Geant4 Simulation in JUNO

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Motivations

Geant4 version used in JUNOSW is quite old (2018). Lots of updates were made on hadronics and electromagnetic physics processes

OBJECTIVE:
Perform comparisons and tests between versions and locate any major discrepancies

Geant4 version	Geant4 v10.4.2	Geant4 v11.2.2
Release date	2018	2024

Outline

Comparison of Geant4 versions

- Electron Simulation
- Hadronic Simulation

Simulation / Data comparison

- AmBe Calibration source
- Selection cuts
- Comparison with Geant4 v11 simulations

Geant4 version comparison

Method

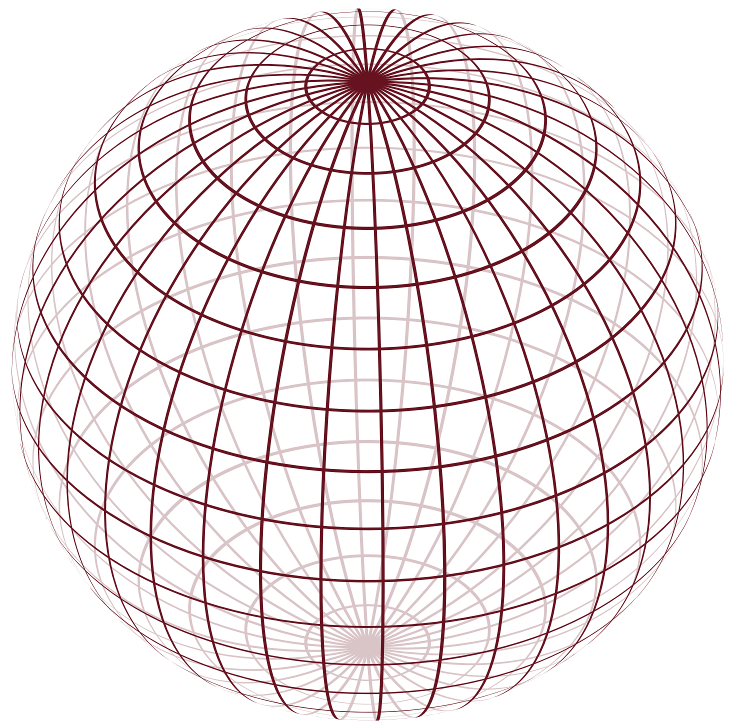
Built a small JUNO detector **(10 m diameter sphere filled with LAB)** using different Geant4 version:

- Geant4 v10.4.2
- Geant4 v11.2.2

Run a full simulation of different types of particles at the center of the sphere and look at basic distributions:

- **Deposited energy per step (dE)**
- **Step Length (dx)**
- **Stopping power per step (dE/dx)**
- **Quenched energy (Qedep)**

EmPhysicsList**: G4EmLivermorePhysics**



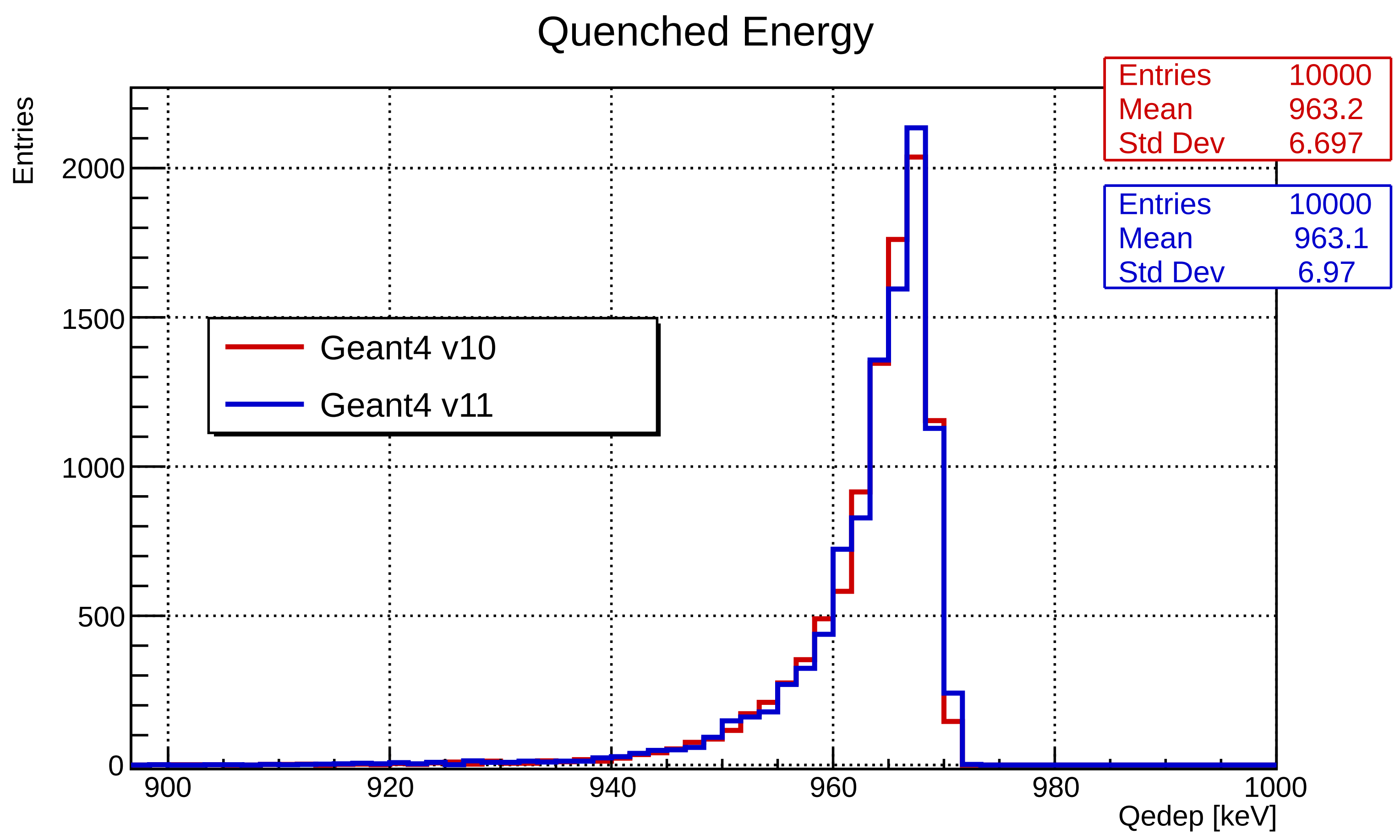
Electron simulation

Electron simulation

FULL SIMULATION OF 10000 EVTS OF 1 MEV ELECTRON

Birks Law: $$Qedep = \sum_{i=1}^{N} \frac{dE}{1 + kB\frac{dE}{dx}}$$

WITHOUT OPTICS



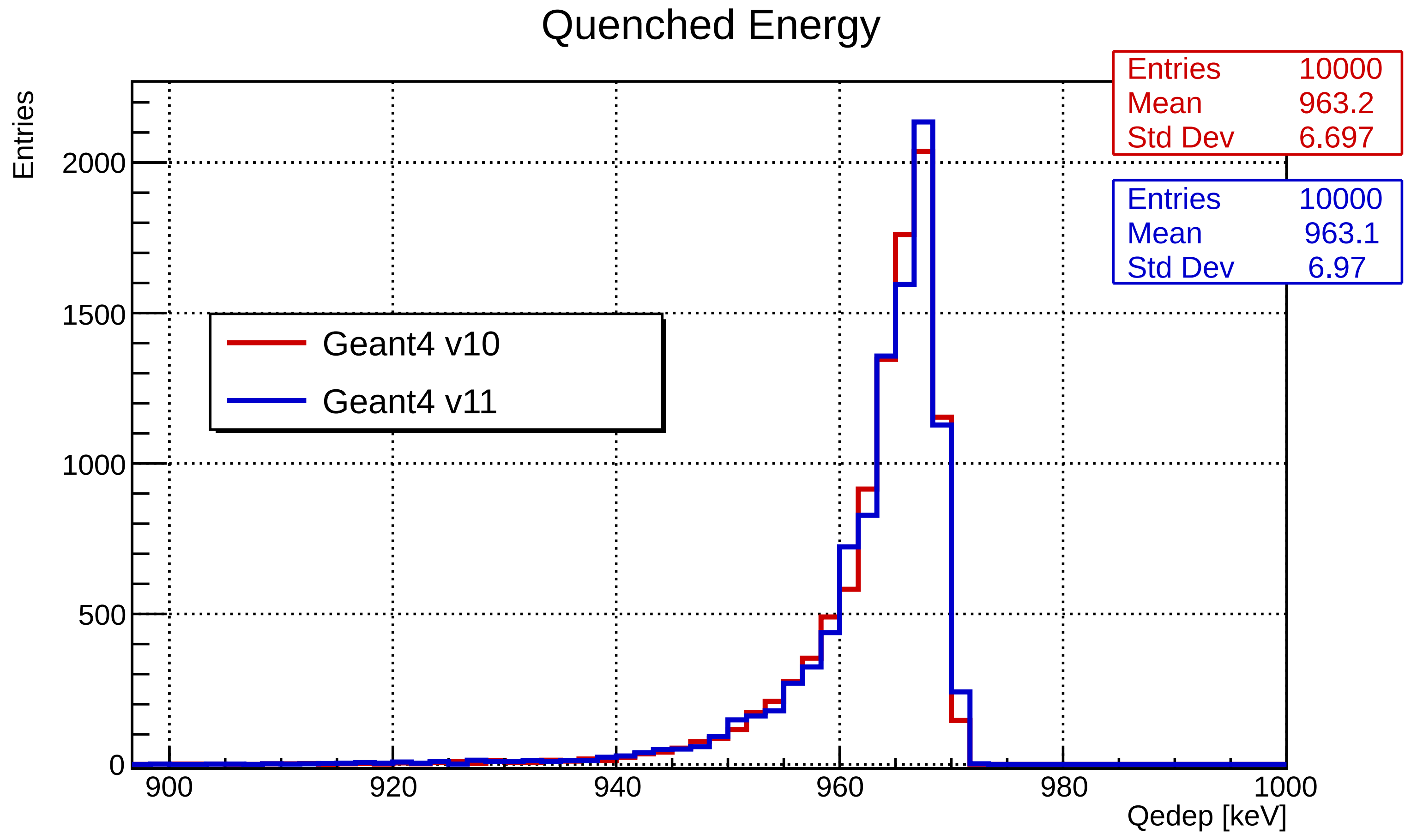
Good agreement between versions without optics

Electron simulation

Full simulation of 10000 evts of 1 MeV electron

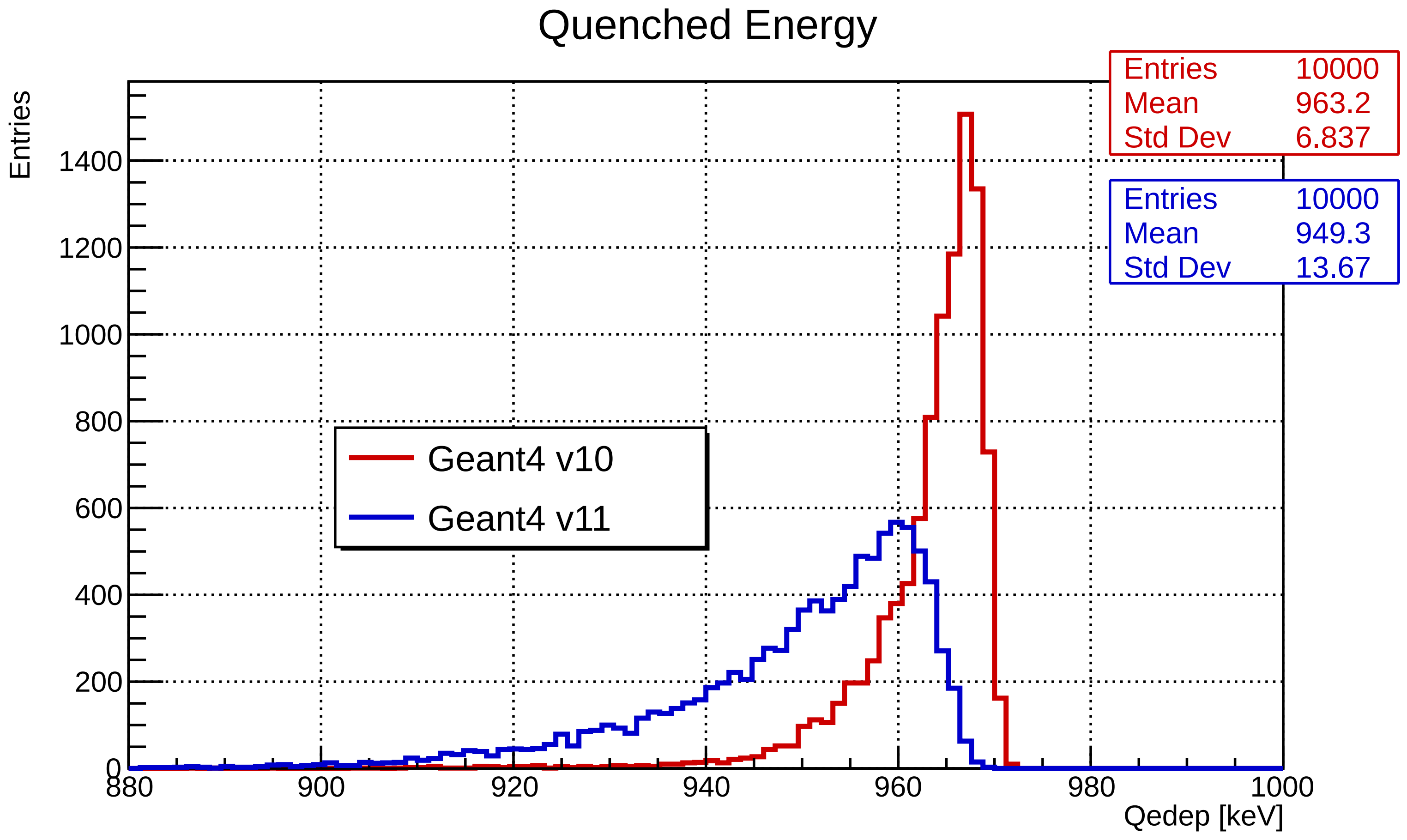
Birks Law: $Qedep = \sum_{i=1}^{N} \frac{dE}{1 + kB\frac{dE}{dx}}$

Without optics



Good agreement between versions without optics

With optics

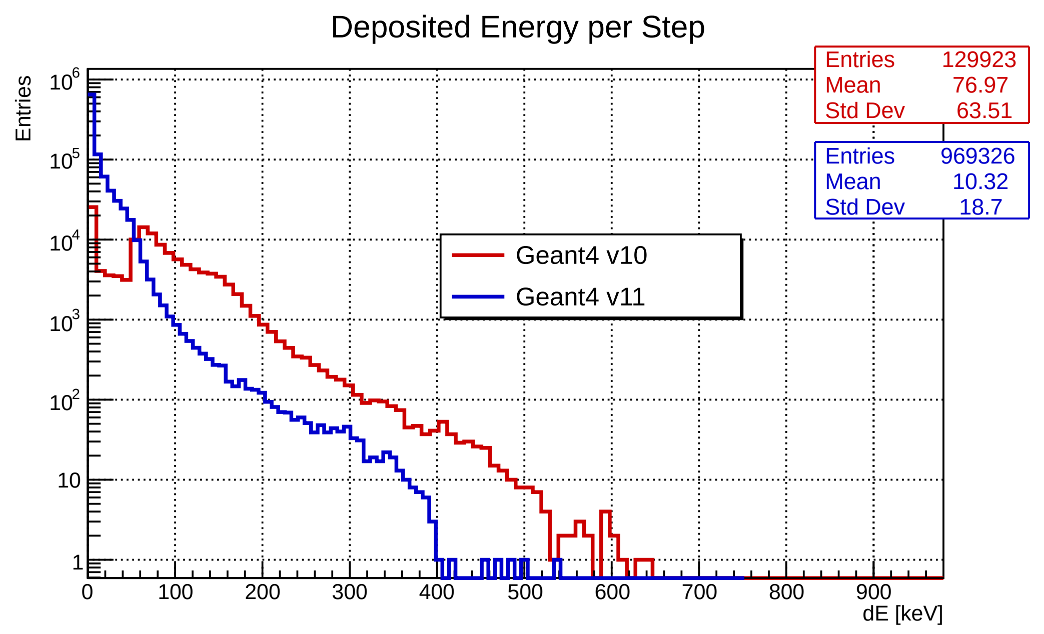


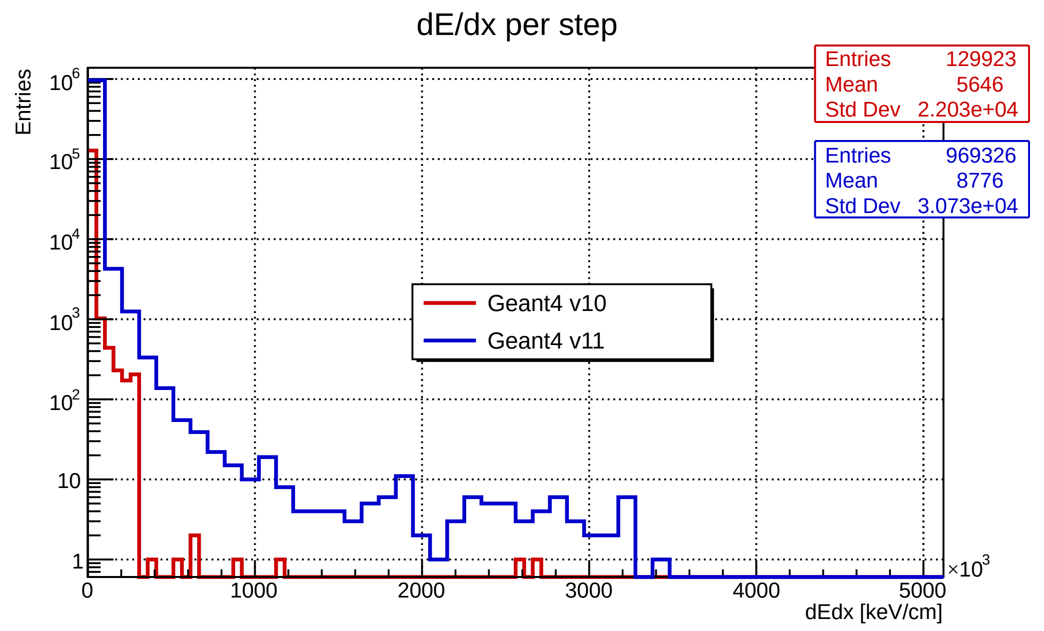
Enabling optical processes modifies Qedep distribution in Geant4 v11

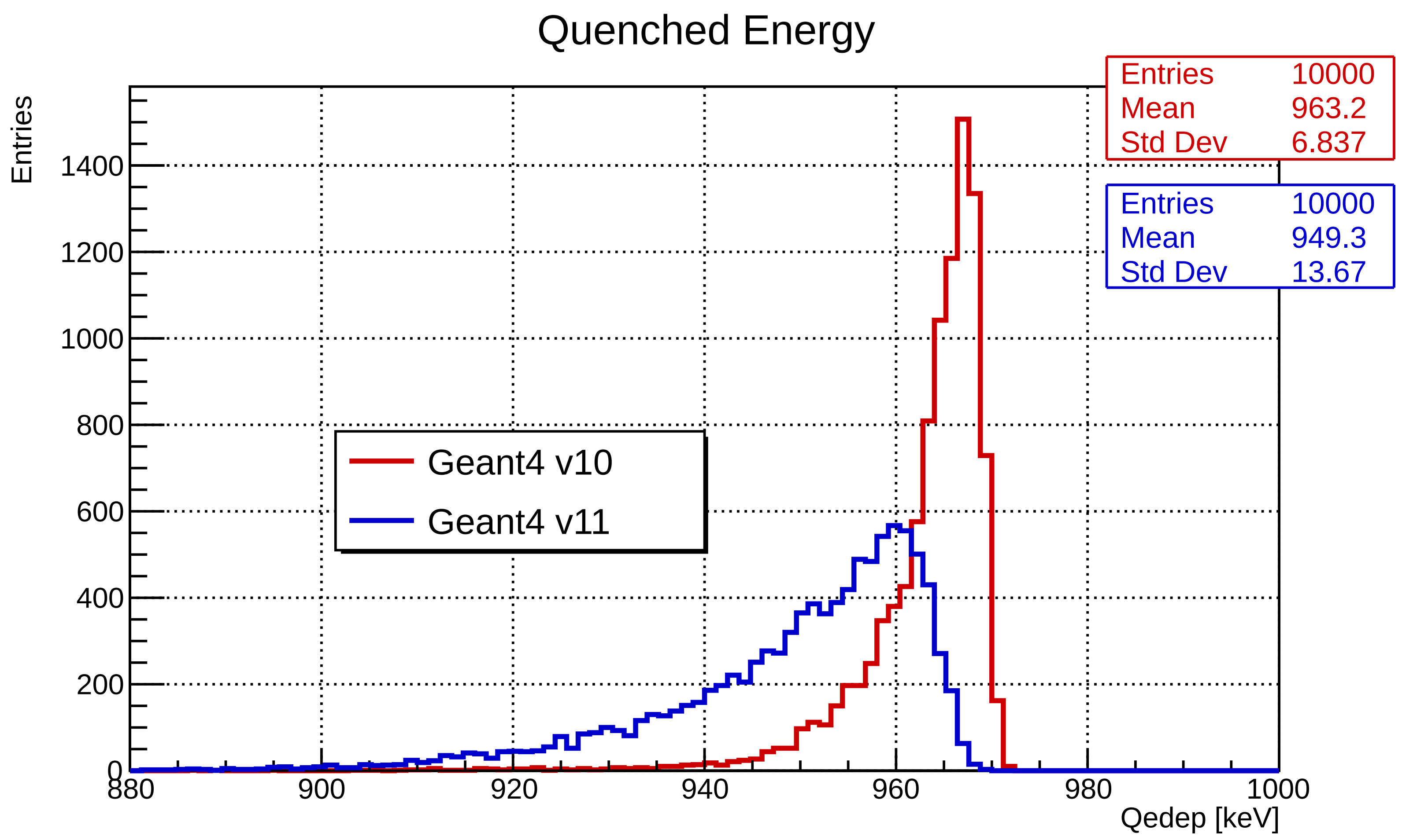
Electron simulation

FULL SIMULATION OF 10000 EVTS OF 1 MEV ELECTRON

Birks Law: $$Qedep = \sum_{i=1}^{N} \frac{dE}{1 + kB\frac{dE}{dx}}$$







Number of steps to track electron has increased in Geant4 v11.2.2 **(~x10)**

The deposited energy per step is smaller thus giving a smaller visible energy

Electron simulation

WITHOUT OPTICS

```
*************************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
*************************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0        0        0        0         1        0        0         0    LSSphere initStep
    1   0.0006        0        0         1 1.62e-05   0.0006    0.0006    LSSphere msc
    2     1.06  0.00238 -0.00465     0.758    0.242     1.15      1.15    LSSphere eIoni
    3     1.83  -0.0613  -0.0508     0.548     0.21    0.851         2    LSSphere eIoni
    4     2.35   -0.108    0.089     0.453   0.0952    0.605      2.61    LSSphere eIoni
    5     2.76   0.0465    0.078     0.382    0.071    0.499       3.1    LSSphere eIoni
    6     3.03     0.12   -0.164     0.308   0.0742    0.423      3.53    LSSphere eIoni
    7     3.29    0.231   -0.275     0.241   0.0676    0.347      3.87    LSSphere eIoni
    8      3.5    0.232   -0.364     0.182   0.0586    0.281      4.16    LSSphere eIoni
    9     3.58    0.328   -0.488     0.123   0.0588    0.227      4.38    LSSphere eIoni
   10      3.6    0.373   -0.589    0.0686   0.0545    0.169      4.55    LSSphere eIoni
   11     3.64     0.35   -0.606         0   0.0686   0.0823      4.63    LSSphere eIoni
```

WITH OPTICS

```
*************************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
*************************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0        0        0        0         1        0        0         0    LSSphere initStep
PRESAFETY = 0
PRESAFETY = 0
    1   0.0019        0        0         1 0.000159   0.0019    0.0019    LSSphere msc
PRESAFETY = 9999.998096944608
PRESAFETY = 10000
    2     0.95   0.0245  -0.0138     0.867    0.133     1.02      1.02    LSSphere eIoni
    :----- List of 2ndaries - #SpawnInStep= 35(Rest= 0,Along= 0,Post=35), #SpawnTotal= 35 ---------------
```

Step 1

```
*************************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
*************************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    2     0.95   0.0245  -0.0138     0.867        0        0      1.02    LSSphere initStep
PRESAFETY = 0
PRESAFETY = 0
    3     1.48    0.658   0.0476     0.763    0.104    0.836      1.86    LSSphere msc
    :----- List of 2ndaries - #SpawnInStep= 30(Rest= 0,Along= 0,Post=30), #SpawnTotal= 30 ---------------
```

Step 2

Without optical processes, the step are limited by Ionisation process and the Qedep distributions match between versions.

However when optics are enabled, steps are limited by msc and we observe the increase in number of steps and discrepancies on Qedep.

Msc models in EmLivermore

Differences in the Multiple Coulomb Scattering (Msc) model used between the different versions of Geant4

G4EmLivermorePhysics (Geant4 v10.4)

```
} else if (particleName == "e-") {

  // multiple and single scattering
  G4eMultipleScattering* msc = new G4eMultipleScattering;
  G4UrbanMscModel* msc1 = new G4UrbanMscModel();
  G4WentzelVIModel* msc2 = new G4WentzelVIModel();
  msc1->SetHighEnergyLimit(highEnergyLimit);
  msc2->SetLowEnergyLimit(highEnergyLimit);
  msc->SetEmModel(msc1);
  msc->SetEmModel(msc2);
```

G4EmLivermorePhysics (Geant4 v11.2)

```
// e-
particle = G4Electron::Electron();

// multiple and single scattering
G4GoudsmitSaundersonMscModel* msc1 = new G4GoudsmitSaundersonMscModel();
G4WentzelVIModel* msc2 = new G4WentzelVIModel();
msc1->SetHighEnergyLimit(highEnergyLimit);
msc2->SetLowEnergyLimit(highEnergyLimit);
G4EmBuilder::ConstructElectronMscProcess(msc1, msc2, particle);
```

The definition of msc1 in G4EmLivermorePhysics changed from **G4UrbanMscModel** to **G4GoudsmitSaundersonMscModel (GS).**

The later model was introduced since Geant4 v10.4 but was optimised recently to be more precise than G4Urban (see M.Novak's presentation) and is now the default msc model in EmLivermore.

Optical process in GS model

G4GoudsitSaundersonMscModel.cc

```
// Possible optimization : if the distance is samller than the safety -> the
// particle will never leave this volume -> dispalcement
// as the effect of multiple elastic scattering can be skipped
// Important : this optimization can cause problems if one does scoring
// in a bigger volume since MSC won't be done deep inside the volume when
// distance < safety so don't use optimized-mode in such case.
if (gIsOptimizationOn && (distance<presafety)) {
   // Indicate that we need to do MSC after transportation and no dispalcement.
   fIsMultipleSacettring = true;
   fIsNoDisplace = true;
```

Presafety parameter plays a key role in the tracking of the particle:

- Indicates the particle distance to the closer volume boundary
- If particle is inside the volume:
  - Multiple scattering mode is activated
  - MSC is called but don't limit the step
- If close to the edge:
  - triggers the safety parameter (fUseSafetyPlus in our case)
  - Goes to single scattering mode (smaller steps)

WITH OPTICS

```
****************************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
****************************************************************************************************

Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    0        0        0        0         1        0        0         0    LSSphere initStep
PRESAFETY = 0
PRESAFETY = 0
    1   0.0019        0        0         1 0.000159   0.0019    0.0019    LSSphere msc
PRESAFETY = 9999.998096944608
PRESAFETY = 10000
    2     0.95   0.0245  -0.0138     0.867    0.133     1.02      1.02    LSSphere eIoni
    :----- List of 2ndaries - #SpawnInStep= 35(Rest= 0,Along= 0,Post=35), #SpawnTotal= 35 ---------------
```

```
****************************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
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Step#    X(mm)    Y(mm)    Z(mm) KinE(MeV)  dE(MeV) StepLeng TrackLeng  NextVolume ProcName
    2     0.95   0.0245  -0.0138     0.867        0        0      1.02    LSSphere initStep
PRESAFETY = 0
PRESAFETY = 0
    3     1.48    0.658   0.0476     0.763    0.104    0.836      1.86    LSSphere msc
    :----- List of 2ndaries - #SpawnInStep= 30(Rest= 0,Along= 0,Post=30), #SpawnTotal= 30 ---------------
```
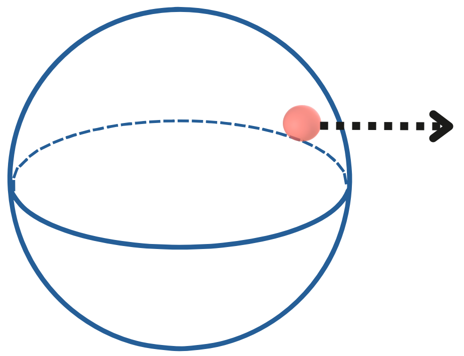

Presafety set to 0 at the beginning of every step **(particle seen as close to the boundary) → Triggers smaller step**

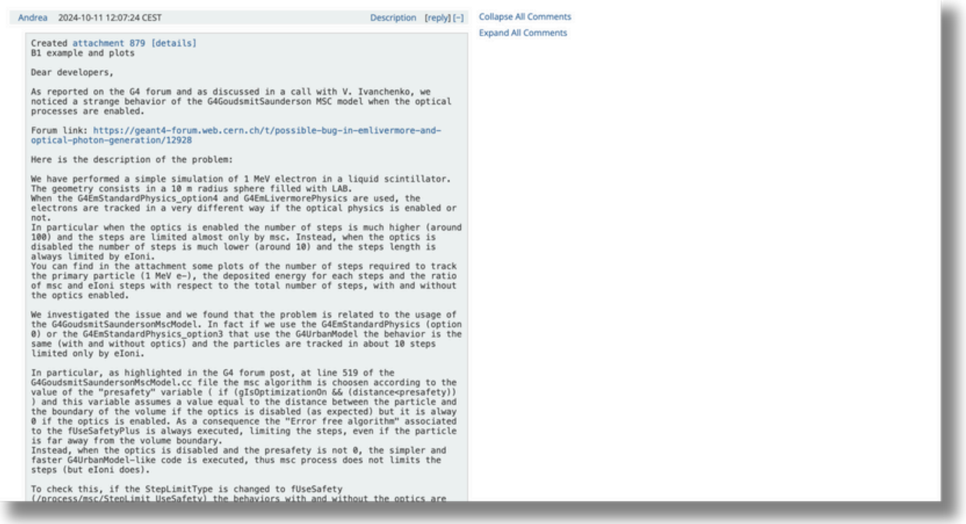
particle virtually seen at the boundary of the sphere at the beginning of every step



Possible solution

Discussion with Geant4 developers to better understand the effect

Geant4 bug report



Andrea 2024-10-11 12:07:24 CEST Description [reply] [-]

Collapse All Comments

Expand All Comments

Created attachment 879 [details]
B1 example and plots

Dear developers,

As reported on the G4 forum and as discussed in a call with V. Ivanchenko, we noticed a strange behavior of the G4GoudsmitSaunderson MSC model when the optical processes are enabled.

Forum link: https://geant4-forum.web.cern.ch/t/possible-bug-in-emlivermore-and-optical-photon-generation/12928

Here is the description of the problem:

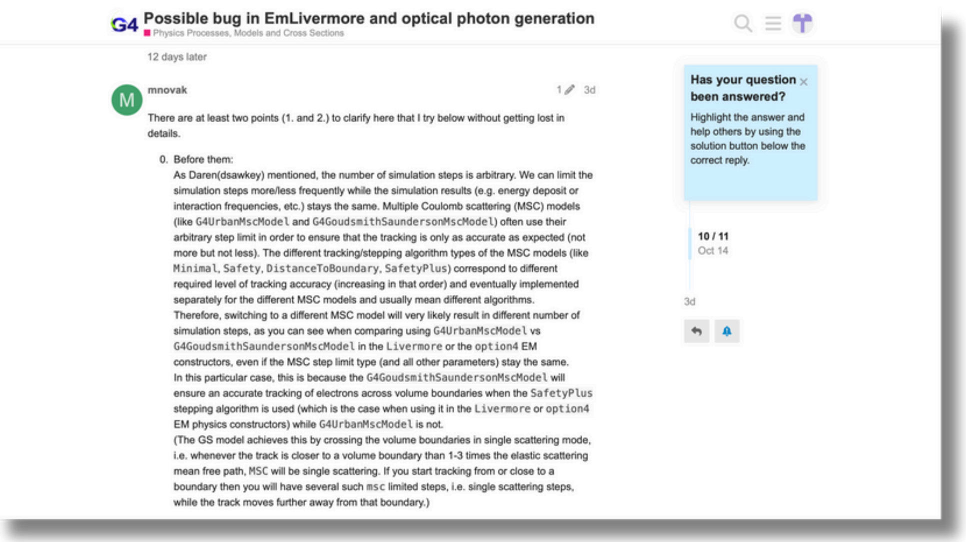
We have performed a simple simulation of 1 MeV electron in a liquid scintillator. The geometry consists in a 10 m radius sphere filled with LAB.
When the G4EmStandardPhysics_option4 and G4EmLivermorePhysics are used, the electrons are tracked in a very different way if the optical physics is enabled or not.
In particular when the optics is enabled the number of steps is much higher (around 100) and the steps are limited almost only by msc. Instead, when the optics is disabled the number of steps is much lower (around 10) and the steps length is always limited by eIoni.
You can find in the attachment some plots of the number of steps required to track the primary particle (1 MeV e-), the deposited energy for each steps and the ratio of msc and eIoni steps with respect to the total number of steps, with and without the optics enabled.

We investigated the issue and we found that the problem is related to the usage of the G4GoudsmitSaundersonMscModel. In fact if we use the G4EmStandardPhysics (option 0) or the G4EmStandardPhysics_option3 that use the G4UrbanModel the behavior is the same (with and without optics) and the particles are tracked in about 10 steps limited only by eIoni.

In particular, as highlighted in the G4 forum post, at line 519 of the G4GoudsmitSaundersonMscModel.cc file the msc algorithm is choosen according to the value of the "presafety" variable (if (gIsOptimizationOn && (distance<presafety))) and this variable assumes a value equal to the distance between the particle and the boundary of the volume if the optics is disabled (as expected) but it is alway 0 if the optics is enabled. As a consequence the "Error free algorithm" associated to the fUseSafetyPlus is always executed, limiting the steps, even if the particle is far away from the volume boundary.
Instead, when the optics is disabled and the presafety is not 0, the simpler and faster G4UrbanModel-like code is executed, thus msc process does not limits the steps (but eIoni does).

To check this, if the StepLimitType is changed to fUseSafety

Geant4 forum post



G4 Possible bug in EmLivermore and optical photon generation

Physics Processes, Models and Cross Sections

12 days later

mnovak 1 3d

There are at least two points (1. and 2.) to clarify here that I try below without getting lost in details.

0. Before them:
As Daren(dsawkey) mentioned, the number of simulation steps is arbitrary. We can limit the simulation steps more/less frequently while the simulation results (e.g. energy deposit or interaction frequencies, etc.) stays the same. Multiple Coulomb scattering (MSC) models (like G4UrbanMscModel and G4GoudsmithSaundersonMscModel) often use their arbitrary step limit in order to ensure that the tracking is only as accurate as expected (not more but not less). The different tracking/stepping algorithm types of the MSC models (like Minimal, Safety, DistanceToBoundary, SafetyPlus) correspond to different required level of tracking accuracy (increasing in that order) and eventually implemented separately for the different MSC models and usually mean different algorithms.
Therefore, switching to a different MSC model will very likely result in different number of simulation steps, as you can see when comparing using G4UrbanMscModel vs G4GoudsmithSaundersonMscModel in the Livermore or the option4 EM constructors, even if the MSC step limit type (and all other parameters) stay the same.
In this particular case, this is because the G4GoudsmithSaundersonMscModel will ensure an accurate tracking of electrons across volume boundaries when the SafetyPlus stepping algorithm is used (which is the case when using it in the Livermore or option4 EM physics constructors) while G4UrbanMscModel is not.
(The GS model achieves this by crossing the volume boundaries in single scattering mode, i.e. whenever the track is closer to a volume boundary than 1-3 times the elastic scattering mean free path, MSC will be single scattering. If you start tracking from or close to a boundary then you will have several such msc limited steps, i.e. single scattering steps, while the track moves further away from that boundary.)

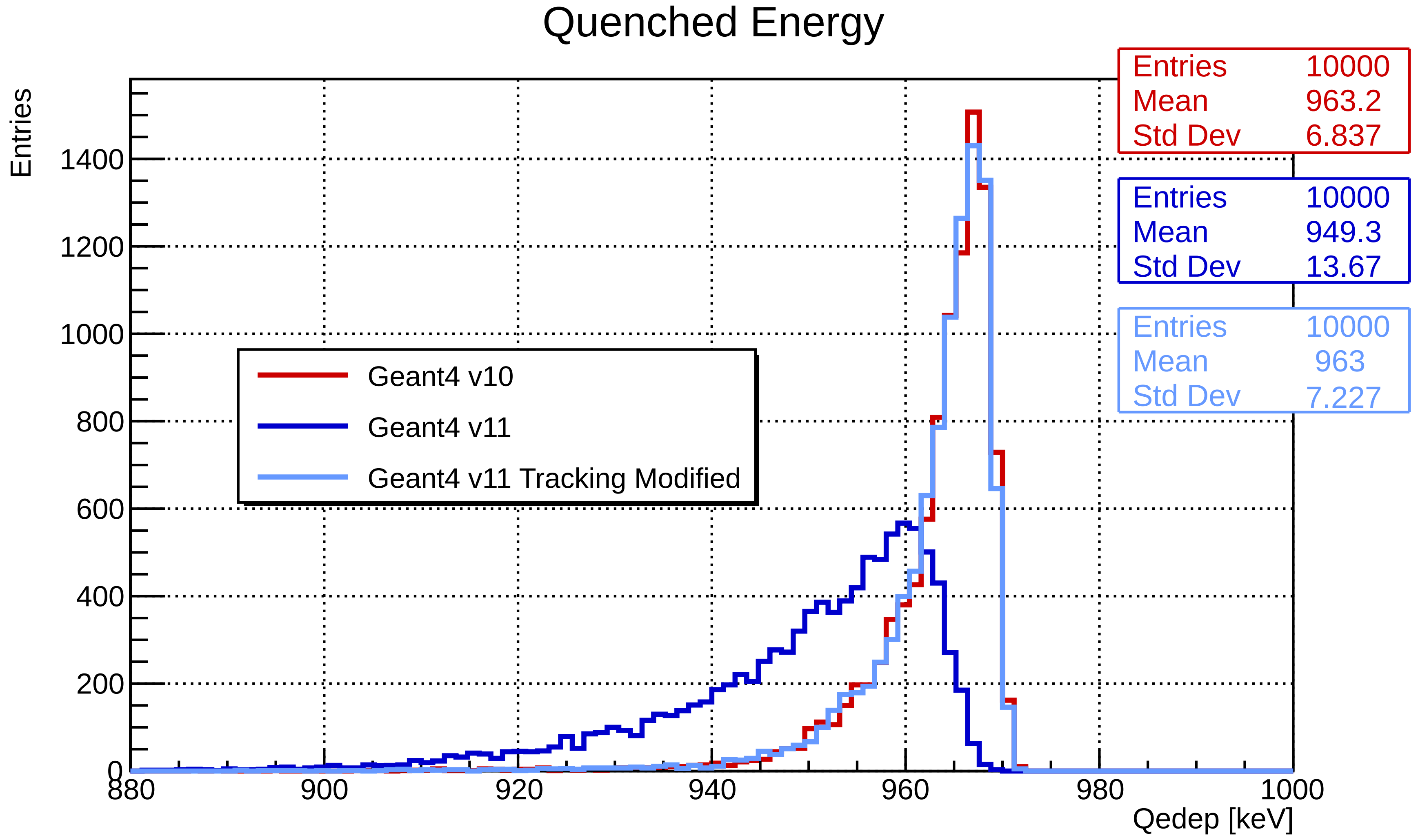
Has your question been answered?

Highlight the answer and help others by using the solution button below the correct reply.

10 / 11
Oct 14

3d

Change the order of tracking → Track secondaries last



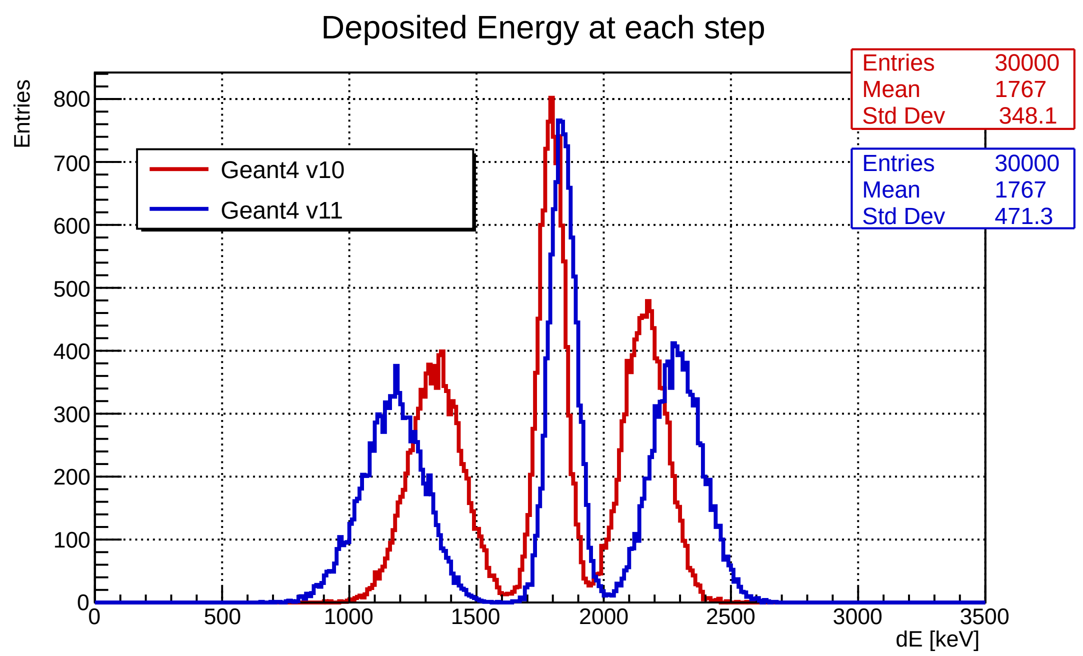
Both versions come to a good agreement
However, for higher energy particles the **computing ressources increase**

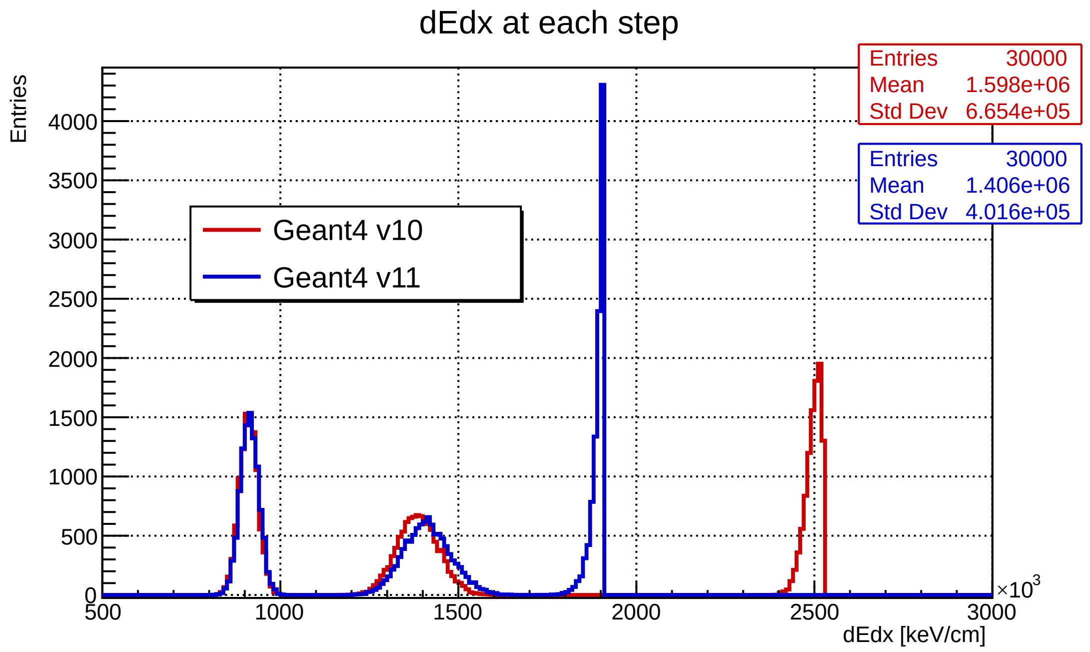
Alpha simulation

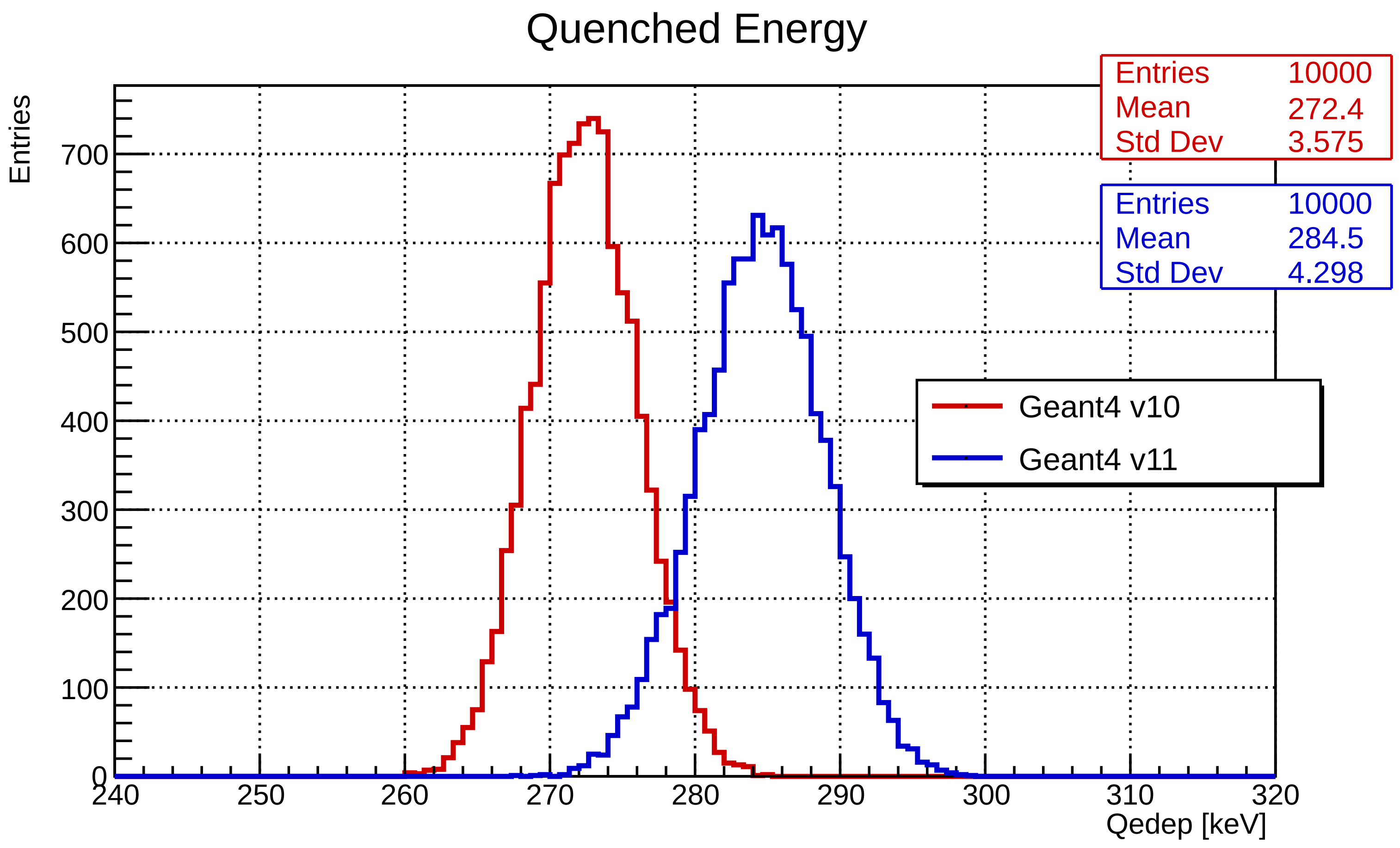
Alpha simulation

FULL SIMULATION OF 10 000 EVENTS OF 5.3 MEV ALPHA

Birks Law: $$Qedep = \sum_{i=1}^{N} \frac{dE}{1 + kB\frac{dE}{dx}}$$





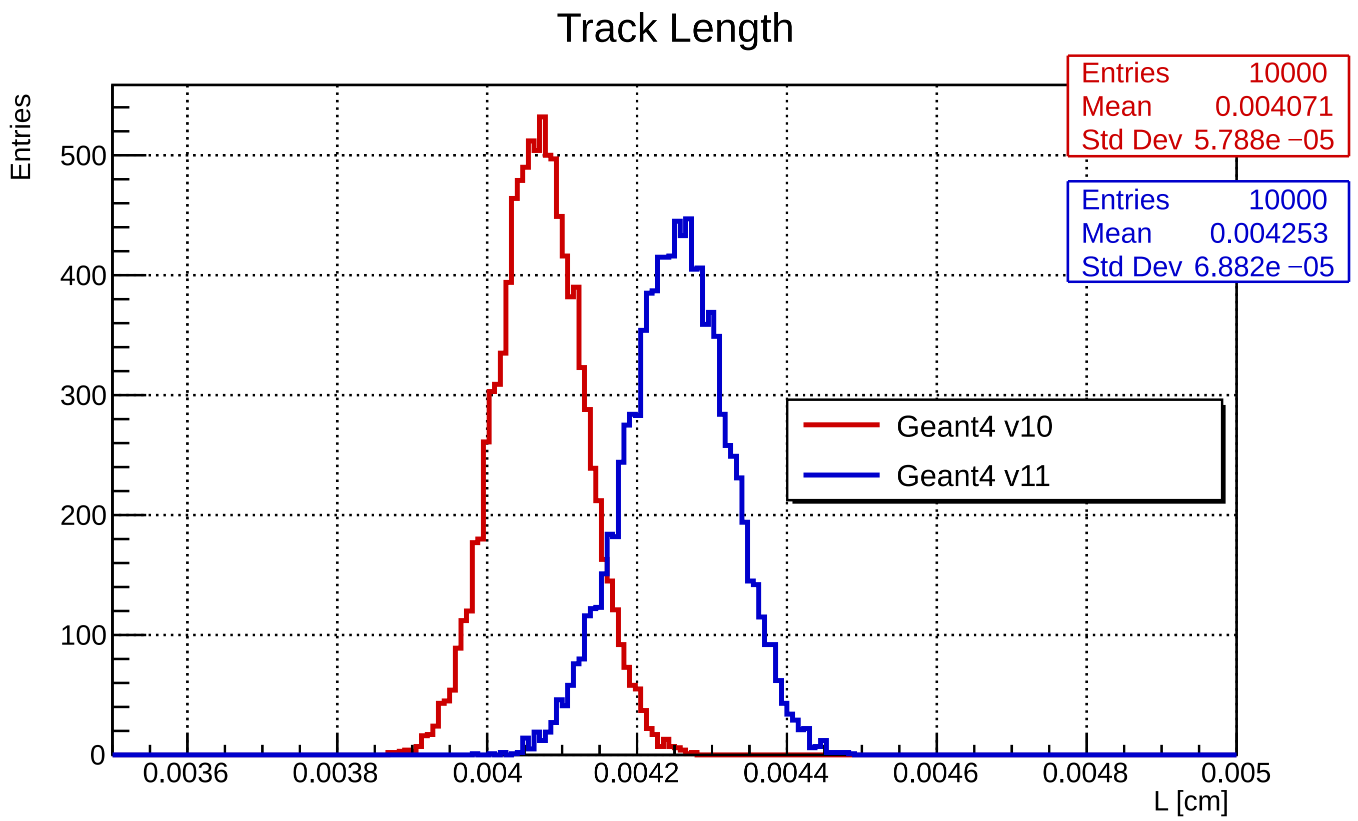


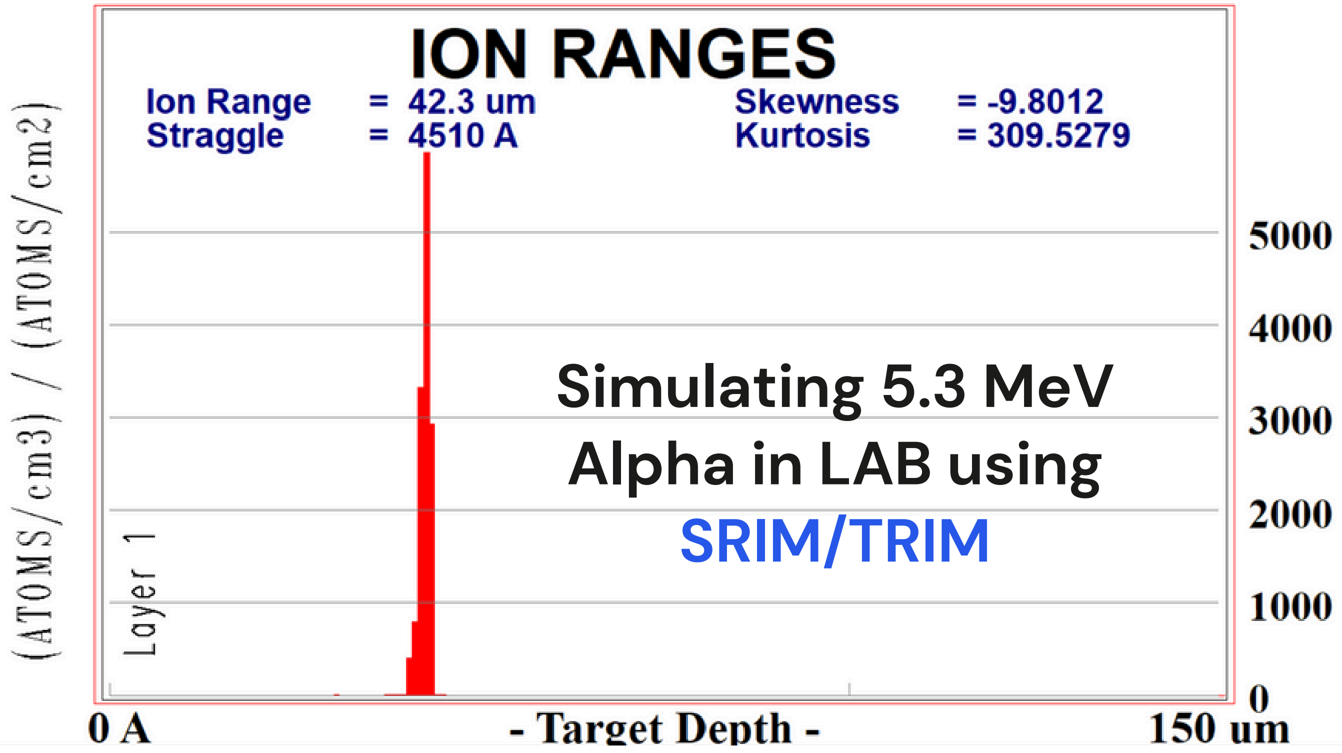
Alpha description is a bit different between versions especially at the **last step → dE/dx smaller in Geant4 v11.2.2**

→ No changements in the physics processes used between versions

Alpha simulation

http://www.srim.org





SRIM uses a group of programs to calculate the stopping and range of ions in matter. A more comprehensive program (TRIM) allows to build complex targets with multiple layers and get various distributions of the ion.

Alpha range obtained with SRIM coincides pretty well with Geant4 v11 (**42.3 µm in SRIM vs 42.5 µm in Geant4 v11.2.2**)

Fix in Geant4 v11.0.0: G4BraggIonModel, G4BetheBlochModel, G4ionIonisation clean-up. Improved implementation of corrections to ion stopping powers: do not apply corrections at the last step of an ion; **do not apply corrections to alpha.** Addressing problem report #2440 (Geant4 v11.0.0 Release Notes)

Simulation/Data Comparison

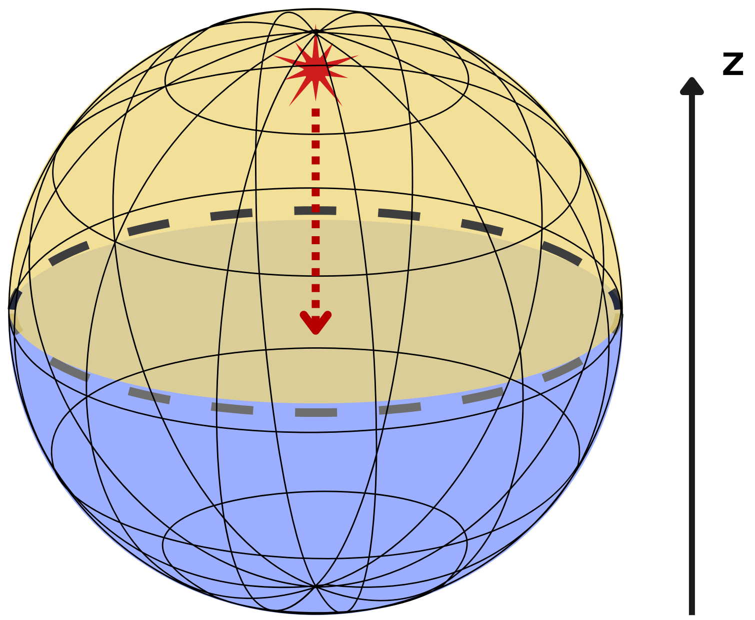
AmBe Calibration source

AmBe chain reaction:

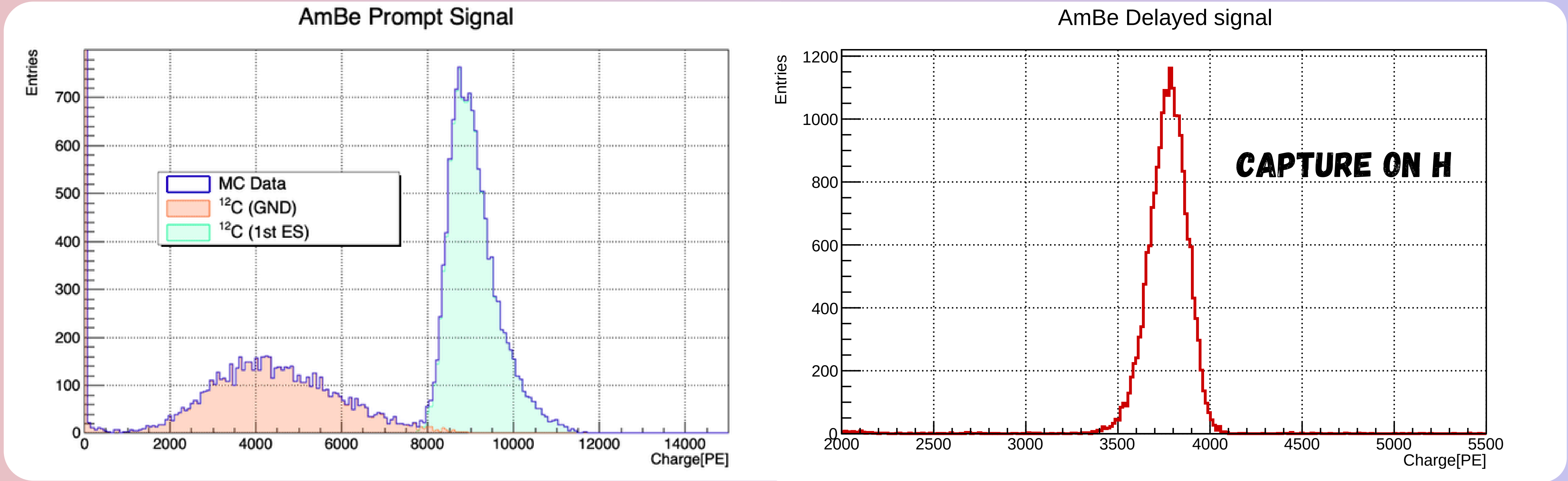
$$^{241}Am \rightarrow \, ^{237}Np + \alpha, \; ^{9}Be + \alpha \rightarrow \, ^{12}C^{*}(or\; ^{12}C) + n$$

Prompt signal: Proton recoils (+ ^{12}C deexitation)
Delay signal: neutron capture on H (or C)

AmBe source
Liquid scintillator
Water



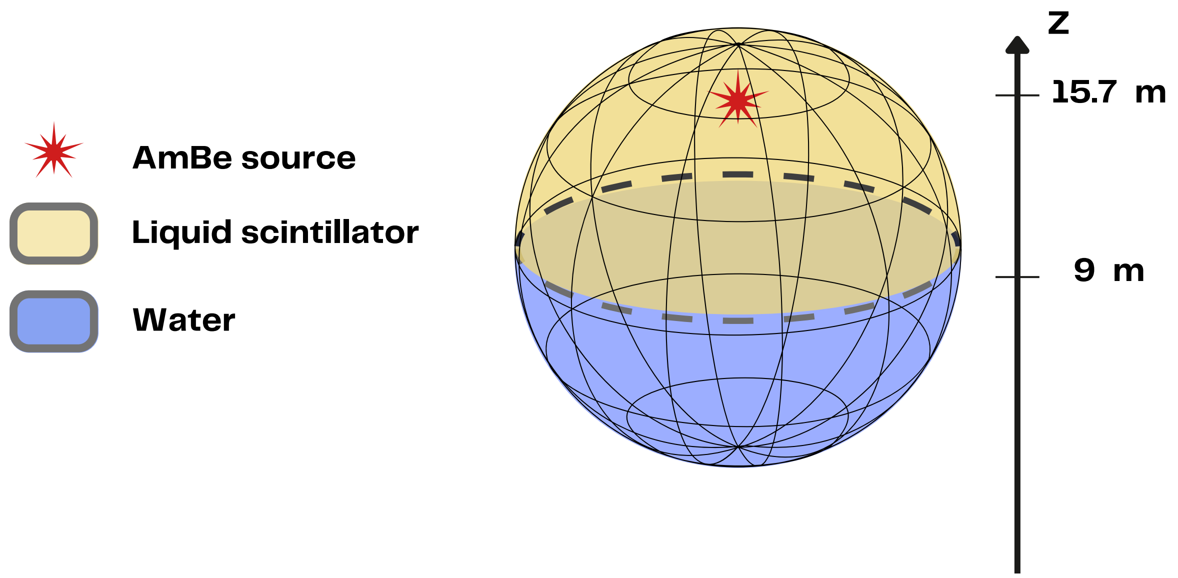
MONTE CARLO

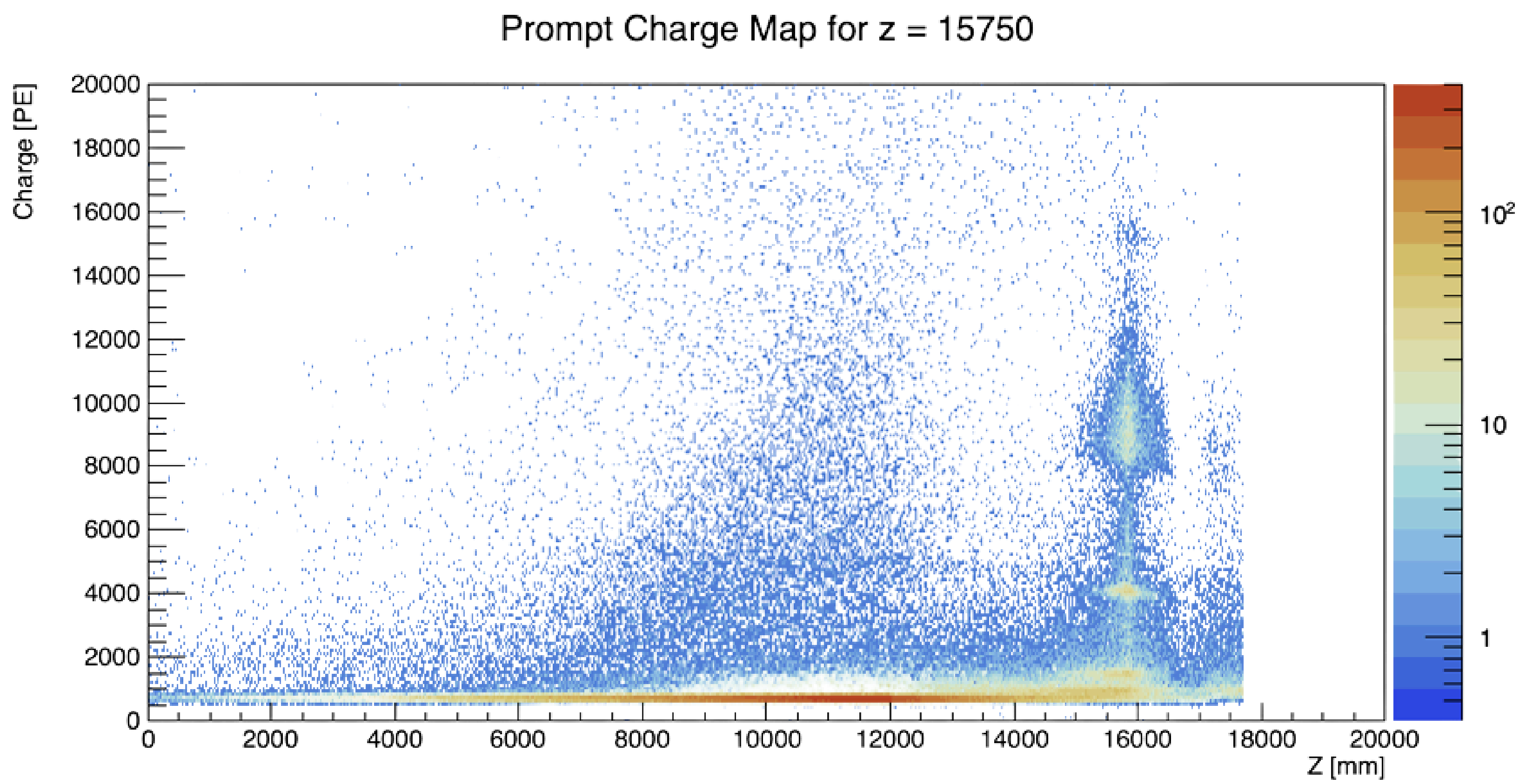


Selection cut on AmBe events

Example of AmBe source placed at **z = 15.75 m** in a detector filled with **3260 m^3 of liquid scintillator**

On top of AmBe events, other type of events can pollute the signal and require a proper selection





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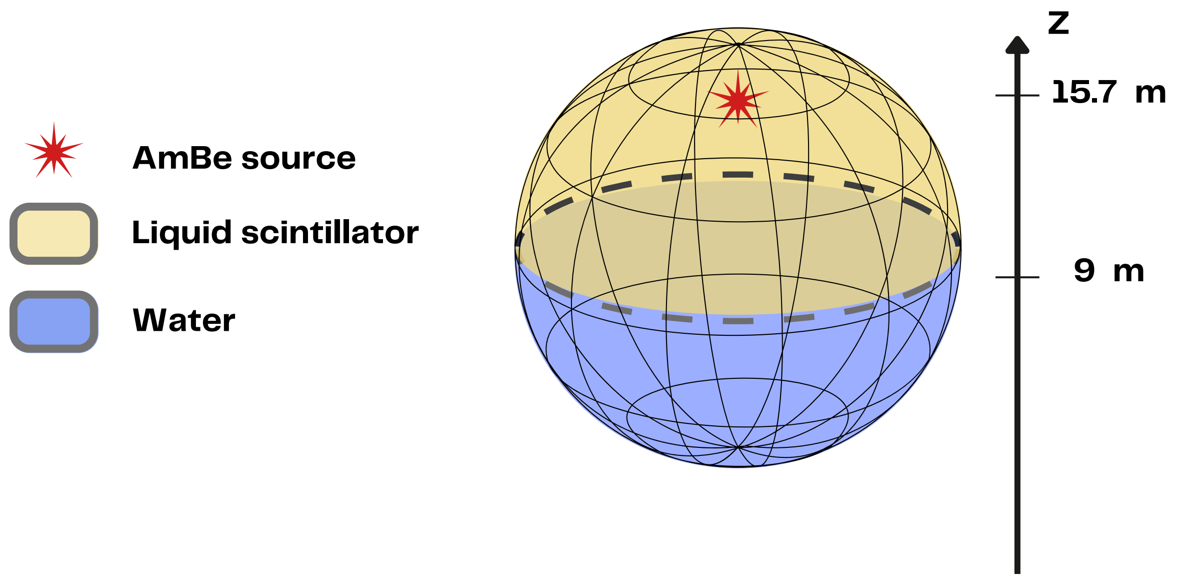
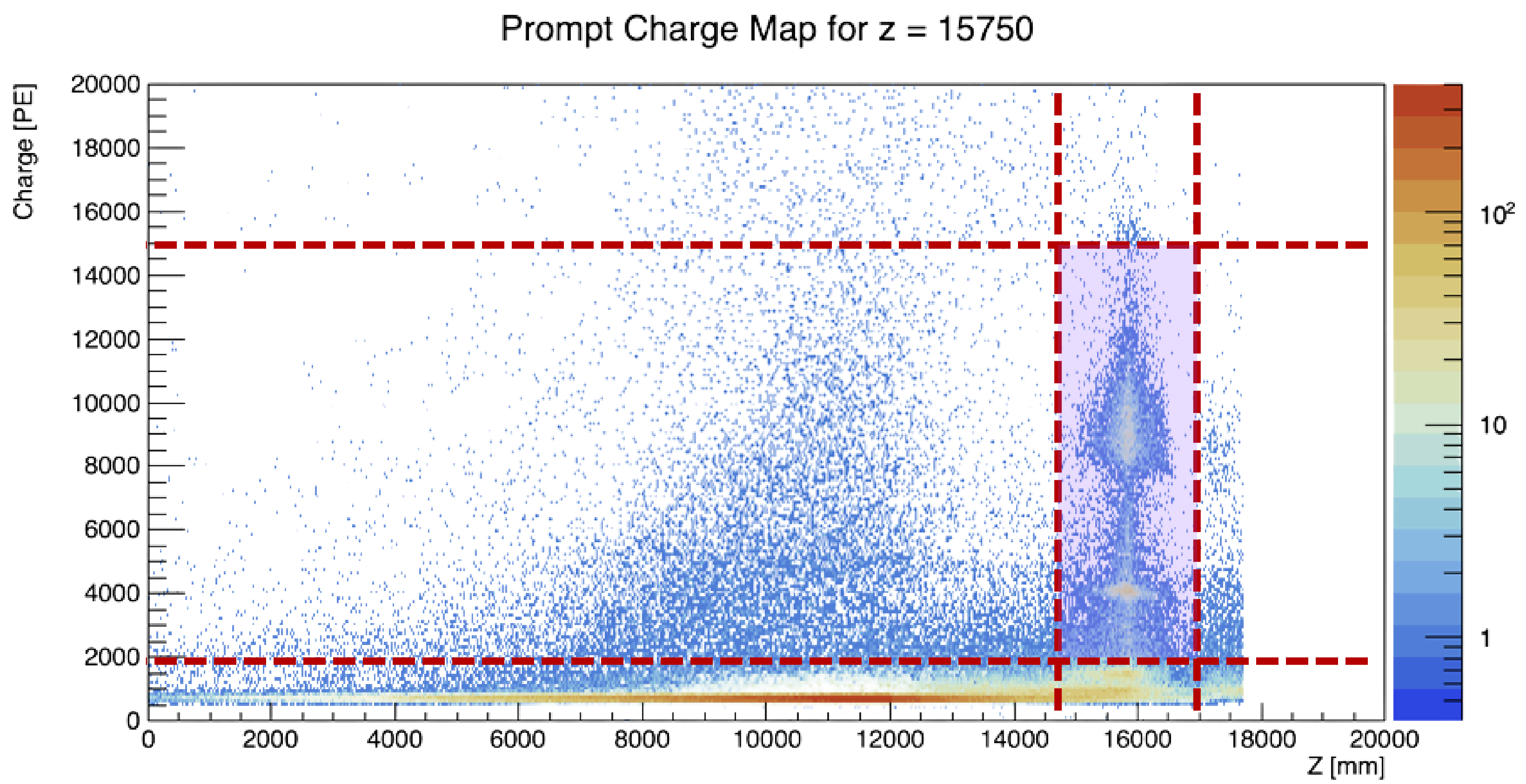
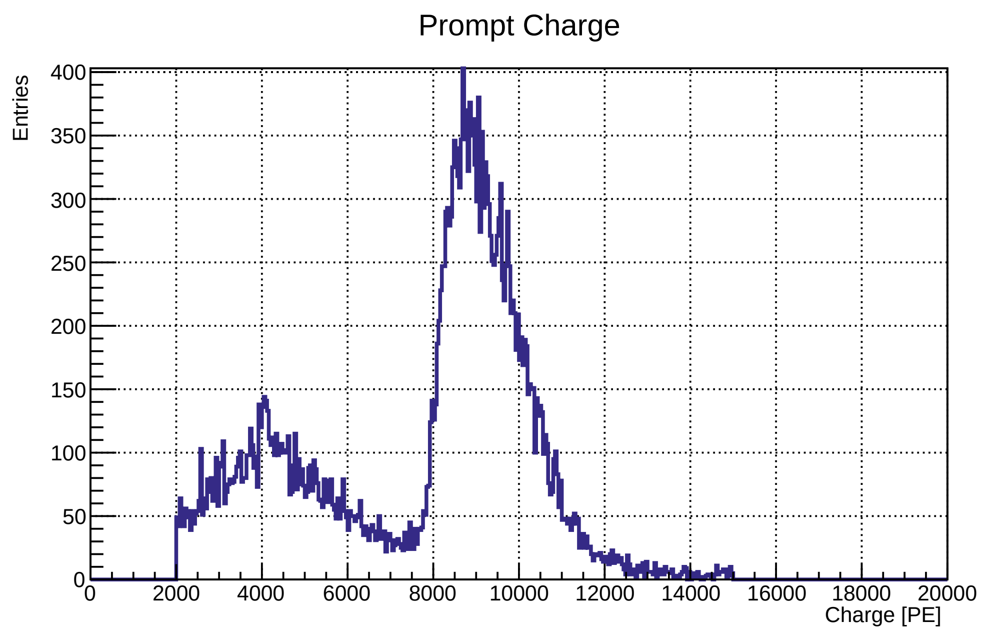




Prompt selection cut:

- +/– 2 m from source position
- Charge > 2000 PE & Charge < 15 000 PE

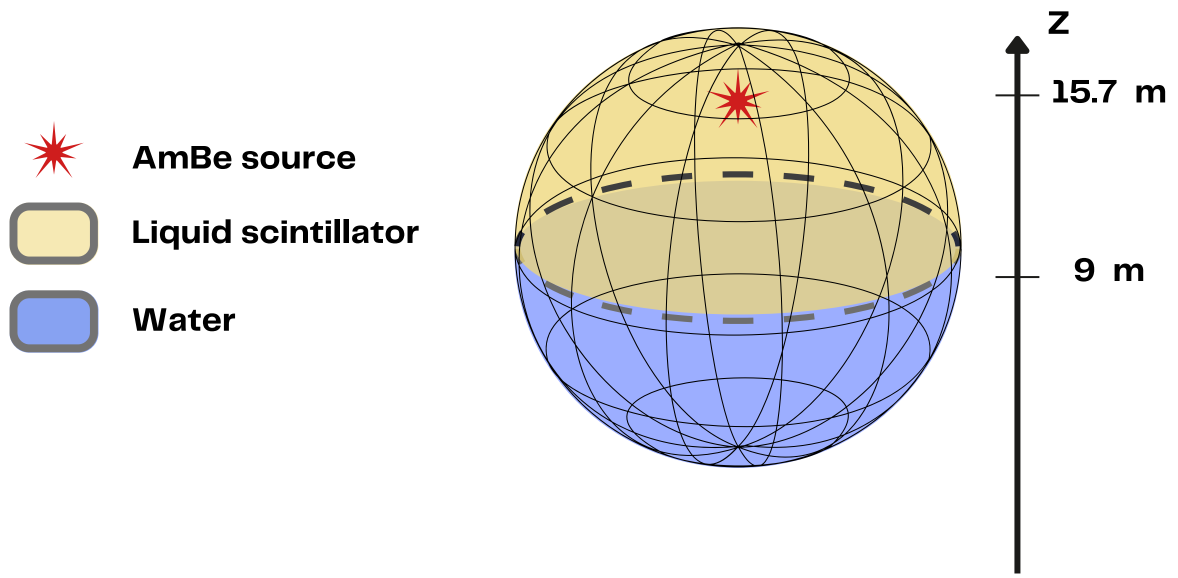


Prompt Charge for AmBe at z = 15.75 m

Selection cut on AmBe events

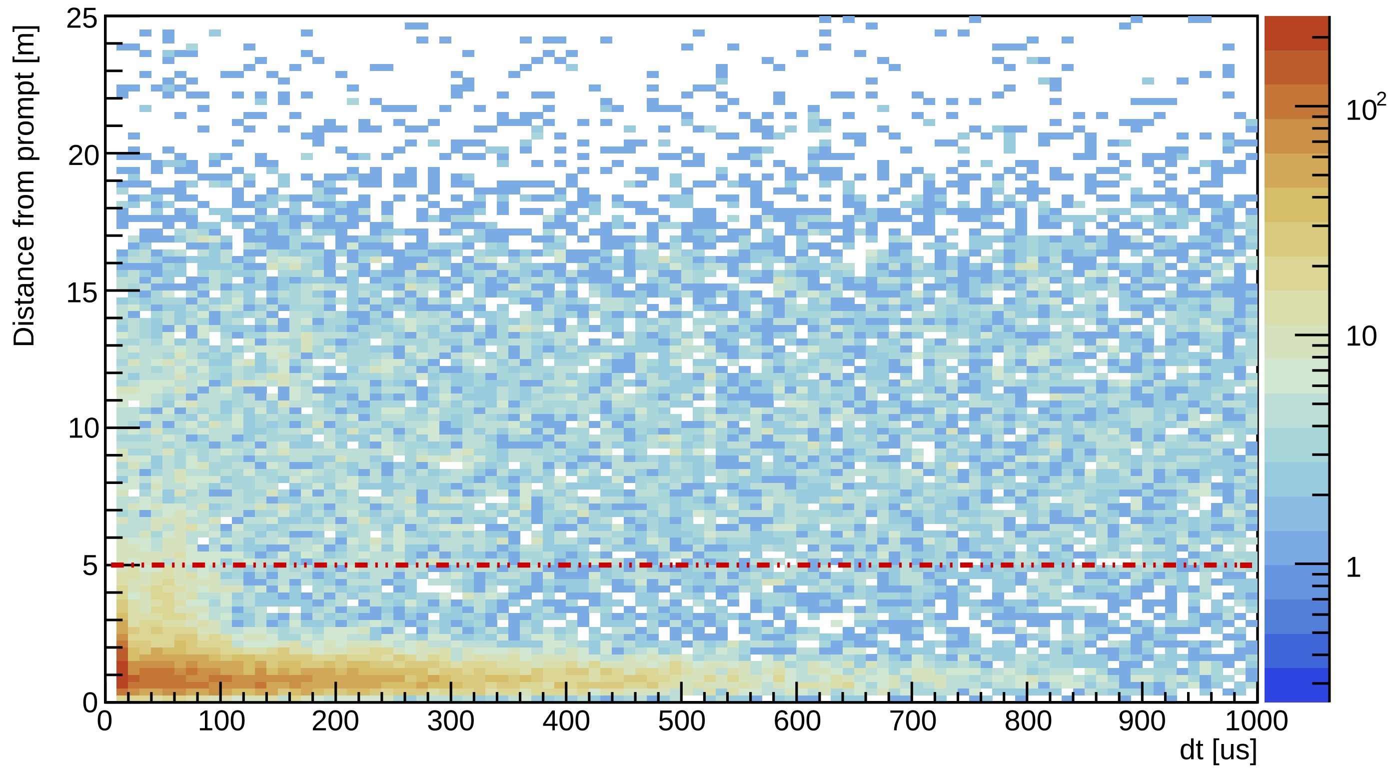
Example of AmBe source placed at **z = 15.75 m** in a detector filled with **3260 m³ of liquid scintillator**

On top of AmBe events, other type of events can pollute the signal and require a proper selection



Delay selection cut:

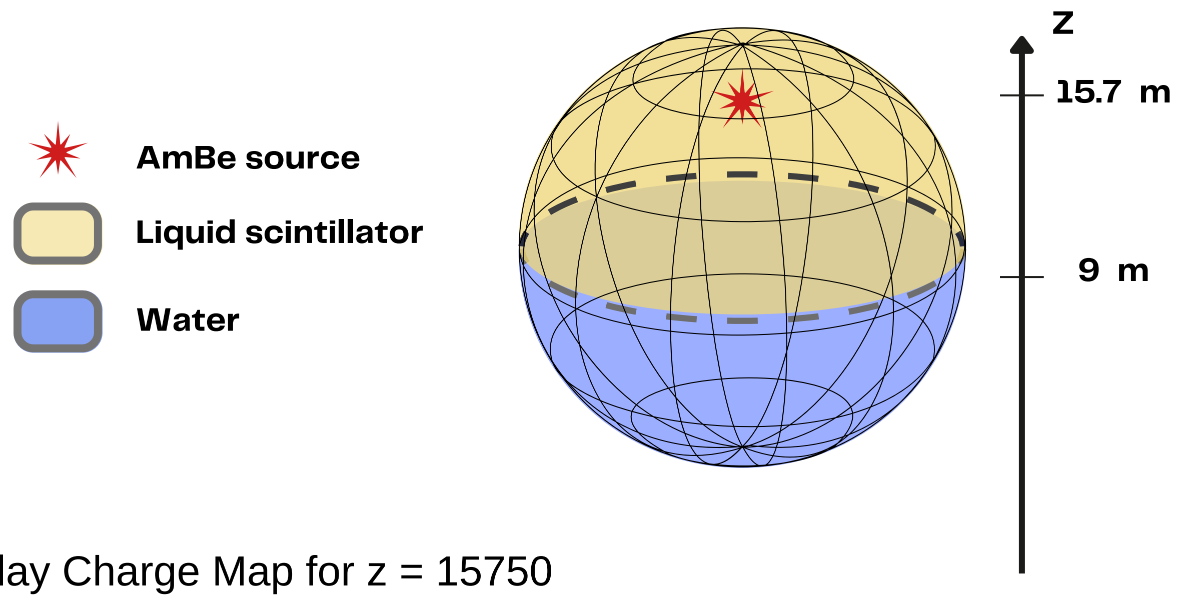
- Time delay < 1000 μs & Time Delay > 10 μs
- Distance from prompt < 5 m



Selection cut on AmBe events

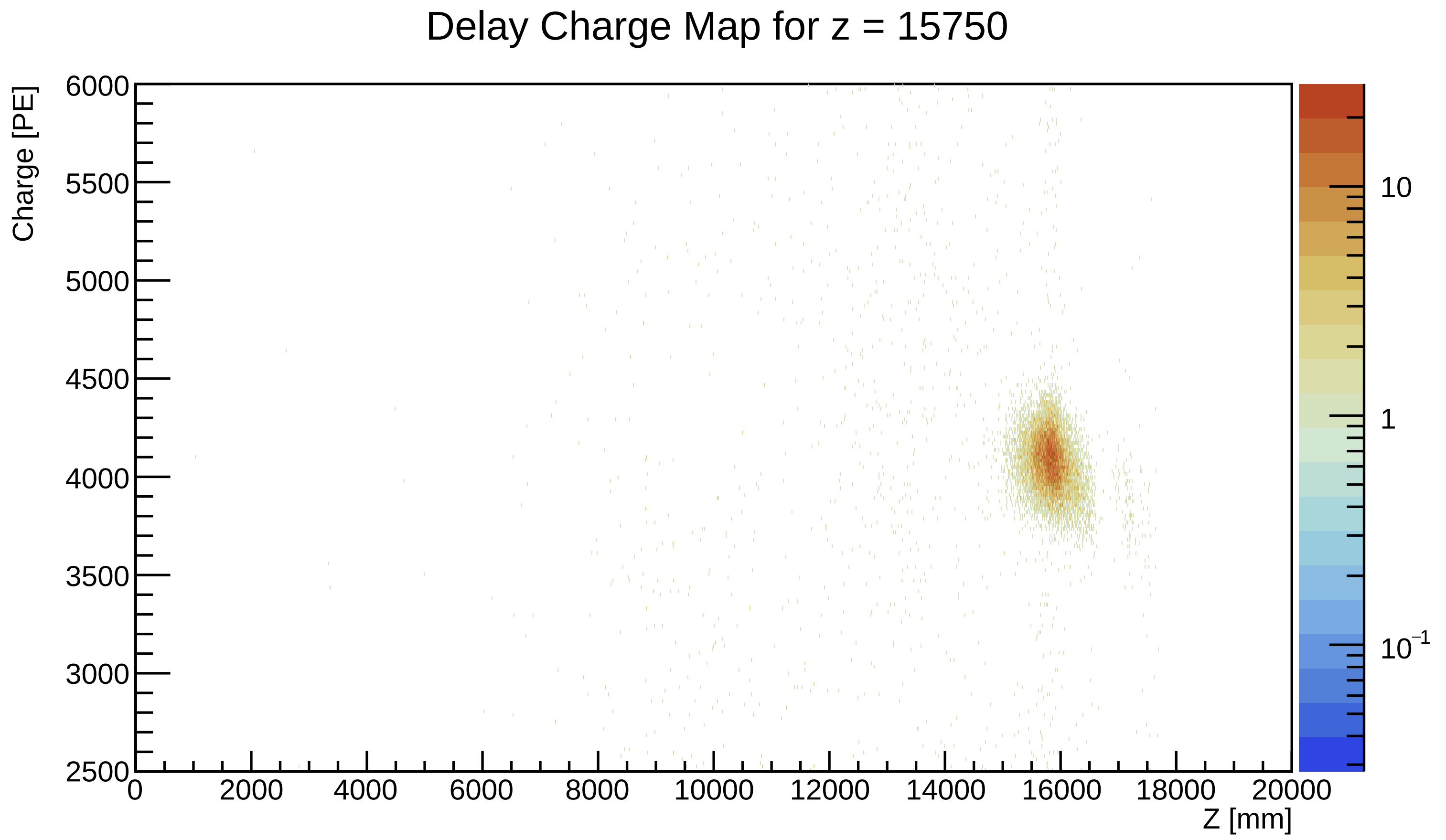
Example of AmBe source placed at **z = 15.75 m** in a detector filled with **3260 m^3 of liquid scintillator**

On top of AmBe events, other type of events can pollute the signal and require a proper selection

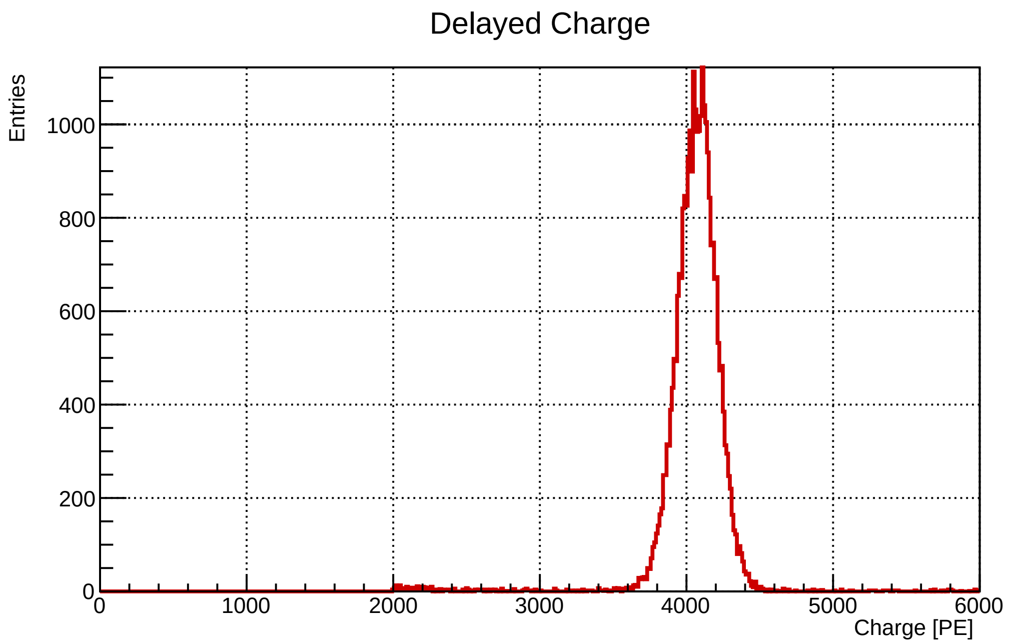


Delay selection cut:

- Time delay < 1000 μs & Time Delay > 10 μs
- Distance from prompt < 5 m
- Charge > 3500 PE & Charge < 5000 PE



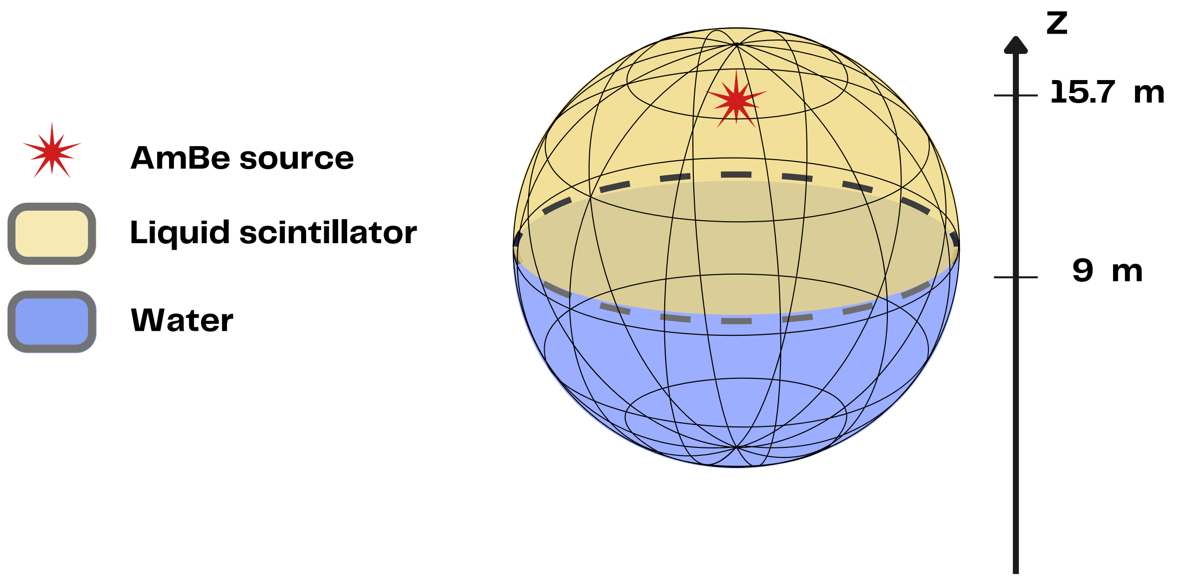
Delay Charge for AmBe at z = 15.75 m

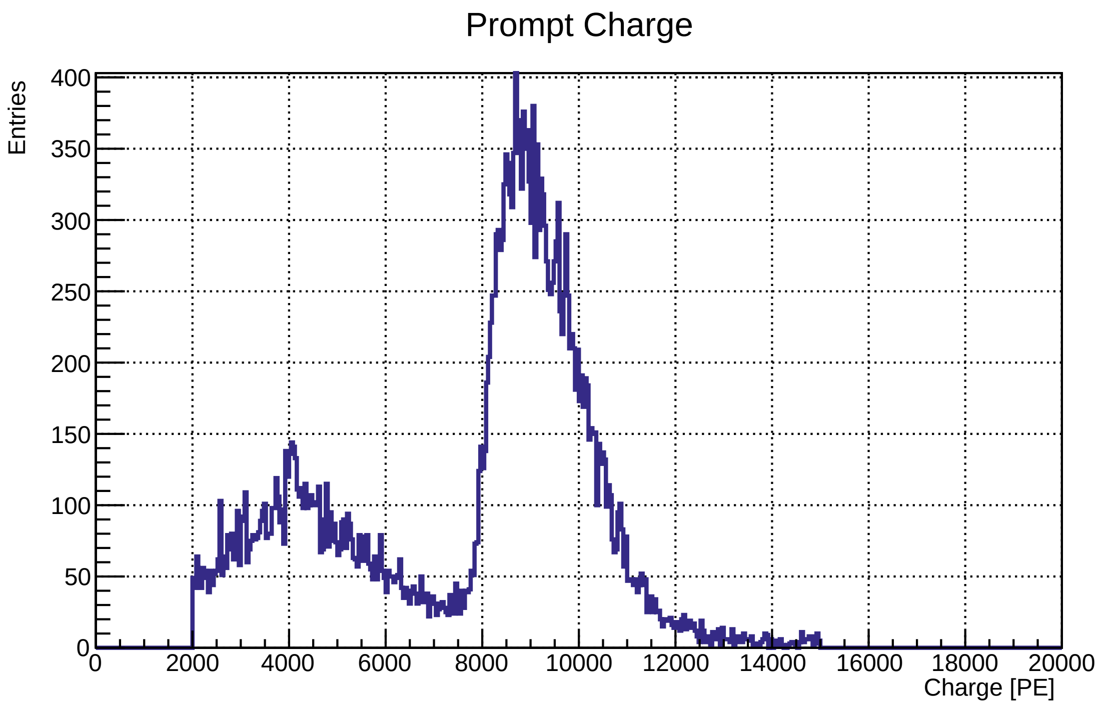


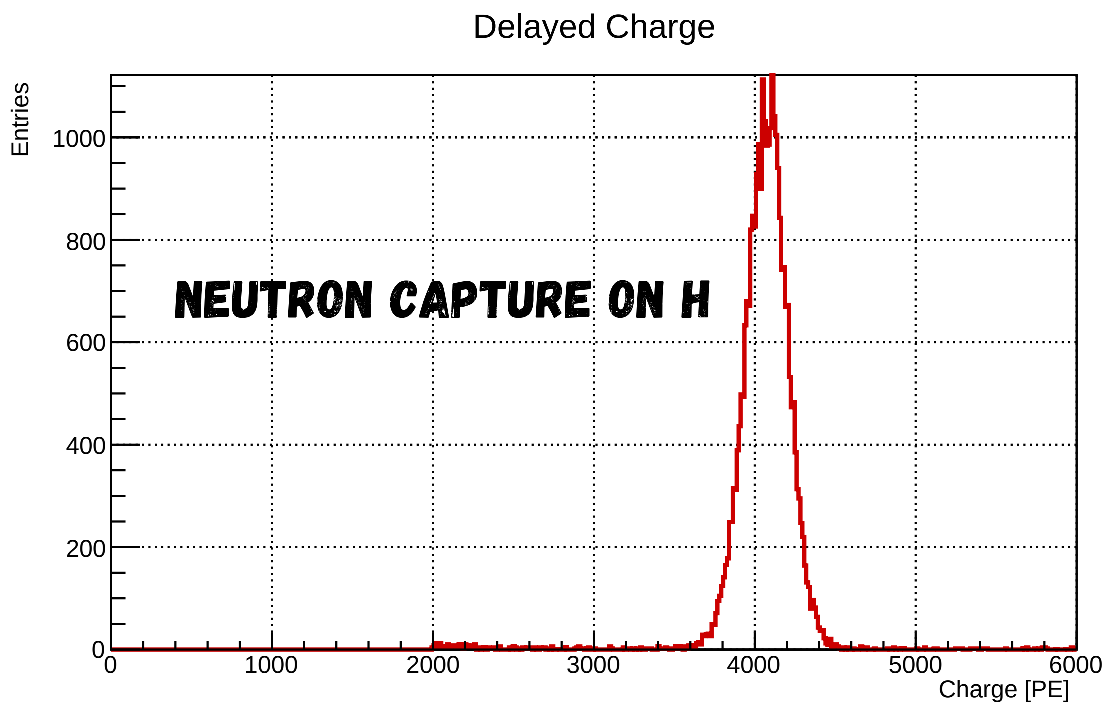
Selection cut on AmBe events

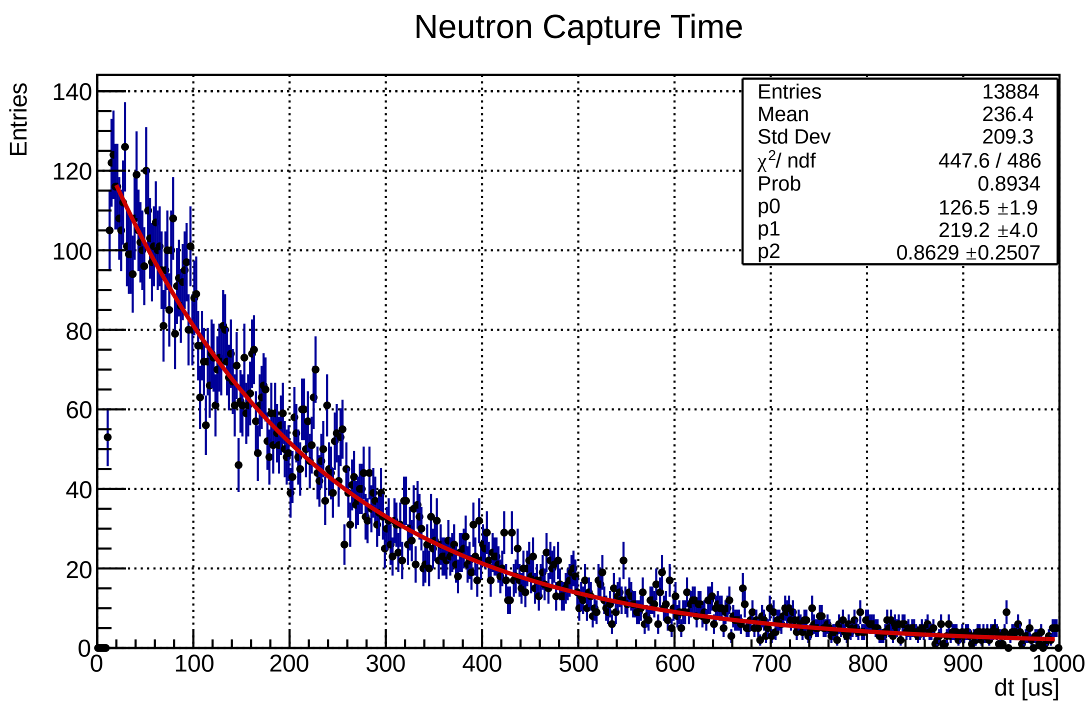
Example of AmBe source placed at **z = 15.75 m** in a detector filled with **3260 m^3 of liquid scintillator**

On top of AmBe events, other type of events can pollute the signal and require a proper selection





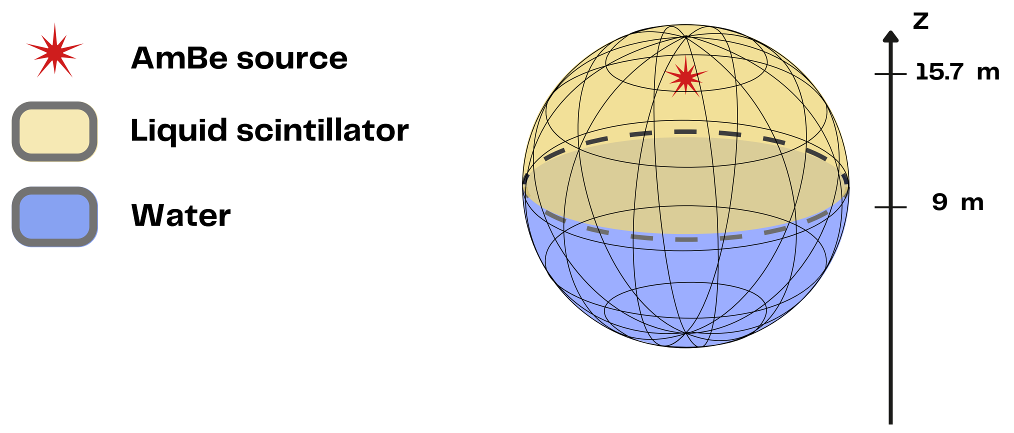


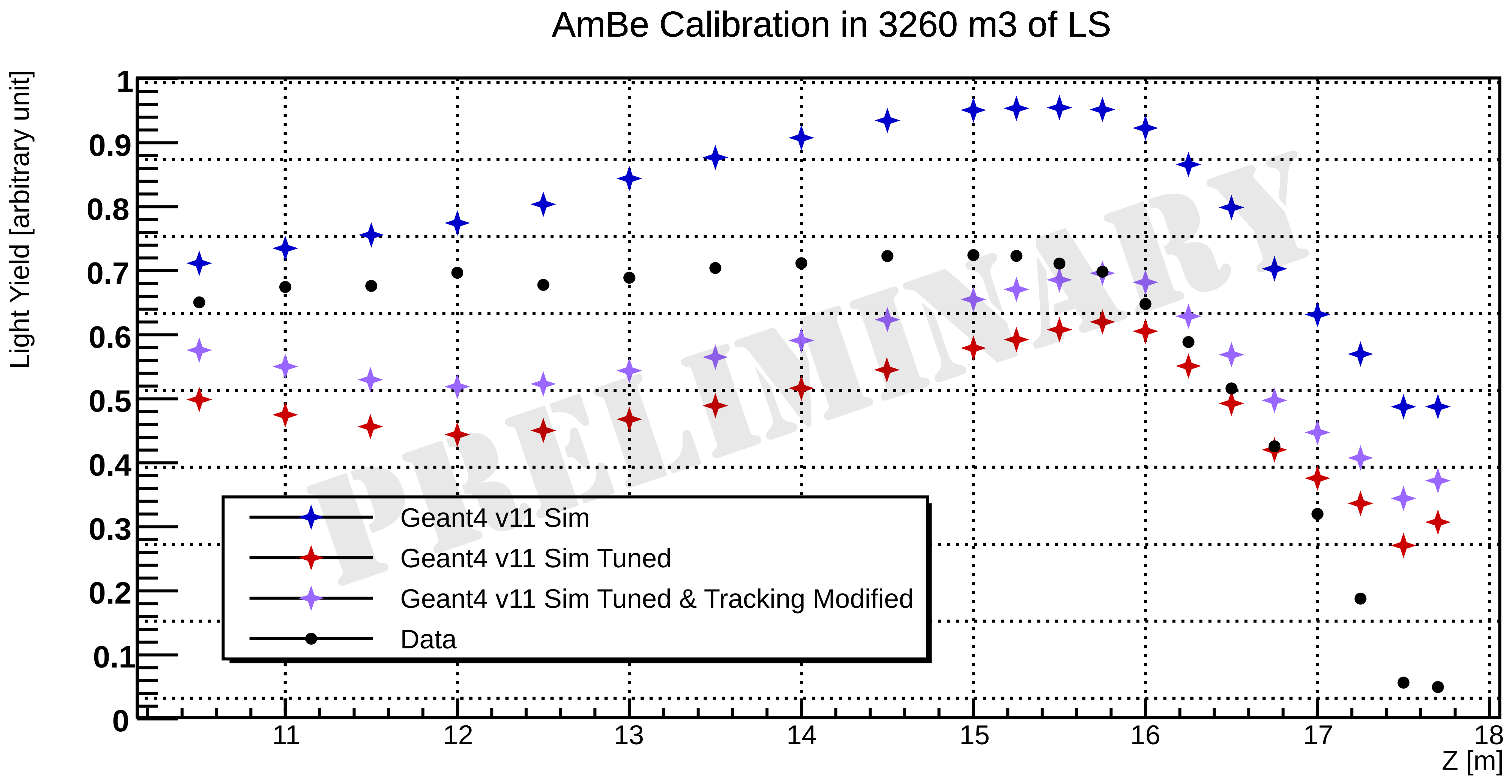


Sim/Data comparison using Geant4 v11

AmBe source placed at different position in a detector filled with **3260 m^3 of liquid scintillator**

Run **simulation with the same configuration** of LS/Water volume and place AmBe source at different Z positions **using Geant4 v11**





Simulation with **Default** Geant4 v11 show good agreement at the interface but deviates from data as we go up in the sphere

Sim/Data comparison using Geant4 v11

AmBe source placed at different position in a detector filled with **3260 m³ of liquid scintillator**

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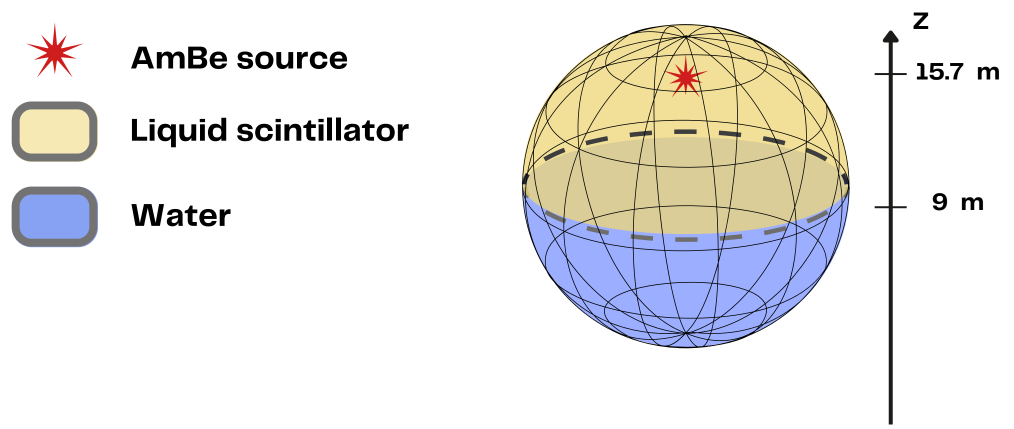
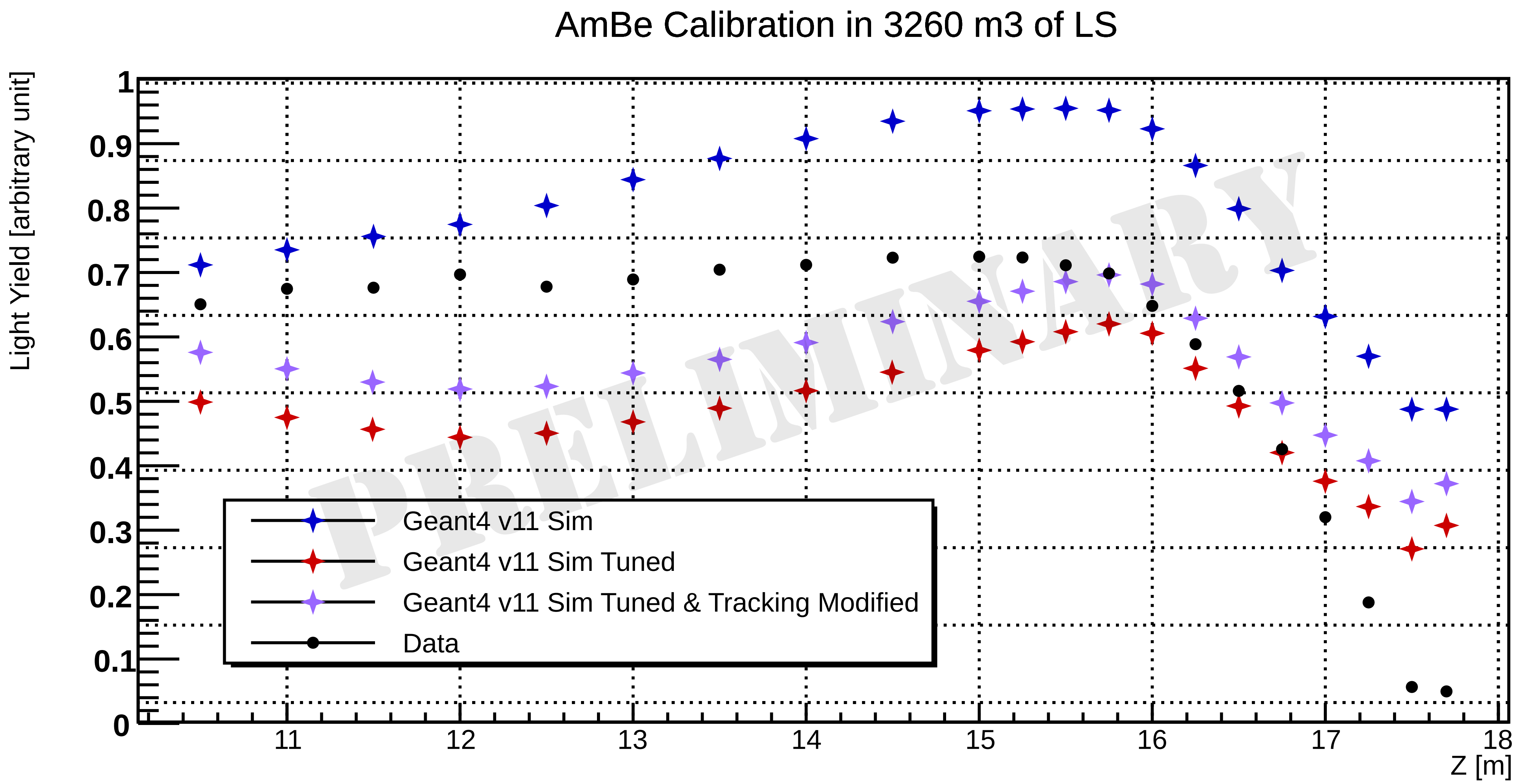
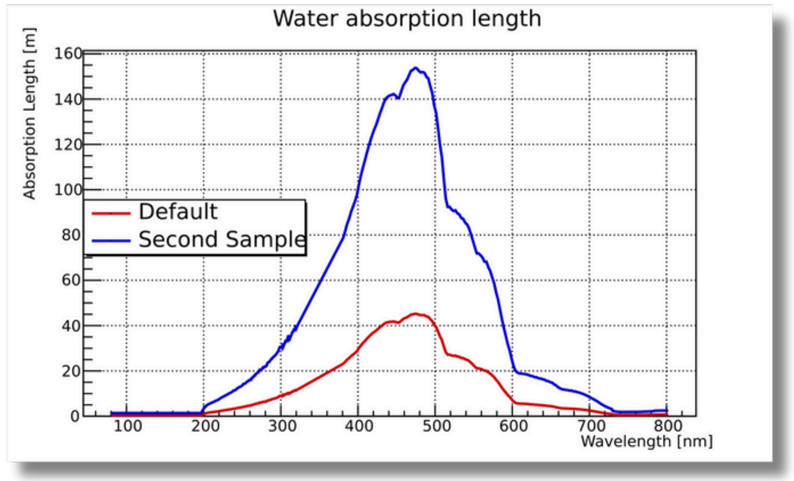




Simulation with **Default** Geant4 v11 show good agreement at the interface but deviates from data as we go up in the sphere

Tune the simulation with **measurement of water/LS absorption length** → Better agreement at interface and top of the sphere but still discrepancies in the middle



Summary and Conclusion

GEANT4 COMPARISON

Hadronic physics has minor discrepancies

Important discrepancies on the description of electrons :

- Different msc model
- Increase in step number
- Different Qedep distribution

Discussion ongoing with Geant4 developers to make sure if any modifications are scheduled

SIM/DATA COMPARISON USING GEANT4 V11

Tuned simulation using Geant4 v11 with modified tracking gives the best agreement with data

→ Still a lot of **improvements to be done on the simulation**

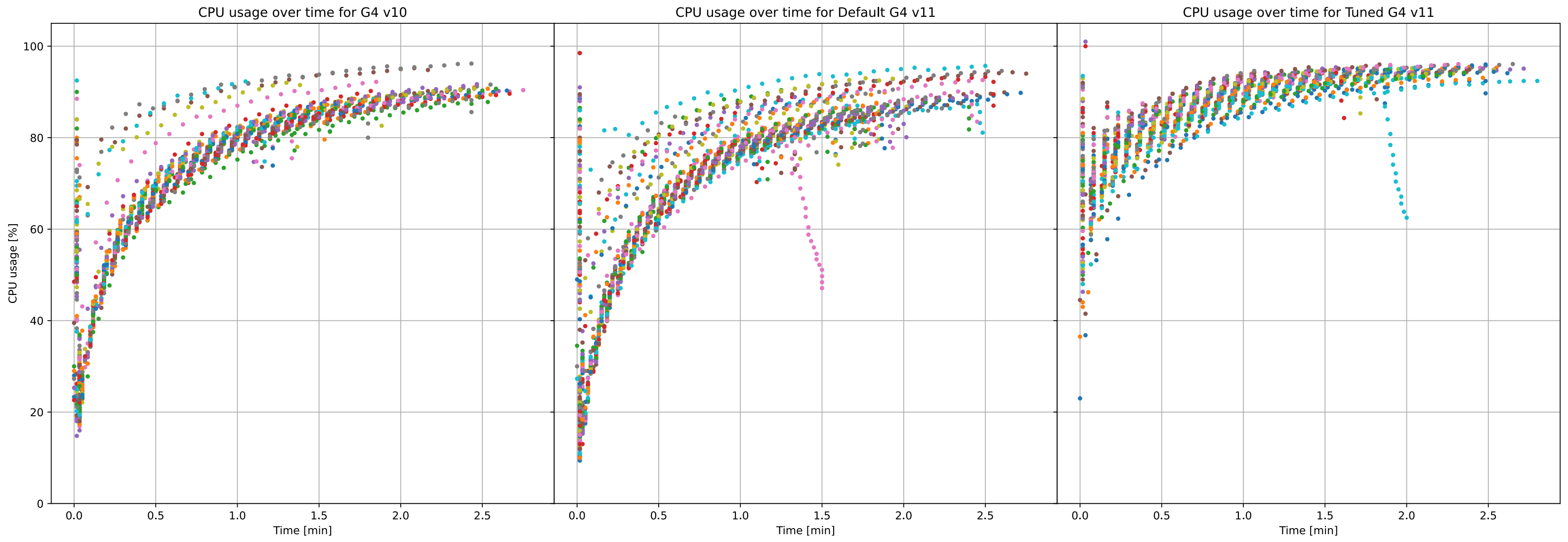
- Measurement of absorption lengths (water/LS)
- Adding detector geometry in the simulation
- DCR measurements
- Tuning of birks constants

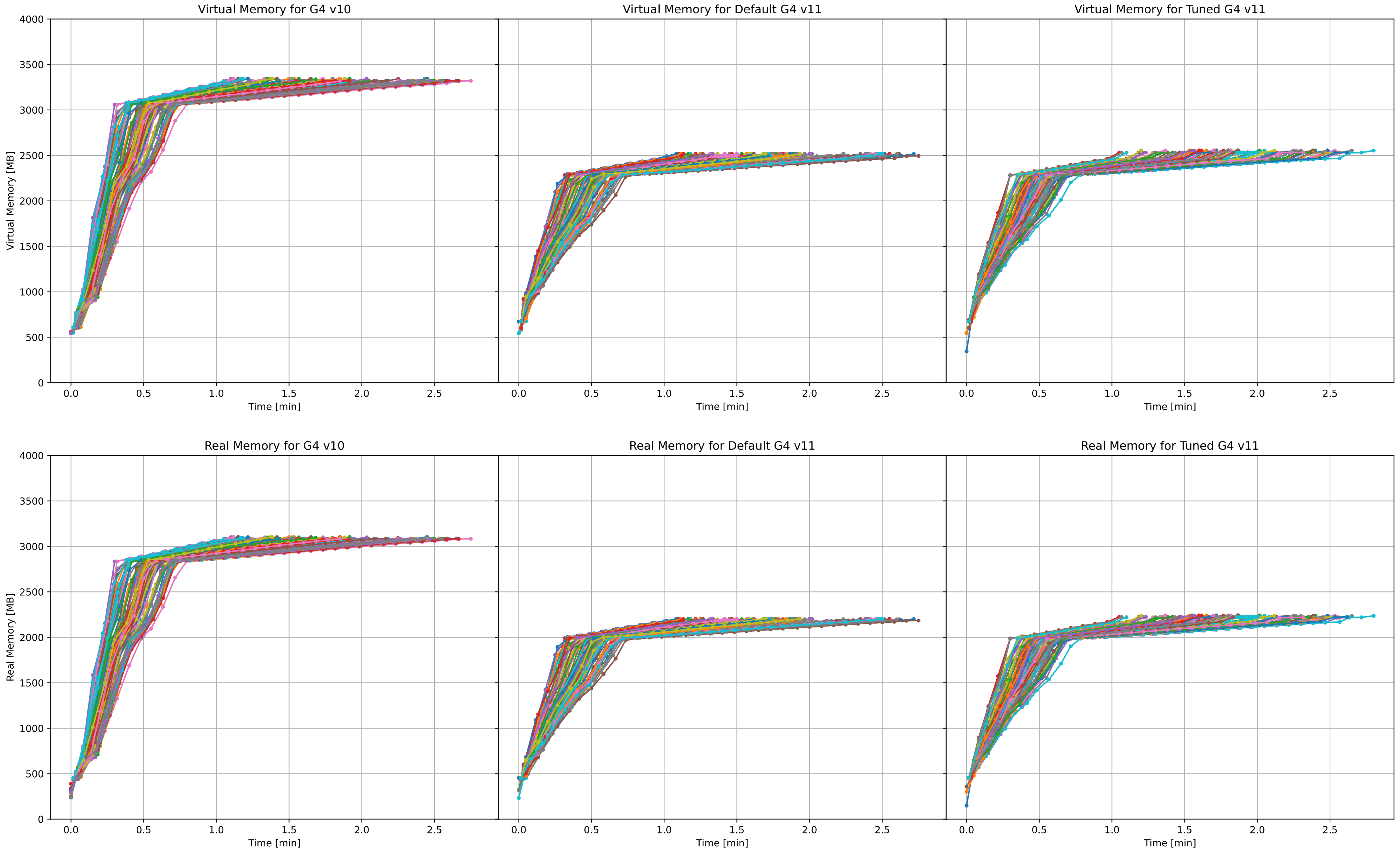
THANKS !

BACK UP

Computation ressources

10 MeV Electron simulation in JUNOSW

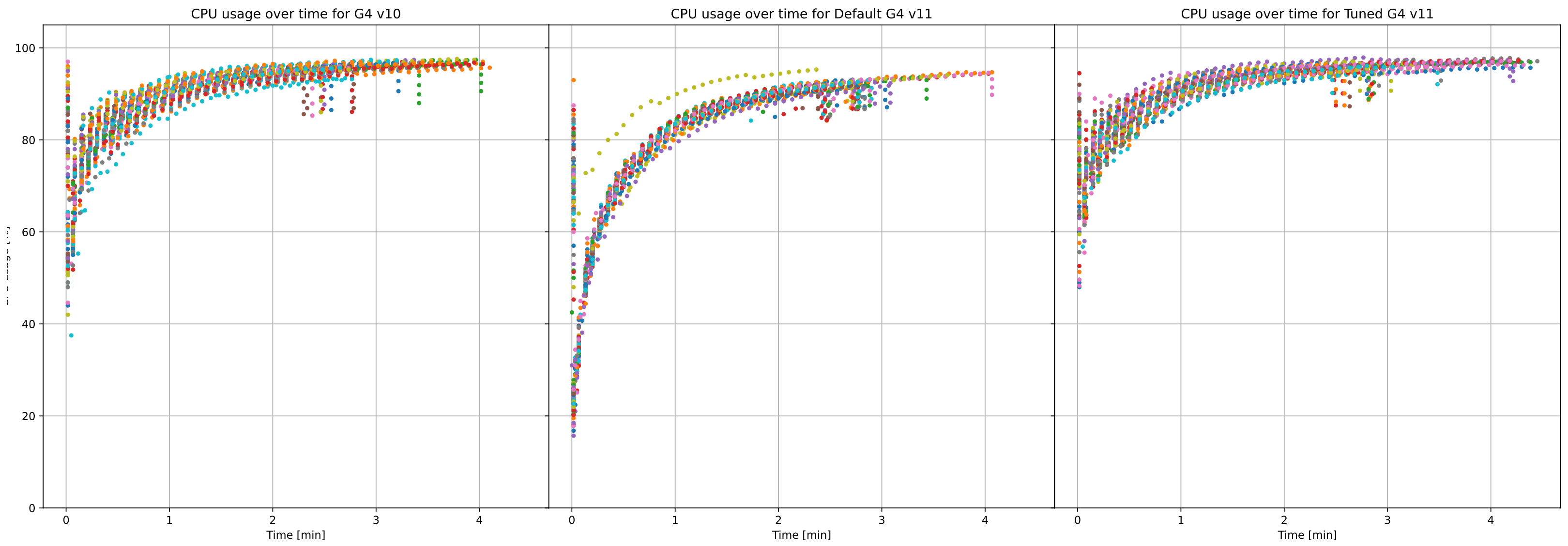


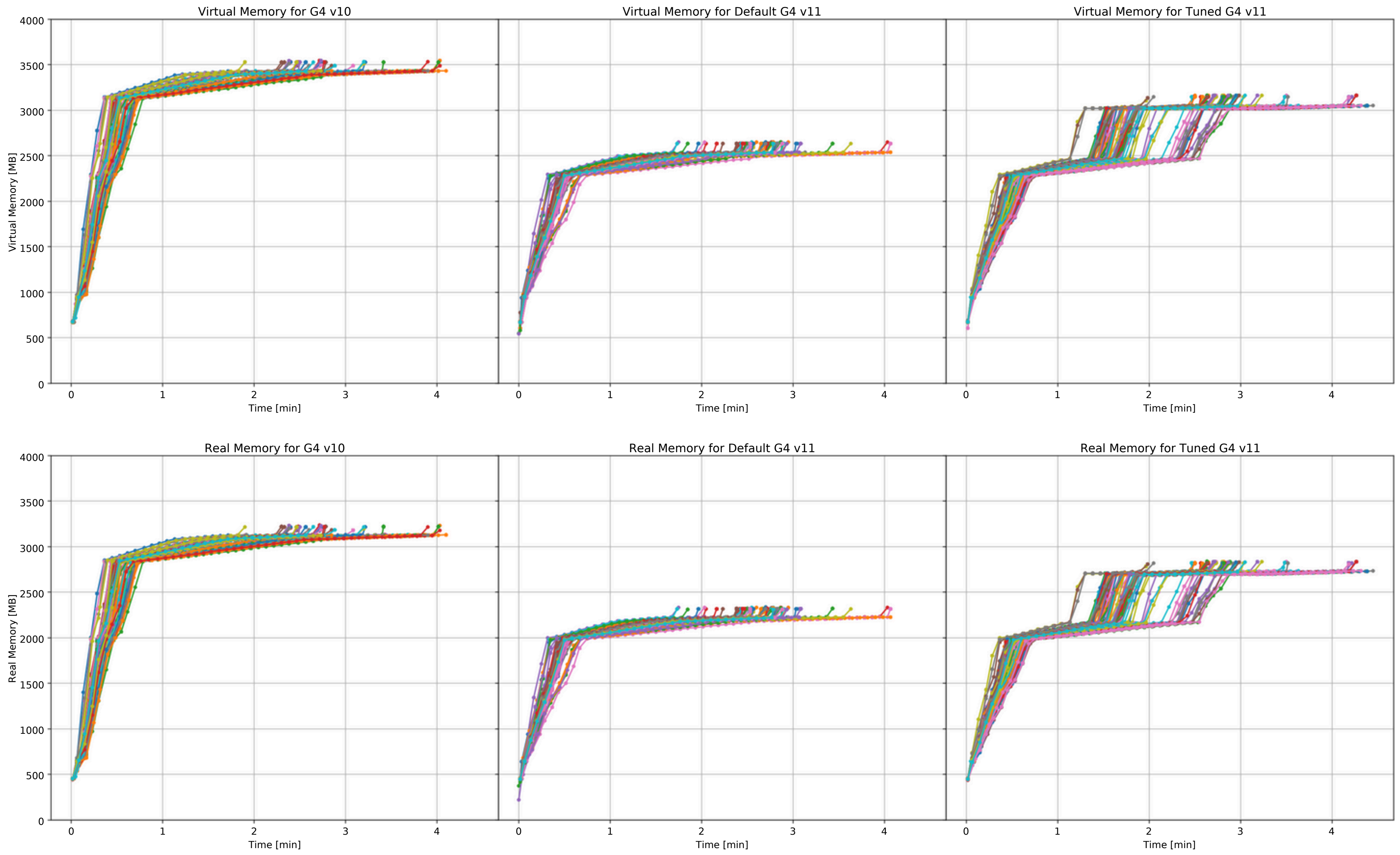


No major differences aside from fast CPU consumption for Tuned Geant4 v11

Computation ressources

100 MeV Electron simulation in JUNOSW

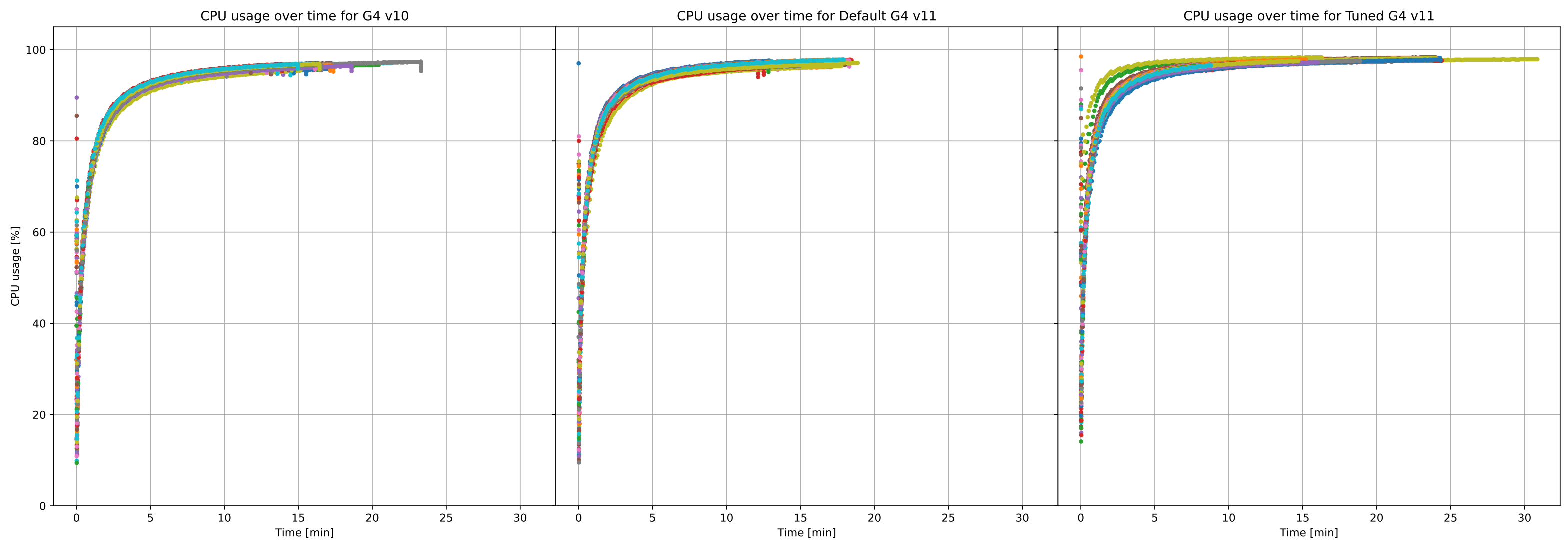


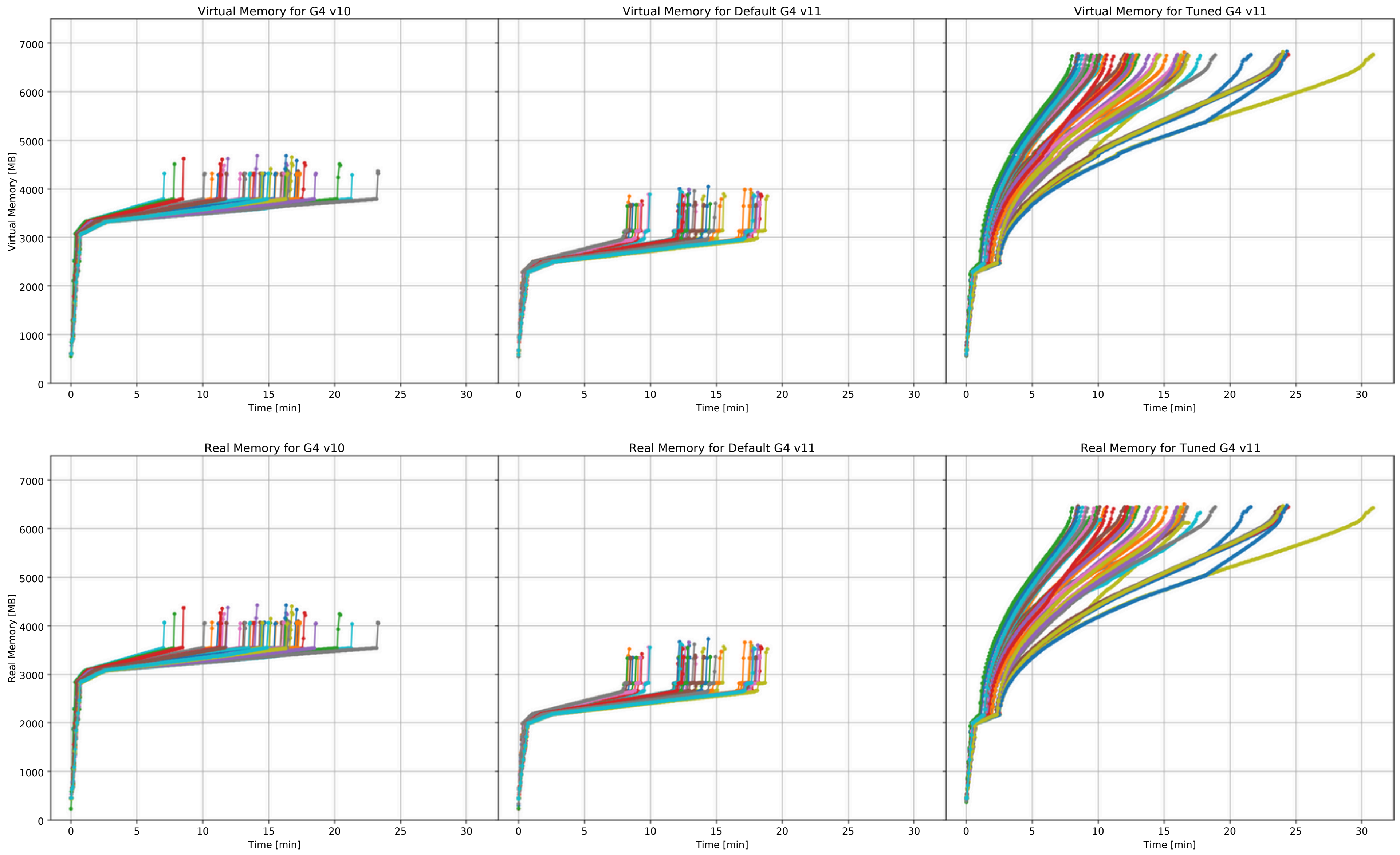


The memory consumption increases but is still lower than Geant4 v10

Computation ressources

1 GeV Muon simulation in JUNOSW



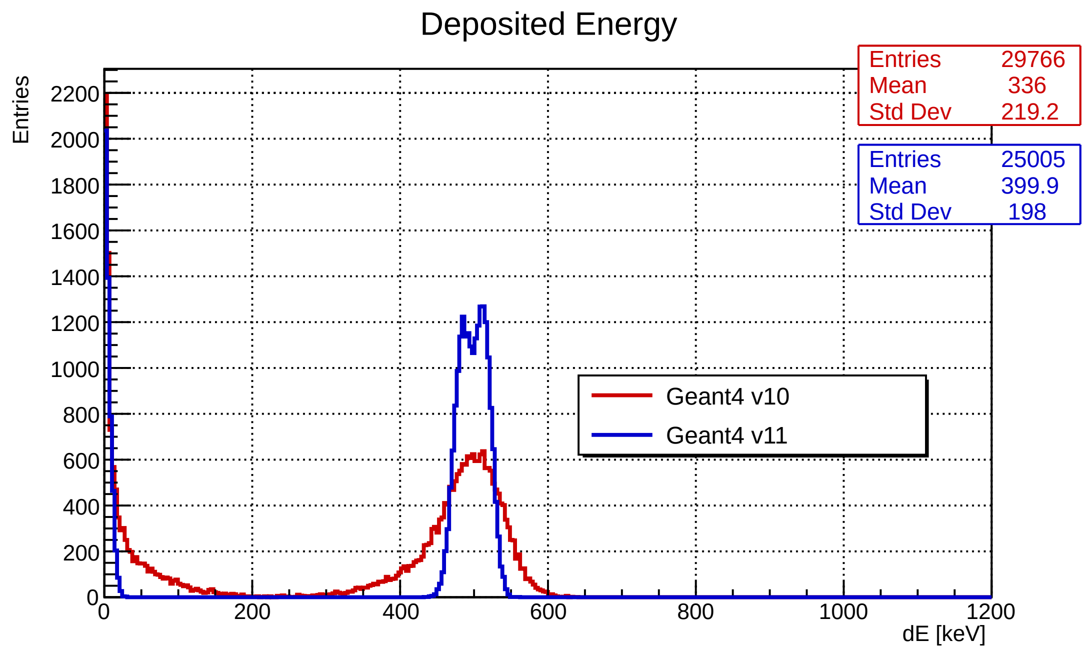


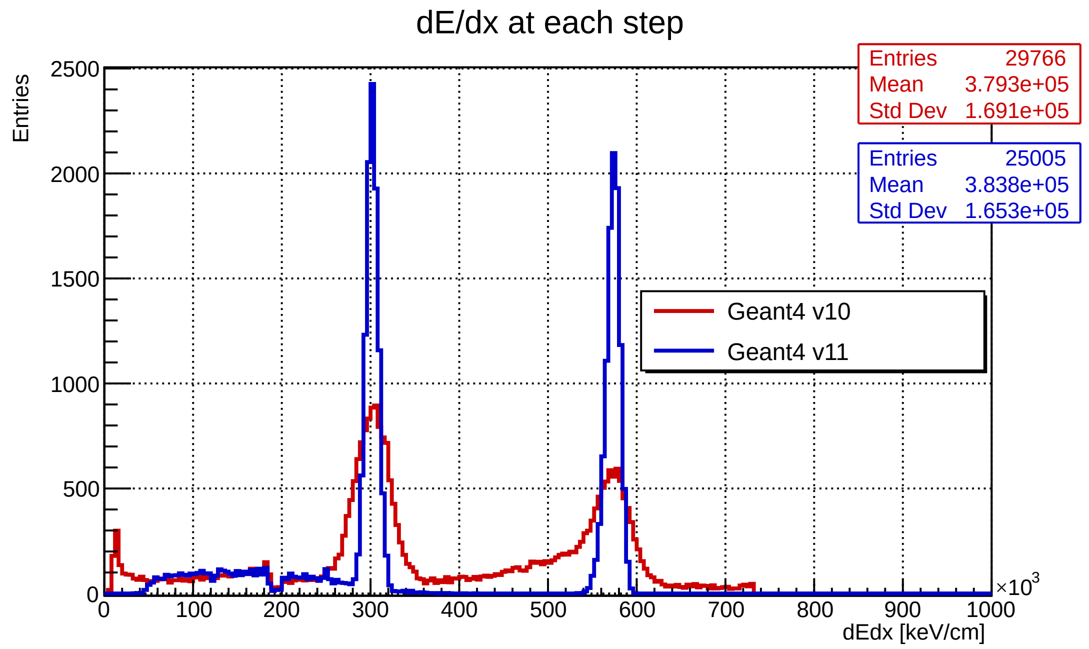
Huge increase in memory consumption in Geant4 v11 tuned when simulating Muons

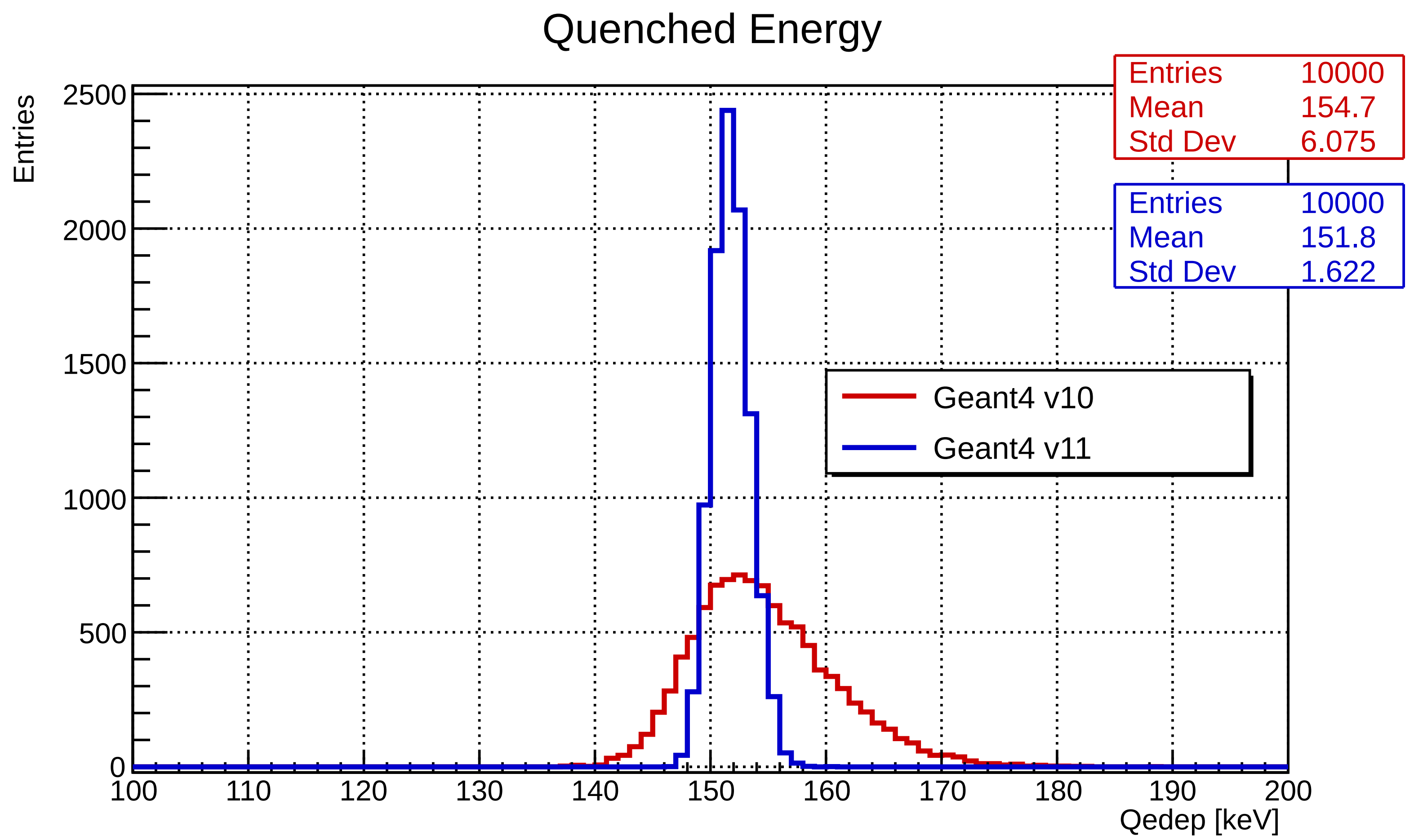
Proton simulation

Full simulation of 10 000 events of 1 MeV proton

Birks Law: $$Qedep = \sum_{i=1}^{N} \frac{dE}{1 + kB\frac{dE}{dx}}$$







On average, Geant4 v11 uses less steps to simulate protons
→ Distributions are narrower
Overall good agreement between versions

Mentions of updated data files and cross section for protons

Fitting kB on gammas

We can suppose that the Qedep distribution from **G4v10 is the "correct"** one and **fit G4v11** to match it

We have dE and dx distributions for each step. We can **recalculate Qedep for different values of kB** and find the value that minimise χ^2

$$Qedep = \sum_{i=1}^{N} \frac{dE}{1 + kB\frac{dE}{dx}}$$

$$\chi^2 = 2\sum_{i=1}^{N} \mu_i(\theta) - n_i + n_i \ln \frac{n_i}{\mu_i(\theta)}$$

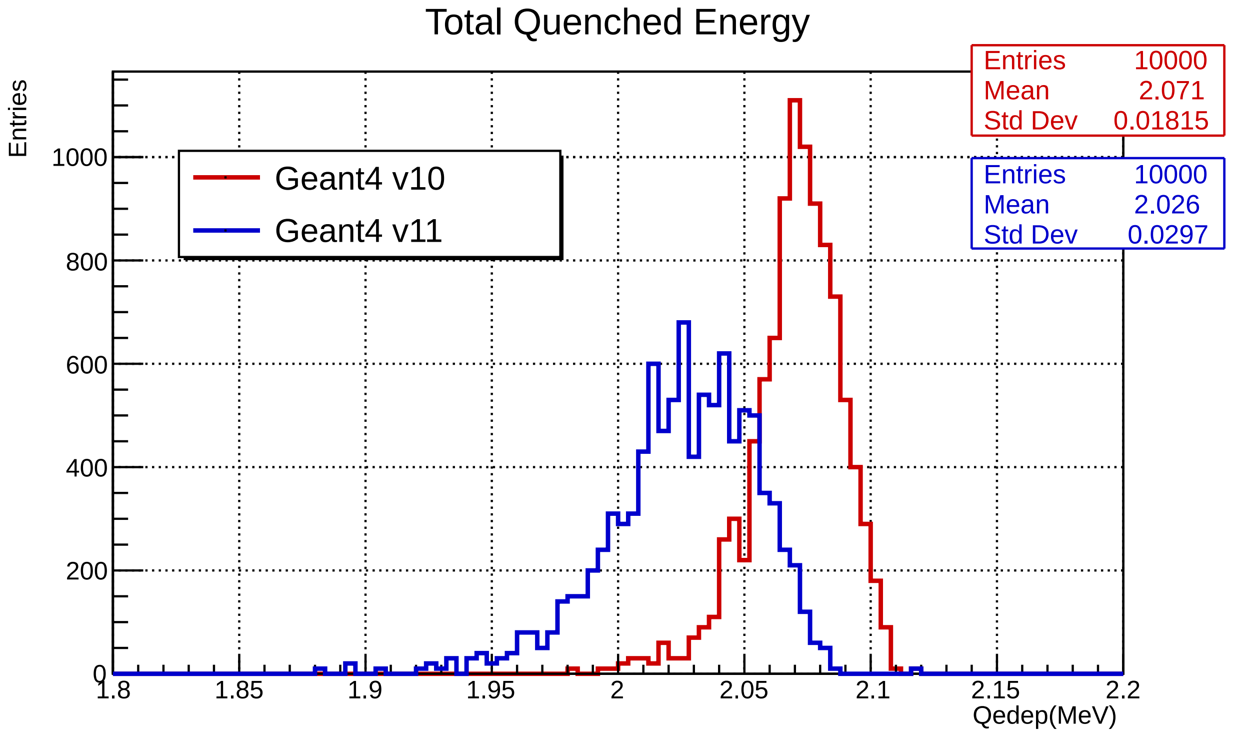
Recalculated Qedep distribution (G4v11)

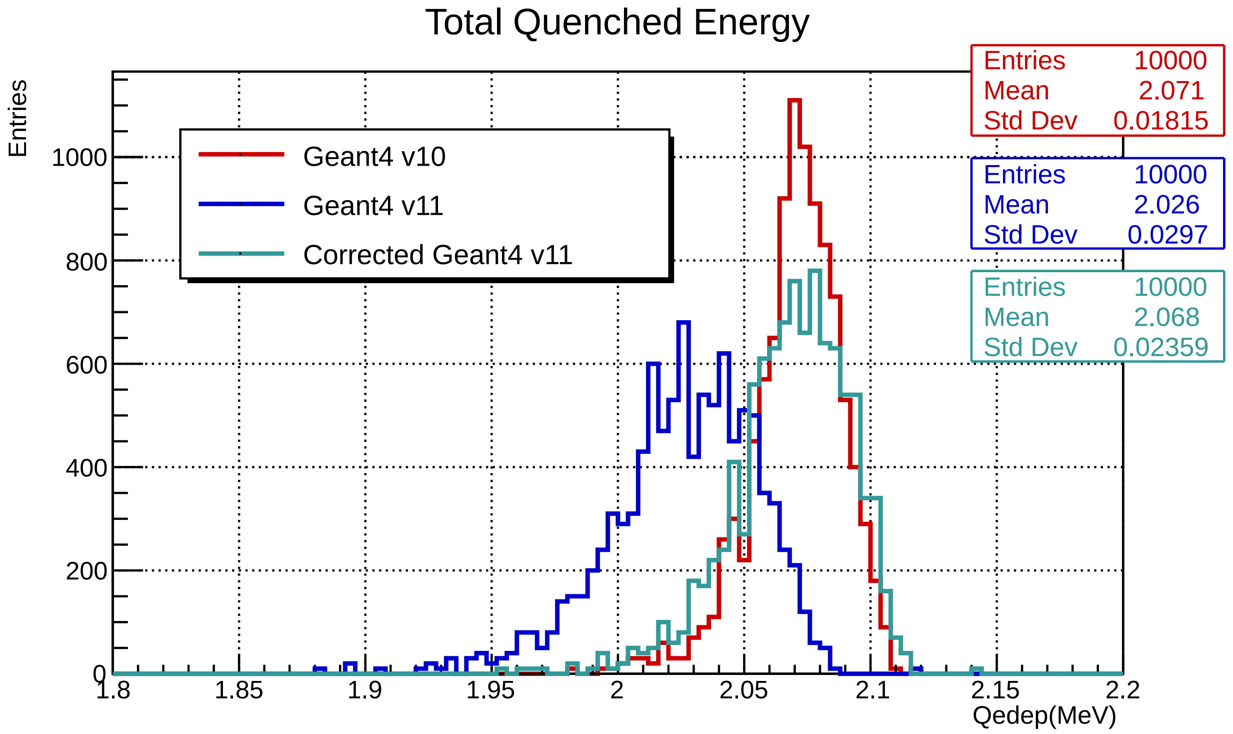
Reference Qedep distribution (G4v10)

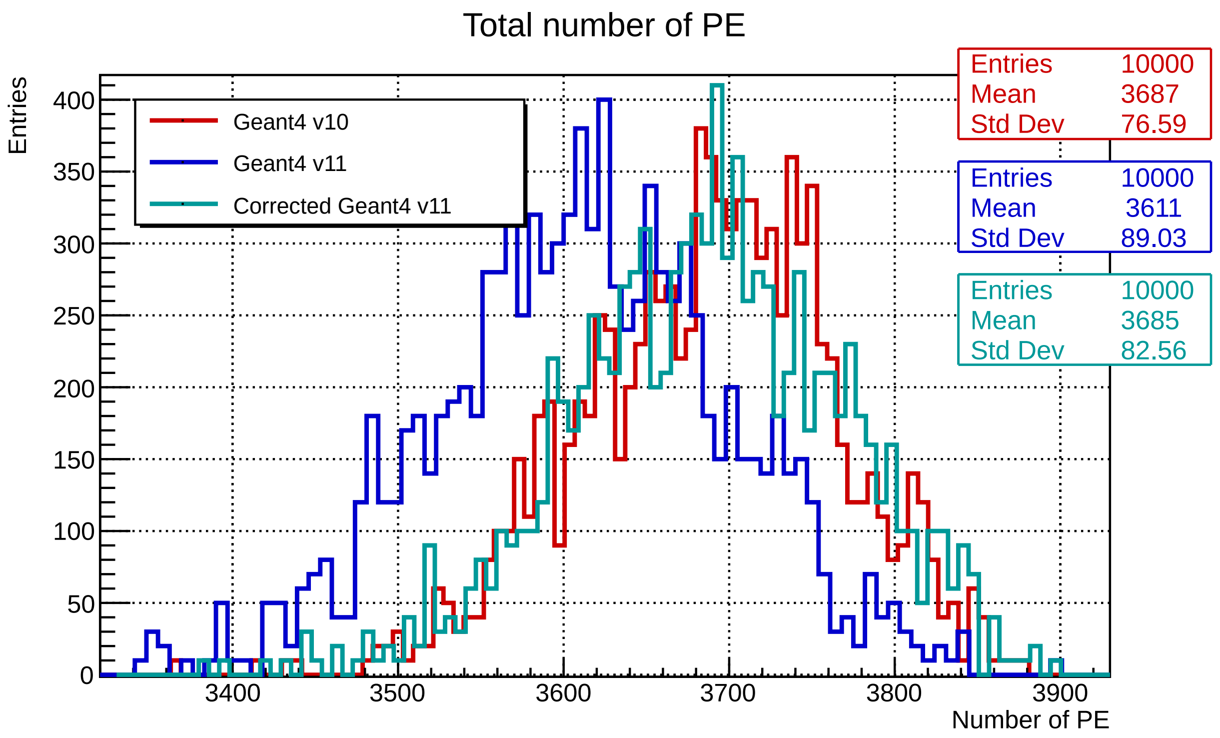
kB = 8.26e-3 g/cm2/MeV

kB = 12.05e-3 g/cm2/MeV

2.2 MeV Gamma





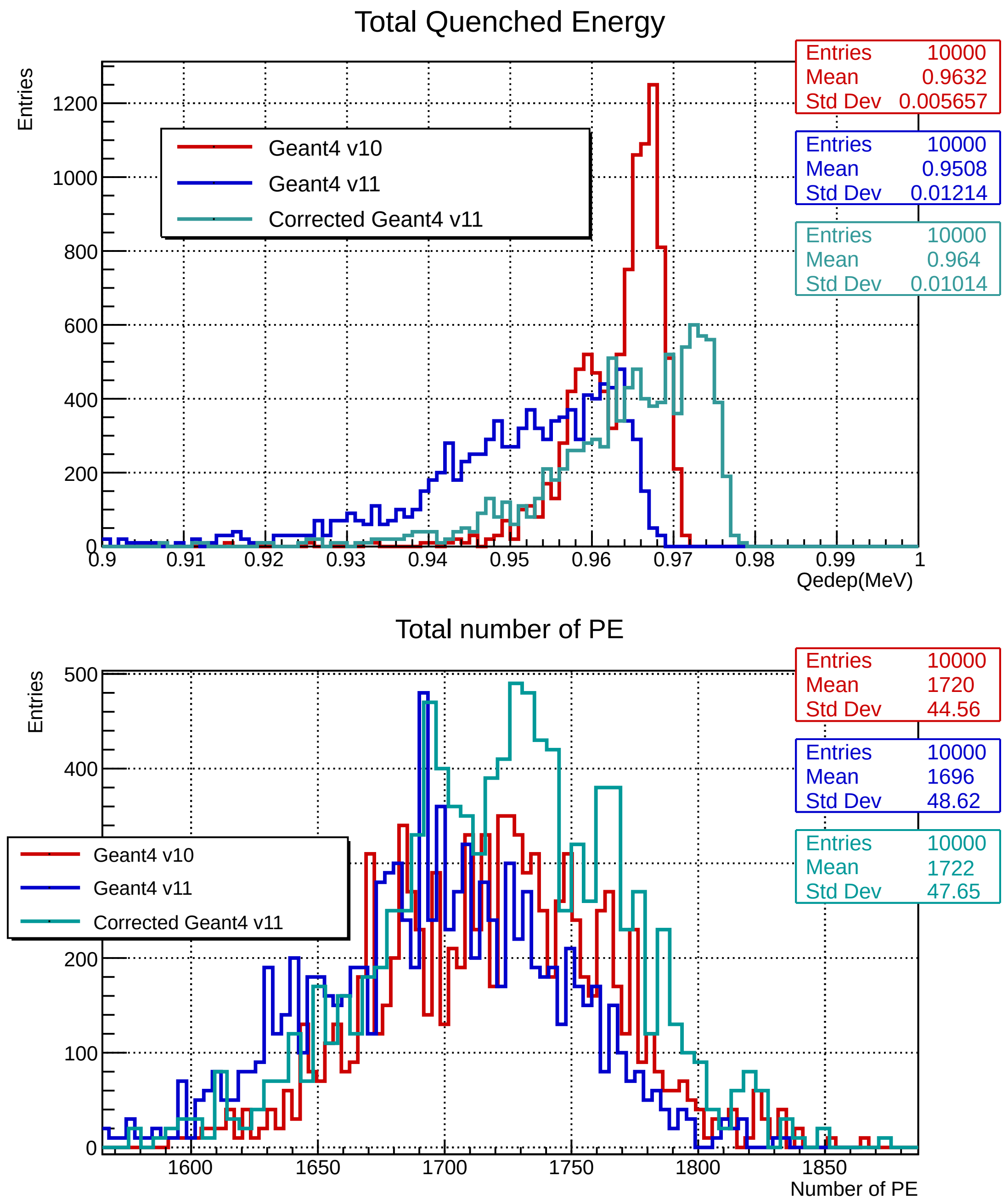


Correcting Qedep for electrons

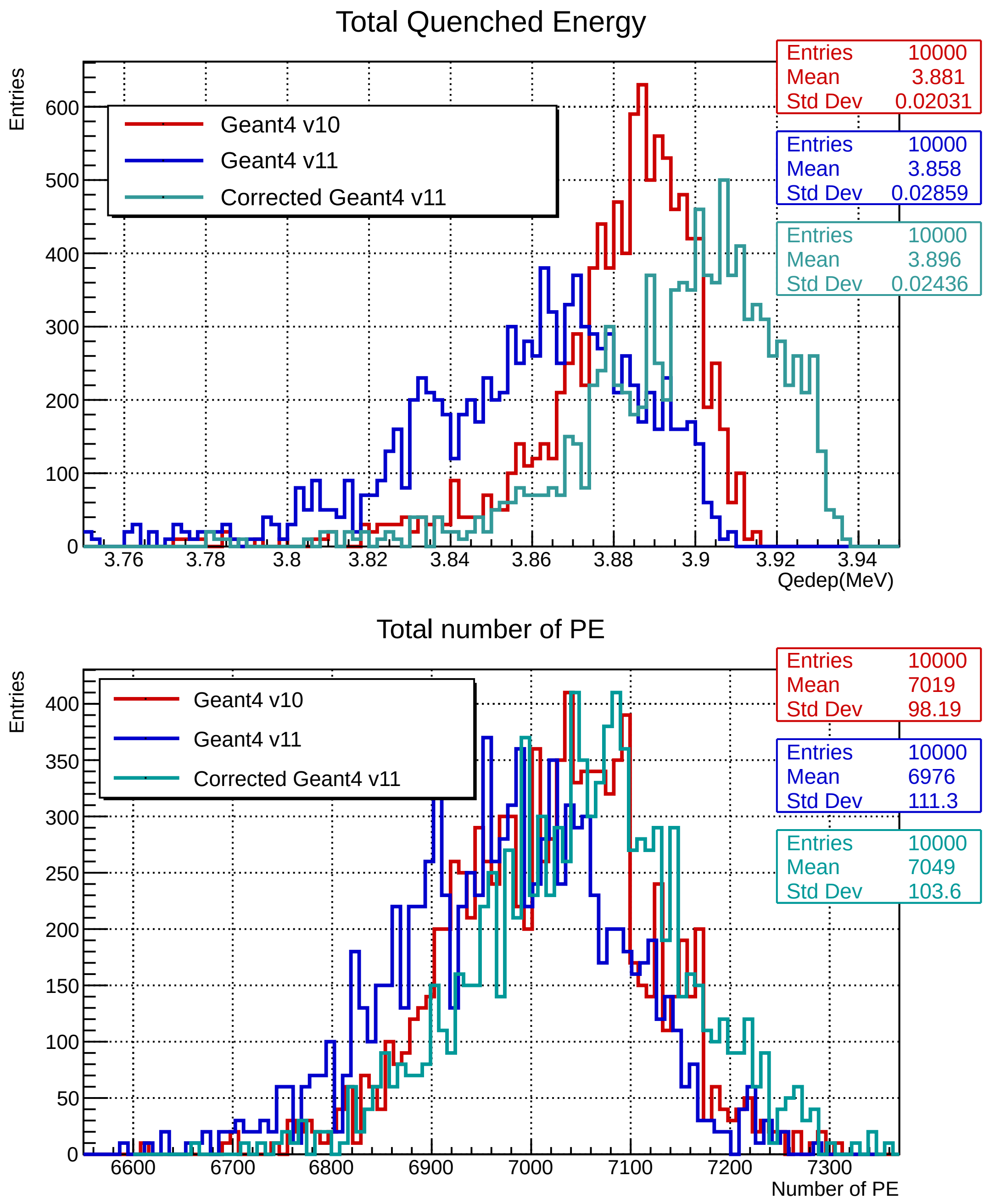
The kB value obtained from the fit on 2.2MeV Gamma is applied to the 1 MeV electron distributions
Even at higher energies the correction is still not good. Total number of PE is increased

kB = 8.26e-3 g/cm2/MeV
kB = 12.05e-3 g/cm2/MeV

1 MeV



4 MeV



10 MeV