Microdosimetry-based calculations of proton dose-averaged LET in liquid water: a novel application with Geant4-DNA.

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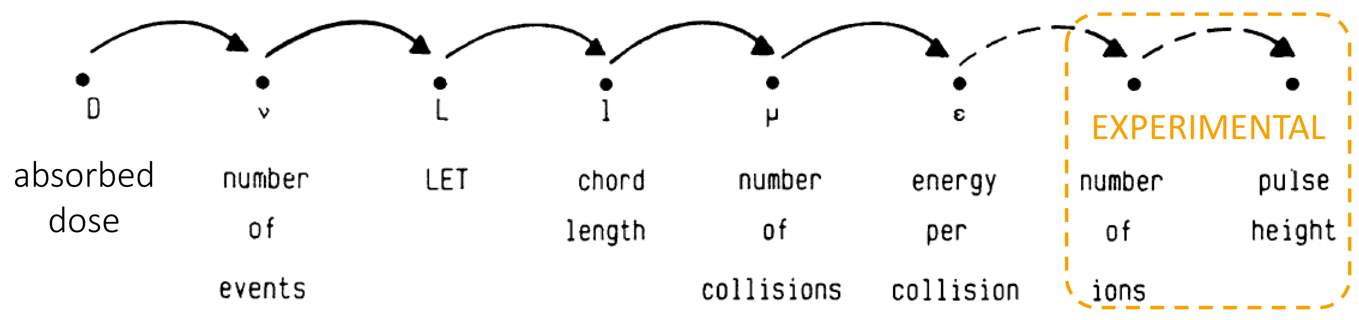
1. Abstract

The spatial distribution of energy deposition events is an essential aspect in the determination of the radiobiological effects of ionizing radiation at the cellular level. Microdosimetry provides a theoretical framework for the description of these events. Recently, several studies have turned to the formalism of microdosimetry to address problems such as the characterization of Linear Energy Transfer (LET) and Relative Biological Effectiveness (RBE) of ion beams for particle therapy applications [1]. Microdosimetry quantities and their distributions can be obtained by means of Monte Carlo simulations. In this work, we present a track structure Monte Carlo application, developed for the computation of microdosimetric distributions of protons in liquid water, based on Geant4-DNA [2,3]. This application provides two sampling methods "uniform and weighted", for the scoring of the quantities of interest in spherical sites, with diameters ranging from 1 to 10 µm. Besides, the distribution of energy deposited per event, the code computes also the distribution of energy imparted to the site per electronic collision of the proton, which has never been included in other microdosimetry examples in the official release of Geant4. With this distribution, the weighted average of the energy imparted per collision of the traversing proton can be computed and used to obtain the macroscopic dose averaged LET as proposed by Kellerer [4].
Finally, results obtained with our application are in good agreement with PARTRAC, which has been taken as the reference track-structure Monte Carlo tool for comparison [5].

2. Theoretical Framework

An **event** in a **site** is defined as the deposition of energy due to particles that are statistically correlated. The shape of the **single event distribution** reflects various stochastic factors [4]:



The influence of the different random factors on the single event distribution (V_1) can be assessed in terms of the **relative variances** of the LET distribution (V_L), the chord length distribution (V_l) and the straggling distribution (V_s):

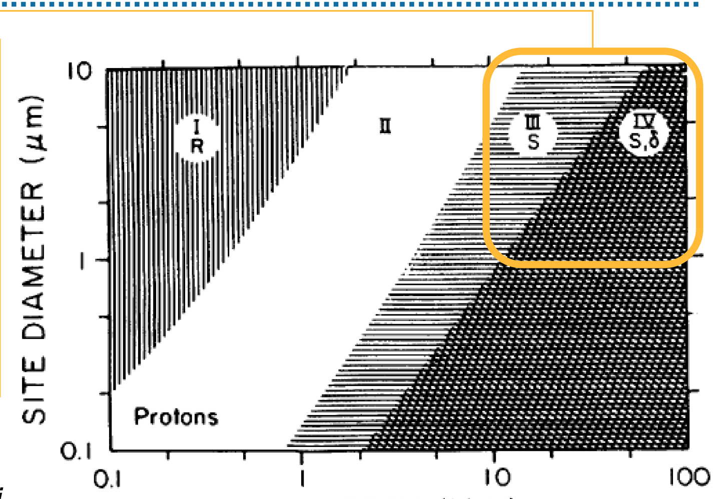
$$V_1 = V_L + V_l + V_L V_l + V_s$$

Assumptions:

- primary particle ranges considerably larger than site dimensions;
- straight track segments.

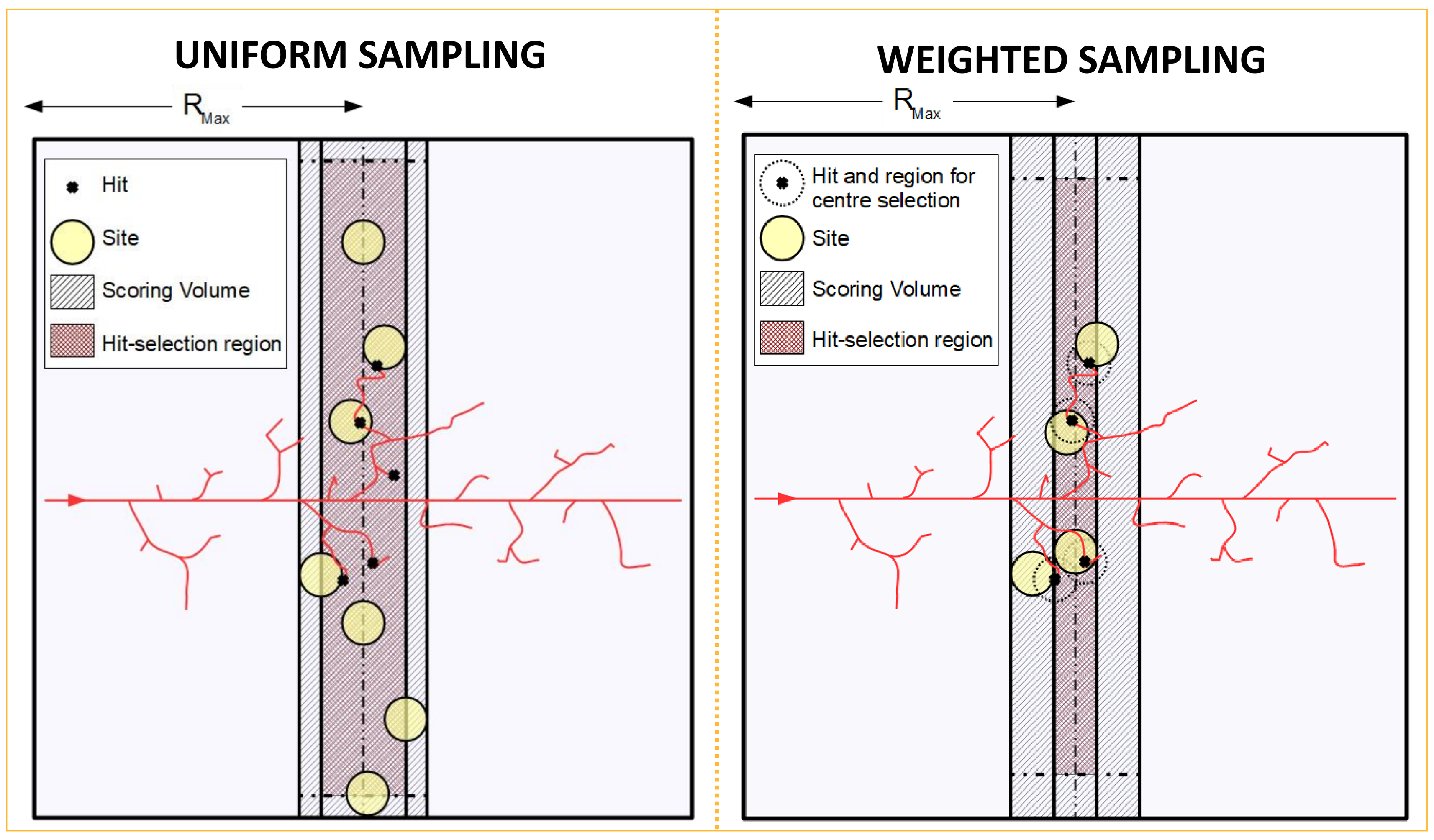
In this region, where energy loss straggling (S) and energy dissipation by delta-rays are relevant to the energy deposition, the formula for the relative variance for spherical sites is:

$$\bar{y}_d = \frac{9}{8}\bar{L}_d + \frac{3}{2d}\delta_2$$

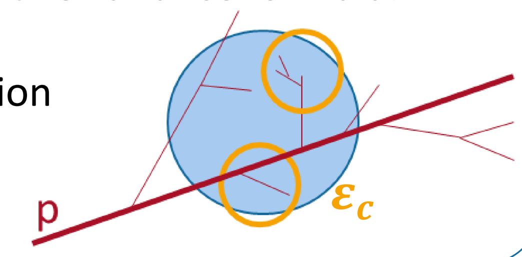


- d is the site diameter (spherical sites).
- $\bar{y}_d$ is the dose mean lineal energy: $\bar{y}_d = \frac{1}{\bar{l}}\frac{\int \epsilon_i^2 f(\epsilon_i)\mathrm{d}\epsilon_i}{\int \epsilon_i f(\epsilon_i)\mathrm{d}\epsilon_i}$.
- δ_2 is the weighted average of the energy imparted to the site per collision (ε_c) of the traversing particle: $\delta_2 = \frac{\int \varepsilon_c^2 w(\varepsilon_c)\mathrm{d}\varepsilon_c}{\int \varepsilon_c w(\varepsilon_c)\mathrm{d}\varepsilon_c}$.

3. Simulations

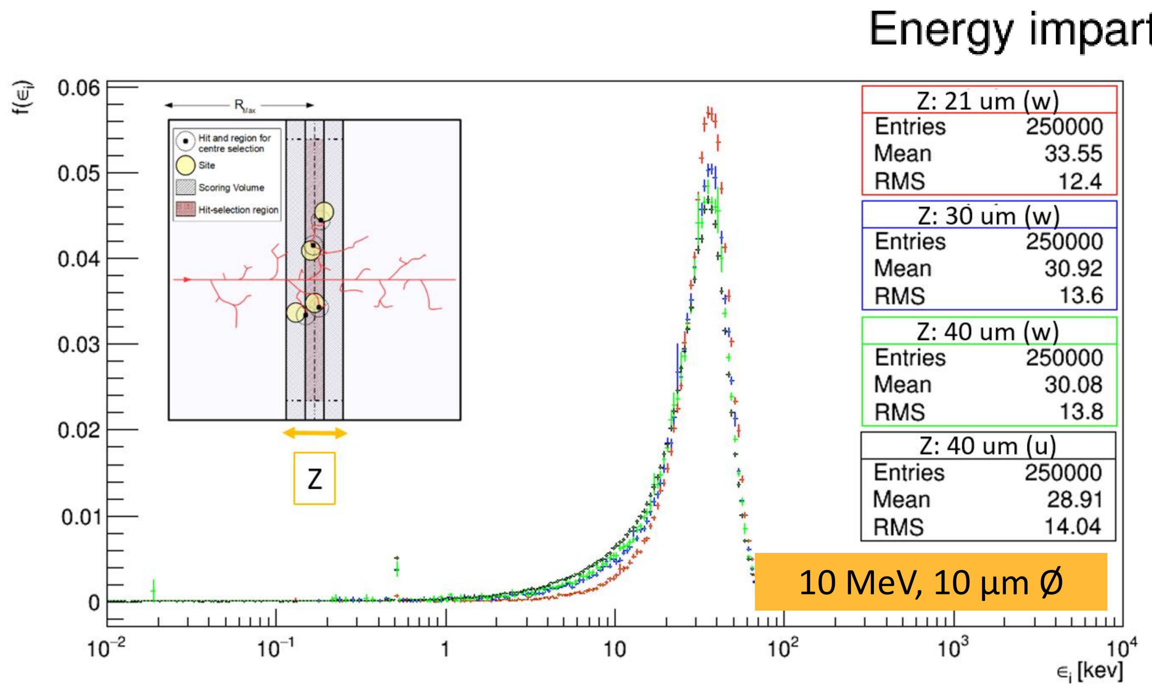


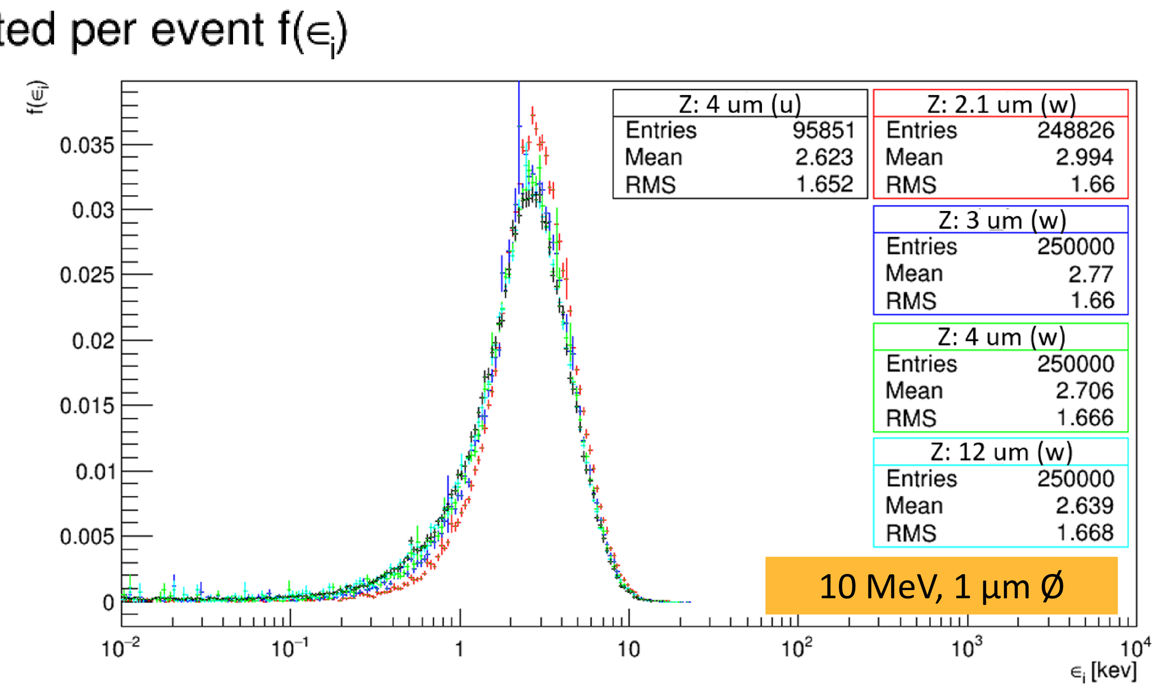
- A user macro allows to select:
  - Dimensions of world volume, scoring volume, hit selection region and site.
  - Beam characteristics (energy distribution and spatial distribution).
  - Type of sampling (uniform or weighted).
  - ROOT output format: histograms or trees with detailed information of tracks.
- The code computes the three distributions involved in the relative variance formula:
  - Distribution of energy deposited per event.
  - Distribution of energy deposited per proton collision
  - Distribution of chord length.

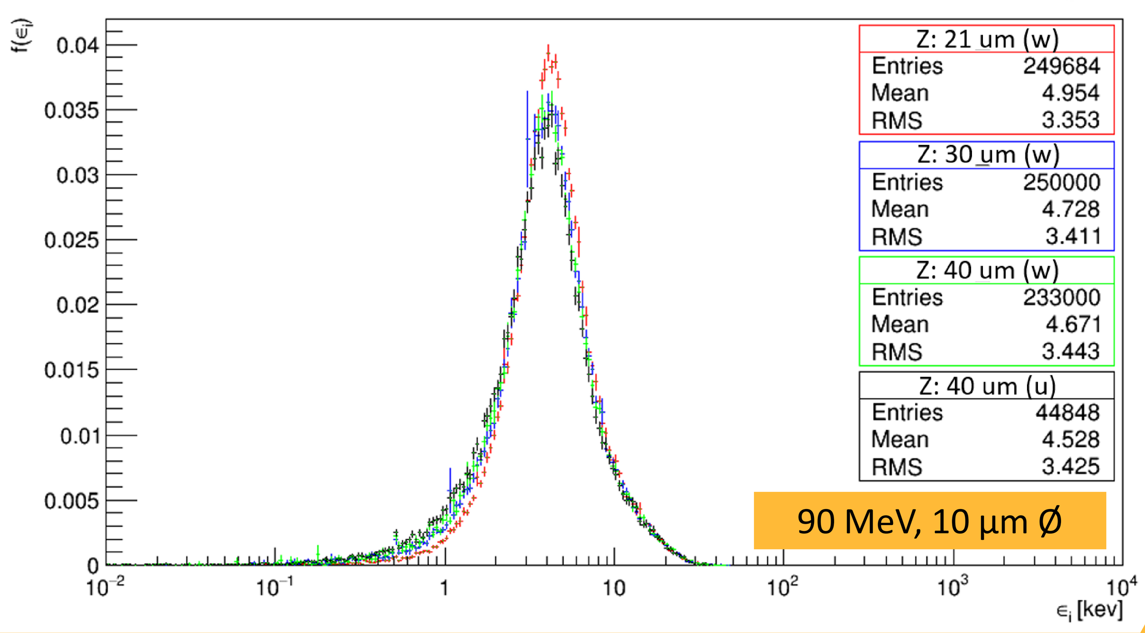


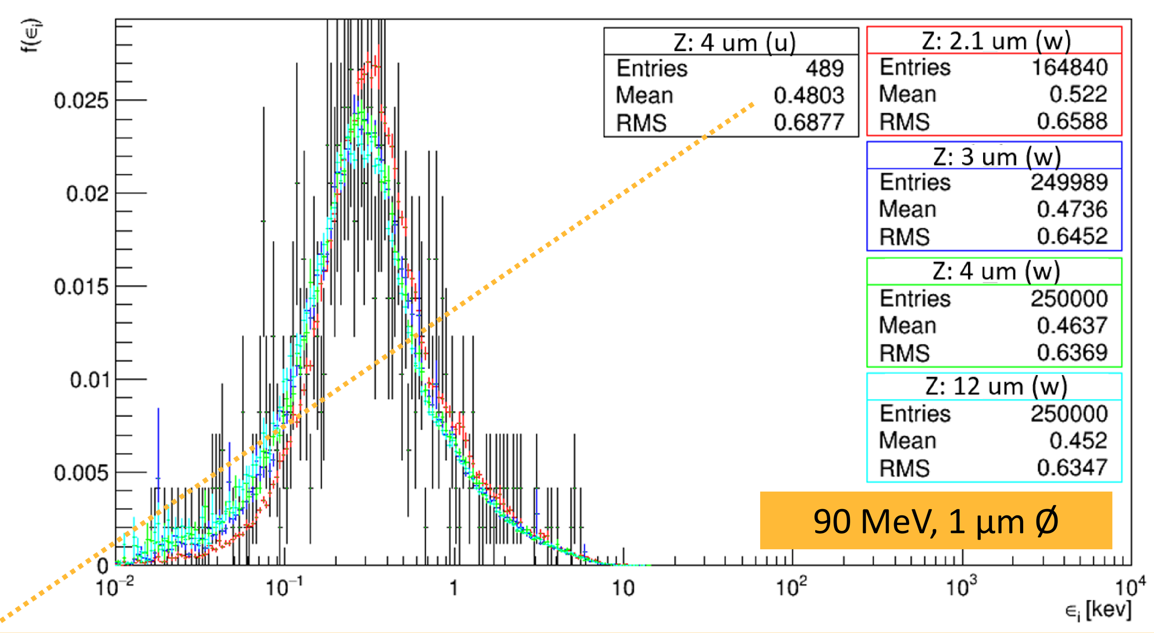
4. Results

Energy imparted per event f(ε_i)

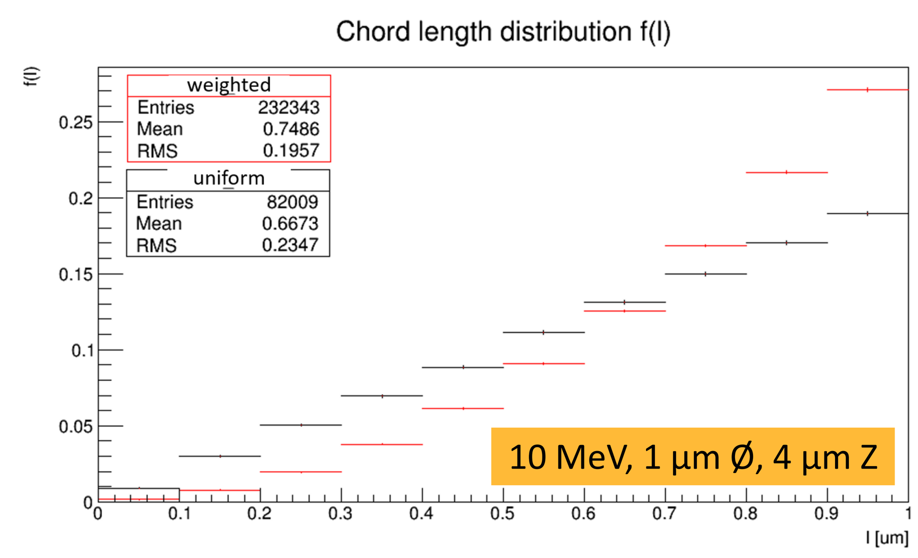




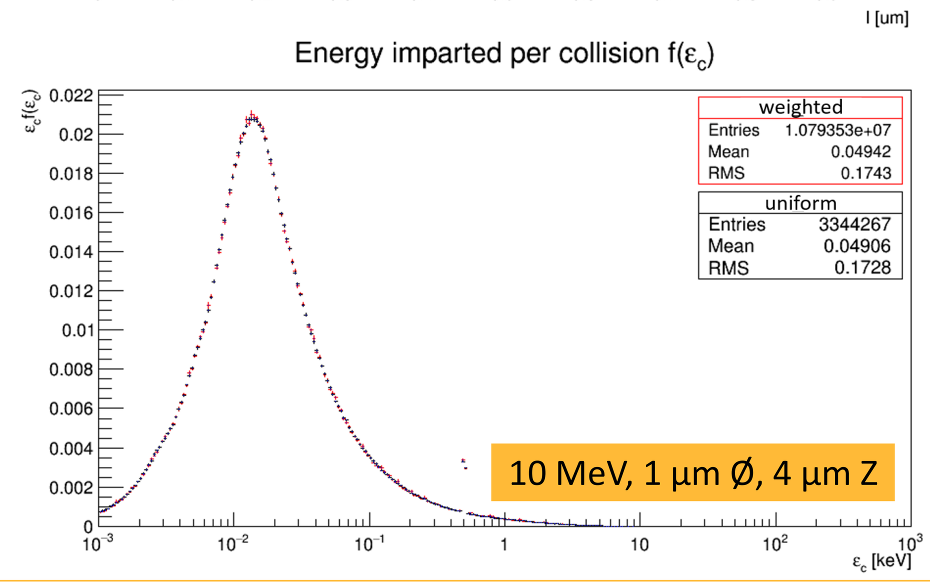




Chord length distribution f(l)

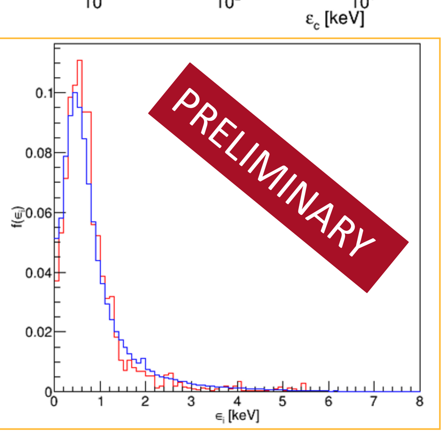


Energy imparted per collision f(ε_c)



Uniform sampling **(u)** is, theoretically, more robust than weighted sampling **(w)**, but highly inefficient when it comes to small sites and high energies. For a of 1 µm diameter and a proton energy of 90 MeV, uniform sampling has an collection efficiency of 0.3%, compared to the 100% efficiency of the weighted sampling method.

PARTRAC COMPARISON: Distribution of f(ϵ_i) computed with our Geant4-DNA application (blue) and compared with PARTRAC (red), for 40 MeV protons in spherical sites of 1 µm diameter.



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