Validation of nuclear de-excitation models of Geant4 toolkit

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Rythme n°1, Robert Delaunay, 1938

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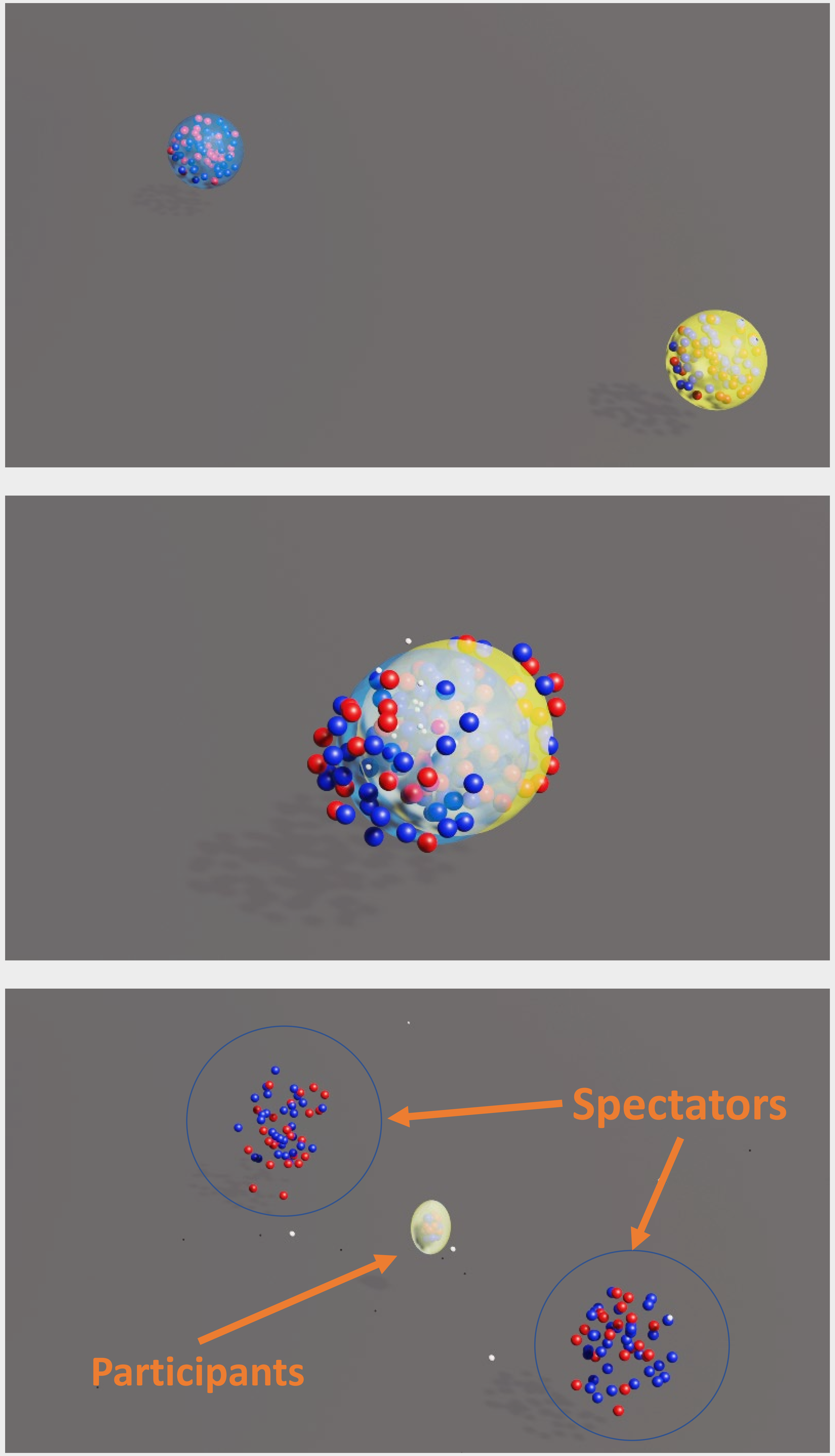
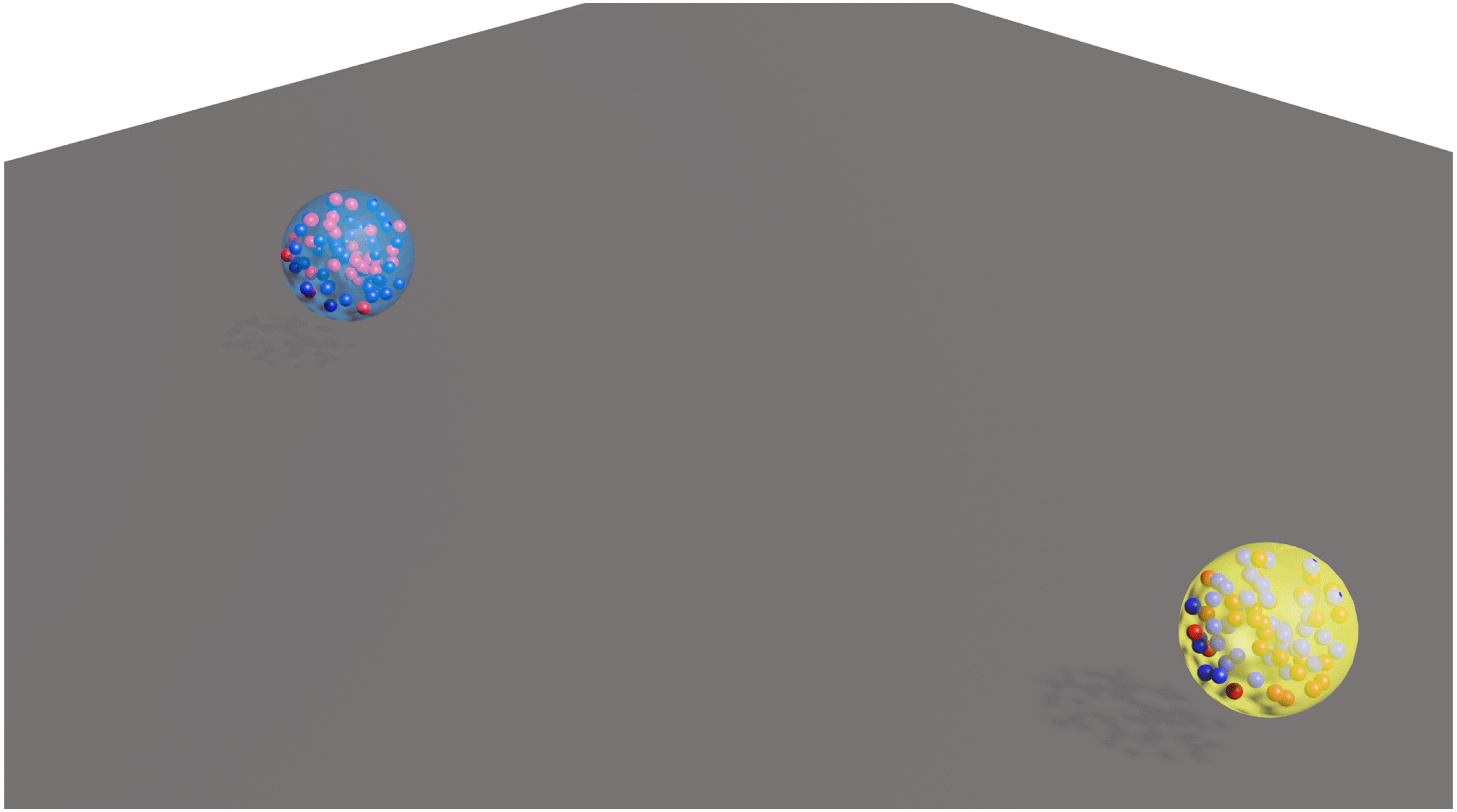
Outline

- Motivation: development of our model — Abrasion Ablation Monte-Carlo for Colliders (AAMCC)
- Examined Geant4 deexcitation models:
  - Evaporation: issues in kinetic energy of light particles in G4Evaporation
  - Multifragmentation (SMM): consideration of Coulomb interaction in G4StatMF
- Comparison of SMM from G4v11.0 with its Fortran version

Visualization of the collision of relativistic nuclei





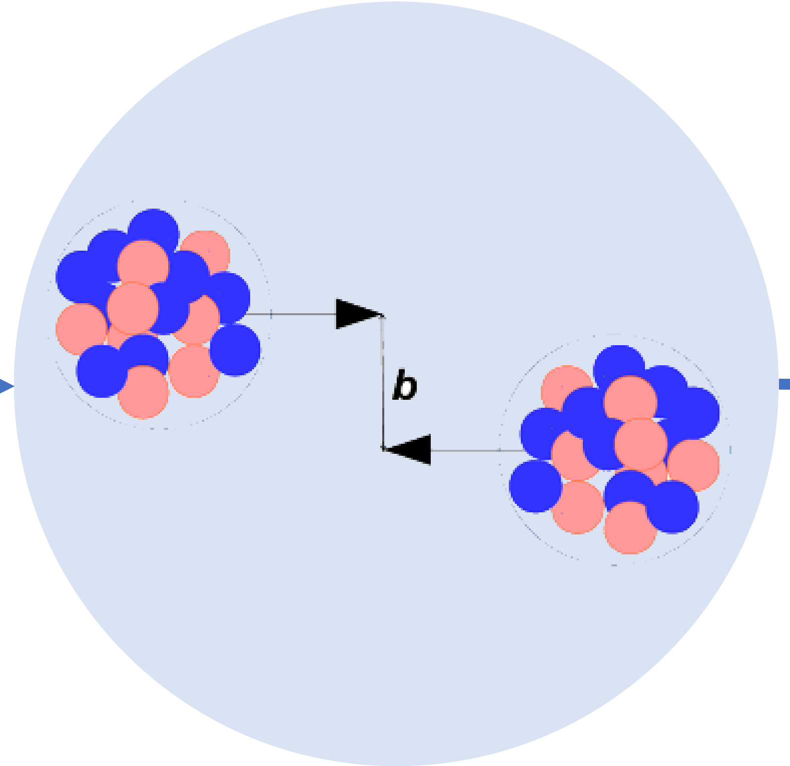
Visualization was made in Blender

- protons
- neutrons

AAMCC model

Abrasion-Ablation Monte Carlo for Colliders*

Abrasion of nucleons



Glauber Monte Carlo

Nucleons' positions sampling

separation of nucleons into spectators and participants

C. Loizides, J. Kamin, D. d'Enterria Phys. Rev. C 97 (2018) 054910

Excitation of prefragments

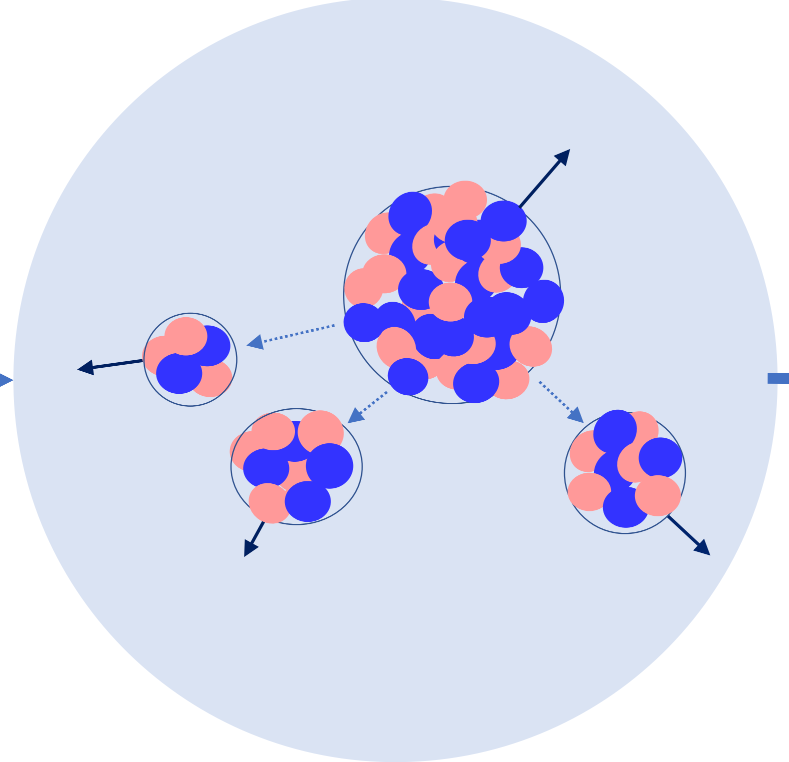
$$\epsilon^* = \frac{E^*}{A}$$

ALADIN parametrization[1]
Ericson formula[2]
Hybrid parametrization

Calculation of the excitation energy using one of the three above-mentioned options

[1]A. Botvina et al. Nuclear Physics A 584 (1995) 737-756
[2]T. Ericson Adv. In Physics 9 (1960) 737-756

Fragmentation of prefragments



Geant4 deex. classes[3]

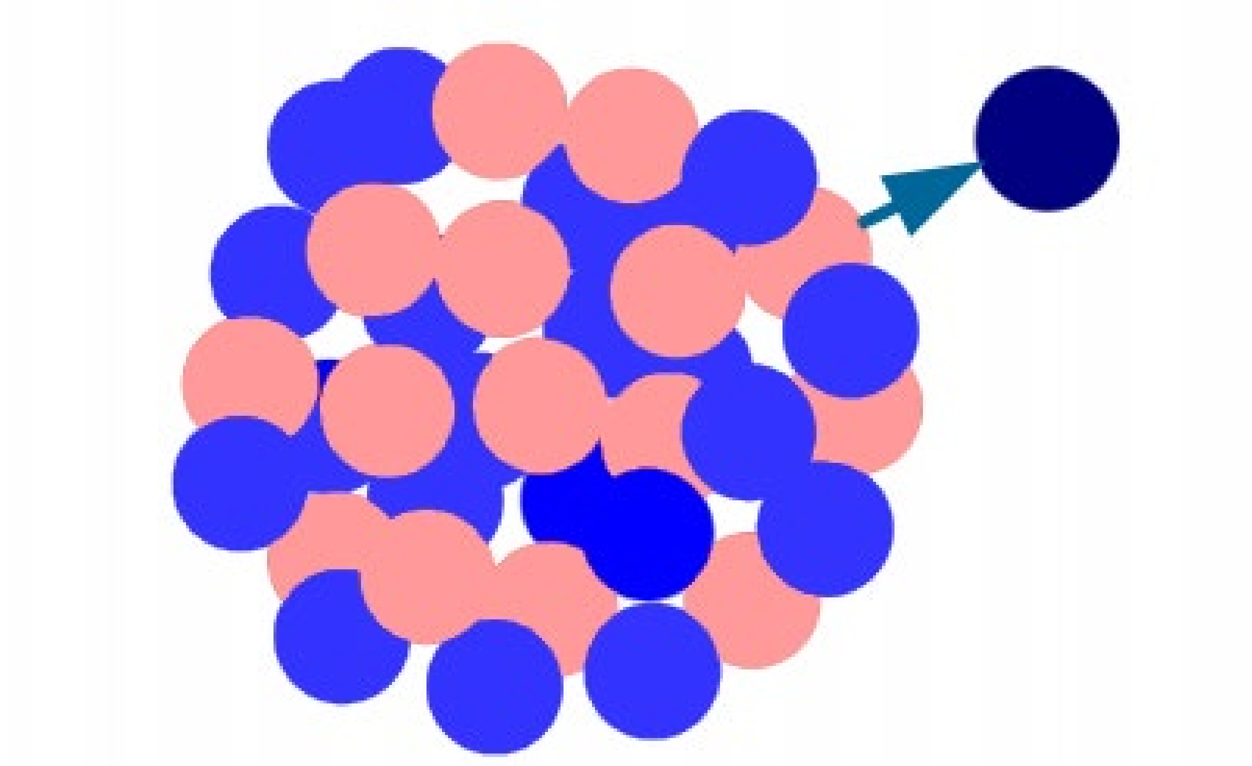
- $\epsilon^* > 4\ MeV/nucl$: Multifragmentation (SMM)[4]
- Evaporation[5]
- Fermi BreakUp $(A < 19)$[6]

[3]J. Alison et al. Nucl. Inst. A 835 (2016) 186-225
[4]J. Bondorf et al. Phys. Rep. 444 (1985) 460-476
[5]V. Weisskopf Phys. Rev. 52 (1937) 295
[6]E. Fermi Progress of Th. Phys. 5 (1950) 570

*A. Svetlichnyi, R. Nepeivoda, I. Pshenichnov Particles. 4 (2021) 227-235

Evaporation model

- Nuclear evaporation is the mechanism process usually employed for a hot intermediate compound nucleus formed in a nuclear reaction
- If the excitation energy is higher than the separation energy, prefragment can eject nucleons and fragments (d, t, ^{3}He, α, others)
- In a conventional treatment of nuclear evaporation, particles are emitted sequentially along an evaporative decay chain



Maximum kinetic energy of the evaporated particle ("j"):

$$\varepsilon_j^{\max} = \frac{(M_i + E^* - \delta)^2 + M_j^2 - M_d^2}{2(M_i + E^* - \delta)} - M_j$$

where
i – compound nucleus
d – residual nucleus ("daughter")
δ – pairing energy correction of the daughter nucleus

Sampling procedure, parametrization and more: Geant4 Physics Reference Manual, section 5.8.5:

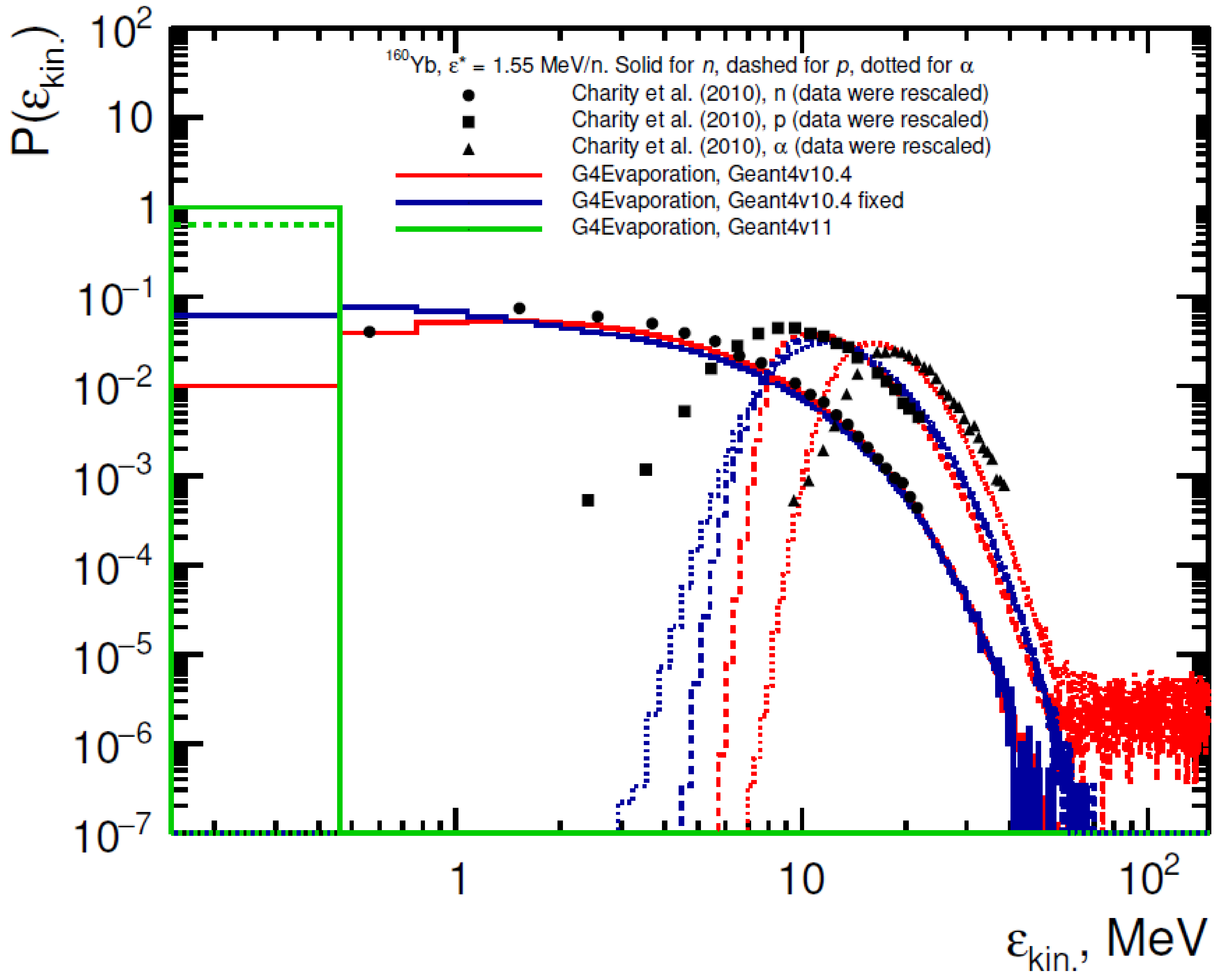
https://indico.cern.ch/event/679723/contributions/2792554/attachments/1559217/2454299/PhysicsReferenceManual.pdf

V. Weisskopf Phys. Rev. 52 (1937) 295

Kinetic energy of light particles in G4Evaporation

- Standalone tests of G4Evaporation from G4v10.4 and G4v11.0 were performed for decaying system: ^{160}Yb, $\varepsilon^* = 1.55$ MeV/n

- Tails of kinetic energy in v10.4 distribution occur due to the low efficiency of the used rejection sampling algorithm
- Calculations with fixed kinetic energy sampler are presented in v10.4 fixed histogram
- Problems with recent v11.0 were reported to Geant4 collaboration*
- We strongly recommend to use our fixed version of G4Evaporation until the official patch of G4 will be released

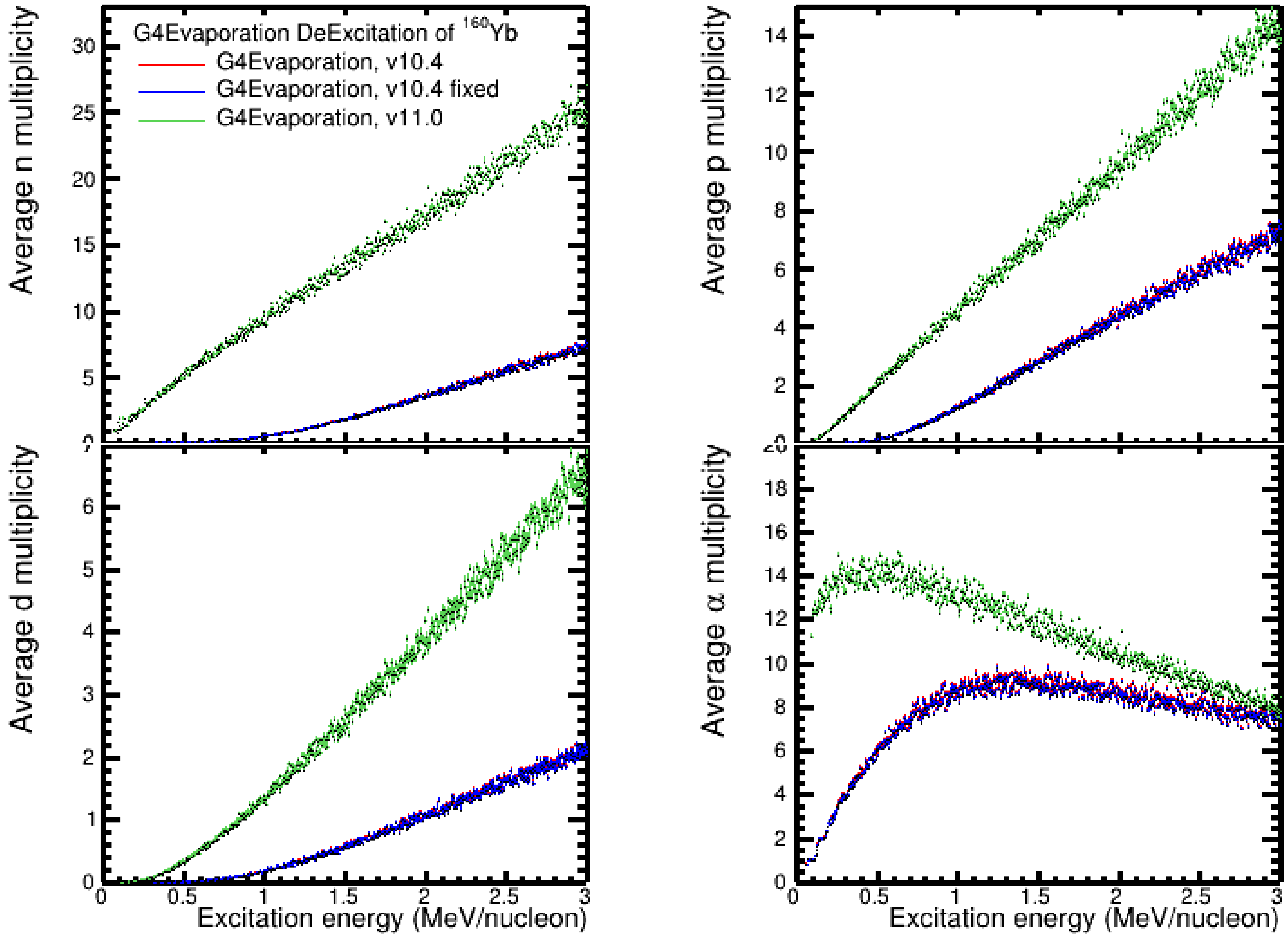


*https://indico.cern.ch/event/1106118/contributions/4693132/

R.J. Charity et al., Phys. Rev. C 82 (2010) 014610

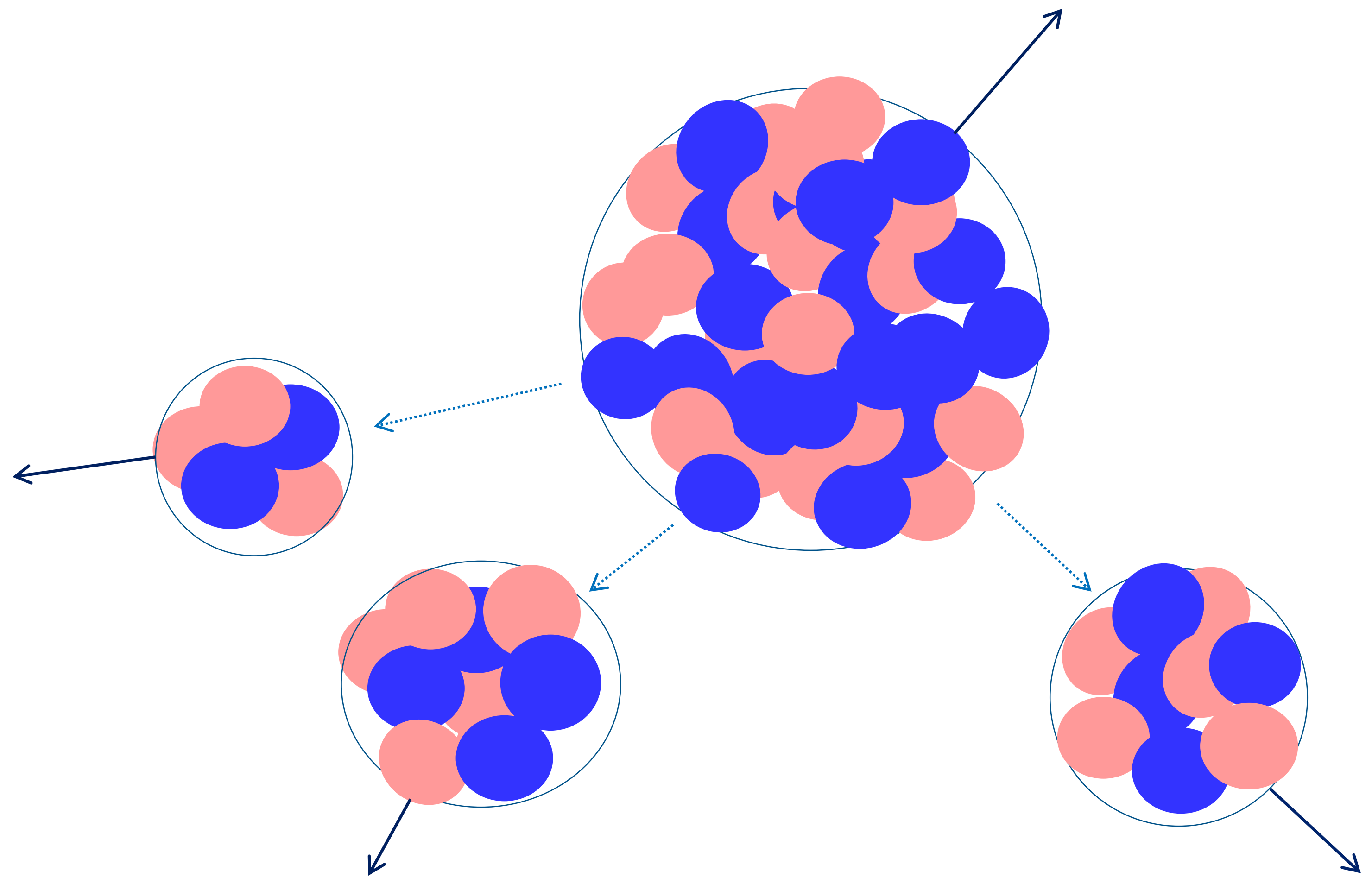
Average multiplicities of light particles in G4Evaporation

- Multiplicities of light particles in v11.0 are overestimated compared to v10.4 and v10.4 fixed
- Calculated multiplicities of α-particles are unrealistic in v11.0. It is up to 14 meaning that 1/3 of the initial nucleus is converted to alphas
- Wrong multiplicities result from the incorrect calculation of the kinetic energy carried away by the evaporated fragments (see prev. slide)
- It's recommended to use v10.4 with the fixes proposed by us



Multifragmentation model

- Multifragmentation is a simultaneous formation of three or more nuclear fragments
- Nuclear system breaks into many nuclear fragments of different masses if its excitation energy is greater than 3-5 MeV/n
- Thermodynamic approach: decaying system is in thermal equilibrium, fragments are described in a liquid drop approximation, channel probability is calculated from the entropy of final states



Kinetic energy of fragments in the rest of decaying system obeys the Boltzmann distribution at a given temperature T_b:

$$\frac{dP(T^f_{kin})}{dT^f_{kin}} \sim \sqrt{T^f_{kin}} \exp\left(-T^f_{kin}/T_b\right)$$

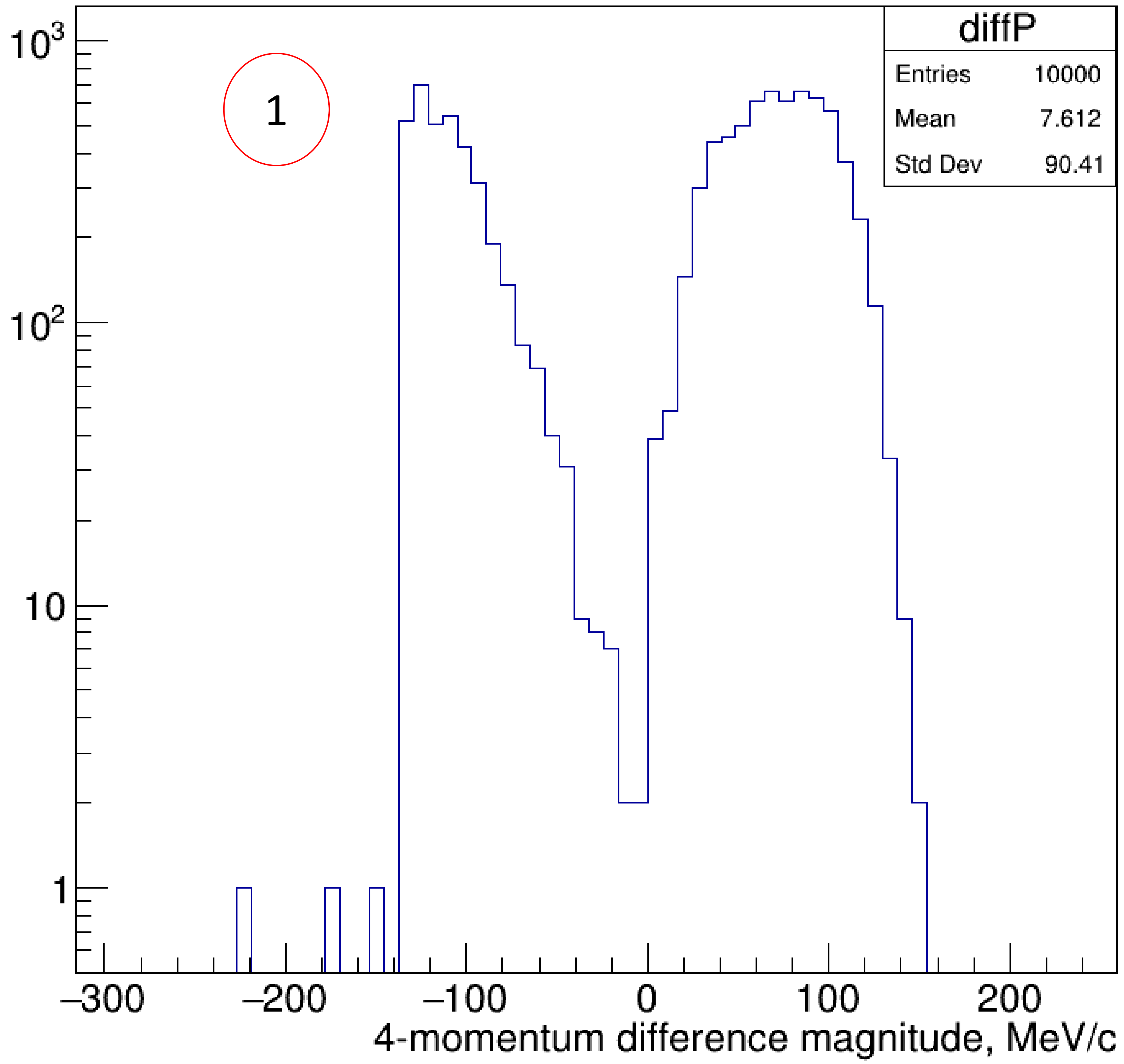
For more: Geant4 Physics Reference Manual, section 5.8.11:

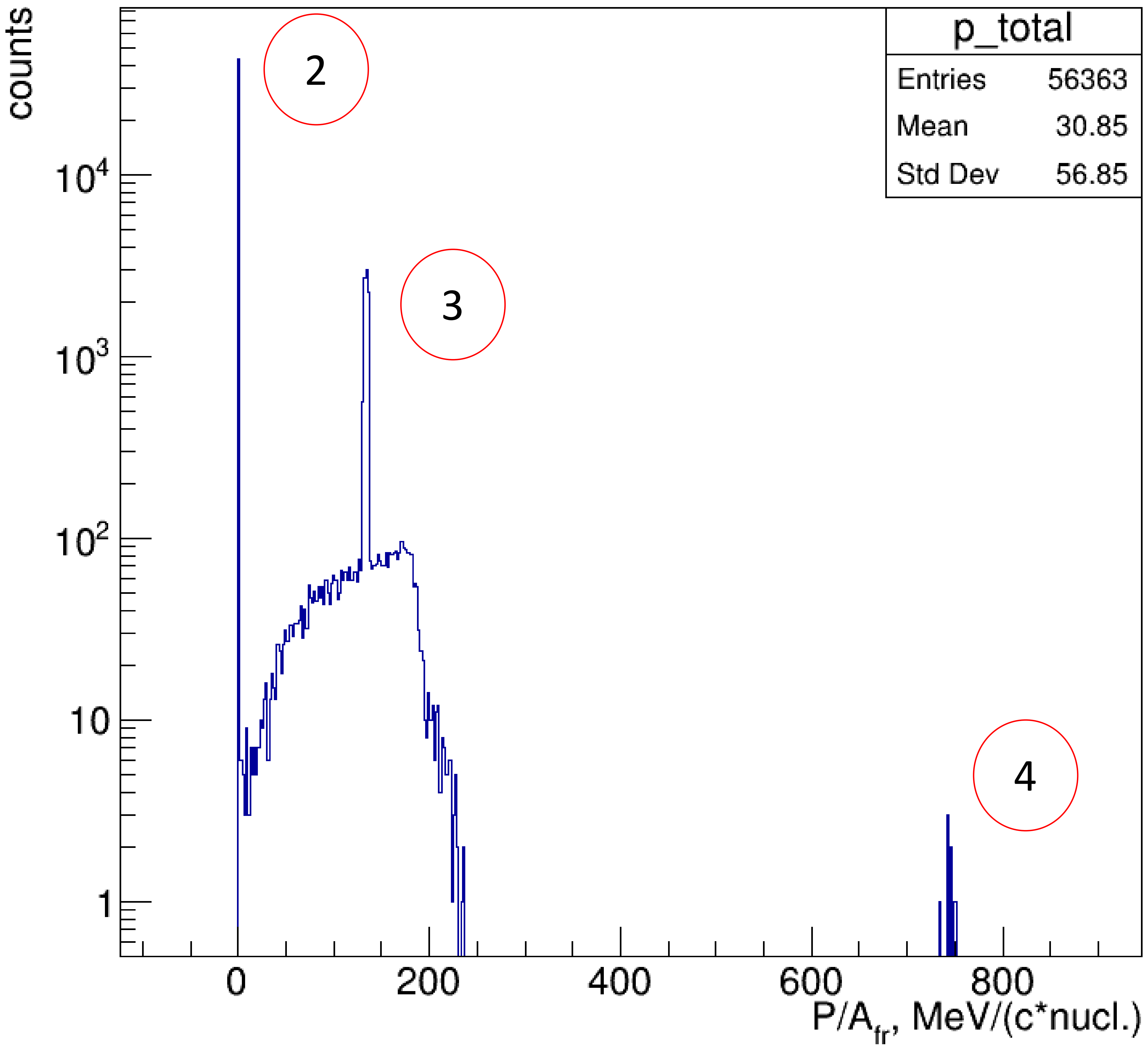
https://indico.cern.ch/event/679723/contributions/2792554/attachments/1559217/2454299/PhysicsReferenceManual.pdf

J.P. Bondorf et al. Physics Reports. 257 (1995) 133–221

Momentum distribution of fragments in G4StatMF

Standalone test of SMM model from G4v10.4 was performed for ^{208}Pb, $\varepsilon^* = 4$ MeV/n





1. 4-momentum is not conserved
2. most of the fragments have zero 3-momentum
3. fragments with “fixed” 3-momentum near 130 MeV/(c*nucl.)
4. fragments with abnormally large 3-momentum

Coulomb interaction between charged fragments in G4StatMF

- The method G4StatMFChannel::SolveEqOfMotion is designed to calculate the evolution of charged fragments in a mutual Coulomb field
- In v10.4 and v11.0, this method is used even in case when there is only one charged fragment, which leads to abnormally large momentum due to the self acceleration
- In the case when there are several charged fragments they lose their 3-momenta due to the set of issues discussed below

Calculation of Coulomb force by G4StatMF::SolveEqOfMotion()

Dimension analysis:

$$\mathbf{V} = \frac{\mathbf{p}}{m} = \mathbf{a} \cdot \Delta t = \frac{\mathbf{F}}{m} \cdot \Delta t \longrightarrow [V] = 1 = \frac{[F]}{[m]} \cdot [\Delta t] \xrightarrow{[\Delta t] = fm/c} [F] = \frac{MeV \cdot c}{fm}$$

$$F = a_x \cdot \frac{Z_1 Z_2}{r^2} \frac{MeV}{fm} \qquad [r] = mm$$

in SI | in c = 1 | in Geant4

$$F = 10^6 \frac{9 \cdot 10^9 \cdot 1.6^2 \cdot 10^{-38} Z_1 \cdot Z_2}{r^2} H = 2.83 \cdot 10^{-22} \cdot \frac{Z_1 \cdot Z_2}{r^2} MeV^2 = a_x \cdot 1.97 \cdot 10^2 \frac{Z_1 \cdot Z_2}{r^2} MeV^2$$

this analysis gives: $a_x = 1.44 \cdot 10^{-24}$

but in Geant4: $a_x = 1.44 \cdot 10^{-12}$

- The overestimation of the Coloumb force should lead to the overestimation of the fragments' momenta
- Why are the resulting momenta essentially underestimated?

Scaling of kinetic energy in G4StatMF::SolveEqOfMotion()

- Typically Coulomb energy is converted into the fragment kinetic energy within ~500 fm/c
- Since by this time fragments are already separated by ~50 fm, the residual Coulomb interaction does not lead later to a noticeable change of the directions of the fragments' motion and the relation between their velocities
- To simplify the calculations, the integration is stopped and the fragment velocities are proportionally scaled at the time when 80% of the Coulomb energy is converted into the fragment kinetic energy

$$T_{tot} = \eta^2 \sum_{i=1}^{N_{ch}} \frac{p_i^2}{2m_i} = 3/2 \cdot N_{ch} \cdot T + E_c$$

$\Delta t \sim 10$ fm/c $\longrightarrow$ $N_{iterations} \geq 50$ in Geant4: $N_{iterations} = 100$

Presently in Geant4:

$$T_{tot} = \eta \sum_{i=1}^{N_{ch}} \frac{p_i^2}{2m_i} = 3/2 \cdot N_{frag} \cdot T + E_c$$

$$V_i \longrightarrow \eta \cdot V_i$$

Should be:

$$T_{tot} = \eta^2 \sum_{i=1}^{N_{ch}} \frac{p_i^2}{2m_i} = 3/2 \cdot N_{ch} \cdot T + E_c$$

$$V_i \longrightarrow \eta \cdot V_i$$

J.Bondorf et al. Phys. Rep, 257 (1995) 133

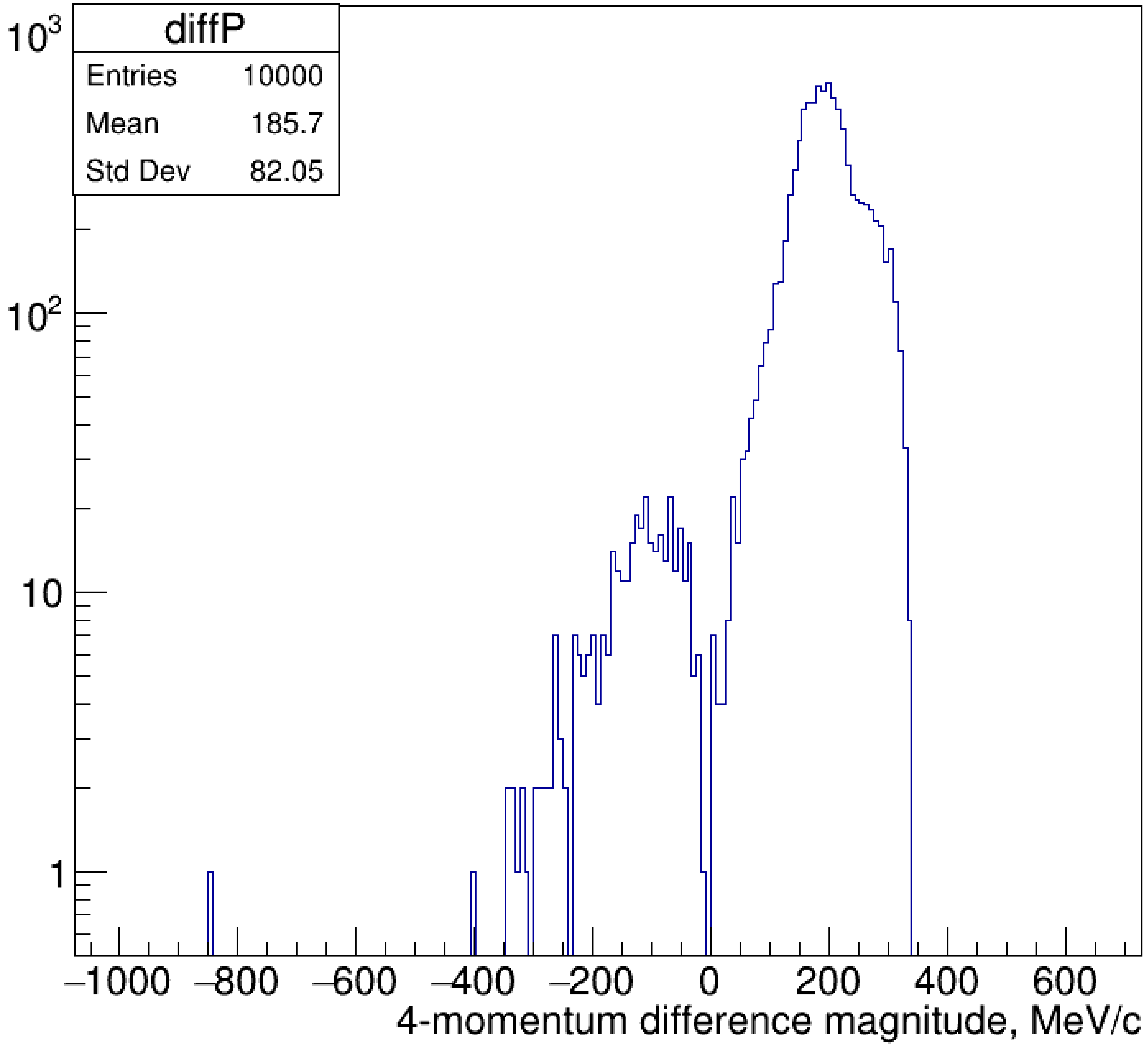
Neutron production in G4StatMF

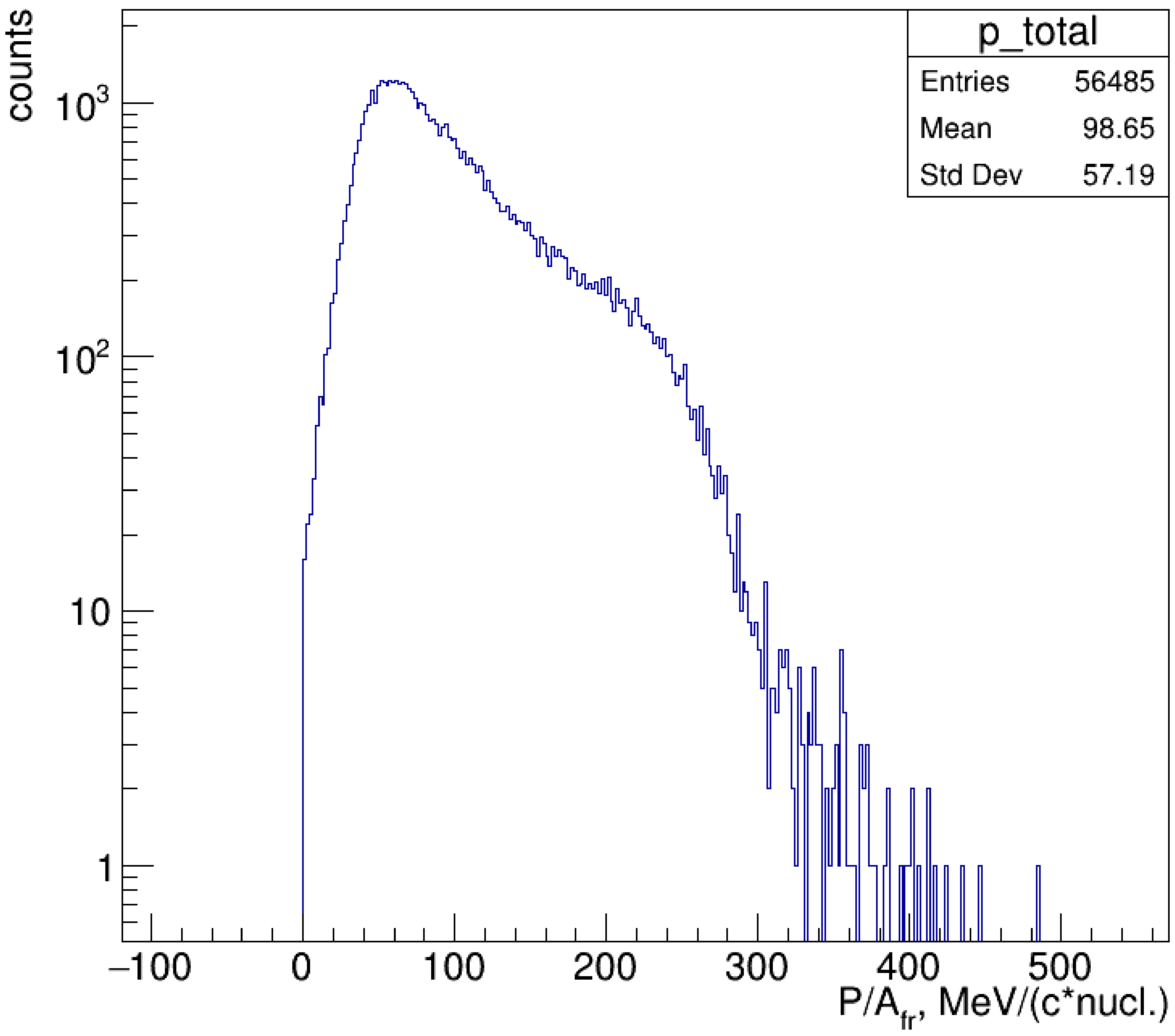
- Momenta of charged and neutral fragments are calculated separately in the G4 v11.0 and v10.4
  - neutral — in G4StatMFChannel::FragmentsMomenta
  - charged — in G4StatMFChannel::CoulombImpulse, using above mentioned method
- In the case there is one charged fragment and also two neutrons in the final state, non-conservation of the full 4-momentum in the decaying system is observed. It is revealed by the sharp peak 3 in the momentum distribution (shown in slide 9)

↓

- In the fixed version of G4StatMF, joint sampling of 3-momentum of charged and neutral fragments has been implemented

Momentum distribution of fragments in G4StatMF after fixes

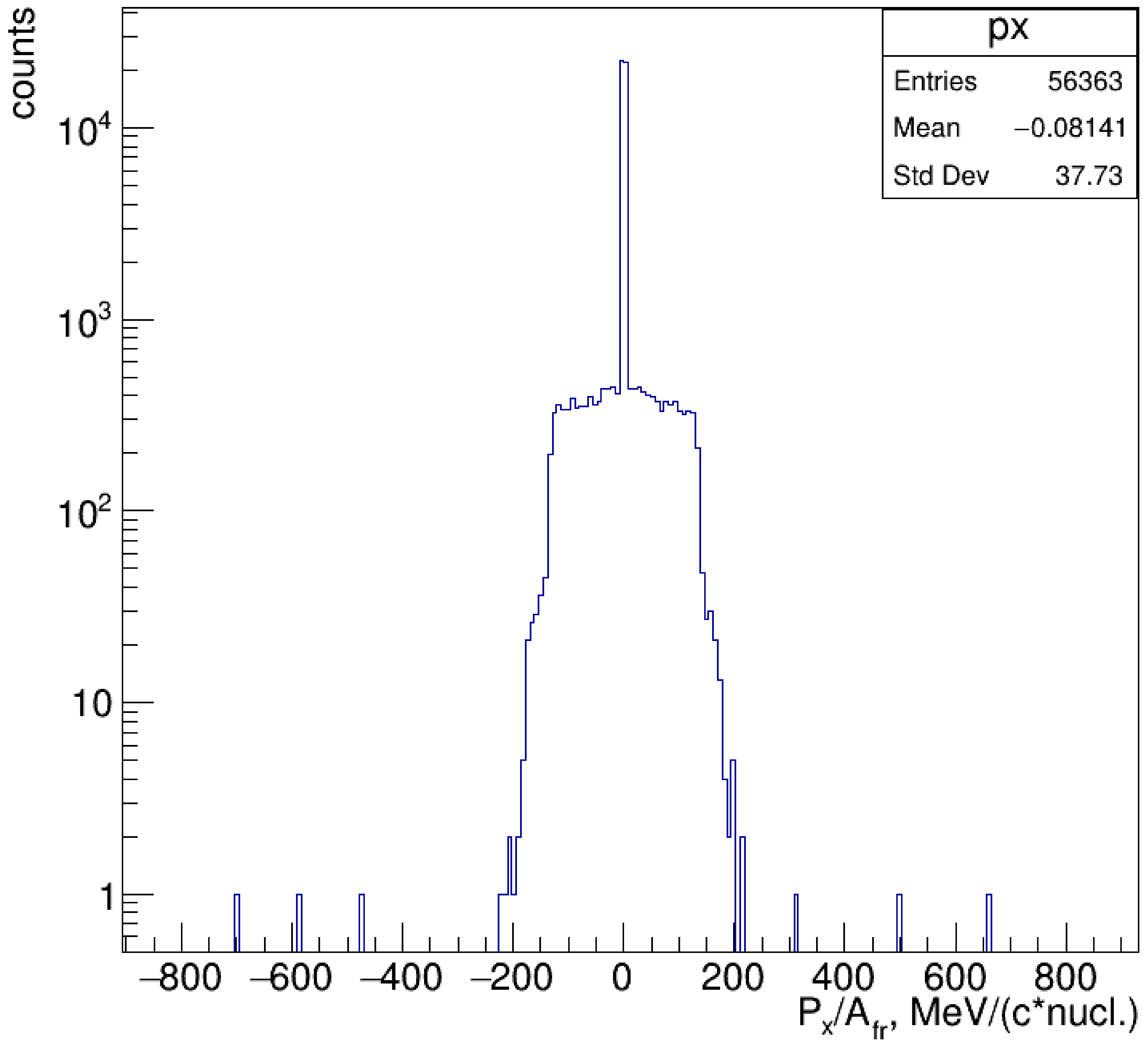




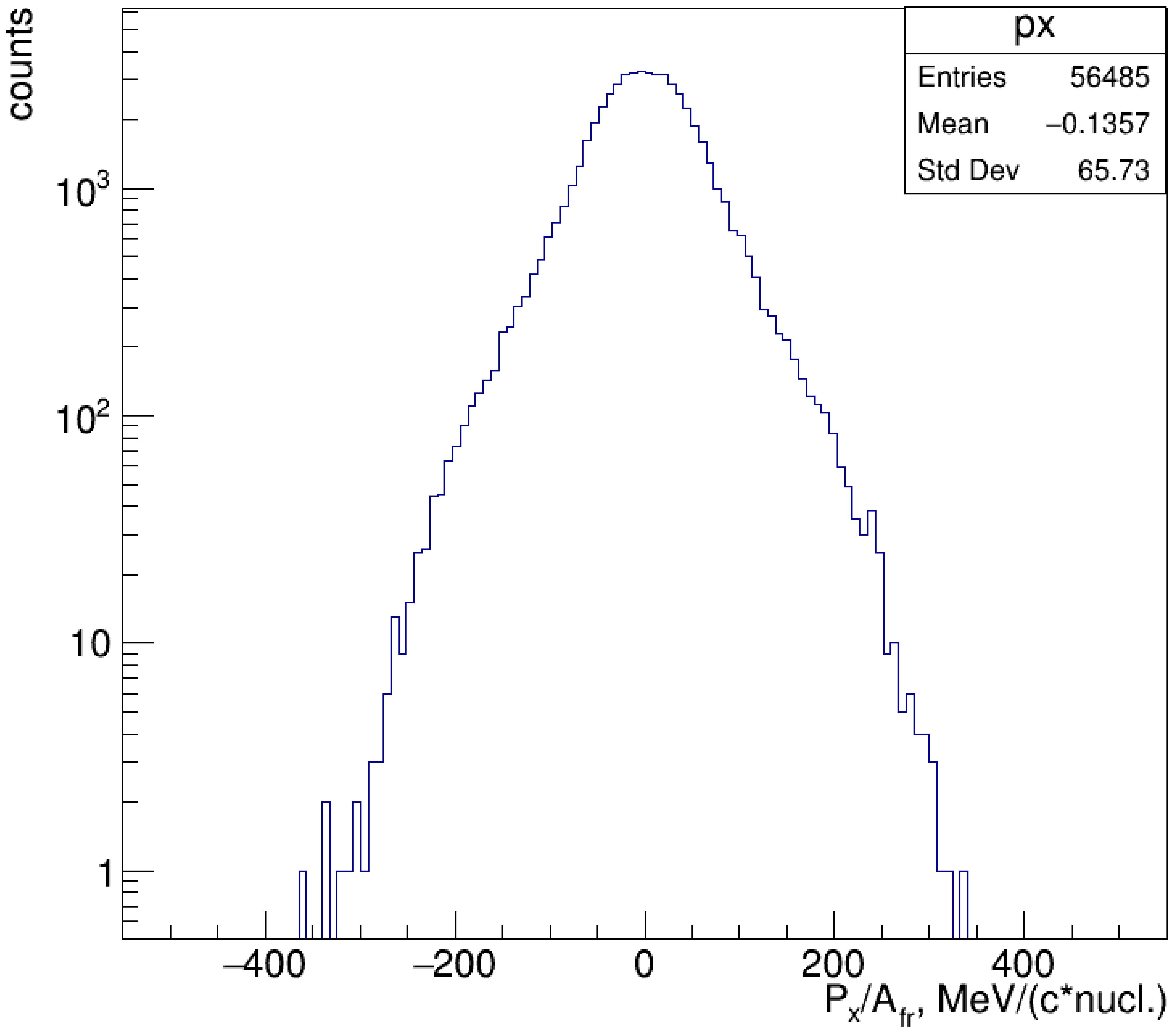
- Problems of the momentum distribution of fragments on the right panel have disappeared
- 4-momentum still doesn't conserve (work in progress)

X component of momentum of fragments

v10.4

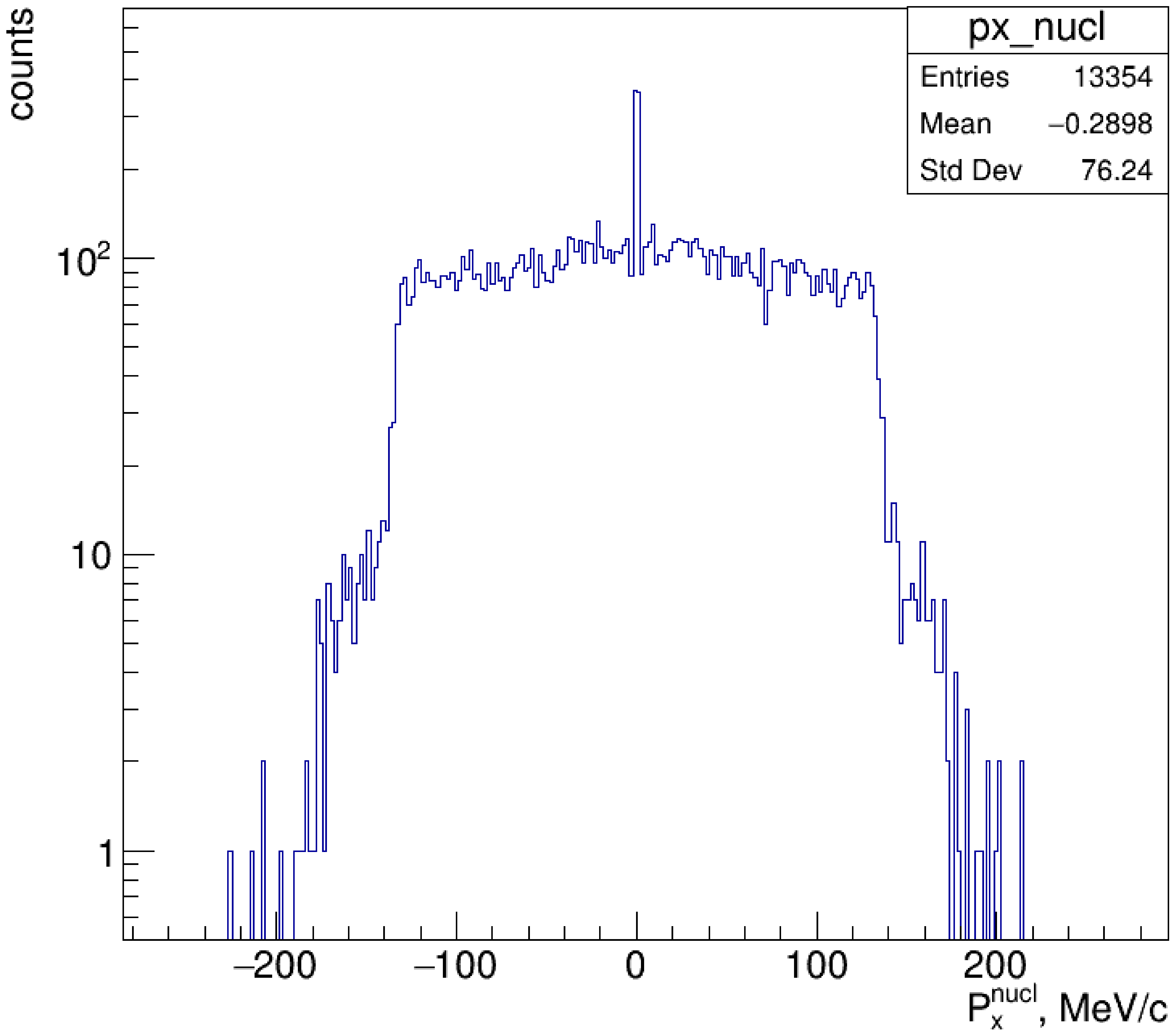


v10.4 fixed

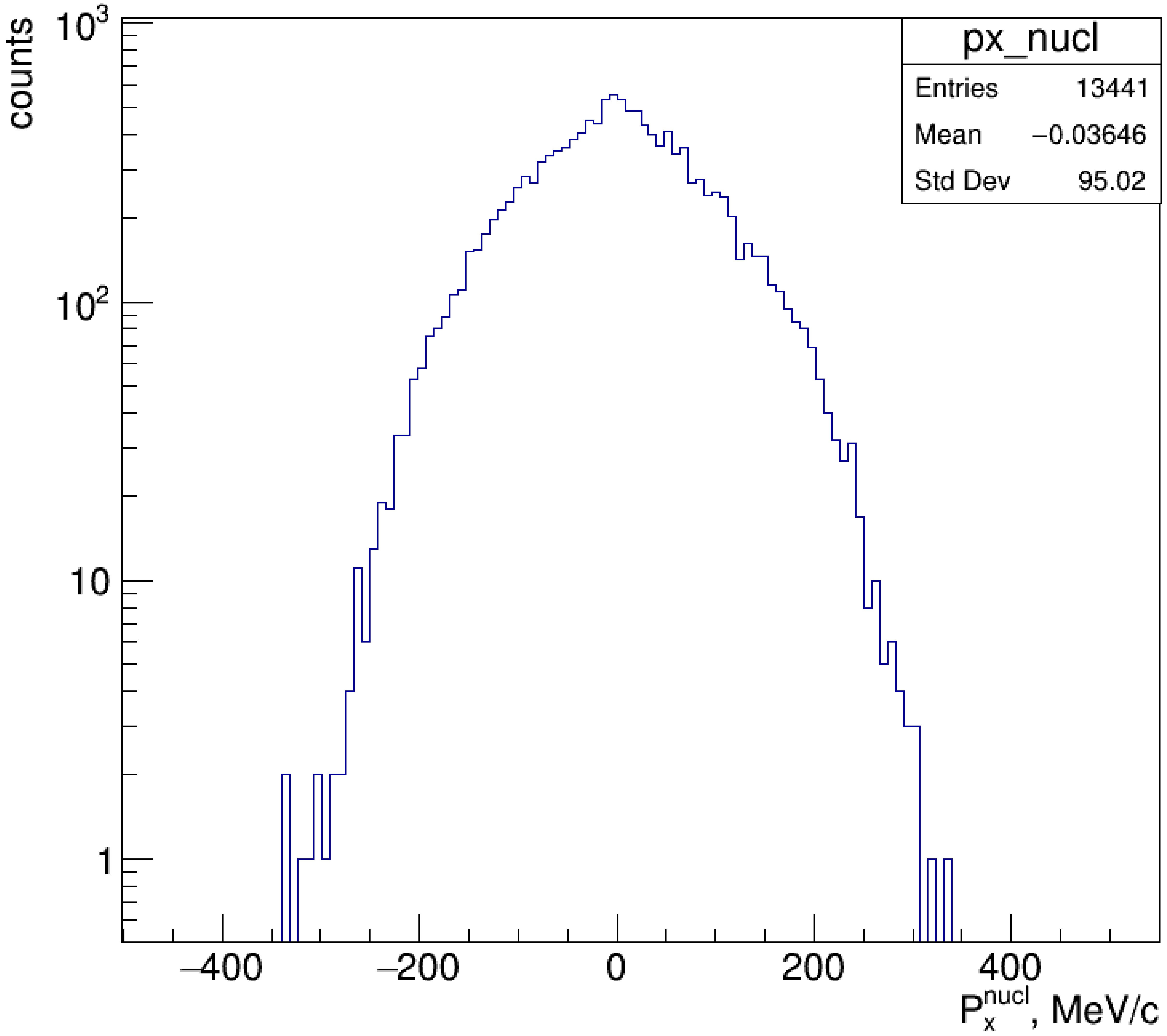


X component of momentum of free nucleons

v10.4

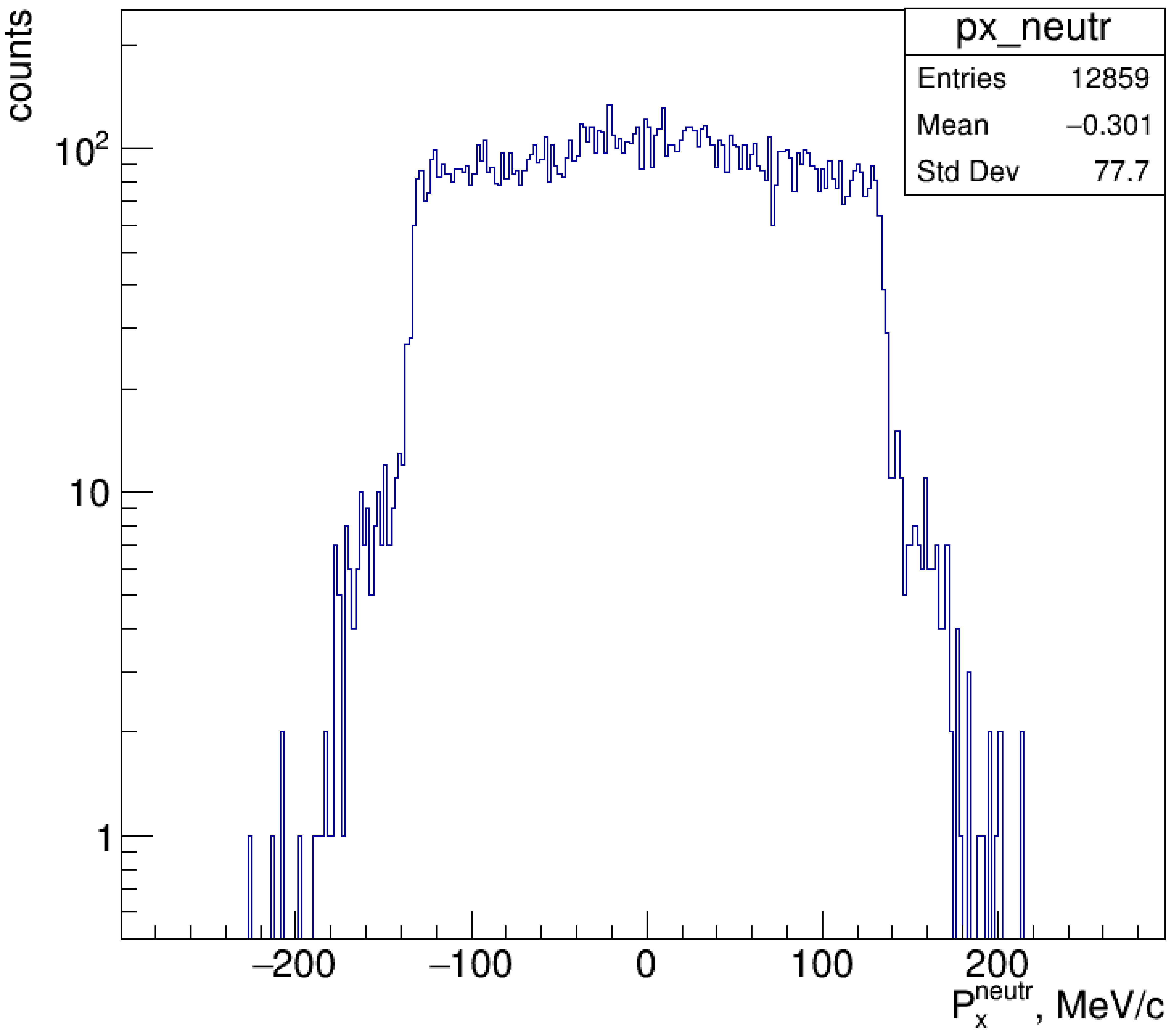


v10.4 fixed

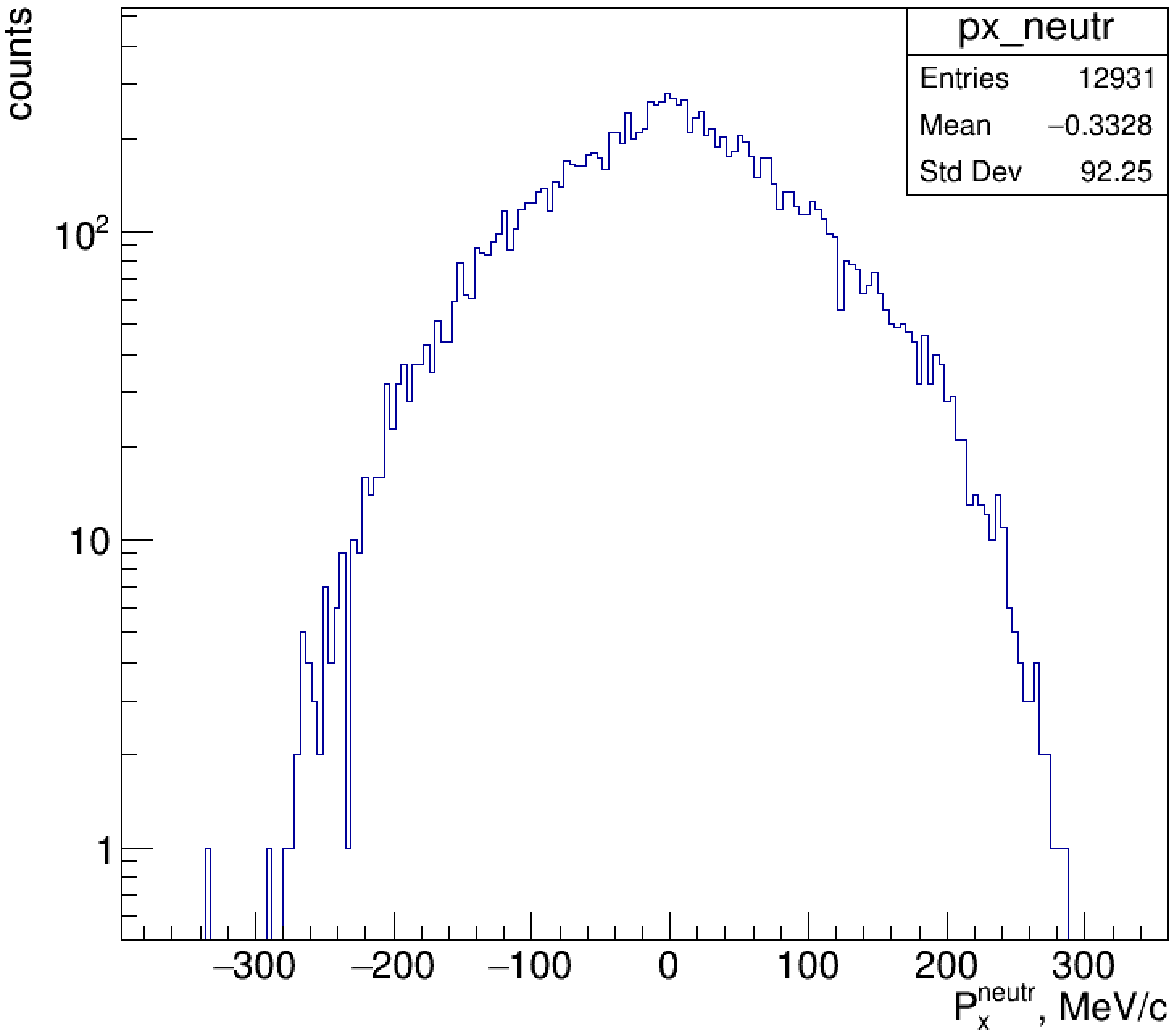


X component of momentum of neutrons

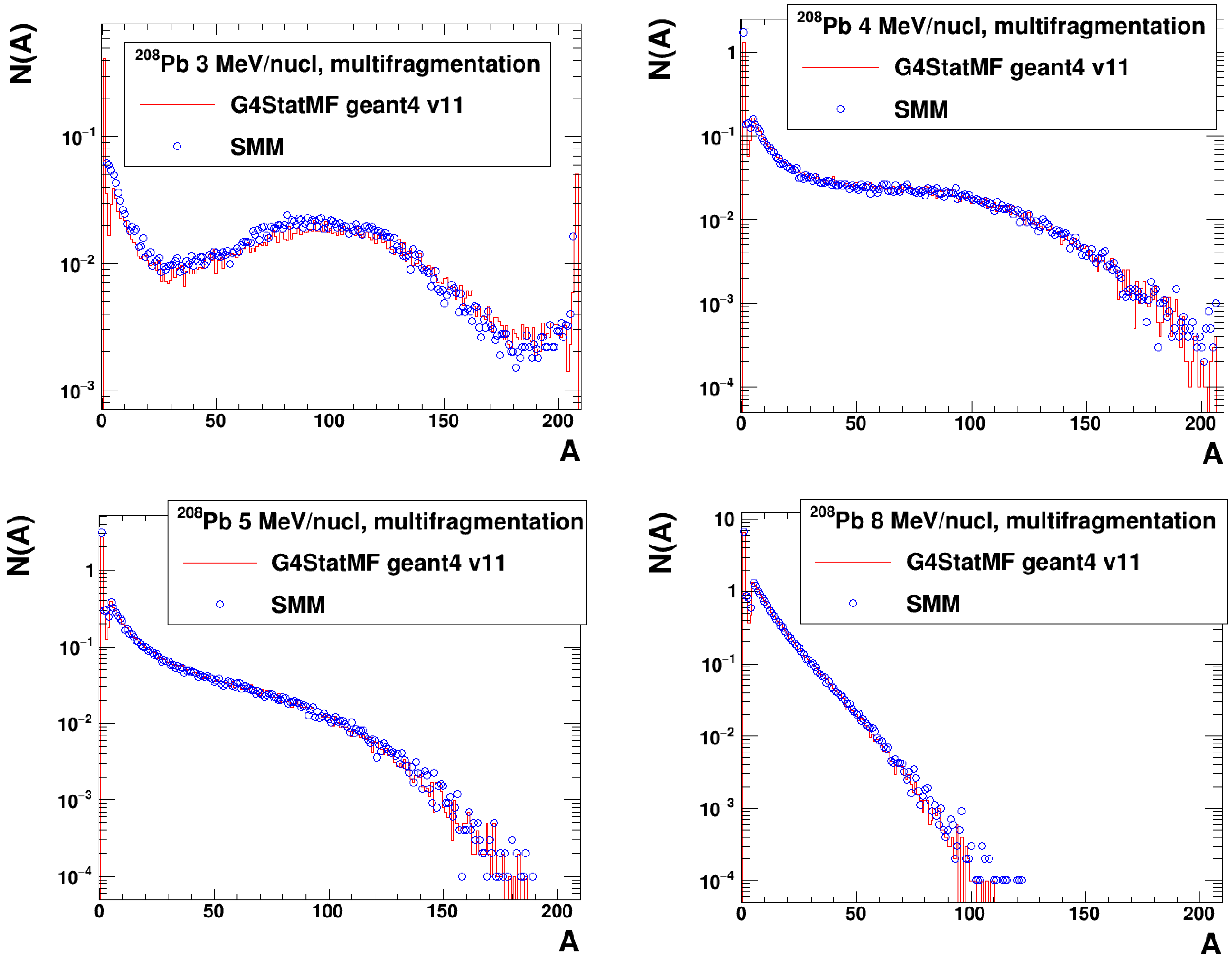
v10.4



v10.4 fixed



Mass distribution of fragments in SMM



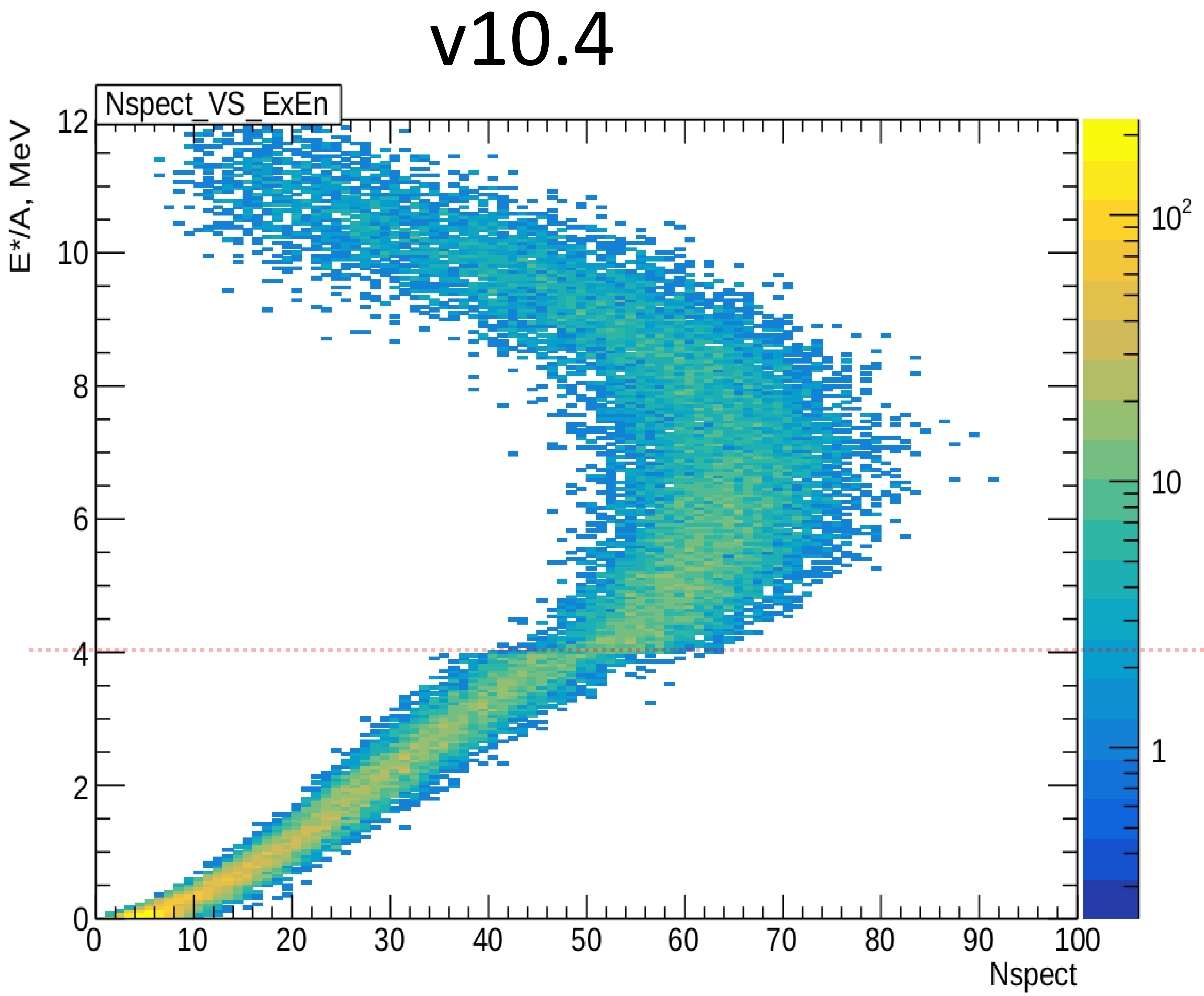
- Comparison of mass distributions in stand alone tests of G4StatMF with Fortran SMM was carried out

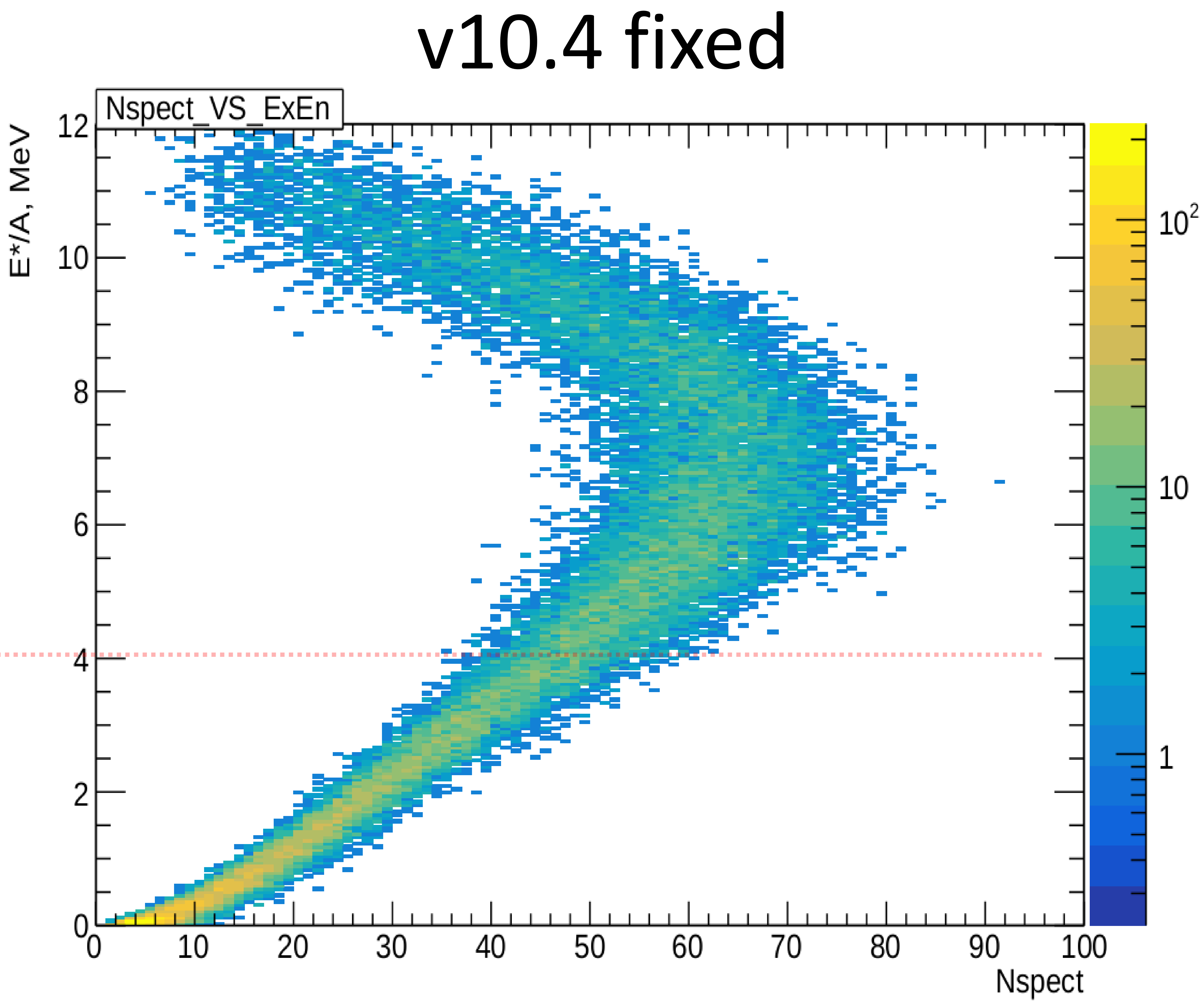
- Decaying system: ^{208}Pb at $\varepsilon^* = 3, 4, 5, 8$ MeV/n

- Good agreement with the Fortran version of SMM is obtained, same as for early versions*

*I. Pshenichnov, A. Botvina, I. Mishustin, W. Greiner, NIMB 268 (2010) 604

Number of spectators in AAMCC model with respect to the excitation energy





- Coulomb energy fix in G4StatMF corrected the SMM channel temperature, thus shifted the multiplicity of spectators
- Smooth transition between deexcitation models in AAMCC is achieved

Conclusion

- Statistical multifragmentation and Evaporation models in the G4 v11.0 and 10.4 were revised
- Issues with momentum distributions were found and fixes were proposed to the Geant4 collaboration:
  - New sampling procedure of fragment's kinetic energy in G4Evaporation
  - Fixed calculation procedure of Coulomb interaction between charged fragments
- Good agreement with the previous Fortran version of SMM is preserved in the fixed version of G4StatMF
- Proposed fixes made it possible to improve the description of spectator matter in AAMCC
- It's recommended to validate G4 models with experimental data prior to using G4 in full-scale simulations of experimental setups
- Geant4 includes more than 2M lines of code. Some of the numerous physics models may contain errors and users are very welcome to report them to the developers

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Thank you for attention!