On the performance of the evaporation and multifragmentation models in Geant4

Spatial force construction,
L.Popova, 1921

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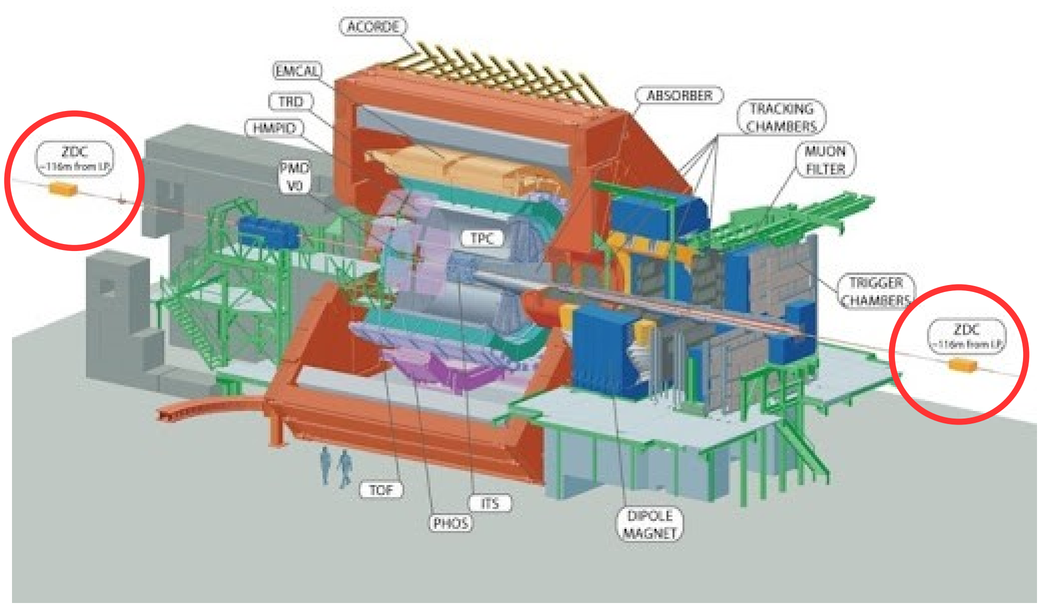
Research

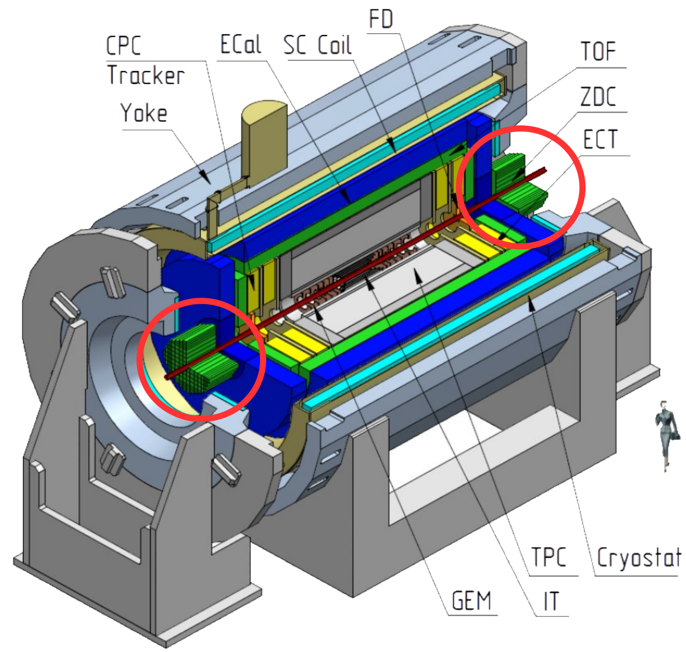
Content

- Our interest in fragmentation models:
  - Our AAMCC model is based on GlauberMC and nuclear de-excitation models from G4
- Momenta of secondary fragments in AAMCC
- Standalone tests of G4StatMF and G4Evaporation:
  - Comparison of kinetic energy spectra from G4Evaporation with experimental data
  - Kinetic energy of charged fragments in G4StatMF is influenced by their Coloumb repulsion

Most of experiments on AA collisions are equipped with forward calorimeters



Neutron and proton ZDCs in ALICE experiment:
C. Oppedisano et al., Nucl. Phys. B **197** (209) 206



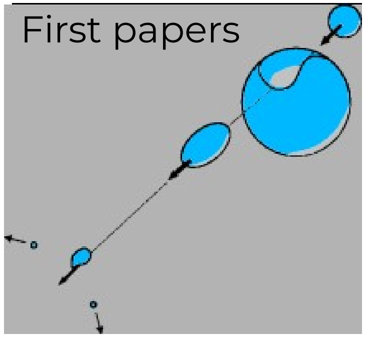
Forward calorimeters of MPD experiment at NICA
A. Sorin et al., Nucl. Phys. A **855** (2011) 510

- Forward calorimeters detect forward going spectator fragments: neutrons and other fragments in some experiments to determine the collision centrality, reaction plane, etc.
- Reliable models are needed for predicting the yields of the spectator fragments and their momenta to model the detector response.

Participant-spectator scenario to model forward matter in nucleus-nucleus collisions

Adopted by abrasion-ablation models, cascade models (ABRABLA, DCM-SMM, LAQGSM-SMM, DPMJET-GEM etc.):

- Interacting (wounded) nucleons and spectator nucleons are distinguished. All the latter are assumed to be inside a nuclear residue (prefragment).
- A realistic prescription for calculating the excitation energy of the prefragment is necessary to obtain a correct composition of decay products.
- A set of prefragment decay models have to be involved.



J. Gosset, H.H. Gutbrod, W.G. Meyer et al., PRC **16** (1977) 629
J. Hüfner, K. Schäfer, B. Schürmann, PRC **12** (1975) 1888

Other abrasion-ablation models:

J.-J.Gaimard K.-H.Schmidt, NPA **531** (1991) 709

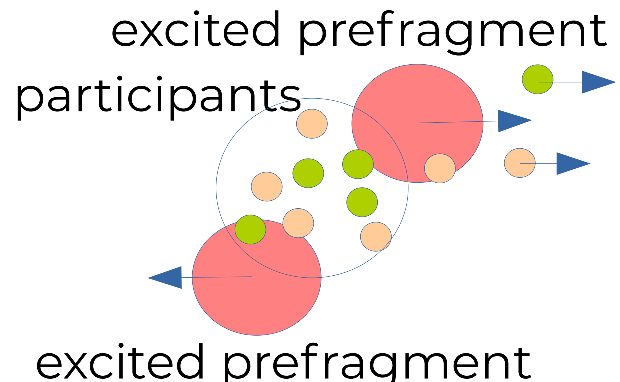
C. Scheidenberger, I.P., K. Sümmerer et al., PRC **70** (2004) 01492

R. Thies et al. (R3B Collaboration)

Phys. Rev. C **93** (2016) 054601

K. Mazurek et al., Phys. Rev. C **97** (2018) 024604

and other papers...

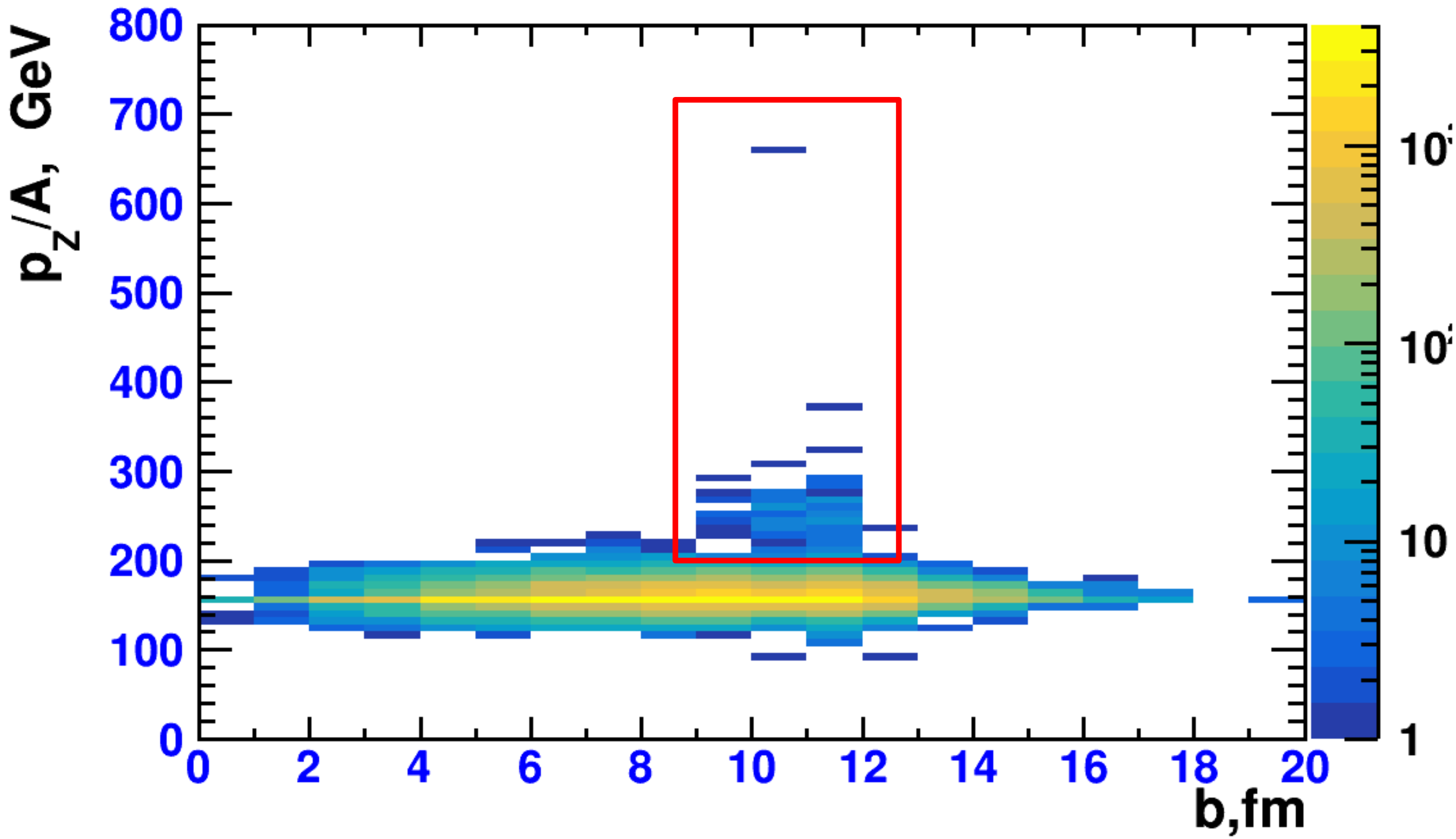


Our model for spectator fragments

- Our model called **Abrasion-Ablation Monte Carlo for Colliders (AAMCC)**[1] is based on the Glauber Monte Carlo v.3.2[2] model, pre-equilibrium decay model based on MST-clustering[3] and models of the decays of excited nuclei from Geant4 toolkit[4] (G4Evaporation, G4StatMF, G4FermiBreakUp).
- GlauberMC is de facto a standard tool adopted by all major experiments on relativistic nucleus-nucleus collisions (ALICE, CMS, ATLAS, STAR, BRAHMS etc.)
- To model the excitation energy a hybrid approach based on the Ericson formula for peripheral collisions and ALADIN parametrization otherwise is used.

1)A.S., I.Pshenichnov. Bull. RAS: Phys. 84 (2020) 1103,
2)C. Loizides, J.Kamin, D. d'Enterria, PRC 97 (2018) 054910
3)R.Nepeivoda, A.S., I.Pshenichnov, submitted to Particles
4)J.M. Quesada,V. Ivanchenko, A. Ivanchenko et al., Prog. Nucl. Sci. Tech. 2 (2011) 936

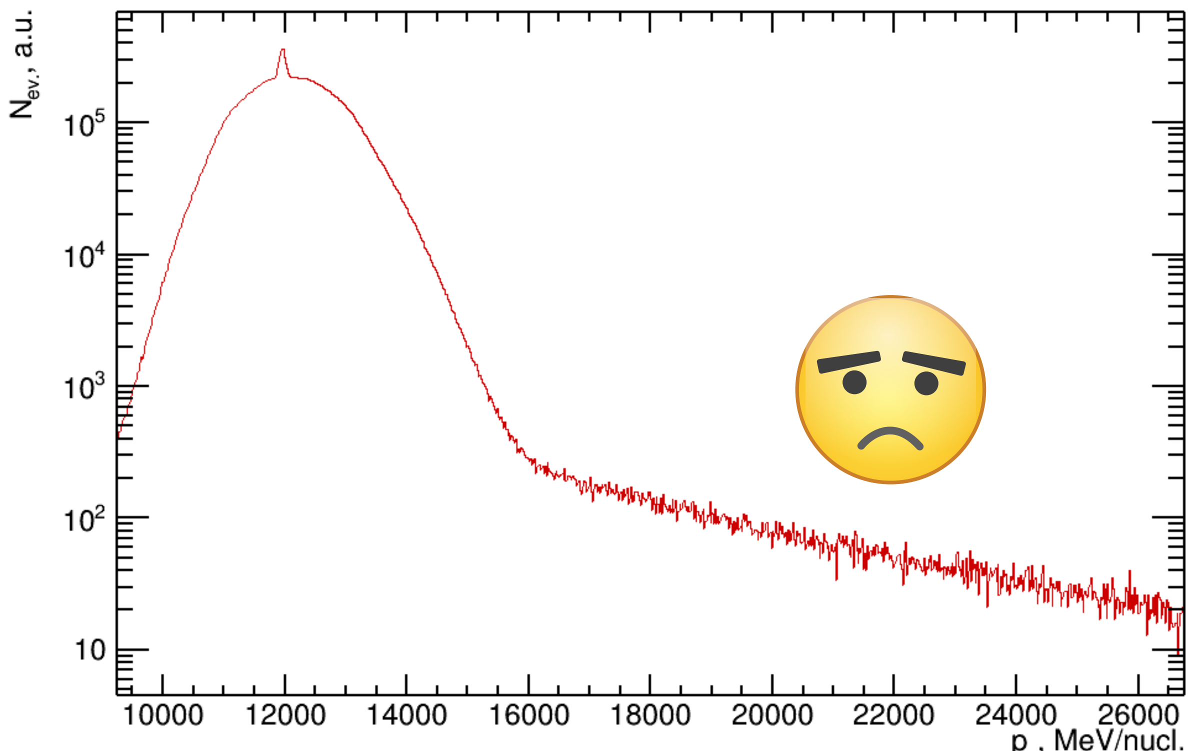
Momenta of secondary fragments in AAMCC



- p_z per nucleon as a function of the impact parameter in AAMCC in collisions of 158A GeV Pb with Pb
- Some strange momenta were found…

Momenta of secondary fragments in standalone test

- Typical size of the spectator prefragment at b ~ 11 fm is A~176 and Z~69.
- We created a standalone test to model the deexcitation of the thulium nucleus ^{176}Tm at the excitation energy of 2.75 MeV/nucleon with p_z = 12A GeV.
- It demonstrates a long tail up to 26 GeV unexplainable by the Lorentz boost



Two techniques to sample kinetic energy in G4Evaporation

- SampleEnergy() method from G4VEvaporation class (by default)
- SampleKineticEnergy() method from G4EvaporationProbability class

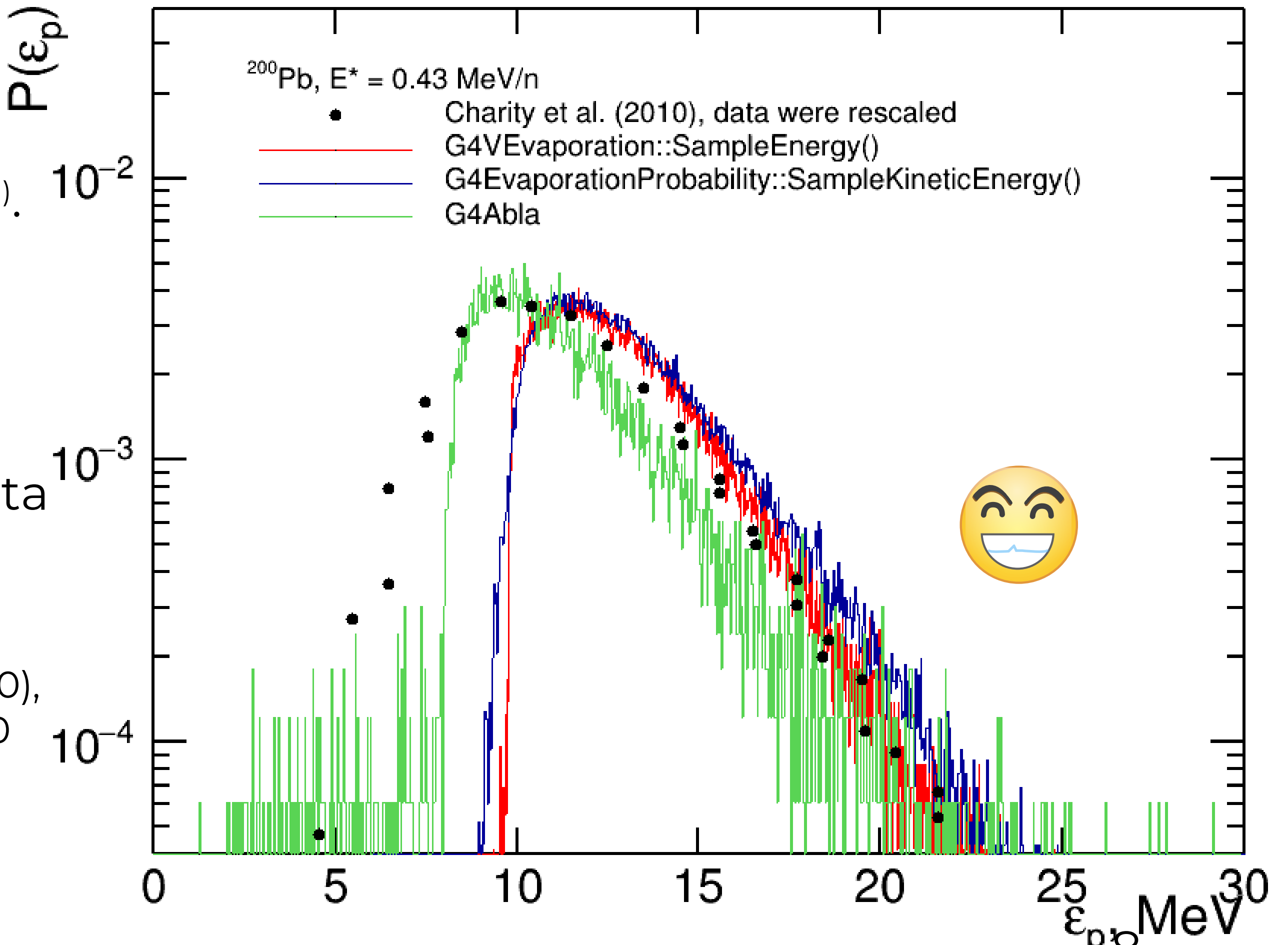
Both were compared with G4Abla and the data

Compared to data by R.J.Charity[1].

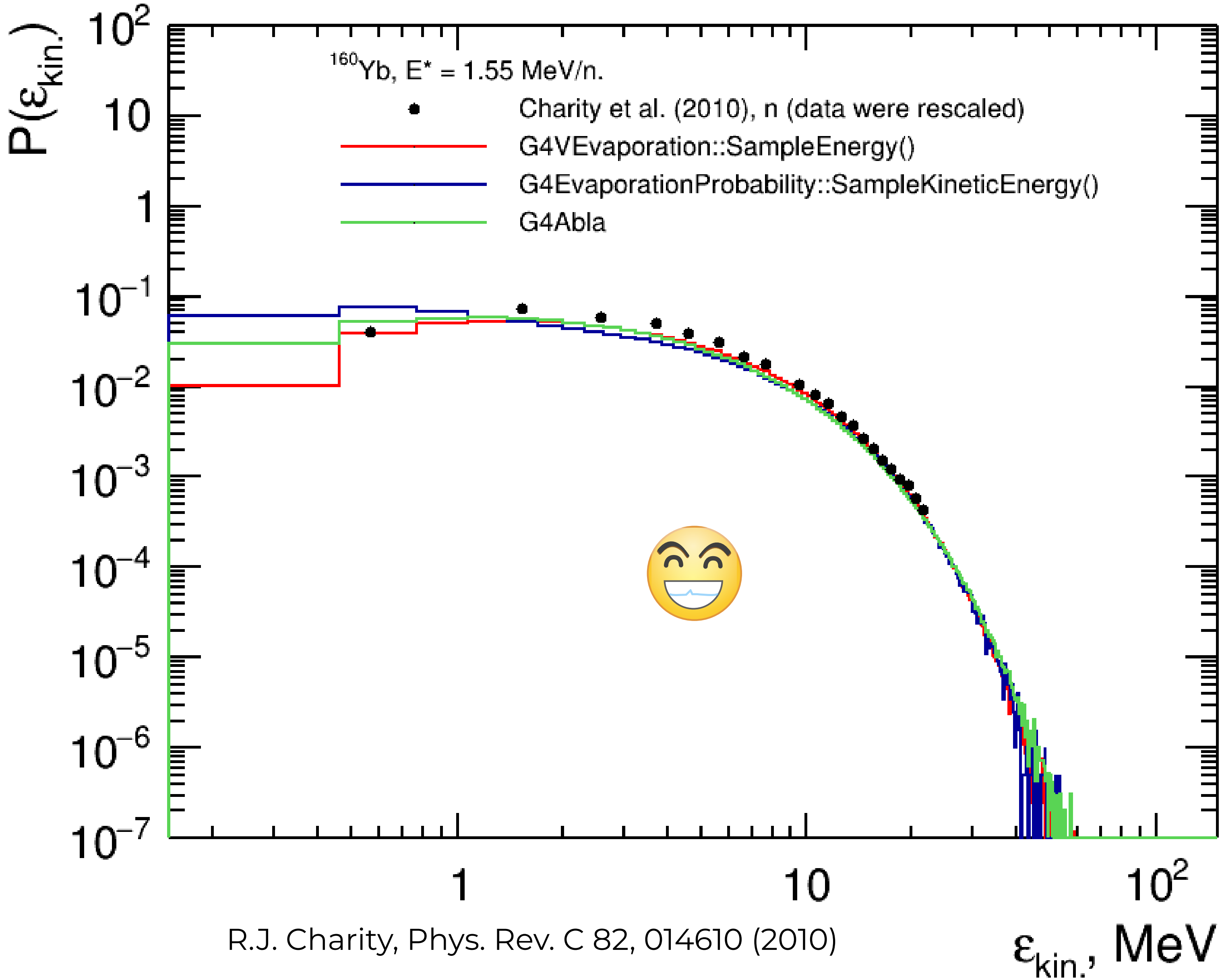
The data were rescaled to fit the peak height

As seen G4Abla describes the data better than G4Evaporation

1) R.J. Charity, Phys. Rev. C 82, 014610 (2010), https://doi.org/10.1103/PhysRevC.82.014610



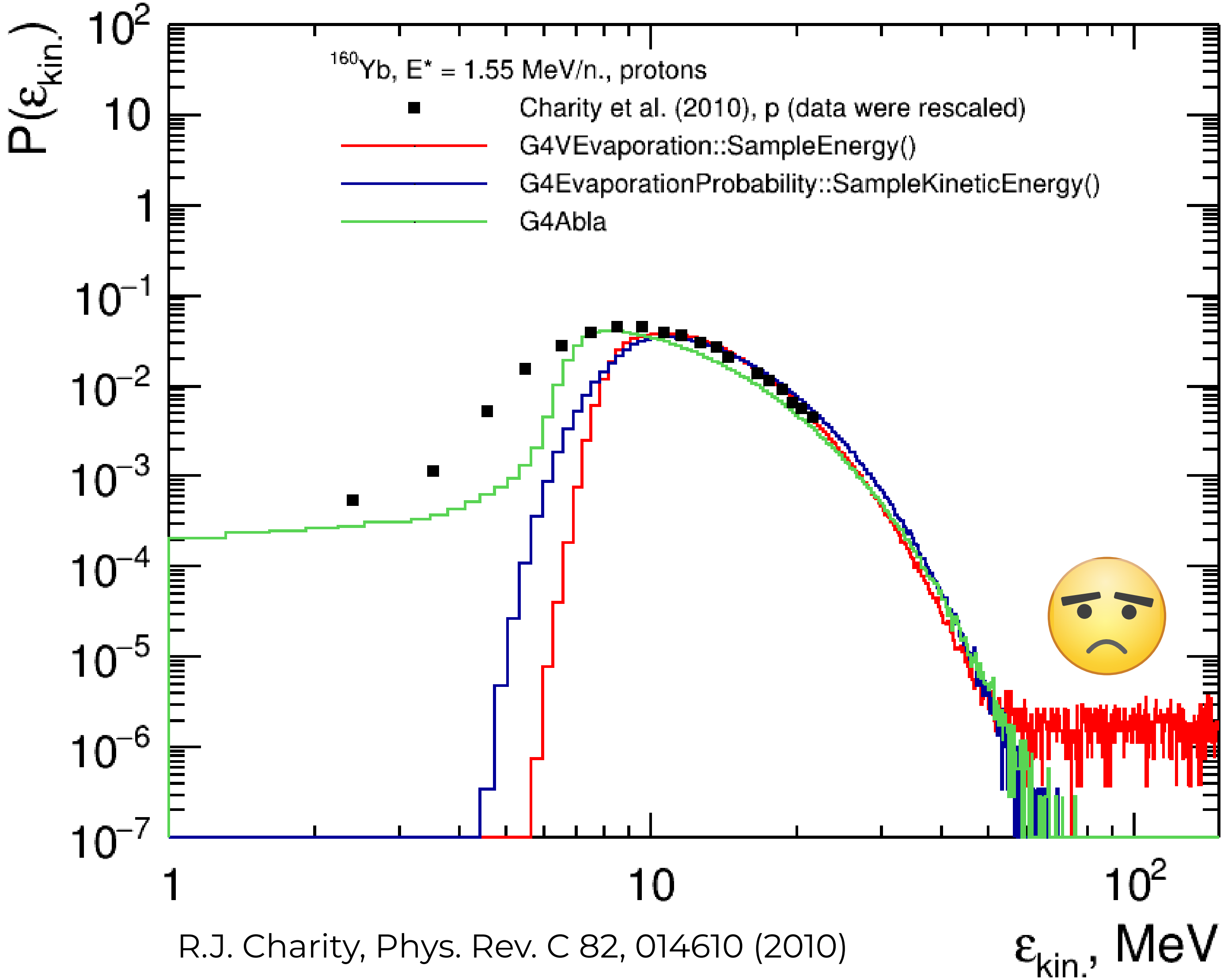
Evaporated neutrons



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

All three models are in good agreement with each other and with the data

Evaporated protons



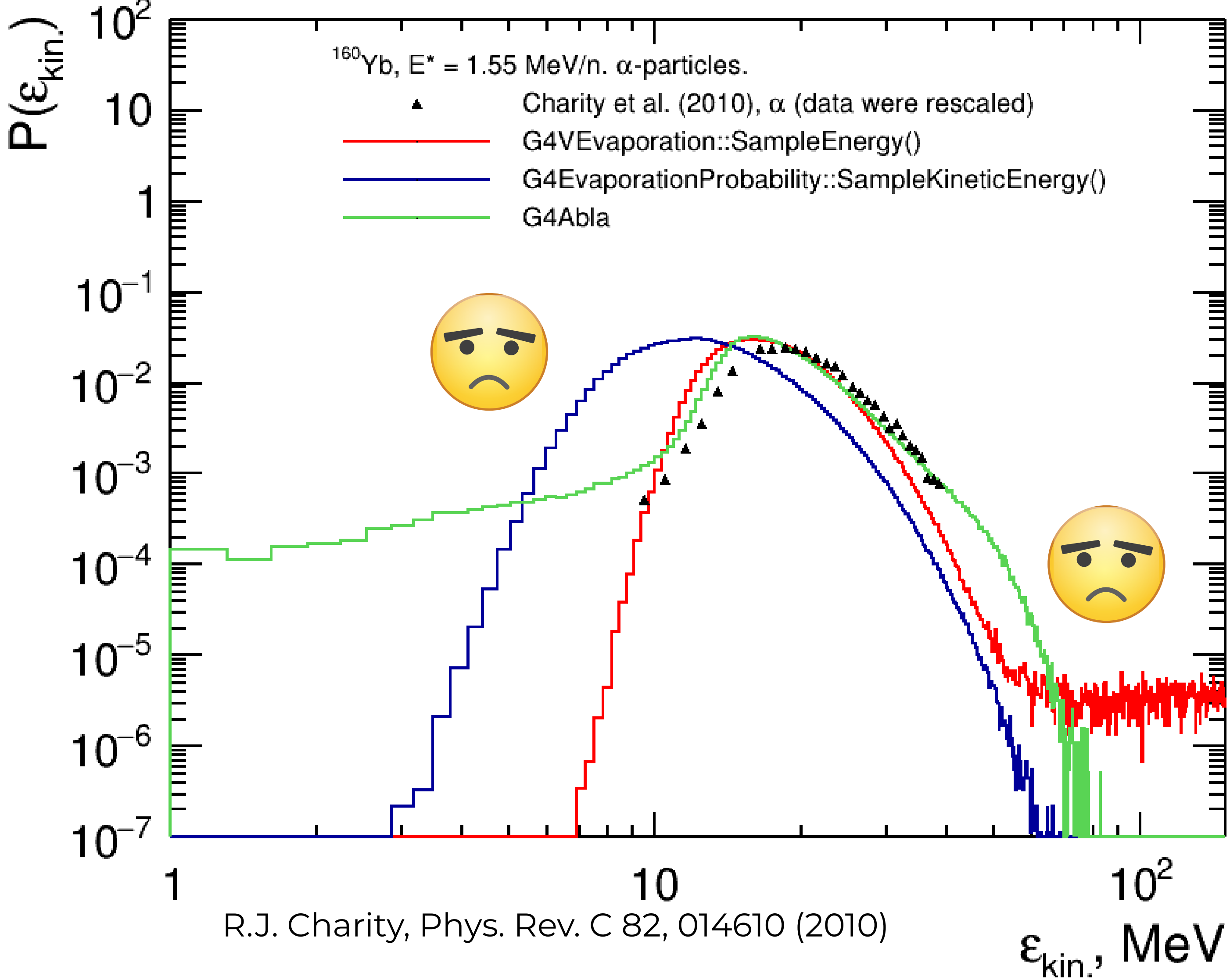
R.J. Charity, Phys. Rev. C 82, 014610 (2010)

G4VEvaporation::SampleEnergy() demostrates a long tail for protons.

G4Abla describes the data slightly better than the others.

G4EvaporationProbability::SampleKineticEnergy() fits the data well.

Evaporated alphas



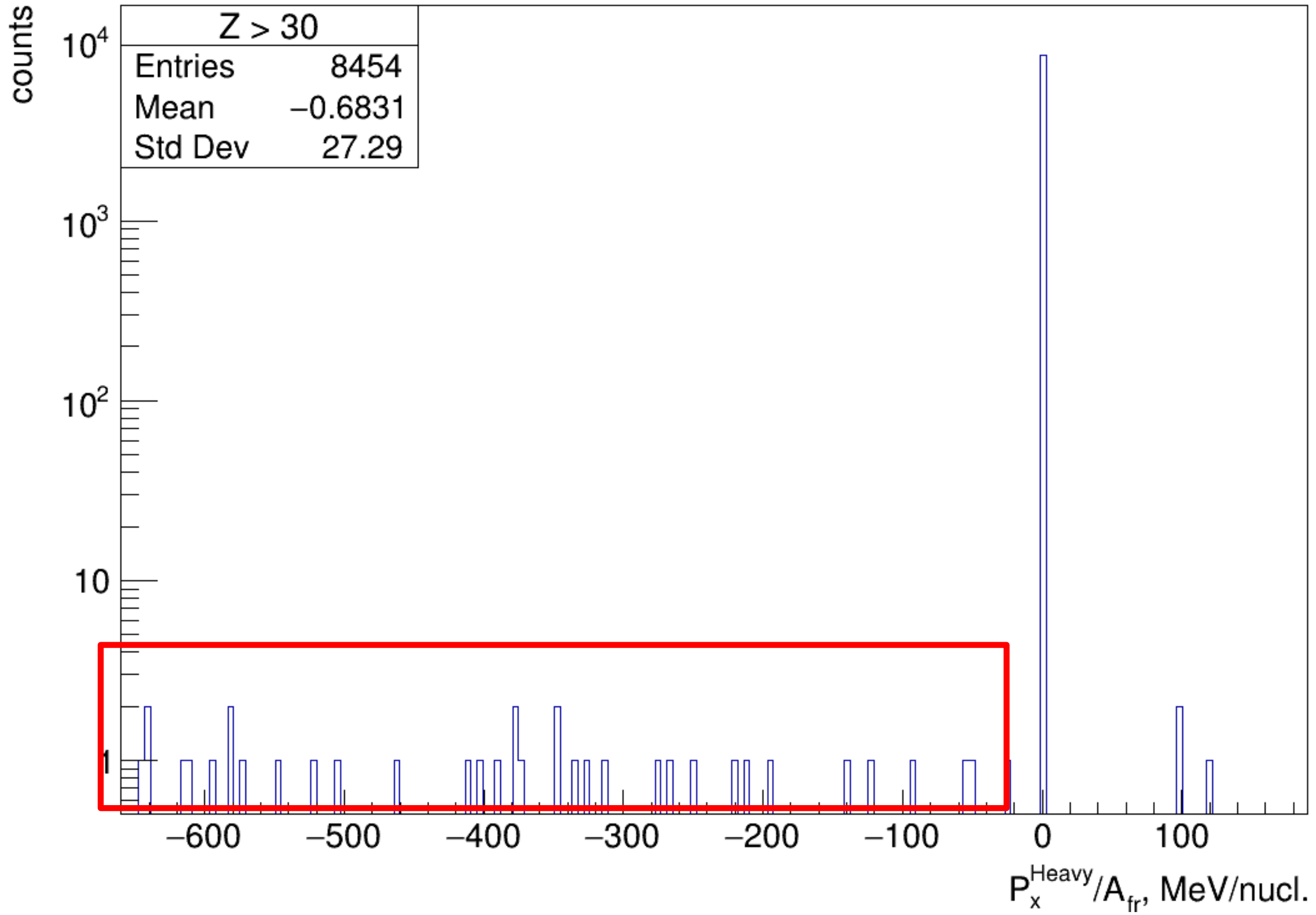
R.J. Charity, Phys. Rev. C 82, 014610 (2010)

G4VEvaporation::SampleEnergy() demostrates long tails for alphas as well as for protons.

G4EvaprotationProbability::SampleKineticEnergy() contradicts the data.

G4Abla is still in a good agreement with the data.

Kinetic energy of a single-produced charged fragment in G4StatMF



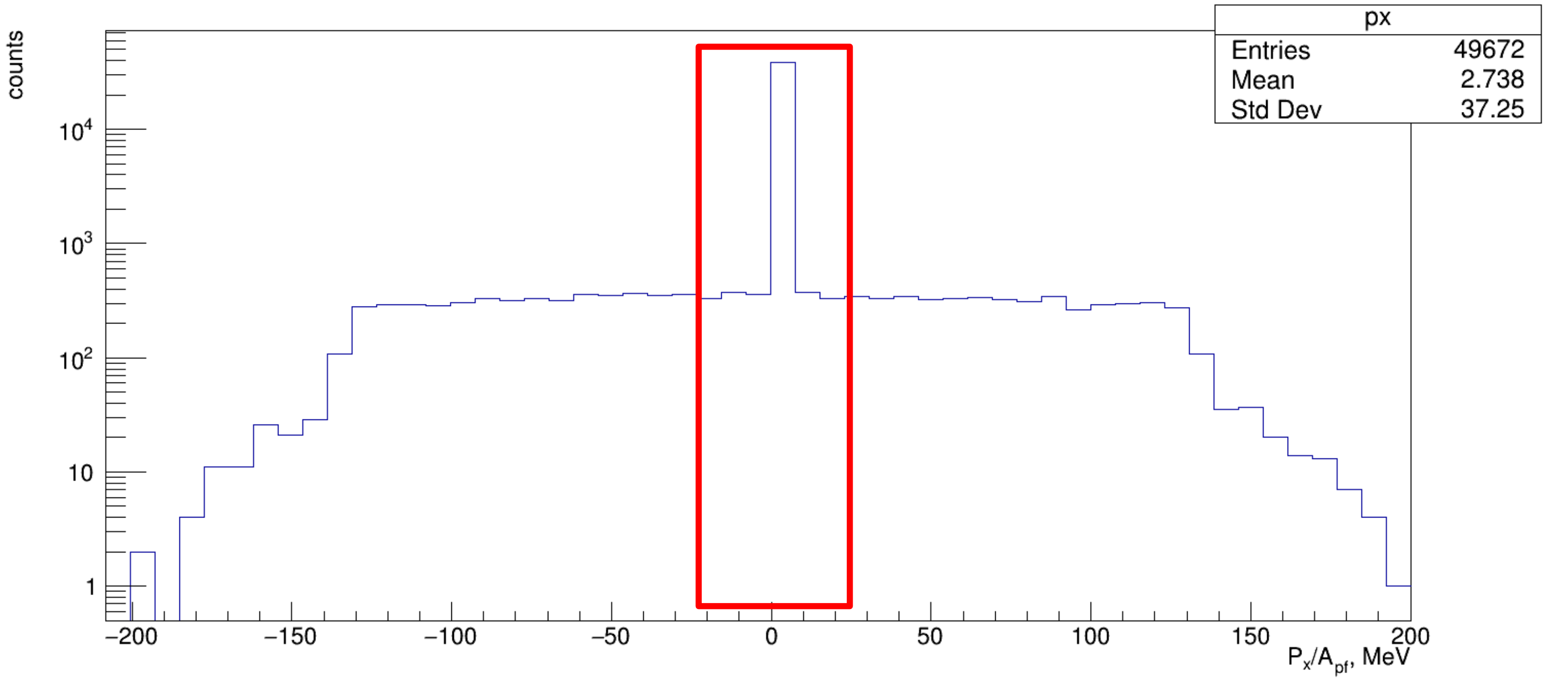
- The decays of ^{176}Tm with E* = 4A MeV in its rest frame were simulated with G4StatMF as a standalone test.
- The results were biased to events with single-produced charged fragment.
- Momenta of produced heavy fragments unexpectedly extend up to 600 MeV/nucleon

Kinetic energy of a single-produced charged fragment in G4StatMF

```
void G4StatMFChannel::CoulombImpulse(G4int anA, G4int anZ, G4double T)
{   …
    SolveEqOfMotion(anA,anZ,T);
    return;
}
```

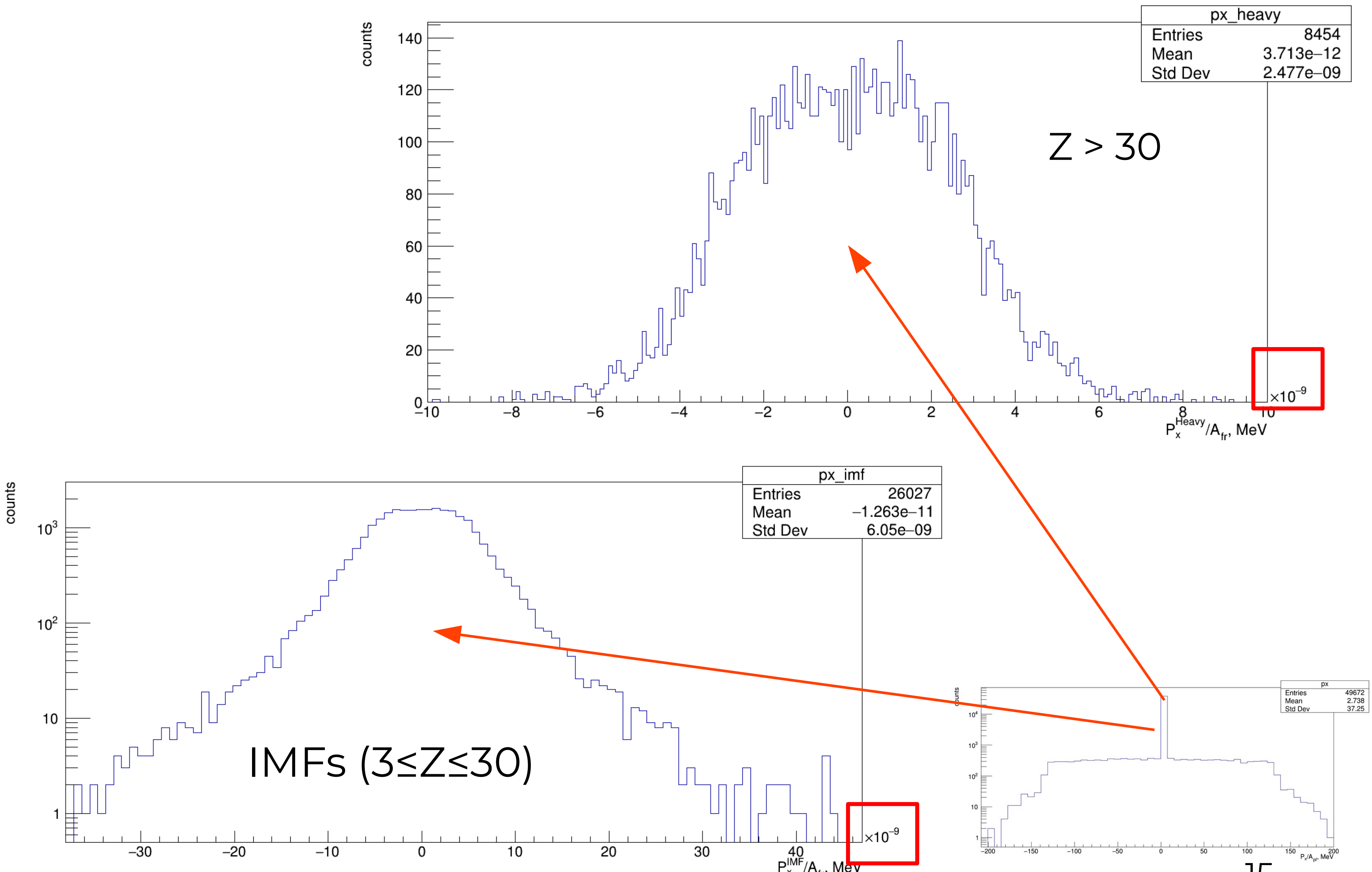
- SolveEqOfMotion method provides an asymptotic momentum due to the Coloumb repulsion of the fragments.
- But it is used even in the case of a single charged fragment!
- This leads to unexpected self-acceleration of this fragment and its momentum is overestimated.

Kinetic energies of multiple produced charged fragments in G4StatMF

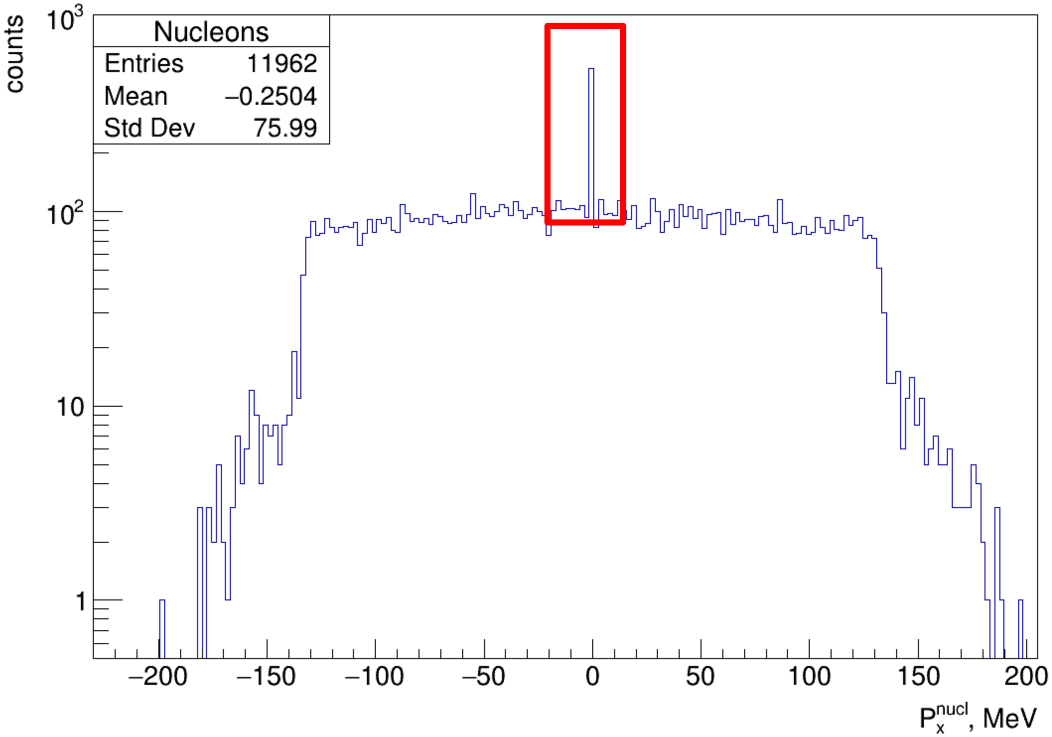


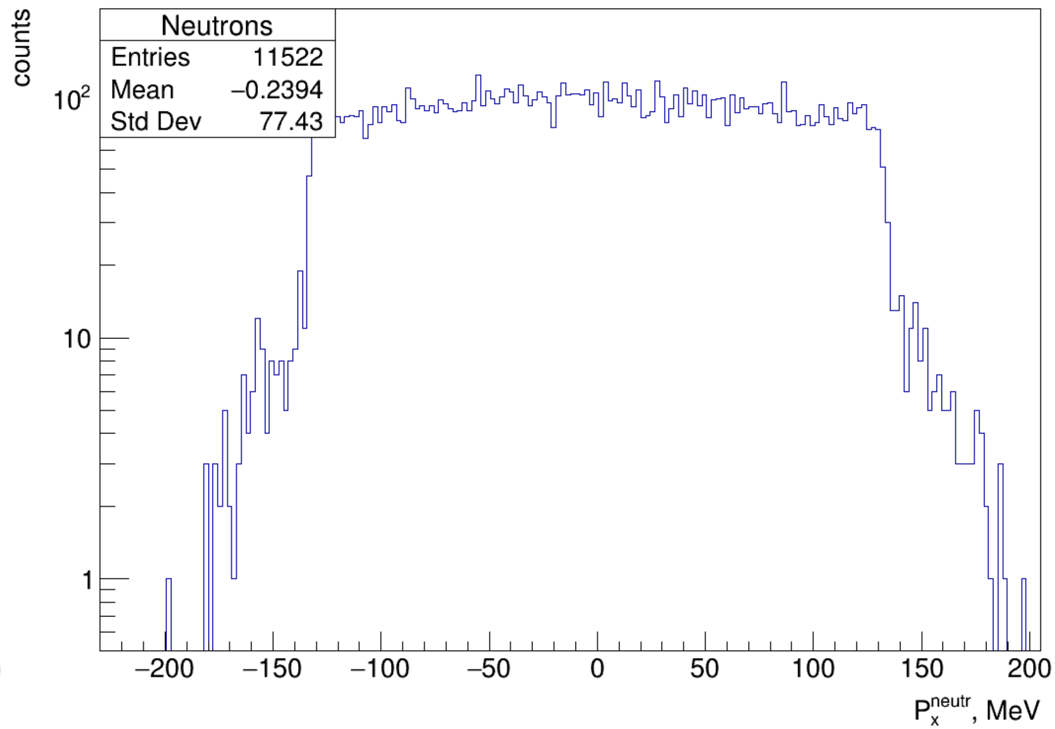
- The decays of ^{176}Tm with E* = 4A MeV in its rest frame were simulated with G4StatMF as a standalone test.
- Momenta of produced fragments extend up to ~200A MeV.
- However, there is unexpected amount of fragments which stay at rest.

Let's look into this peak



All protons, IMFs and heavy fragments have unexpectedly low momenta





- All the charged fragments possess the momentum of the order of magnitude 10^{-9} MeV/nucleon.
- What is the reason for that?

Calculation of 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 overestimation of the momenta.
- But the rescaling procedure applied in G4StatMF::SolveEqOfMotion() results in strong underestimation.

Scaling of kinetic energy in G4StatMF::SolveEqOfMotion()

- Typicaly Coulomb energy is transferred 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 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 transferred 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:

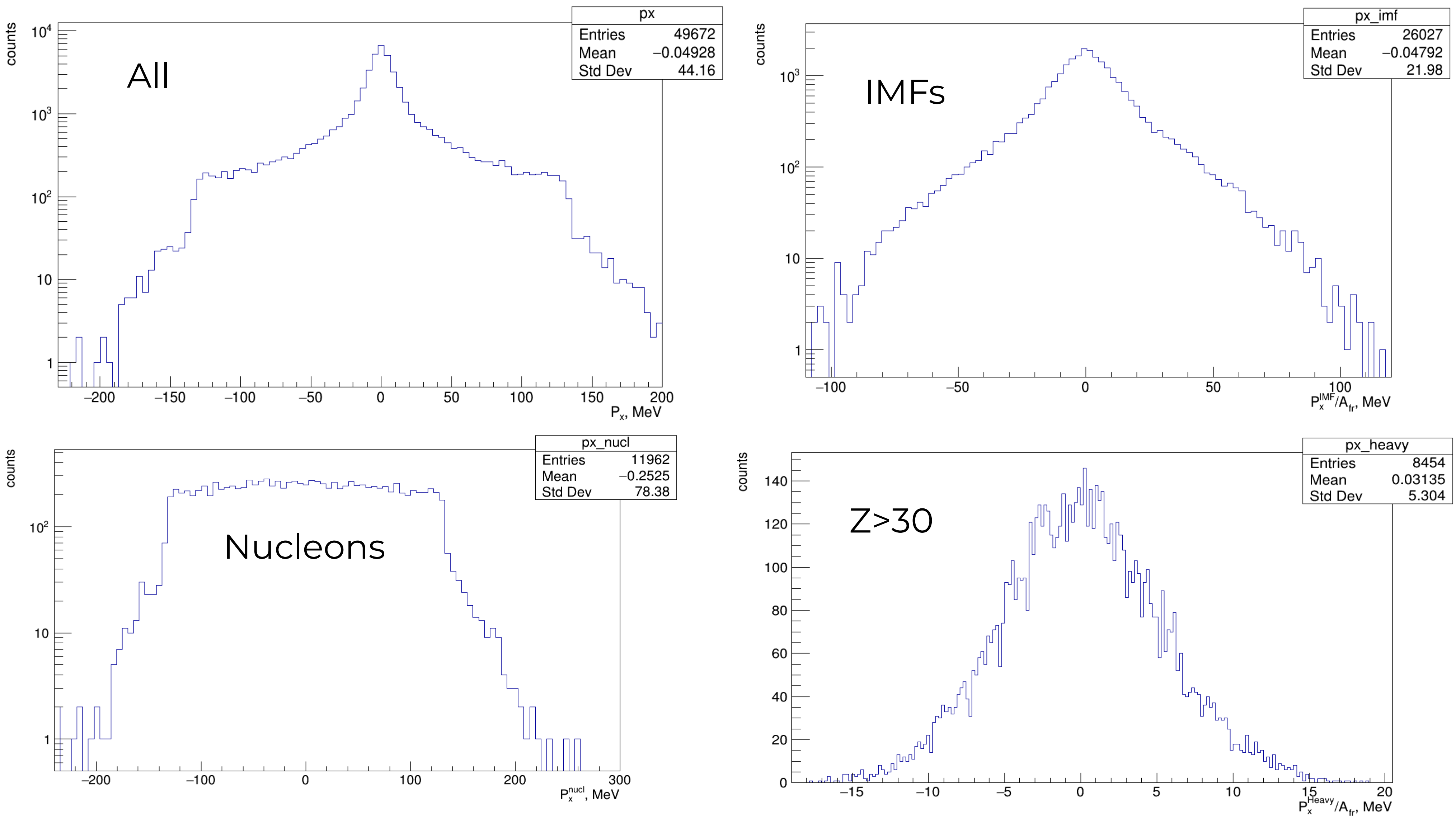
$$T_{tot} = \eta^2 \sum_{i=1}^{N_{ch}} \frac{p_i^2}{2m_i} = 3/2 \cdot N_{ch} \cdot T + E_c$$

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

J.Bondorf et al. Phys. Rep, **257** (1995) 133
https://doi.org/10.1016/0370-1573(94)00097-M

Results without Coloumb repulsion

Modeling the decays of ^{176}Tm with E* = 4A MeV in the rest frame with G4StatMF.



The unexpected peaks at zero momenta disappeared!

Summary

- Kinetic energies of the secondary fragments from the evaporation by G4Evaporation demostrate several oddities:
  - The energy spectra of evaporated protons and alphas have long tails up to hundreds MeV while sampled with G4VEvaporation::SampleEnergy(), which is the default option in G4
  - The spectrum of evaporated alphas contradicts the respective data while sampled with G4EvaporationProbability::SampleKineticEnergy()
- The momenta of fragments produced in the multifragmentation model G4StatMF demonstrate irregularities due to issues in modelling the Coloumb repulsion:
  - The Coloumb repulsion is simulated even for a single-produced charged fragment leading to its unexpectedly high momentum
  - An overestimation of the Coloumb force is found, but a wrong rescaling procedure applied to the momenta of multiply produced charged fragments sets these momenta close to zero.
- We are at your service to provide all additional materials related to this talk

Thank you for attention!

Vasiliy Kandinsky, Several circles 1926

Current status: evaporation

- Problems with G4Evaporation were reported at Geant4 User Forum in November 2021
  - https://geant4-forum.web.cern.ch/t/strange-distribution-of-kinetic-energy-of-evaporated-fragments-in-g4evaporation/6505
- Also reported with Geant4 Problem Tracking System
  - https://bugzilla-geant4.kek.jp/show_bug.cgi?id=2443
- We are at your service to provide all materials for the comparison with data.

Closer look at the Coloumb repulsion

```
START vel: (-2.246150e-02,-5.385208e-02,5.557219e-02)
```

```
) START momentum: (-2.094648e+02,-5.021978e+02,5.182387e+02) Frag num: 3
```

Calculating Force, its too big!

```
force (-1.837190e+12,5.367133e+11,-1.196018e+12) distance (-4.997954e-12,8.513387e-13,-1.286354e-11) Iteration: 0
```

Than, the velocity is too high

```
accel (-2.046037e+08,4.796596e+07,-1.531513e+08)
vel: (-2.046037e+09,4.796596e+08,-1.531513e+09) Frag num: 3 Iteration: 0
```

The next iteration: force is small (due to big distances) so velocity does not change anymore.

```
force (-1.220325e-30,4.539924e-31,-5.308031e-31) distance (-1.242088e+10,4.620890e+09,-5.402696e+09) Iteration: 1
force (-1.223984e-30,4.552363e-31,-5.890625e-31) distance (-1.524771e+09,5.183146e+08,-2.427550e+10) Iteration: 1
force (-1.252195e-30,4.342242e-31,-6.117674e-31) distance (-1.767236e+10,-1.316273e+10,-1.422319e+10) Iteration: 1
force (-1.227597e-30,3.750985e-31,-7.241393e-31) distance (2.538343e+09,-6.101300e+09,-1.159587e+10) Iteration: 1
accel (-1.316386e-34,4.022286e-35,-7.765149e-35)
vel: (-2.046037e+09,4.796596e+08,-1.531513e+09) Frag num: 3 Iteration: 1
```

Impulses are low in result cause of “scaling”:

```
Frag num: 3 berfore (-2.094648e+02,-5.021978e+02,5.182387e+02)
Frag num: 3 after (-6.626221e-08,1.553408e-08,-4.959901e-08)
```