Nuclear recoils simulations with SRIM

CYGNO SIMULATION MEETING – 23/11/2020

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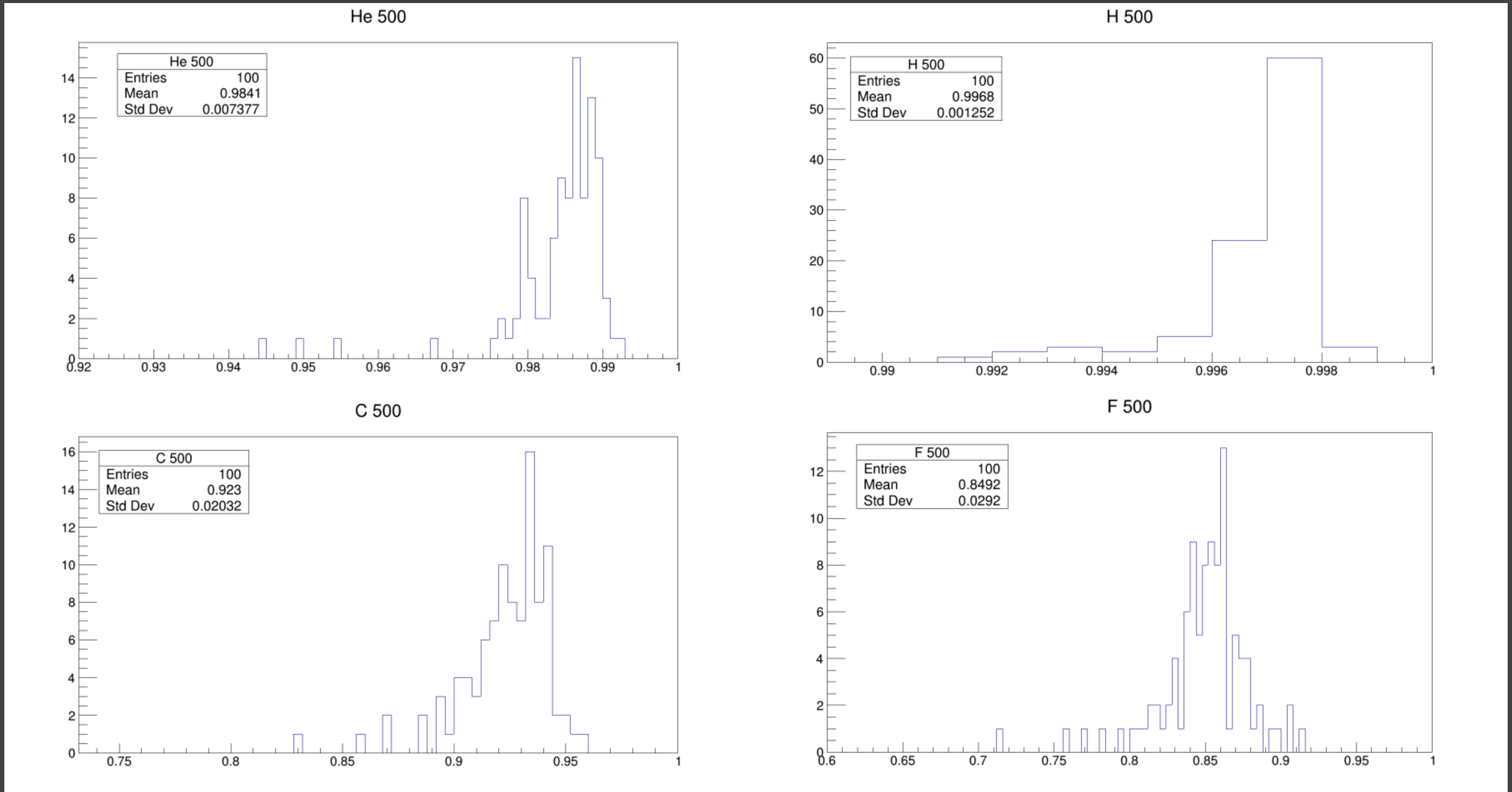
pySRIM simulation

- We managed to run pysrim
- 100 ions for each energy (1->500 keV) for each element (H, He, C, F)
  - It took a total of 6 days…
- Quenching factor evaluation
- Spatial distribution of ionization electrons

Quenching factor



For each element of each energy we considered the distribution of $\frac{E_{ioniz}}{E_{tot}}$

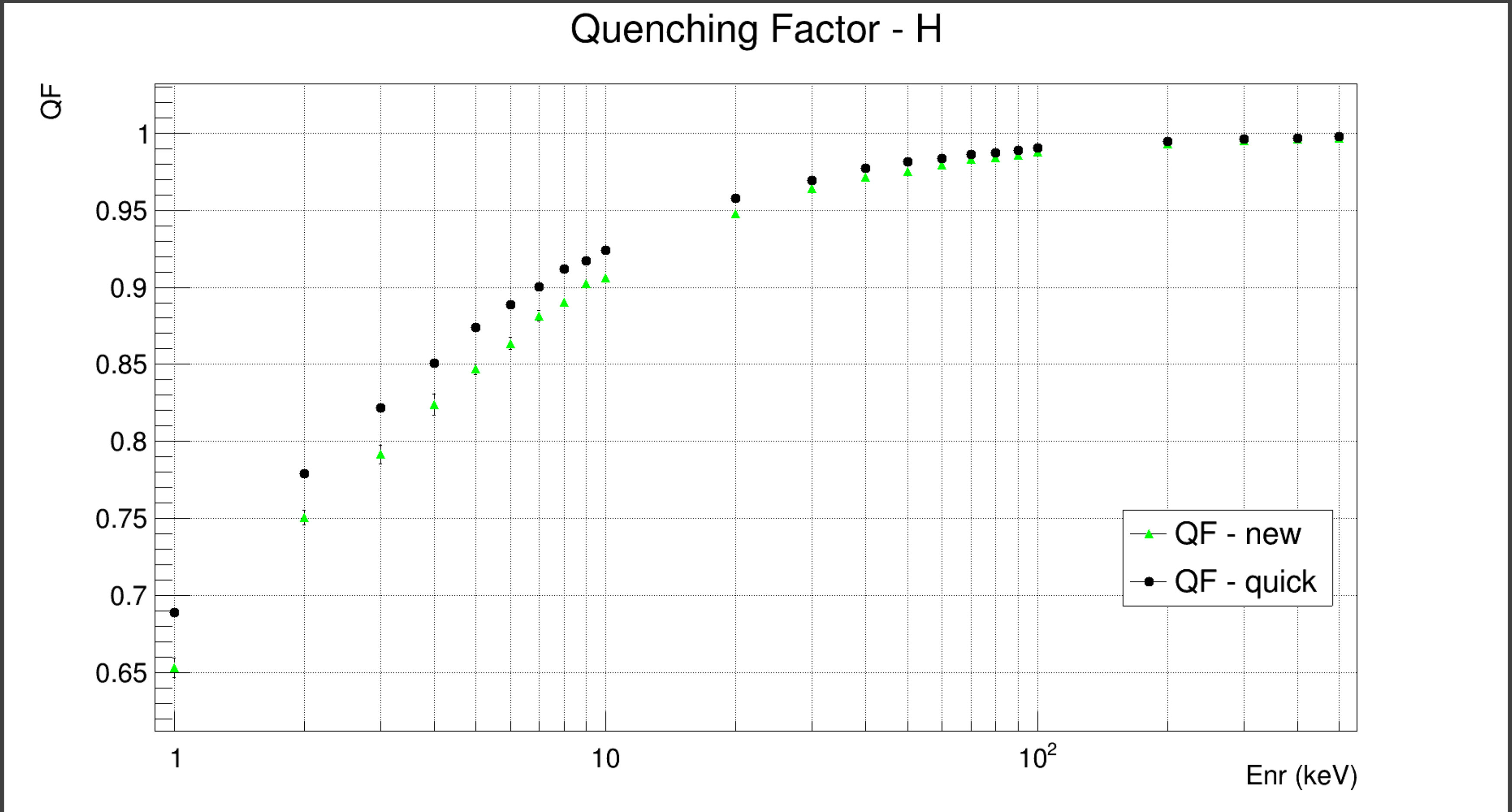
From each histogram we take the mean and the standard deviation

Output file:

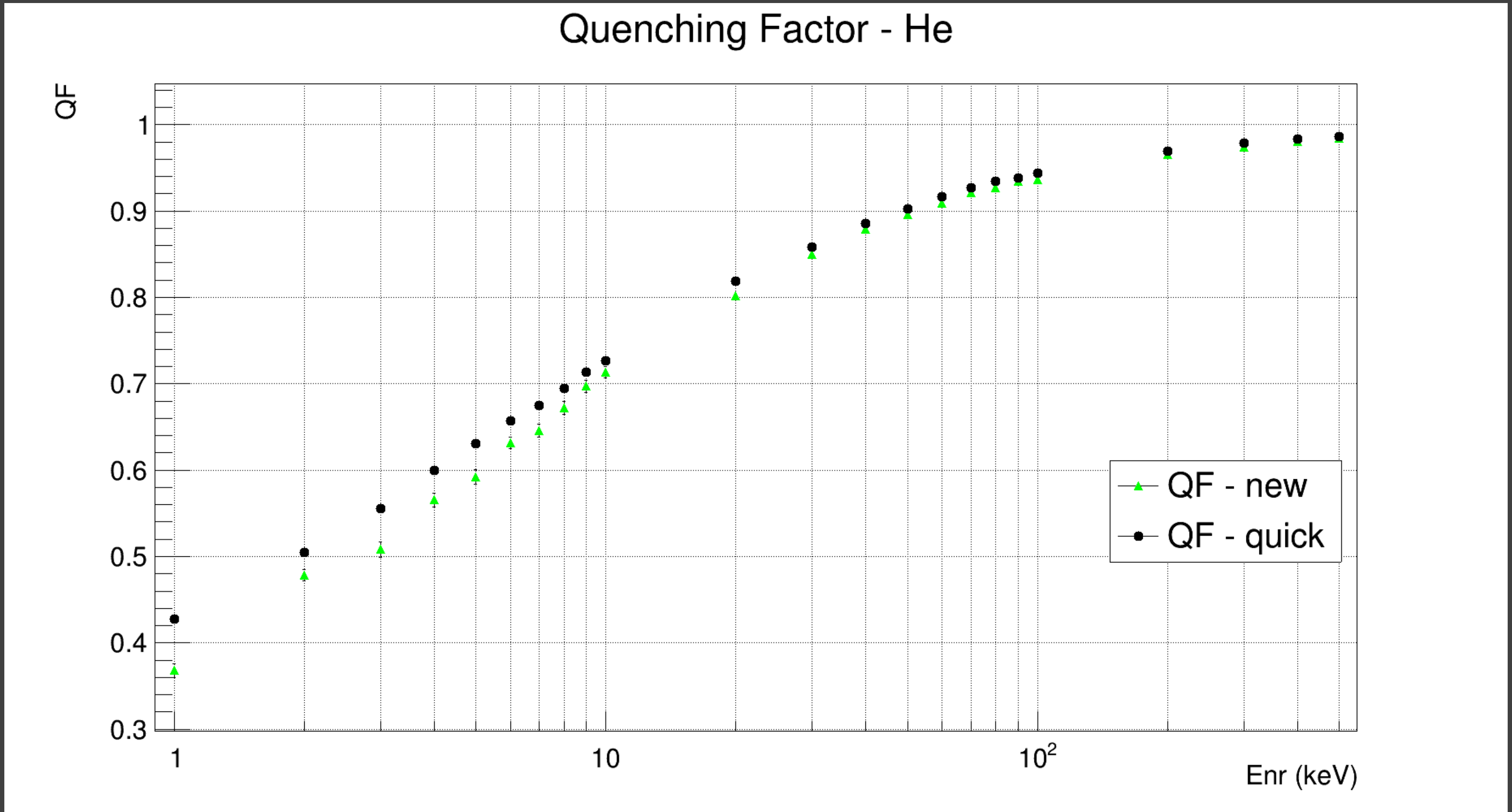
E[keV]	QF	ΔQF
1	0.367841	0.00752661
2	0.478328	0.00690195
3	0.508106	0.00915467
4	0.565443	0.00793515
5	0.592212	0.00814013
6	0.631556	0.00671801
7	0.645395	0.00743269
8	0.672503	0.00758357

where $\Delta QF = \sigma/\sqrt{n}$

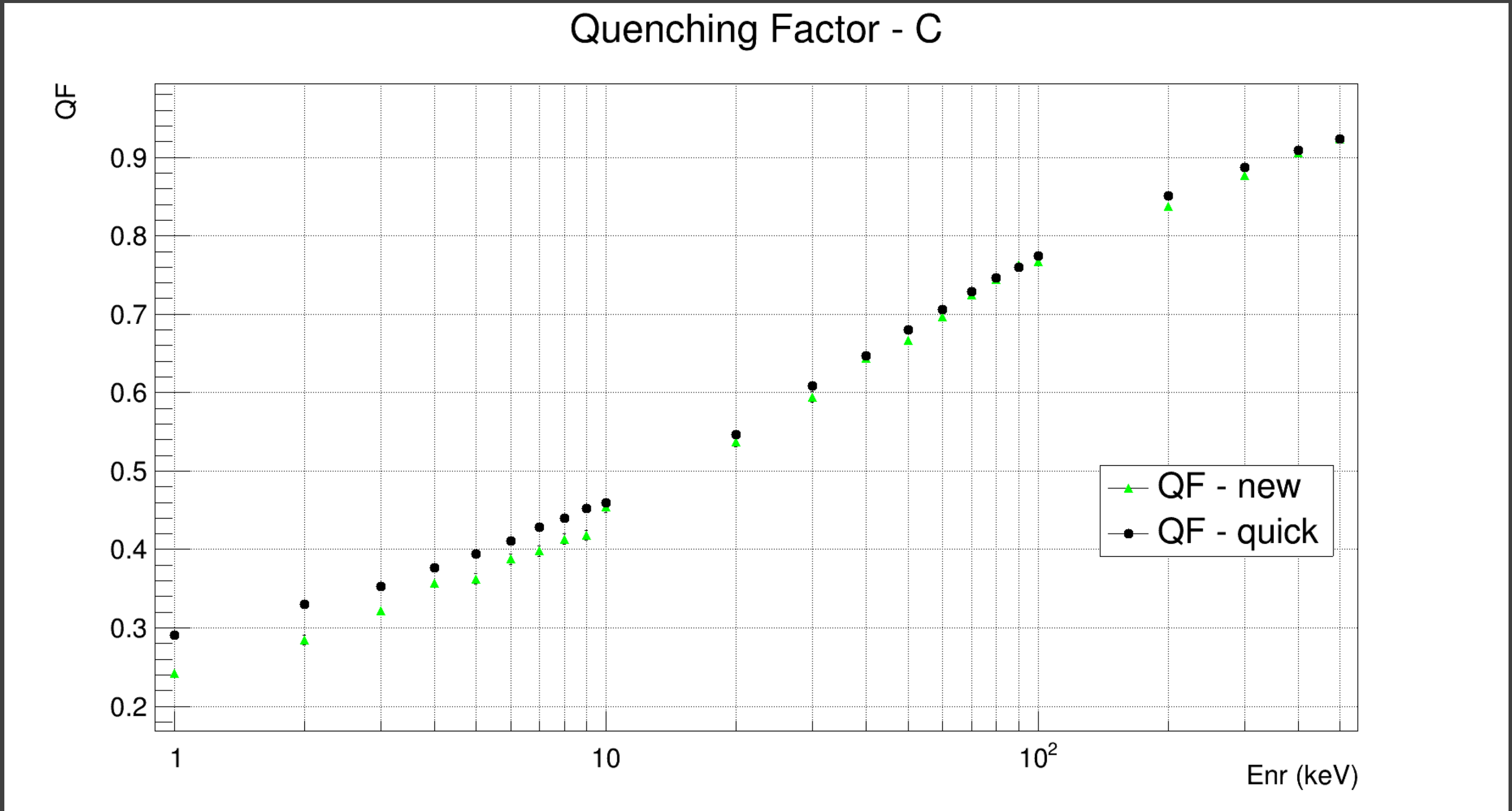
Quenching factor



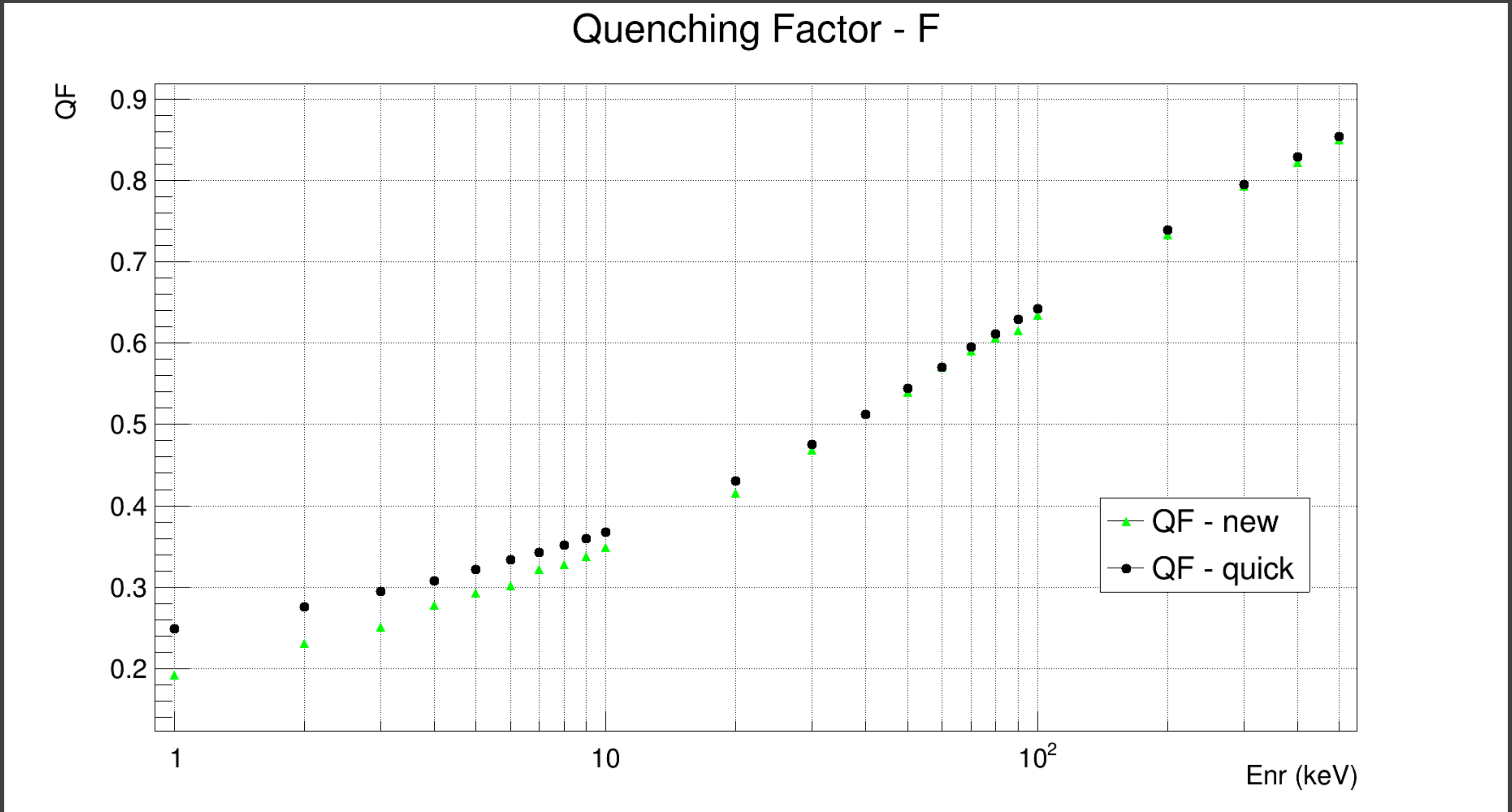
Quenching factor



Quenching factor



Quenching factor



Ionization profile

- SRIM was not developed to reconstruct the (ionization) energy loss along the track
- We thought we could retrieve the information we need from **Ioniz-3D.txt** (ionization energy losses as a function of 2D position)
  - But it's likely to have ambiguity anyway (points in the track with the same x and y coordinates)
- Two possible solutions:
  - <u>with the QF</u>: the product of energy loss and QF gives the energy lost by ionization; dividing by the ionization potential results in the average number of electrons
  - <u>with the w-value</u>:

$w = \frac{T}{N}$ T = energy of incident ion, N = number of electron-ion pairs formed

The ratio between *total* energy lost and the w-value is the average number of electron-ion pairs

Once we obtain the average number of electron-ion pairs produced at each position, we can extract, at each step, the number of electrons along the track from a Poisson distribution

COLLISON.TXT

Primary ion

Coordinates of recoil

Energy of recoil

```
³00001³19.56E+00³11135.E+03³-2753.E+02³-1404.E+03³0000.00³  F ³35134.E-03³ <== Start of New Cascade  ³
===================================================================================================
  Recoil  Atom  Energy(eV)   X (A)       Y (A)       Z (A)    Vac  Repl  Ion Numb 00001=
Û 00001    09   35134.E-03 1113.E+04 -2753.E+02 -1404.E+03  1    00 Û<ÄPrime RecoilÛ
Û 00002    02   66796.E-04 1114.E+04 -2720.E+02 -1400.E+03  1    00 Û
Û 00003    02   38494.E-06 1114.E+04 -2719.E+02 -1400.E+03  0    01 Û
Û 00004    02   56120.E-04 1114.E+04 -2719.E+02 -1400.E+03  1    00 Û
===================================================================
```

Primary recoil

Energy loss =
(Energy lost to cascade) + other

We use these information to take into account the contribution of the cascades to the track

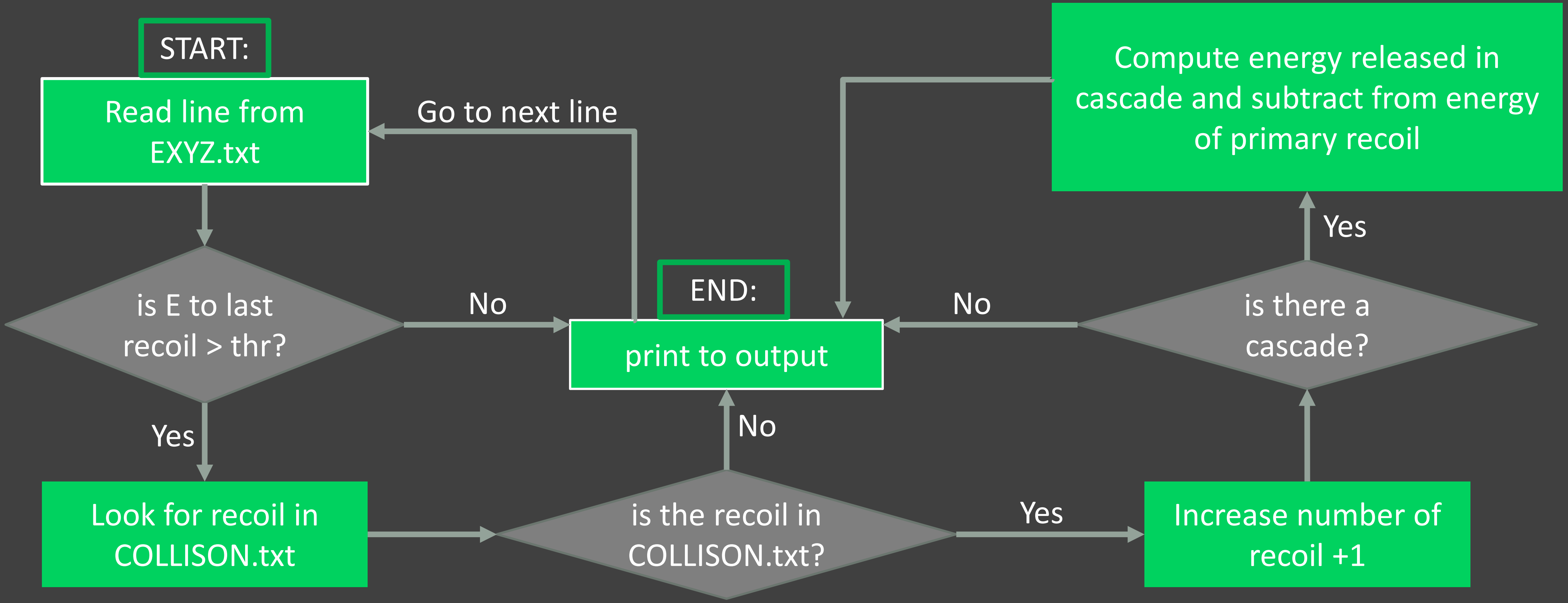
Secondary recoils (cascade)

EXYZ.TXT

- Ion energy as a function of its position in 3D
- *Energy lost to the last recoil* is also given
    - We can merge with the info from COLLISON.TXT
- The step is defined by an energy interval (set by the user)
    - We use a multiple of the **w value** (~42 eV)

```
=====================================================================
=                    Ion Energy vs Position File                    =
=====================================================================
=   AXIS DEFINITIONS: X=Depth, Y,Z= Lateral plane of target surface.=
=   (If beam enters target at an angle, this tilt is in Y direction)=
=   Shown are: Ion Number, Energy (keV), X, Y, Z Position           =
==================  CALCULATION   DATA  =============================
 Ion Data: Name, Mass,    Energy , Energy Interval
           H     001.01  100keV     130eV
=====================================================================
Ion        Energy     Depth (X)      Y           Z       Electronic   Energy Lost to
Number     (keV)     (Angstrom)  (Angstrom)  (Angstrom)  Stop.(eV/A)  Last Recoil(eV)
------- ---------- ---------- ---------- ---------- ----------- --------------
0000001 1.0000E+02  0.0000E+00  0.0000E+00  0.0000E+00  8.3750E-03  0.0000E+00
0000001 9.9840E+01  1.7918E+04  6.8529E+00  7.8415E+00  8.3745E-03  6.8090E-08
0000001 9.9710E+01  3.3455E+04  2.5936E+01  8.0856E+00  8.3740E-03  1.3046E-08
0000001 9.9580E+01  4.8717E+04  4.8929E+01 -3.1712E+00  8.3736E-03  2.3807E-08
0000001 9.9450E+01  6.4254E+04  7.4421E+01 -3.1579E+01  8.3732E-03  6.7205E-09
0000001 9.9320E+01  7.9742E+04  1.0286E+02 -6.6138E+01  8.3727E-03  3.4368E-07
```

Spatial energy distribution reconstruction



Cascades are not what they seem…

Cascades in COLLISON.txt are actually made of sub-cascades

The collisions that are listed are either a secondary recoil, or a tertiary recoil, etc…

→ If we can't reconstruct the cascade correctly, we would lose information on the spatial distribution of energy deposition

Compute energy released in cascade and subtract from energy of primary recoil

```
=================================================================================
  Recoil Atom Energy(eV)   X (A)      Y (A)      Z (A)    Vac Repl Ion Numb 00001=
Û 00001   09  21960.E-02 4327.E+02  2034.E+02  2779.E+02  1   00 Û<ÄPrime RecoilÛ
Û 00002   02  12227.E-03 4326.E+02  2069.E+02  2692.E+02  1   00 Û
Û 00003   02  17265.E-03 4326.E+02  2068.E+02  2694.E+02  1   00 Û
Û 00004   02  16205.E-03 4325.E+02  2067.E+02  2698.E+02  1   00 Û
Û 00005   02  15620.E-03 4322.E+02  2057.E+02  2724.E+02  1   00 Û
Û 00006   09  12919.E-02 4324.E+02  2031.E+02  2769.E+02  1   00 Û
Û 00007   09  25285.E-03 4267.E+02  2017.E+02  2553.E+02  1   00 Û
Û 00008   02  80912.E-04 4289.E+02  2007.E+02  2656.E+02  1   00 Û
==================================================================
```

Output file

Ion number	Recoil number	3D position (µm)			Deposited energy (eV)	Number of electrons	
4	4	22.5	21.18	-3.777	40.585	0	
4	4	22.498	21.185	-3.7765	110.415	2	
4	4	23.401	27.417	-5.1701	100.85	4	Cascade
4	4	24.3	35.862	-6.4363	134.88	3	
4	4	23.656	41.803	-8.2294	129.17	3	
4	5	24.21	50.06	-8.685	25.158	1	Primary recoil
4	5	24.47	50.3	-8.322	11	0	
4	5	24.211	50.065	-8.6848	115.262	3	Cascade
4	5	25.058	56.019	-6.0328	104.51	2	
4	6	25.71	59.44	-2.876	128.289	2	Primary recoil
4	6	29.43	58.99	2.241	43.408	2	
4	6	26.82	60.39	-2.109	7.6507	0	
4	6	26.61	60.21	-2.772	47.962	1	Cascade
4	6	25.711	59.437	-2.8757	77.375	3	
4	6	28.409	56.601	-4.6383	85.285	0	

Conclusions and future work

- We evaluated the quenching factor from a sample of 100 ions per energy per element
  - To do: larger sample for higher accuracy
- We can reconstruct the energy loss along the track, but we lose the details of the spatial distribution for some cascades
  - To do: understand how to *identify the tertiary* (and higher order) recoils OR make some assumptions on the deposited energy distribution along the secondary tracks (and lose some information/precision)
    - We could use the stopping power to estimate the fraction of energy lost at each position
    - or identify the recoils that give rise to secondary cascades and discard the details of the tertiary
    - or optimize the energy deposited in the cascade at each step to match the total energy
    - or distribute the total charges in a region around the primary collision point
    - The choice also depends on the spatial resolution (O(100μm))
    - …?
- Suggestions?