Geant4 Validation for n3He

Description of the simulation process:

In Geant4 you specify:

- Volumes with material attributes
  - elemental composition, density, temperature, phase, pressure
- Particles of interest that interact with the material
  - primaries, secondaries (without specifying them G4 does not make them!)
- For each particle you specify a list of processes/interactions you are interested in
  - Elastic, inelastic, E&M, hadronic, high energy, low energy, etc.

Geant4 execution:

- Primaries and tracks them in steps through the geometry
- Track step lengths are limited by the process with the shortest mean free path (*)
- If applicable secondaries are generated along the track and/or at the end of the track
- For stopped particles, the final state of *it* and any final products is calculated based on the processes and models that were registered for the particles (*)
- Along the track energy deposition and momentum changes can be extracted
- Final state energy, momentum, positions, … can all be extracted

Geant4 Validation for n3He

Description of the n3He simulation setup:

As of yet simple geometry …

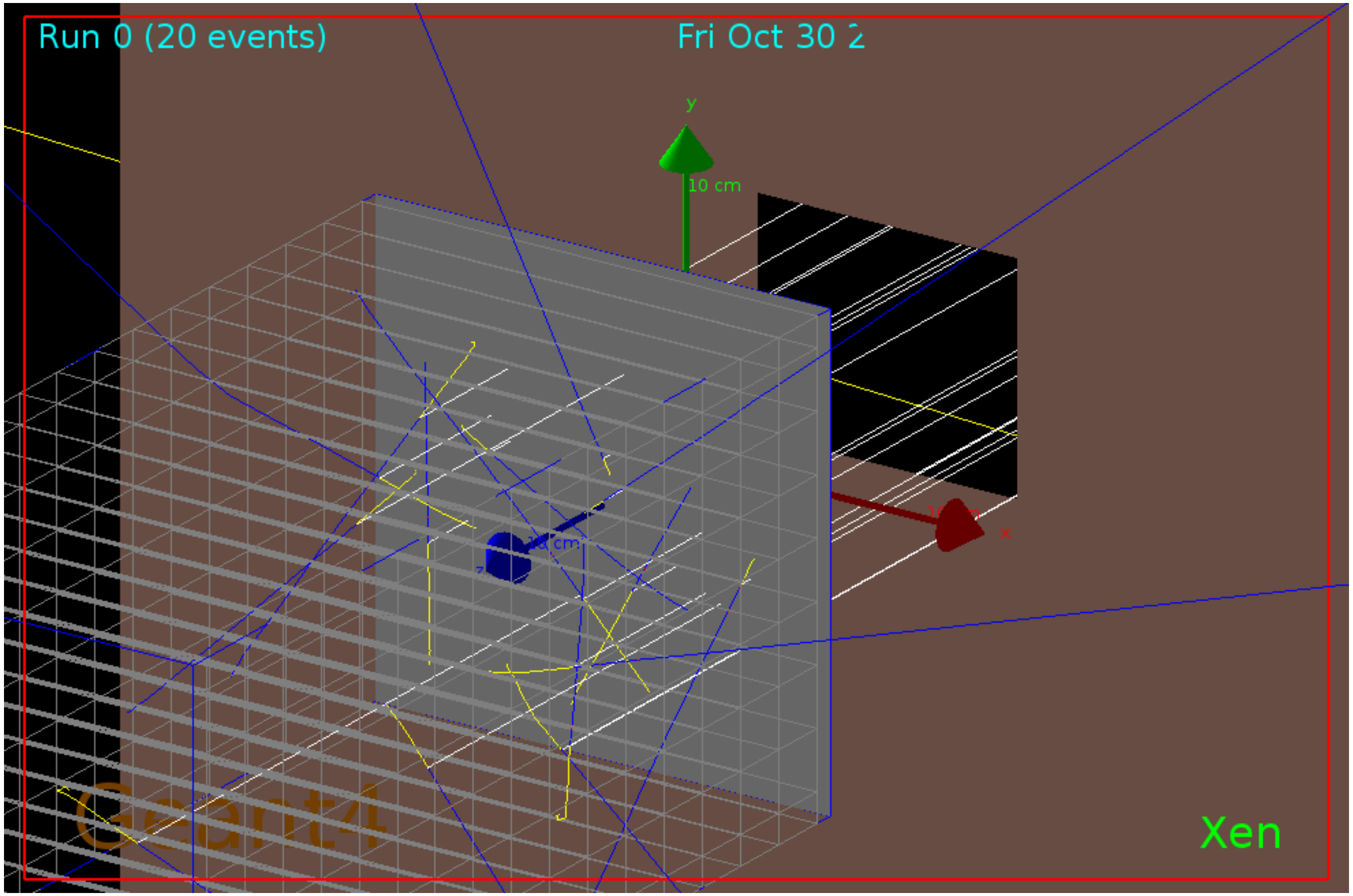
Coordinates:

Z – beam direction
Y – beam up
X – beam left

Each cell is an individual sensitive detector
(easy to implement twist)

White = neutrons
Blue = protons
Yellow = tritons

alphas, gammas, electrons, are not drawn



Registered processes: Neutrons: elastic, inelastic, capture-gamma, radioactive decay, fission
Protons: low energy ionization, elastic, bremsstrahlung
Tritons: low energy ionization, elastic, low energy hadronic (inelastic) and radioactive decay

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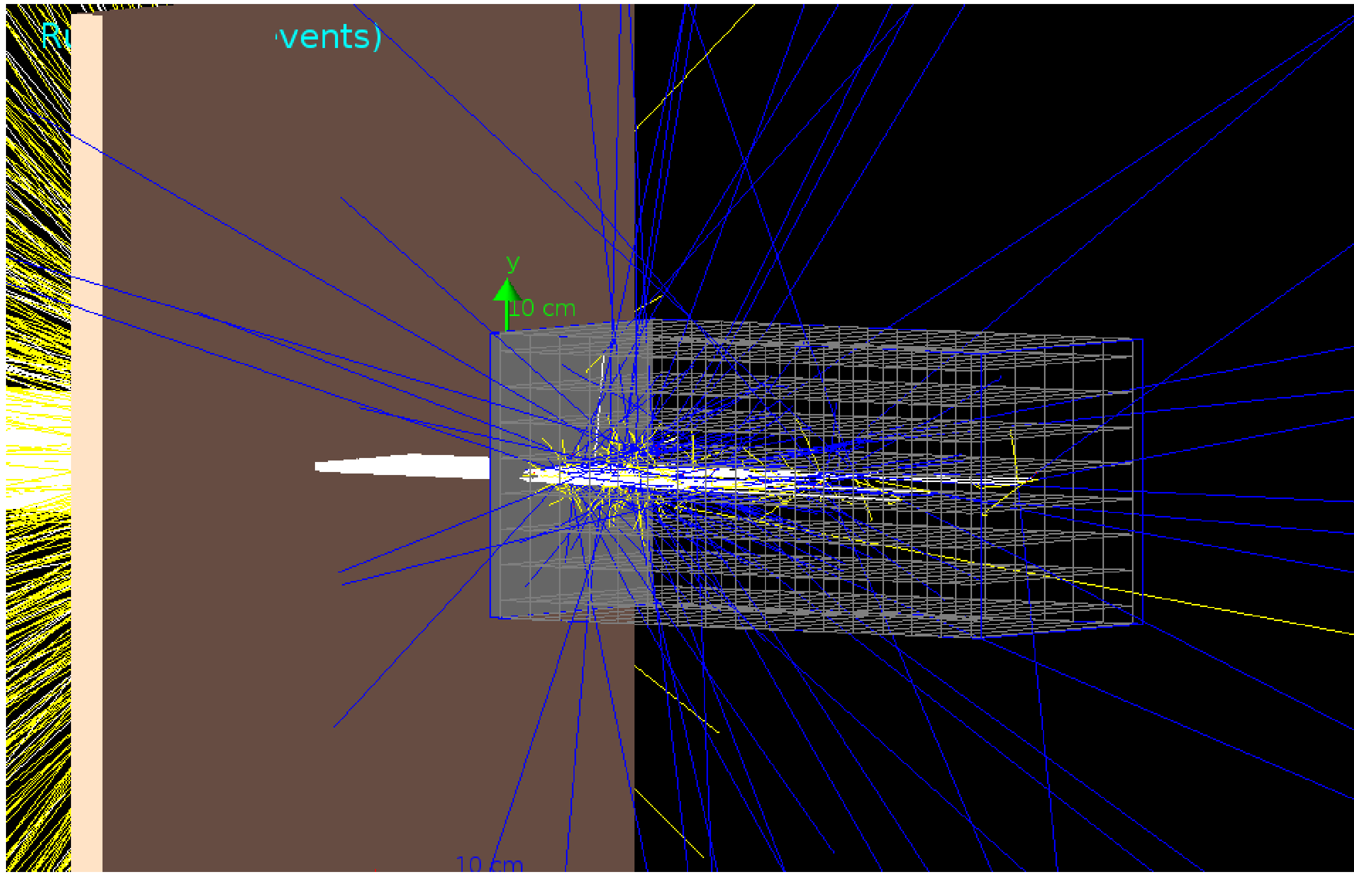

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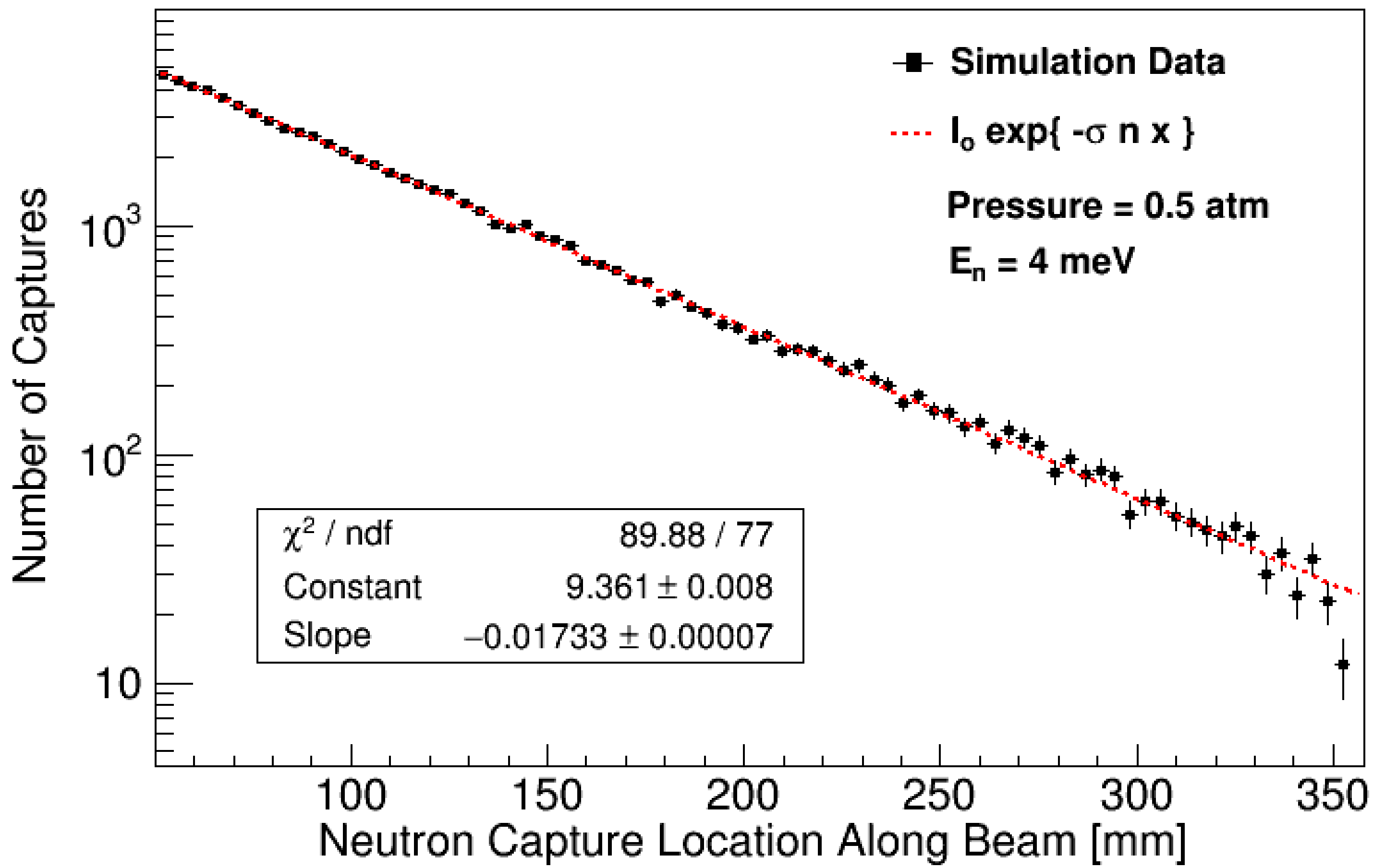
Simulation output verification:

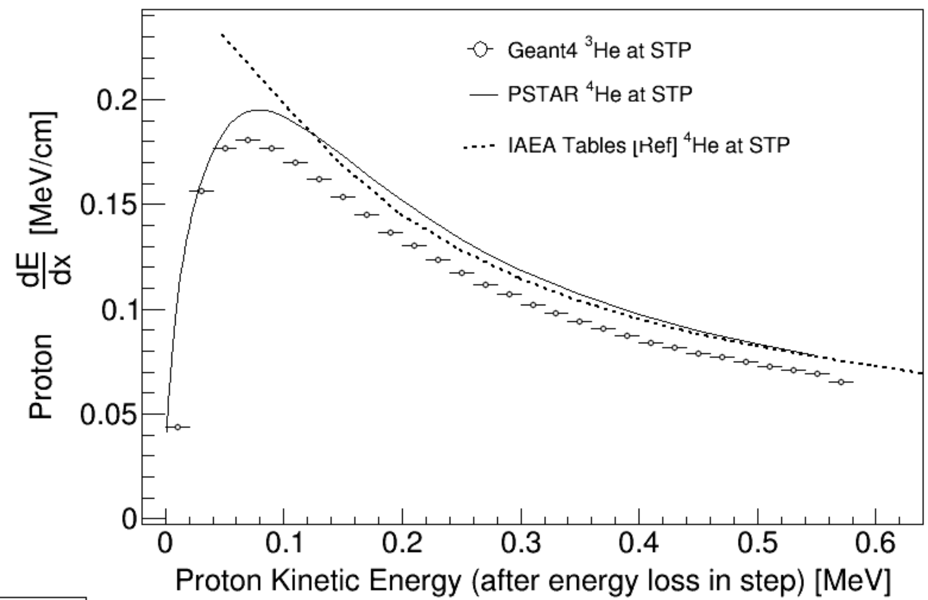
1) Neutron capture profile:

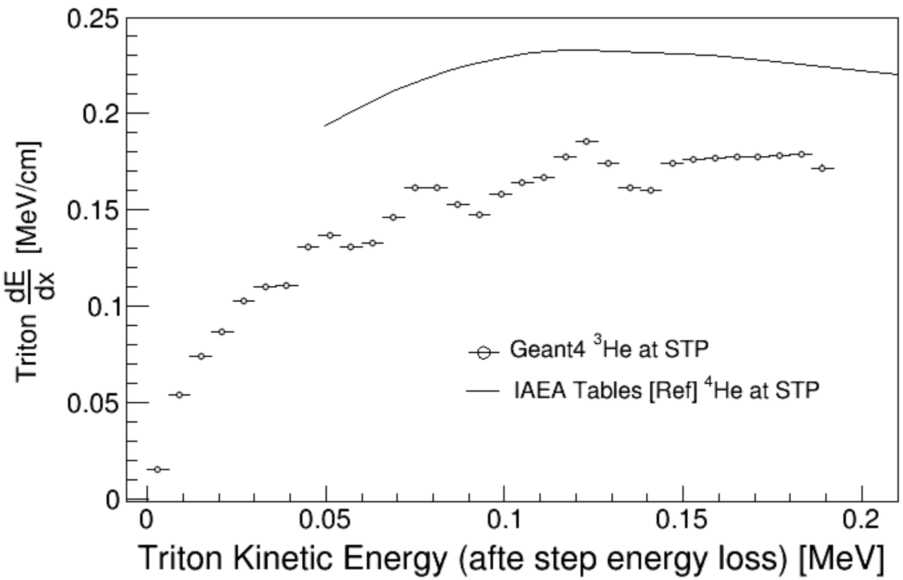


Geant4 Validation for n3He

Simulation output verification:

2) Proton / triton energy deposit:

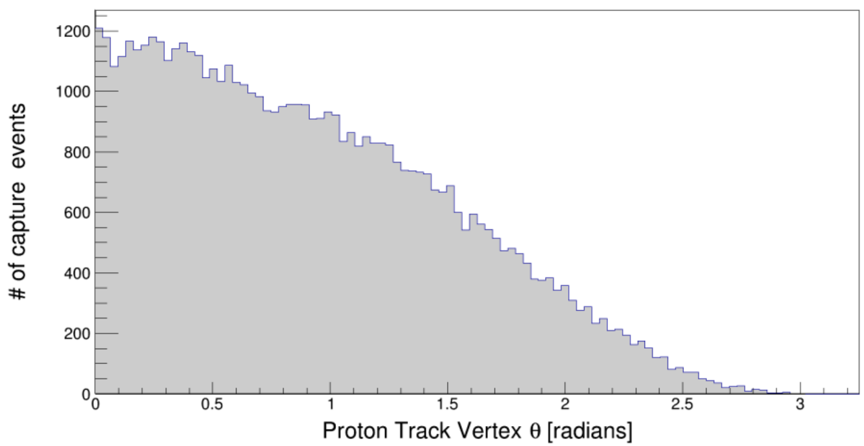


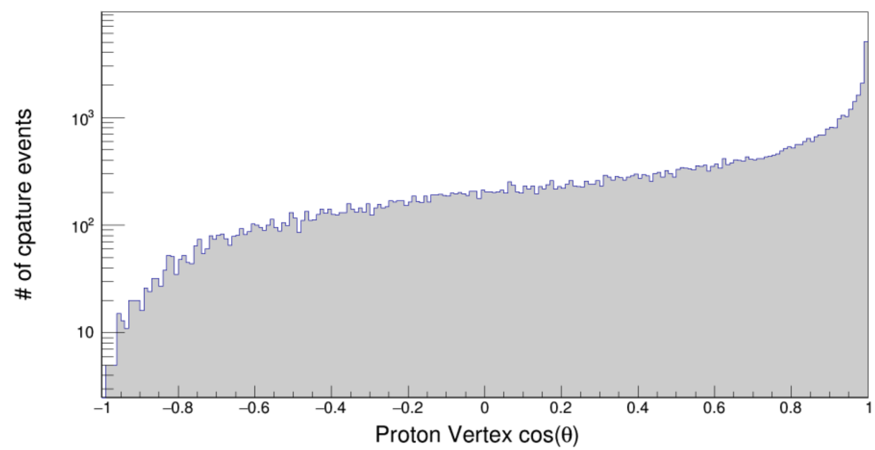


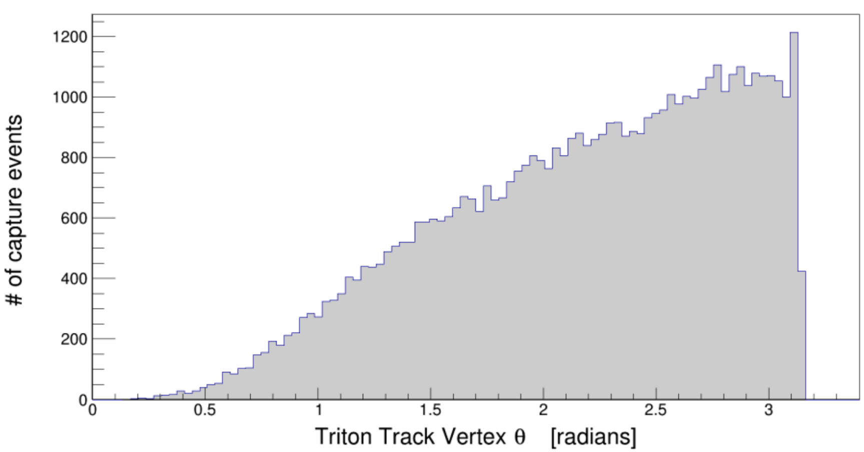
Geant4 Validation for n3He

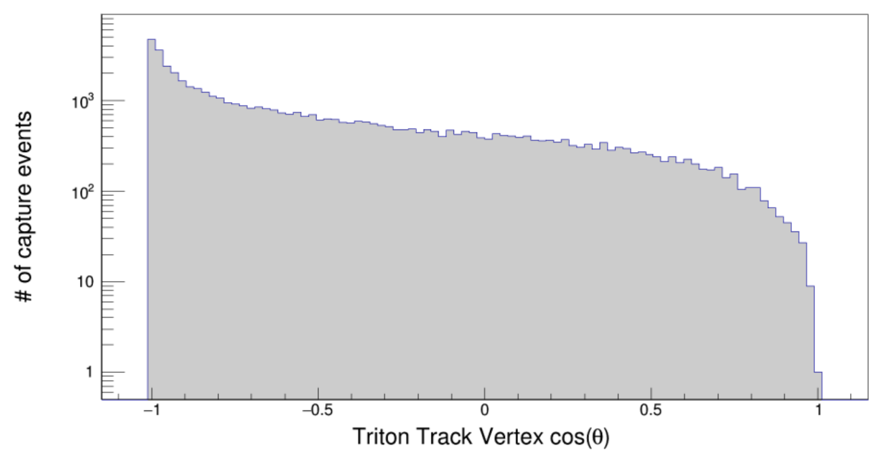
Simulation output verification:

3) **Proton / triton momentum and angle distributions don't correspond to what is expected (recall that the beam neutron momentum is in the z direction and θ is the polar angle):**







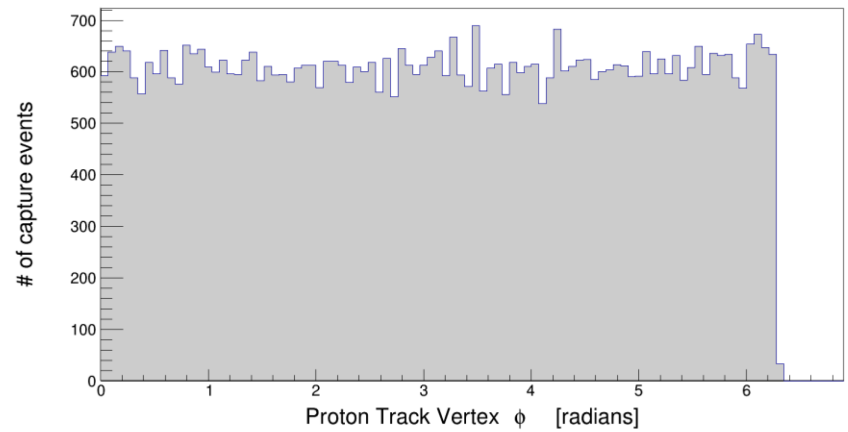


Geant4 Validation for n3He

Simulation output verification:

4) Proton / triton momentum and angle distributions don't correspond to what is expected (recall that the beam neutron momentum is in the z direction and θ is the polar angle):

Phi looks okay!



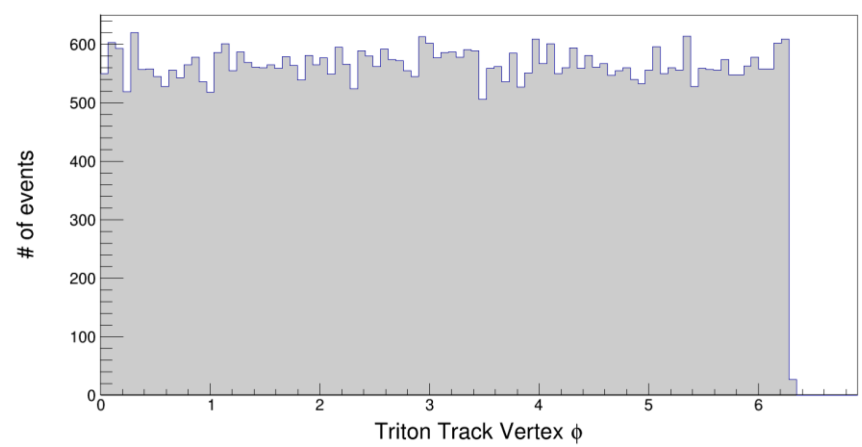
But my question was where the theta distribution comes from…

To answer that I had to look into the part of the G4 code that generates the final states.

The relevant G4 class for our process is

G4ParticleHPInelasticCompFS::

CompositeApply(…)



Geant4 Validation for n3He

Simulation output verification:

The simulation process:

1. G4 takes thermal motion into account: The helium-3 atom momentum is Gaussian distributed (**The relevant G4 class is: G4Nucleus**):

$$\left\langle p_{x,y} \right\rangle_{^3He} = 0 \qquad \sigma_{x,y} = \sqrt{k_B T M_{3He}}$$

$$\left\langle p_z \right\rangle_{^3He} \simeq 2 \, keV/c \qquad \sigma_z \simeq \sqrt{k_B T M_{3He}}$$

The z-distribution (because it is the direction of the incoming neutron) is biased with

$$\frac{\left| \vec{v}_{^3He} + \vec{v}_n \right|}{15\sqrt{\frac{k_B T}{M_{3He}}} + v_n} \geq urand[0,1]$$

?

This expression sits inside a loop that exits when this condition is met and a new helium-3 momentum is sampled in each iteration. This way the selected momentum is biased toward larger values. For T = 0, the sampled $\vec{v}_{^3He}$ is always zero and the above condition is always satisfied.

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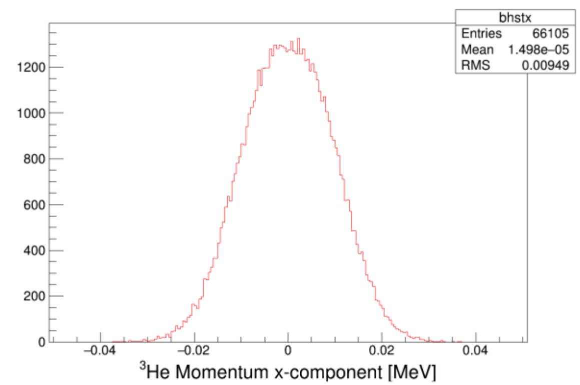
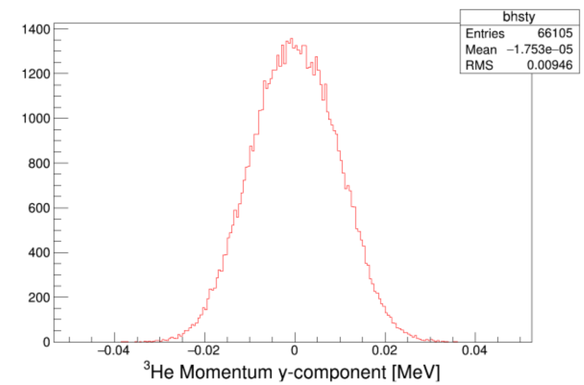
Simulation output verification:

The simulation process:

1. G4 takes thermal motion into account: The helium-3 atom momentum is Gaussian distributed (**The relevant G4 class is: G4Nucleus**):

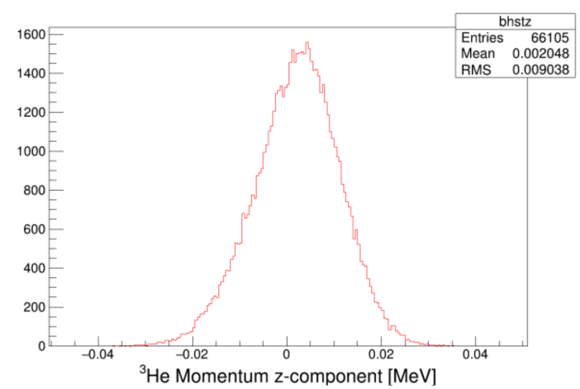
The z-component is biased by the neutron momentum. **I don't understand the reason for this entirely yet, but I think it is related to the transformation into the CM frame before interaction.**

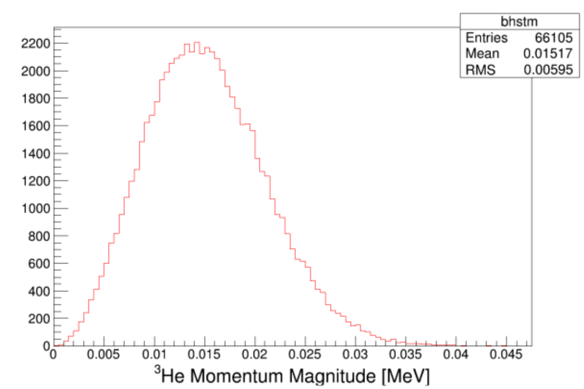




The total momentum has the expected Maxwell-Boltzmann distribution.

All units are MeV/c with c=1





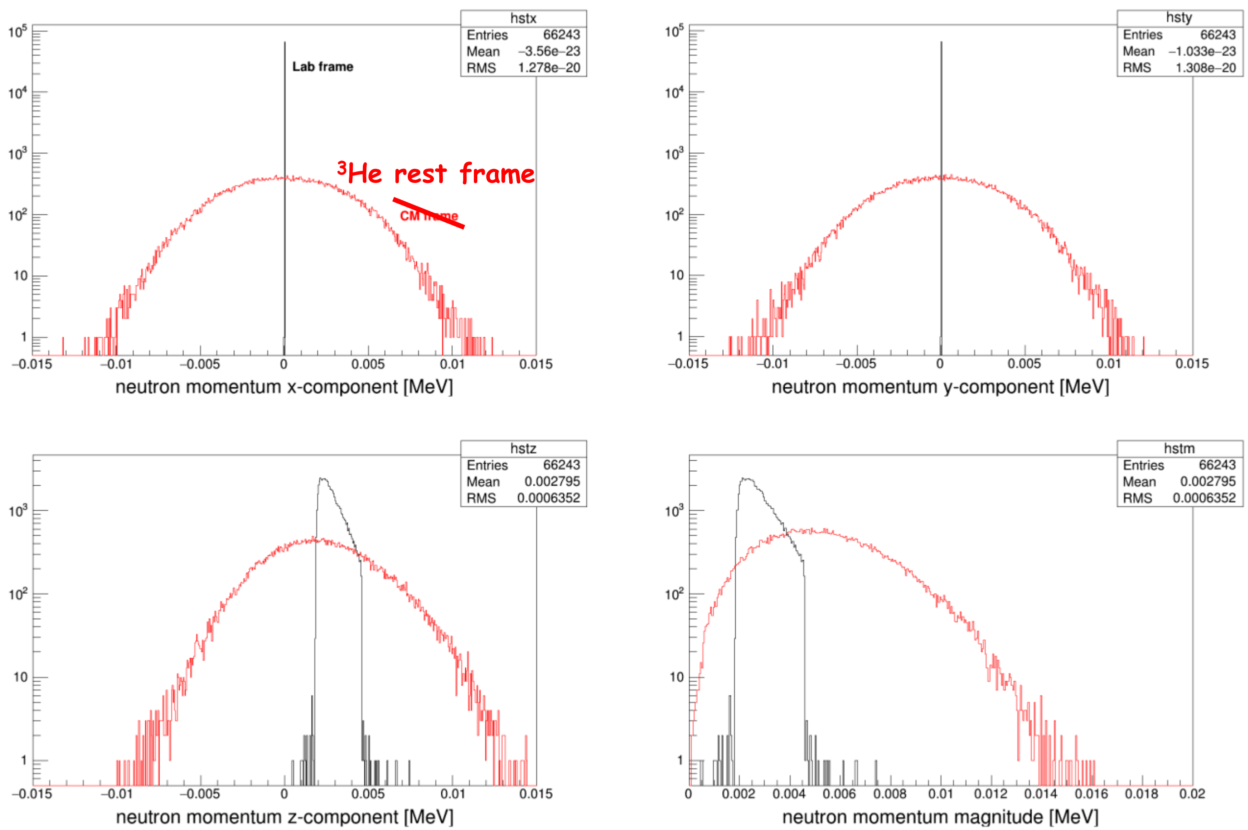
Geant4 Validation for n3He

Simulation output verification:

The simulation process:

2. The neutron is boosted into the target rest frame:

The neutron momentum distribution in the target rest frame is shown in red.



Geant4 Validation for n3He

Simulation output verification:

The simulation process:

3. The target frame neutron momentum is rotated to be along the z-direction in that frame.

4. The secondary particle momentum (in our case the proton or the triton) is set as

$$\vec{p}_p = \left(0, p_p\sqrt{1-\omega^2}, p_p\omega\right) \qquad \text{where} \qquad p_p = \sqrt{\left(E_p - M_p\right)^2 - M_p^2}$$

and

$$\omega = \frac{1+\beta\mu}{\sqrt{\beta^2+1+2\beta\mu}} \qquad \mu = urand\left[-1,1\right]$$

$$E_p = \frac{A_p}{\left(1+A_{3He}\right)^2}\left(\beta^2+1+2\beta\mu\right)E_n \simeq \frac{1}{16}\left(\beta^2+1+2\beta\mu\right)E_n$$

$$\beta = \sqrt{\frac{A_{3He}\left(A_{3He}+1-A_p\right)}{A_p}\left(1+\frac{\left(1+A_{3He}\right)Q}{E_n A_{3He}}\right)} \simeq 3\sqrt{\left(1+\frac{4}{3}\frac{Q}{E_n}\right)}$$

Geant4 Validation for n3He

Simulation output verification:

The simulation process:

5. This momentum is then inverse-rotated with the same matrix that was used to rotate the neutron momentum to lie along and the z-direction in the target rest frame.

6. The secondary (proton) is boosted back into the laboratory frame.

7. The lab frame proton (or triton) becomes the new particle to track in the rest of the G4 simulation

8. Simulation of subsequent energy deposition and ionization depends on initial angular track distribution …

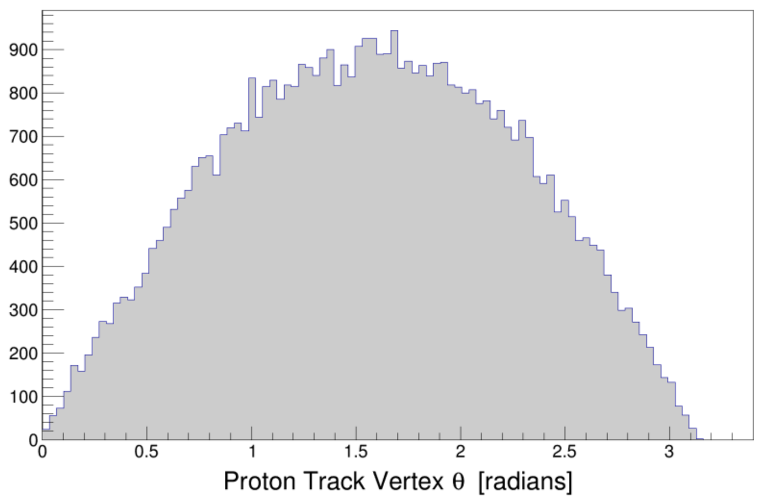
Geant4 Validation for n3He

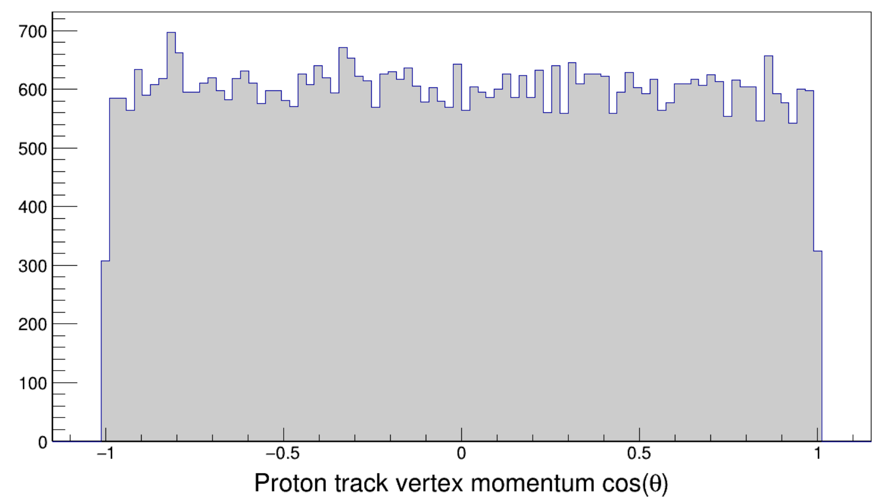
Simulation output verification:

The basic observations are that:

1) The distributions on slide 6 depend on the helium-3 temperature and the associated boost into the target restframe:

   When I set either T = 0 K, or I modify the code and remove the boost, I get:





The phi distribution looks uniform, as before. In the simulation, the theta distribution from slide 6 is caused by the helium thermal motion and the neutron momentum …

So the particular distributions seen under normal circumstances could be accurate and may need to be taken into account when calculating the geometry factors !?