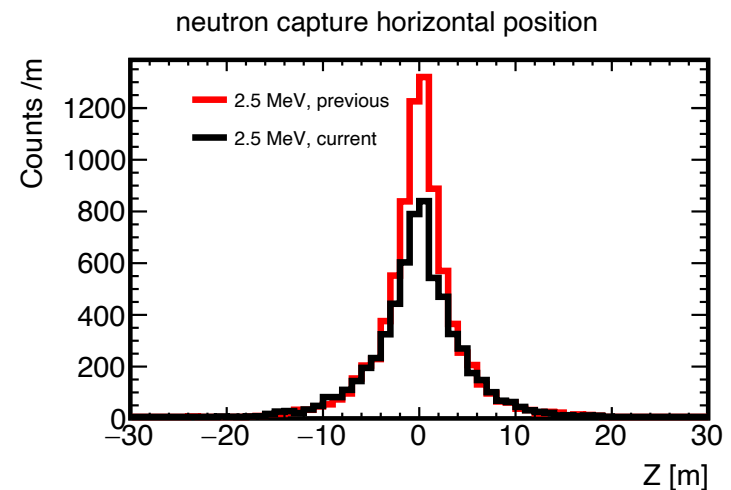
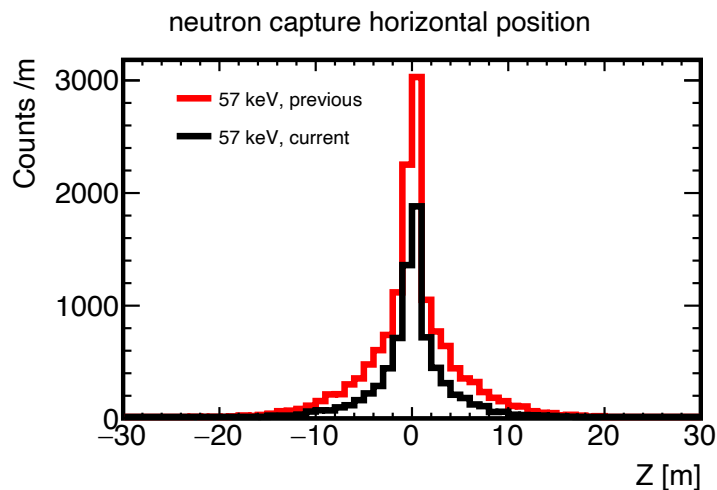
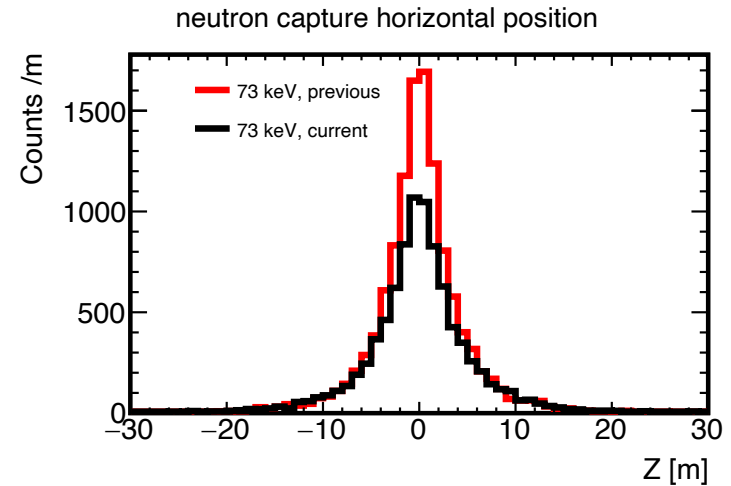
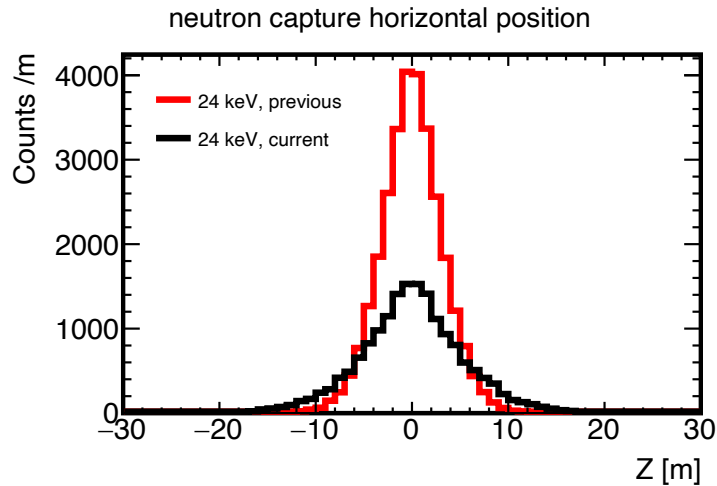
- **Cryostat Insulator is set to be pure polyethylene.** Neutrons hitting the insulator could scatter back to liquid argon volume
- As the back-scattered neutrons are thermal, they cannot travel very deep into the TPC. A fiducial volume selection is expected to be efficient to cut off these neutrons (to be verified by simulation)



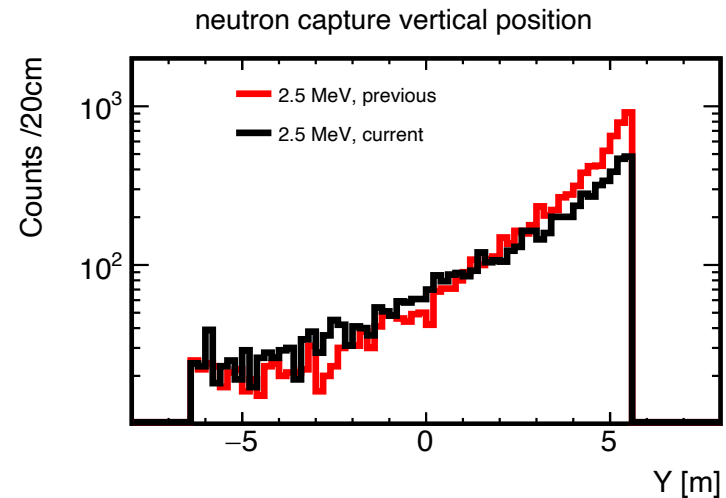
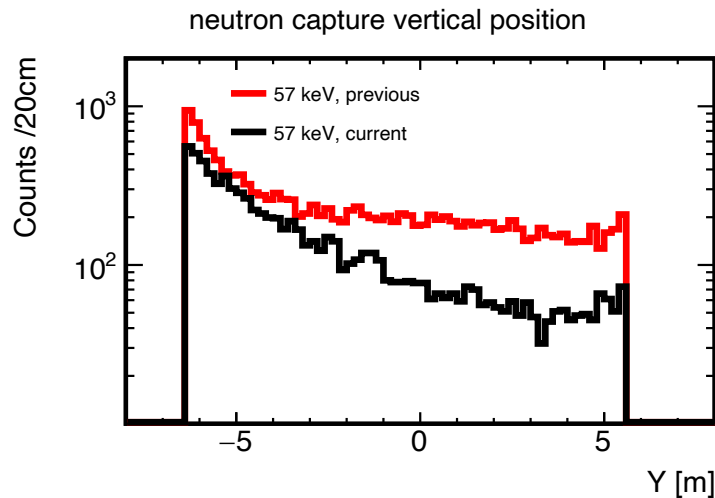
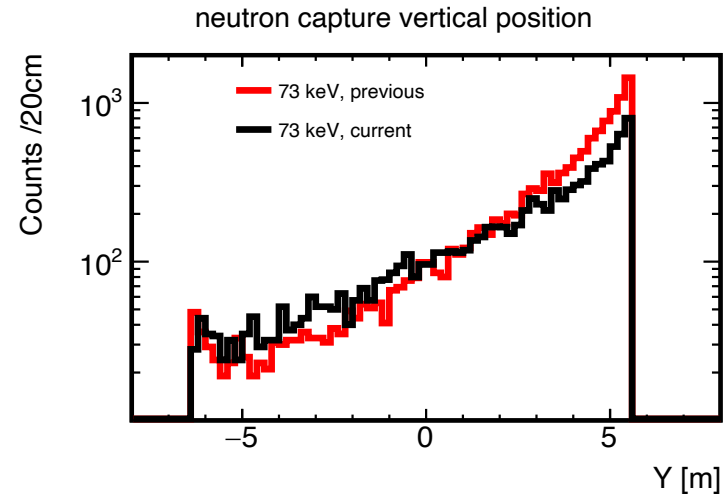
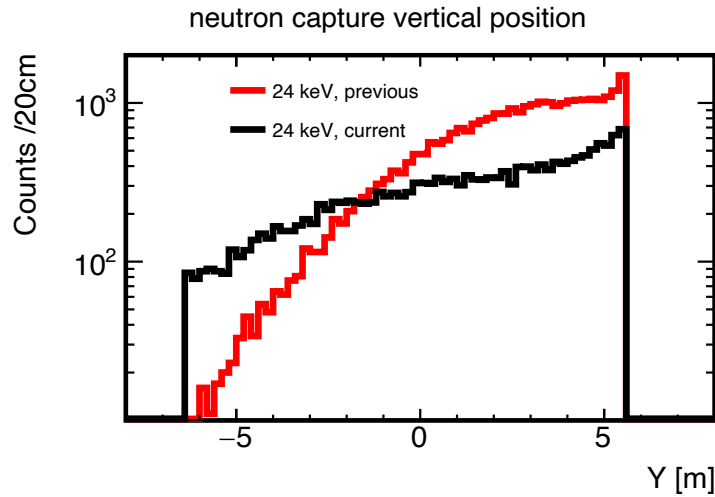
Affect due to the bug fix



Horizontal Position

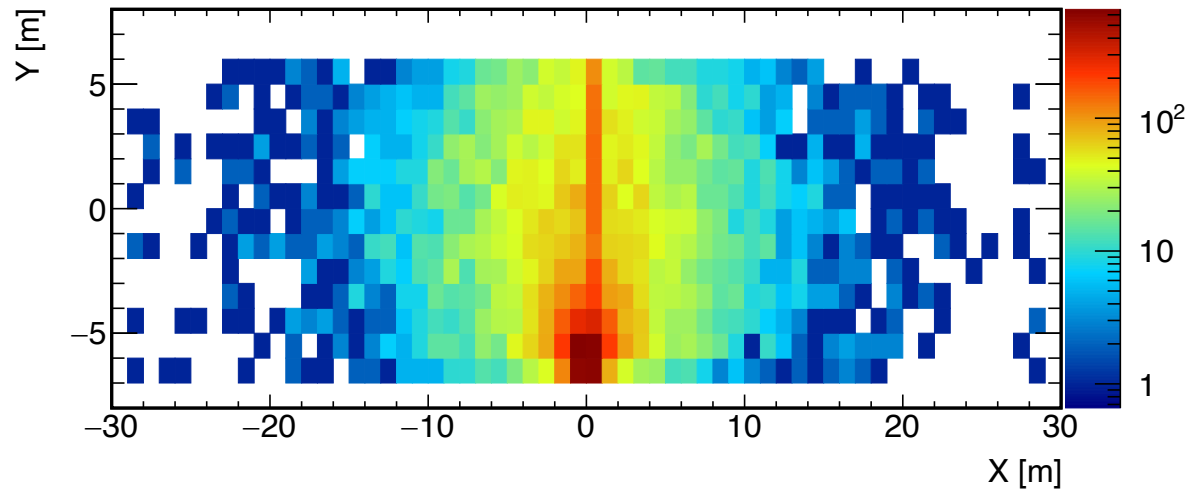


Vertical Position



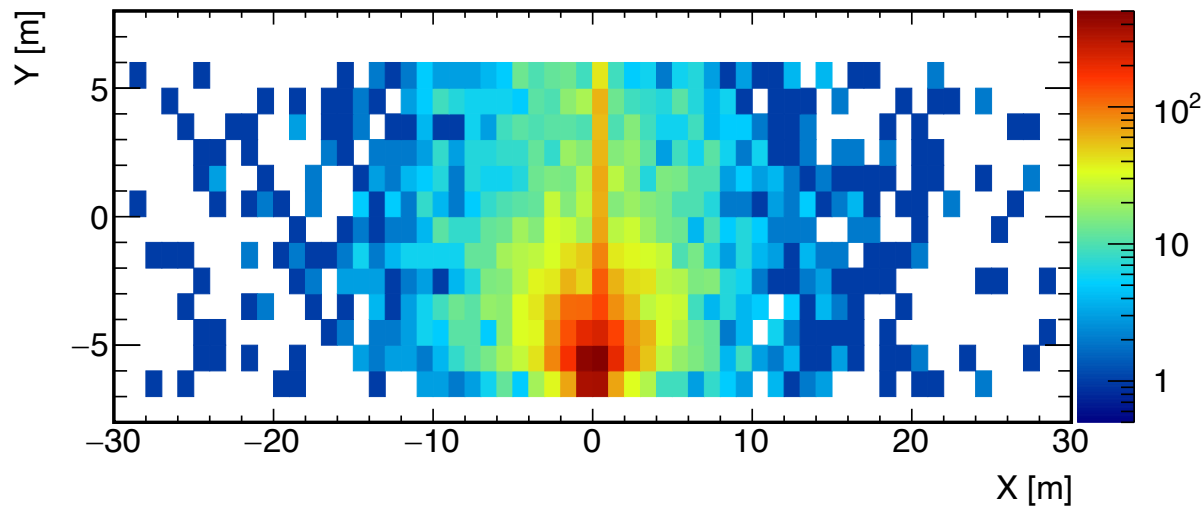
57 keV, Side View

neutron capture side view, 57 keV



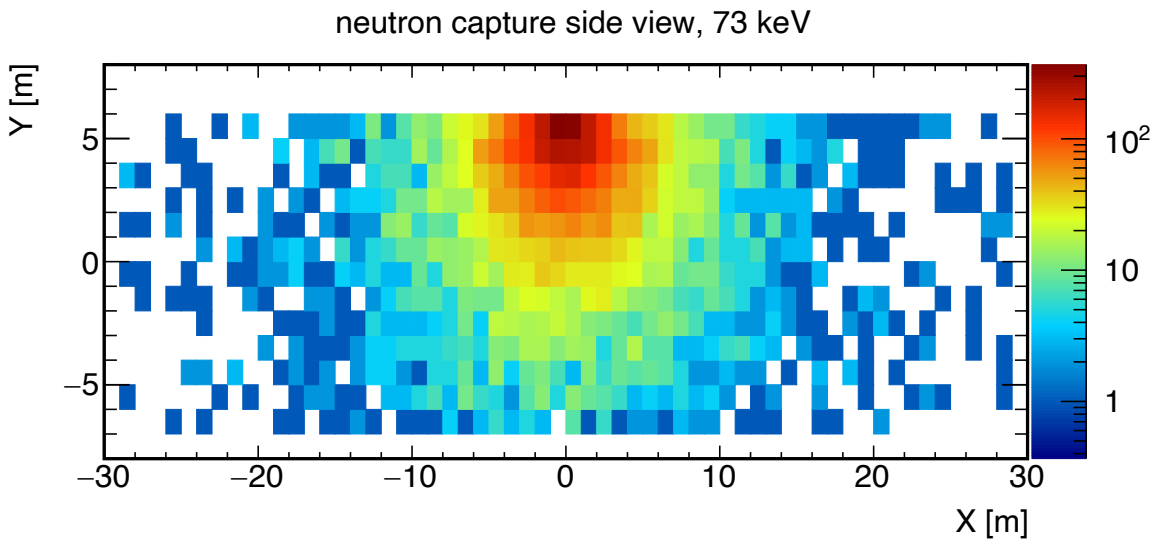
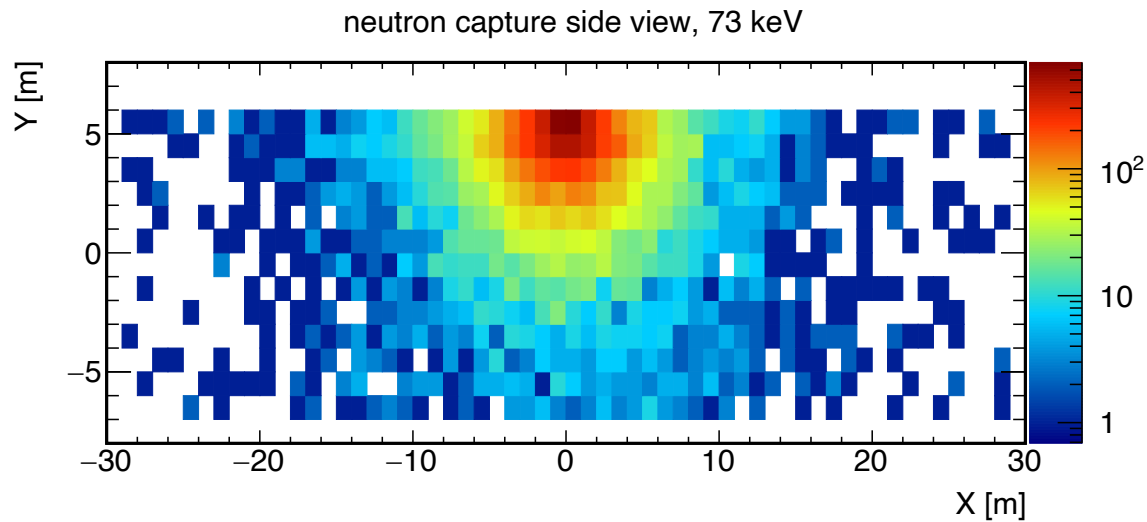
with bug

neutron capture side view, 57 keV

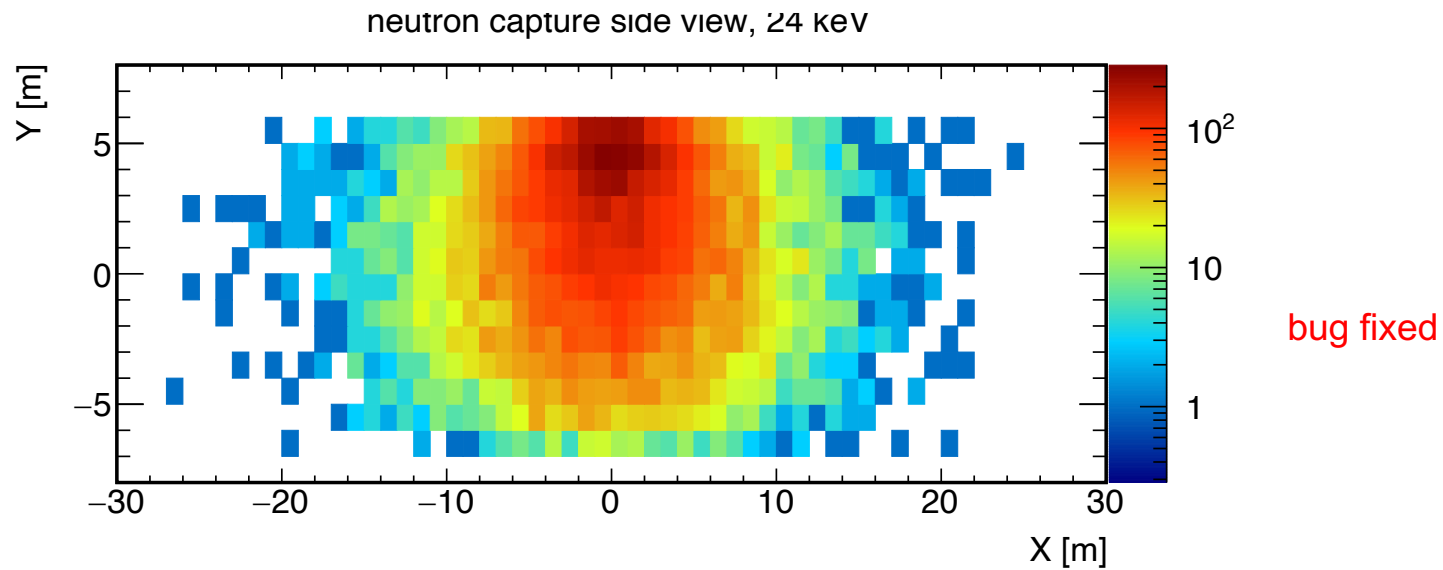
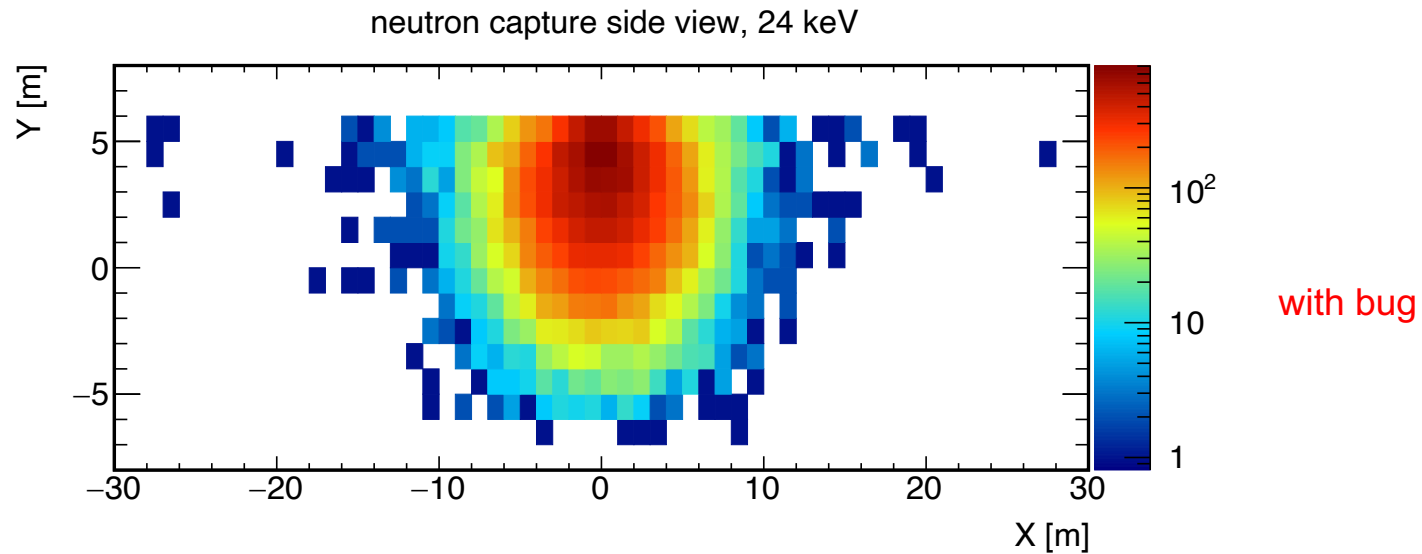


bug fixed

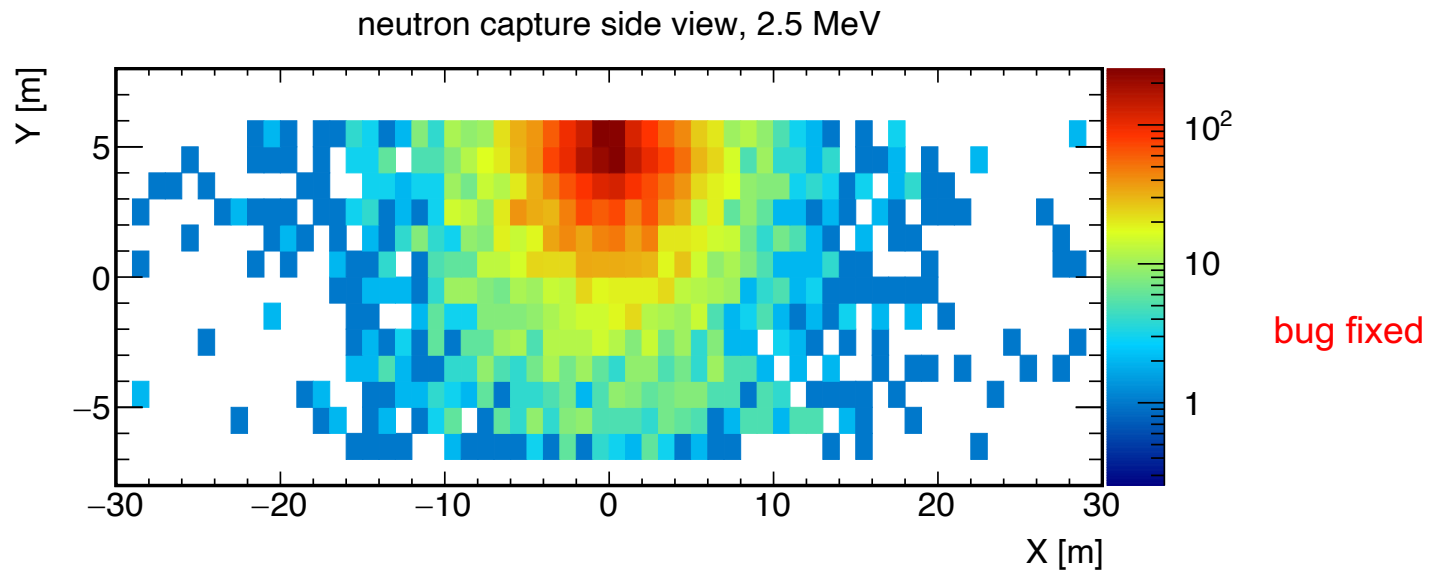
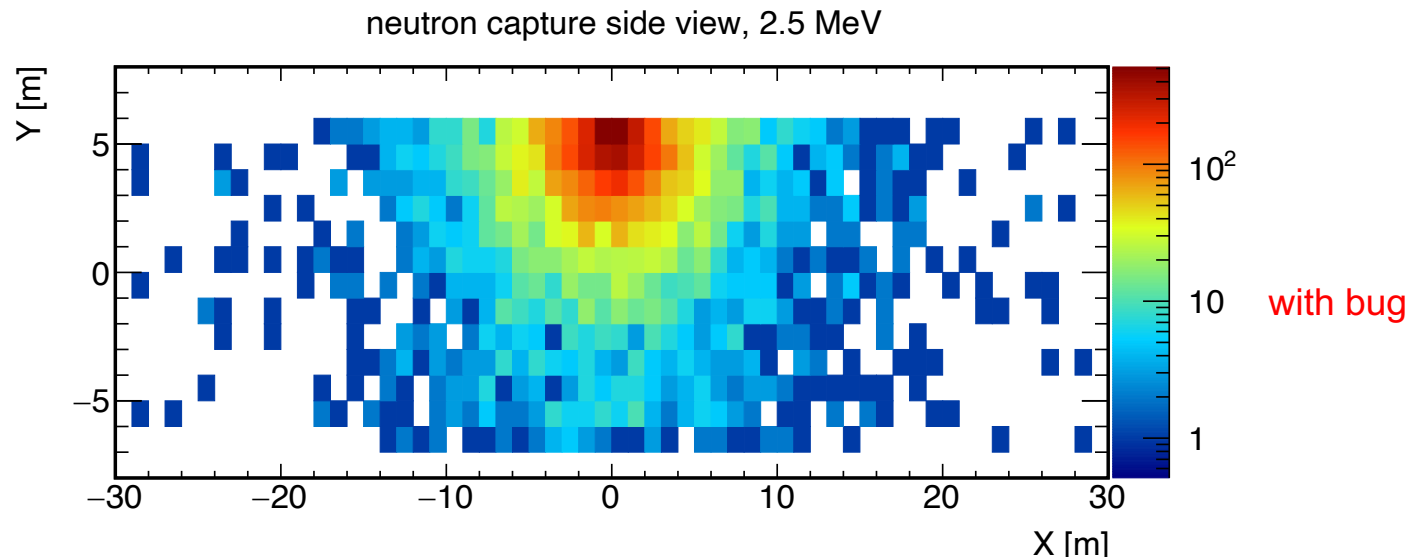
73 keV, Side View



24 keV, Side View



2.5 MeV, Side View



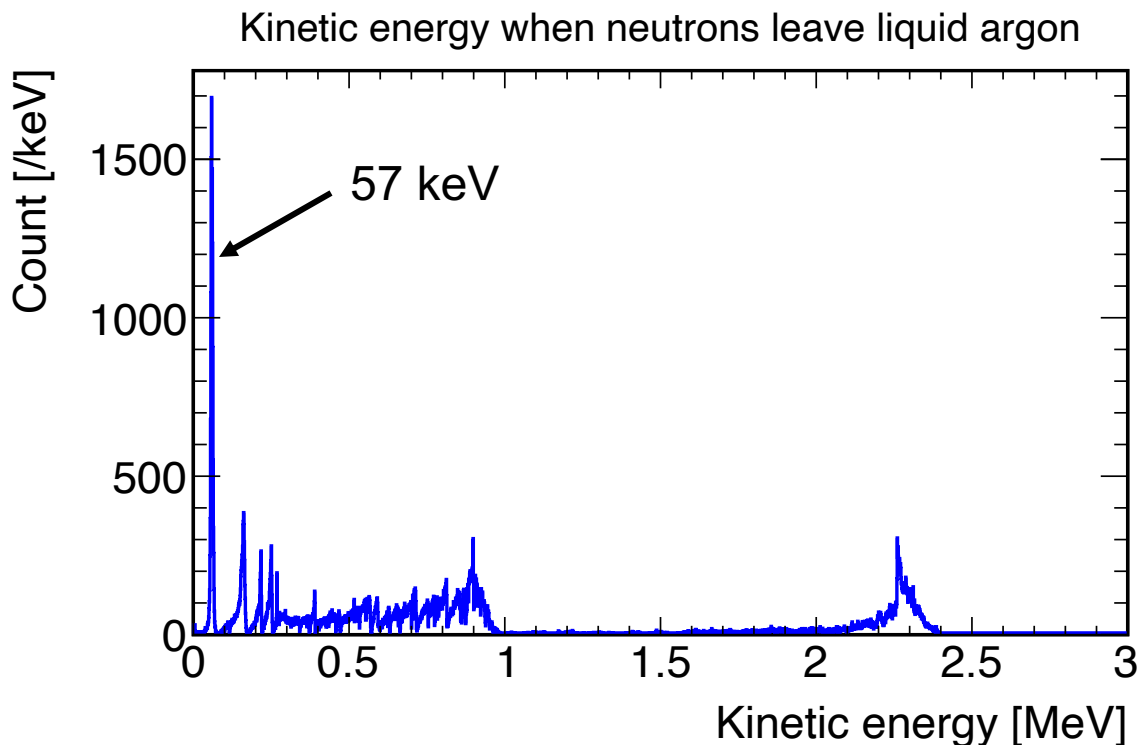
Number of Captures in LAr

Total number of primary neutrons: 100,000

	24 keV	57 keV	73 keV	2.5 MeV
Previous sim	29631	14672	11806	8169
Current sim	17137	8097	8985	6431

How many 73 keV neutrons fall into antiresonance?

- In infinite LAr volume, almost all the 2.5 MeV neutrons can fall into the 57keV antiresonance dip.
- However, in DUNE-size LAr volume, about 87% of the neutrons leave the detector before falling down to 57 keV



What if Winter's data is correct?

- To be simulated
- The cross-section at 57 keV is expected to have little effect, because most of the neutrons will not reach 57 keV in DUNE-size liquid argon volume.

Moderator Design

- Does the previous design work? **No**
- What would be the new design?
- Is a moderator really needed?

Possible Solutions:

1. Use 2.5 MeV DD generator neutrons. No moderator is needed
2. Use liquid argon moderator to produce near 57 keV neutrons. Need new simulation
3. Use Fe-Al moderator to produce near 24 keV neutrons. Need new simulation

Shield Design

- We need to redo the shield simulation for the DD generator test at CERN

Summary

- There is a bug in the previous physics list, which affects the moderator design and the neutron transport in liquid argon
- The new simulation indicates a wider neutron spread inside the liquid argon volume.
- In new simulation, the neutron capture time is $307 \mu s$ in infinite LAr volume, and is $240 \mu s$ in DUNE-size TPC. We need a measurement to confirm.
- We need to change the moderator and shield designs. Several options are being considered.