Nuclear recoil simulation with SRIM

CYGNO simulation meeting
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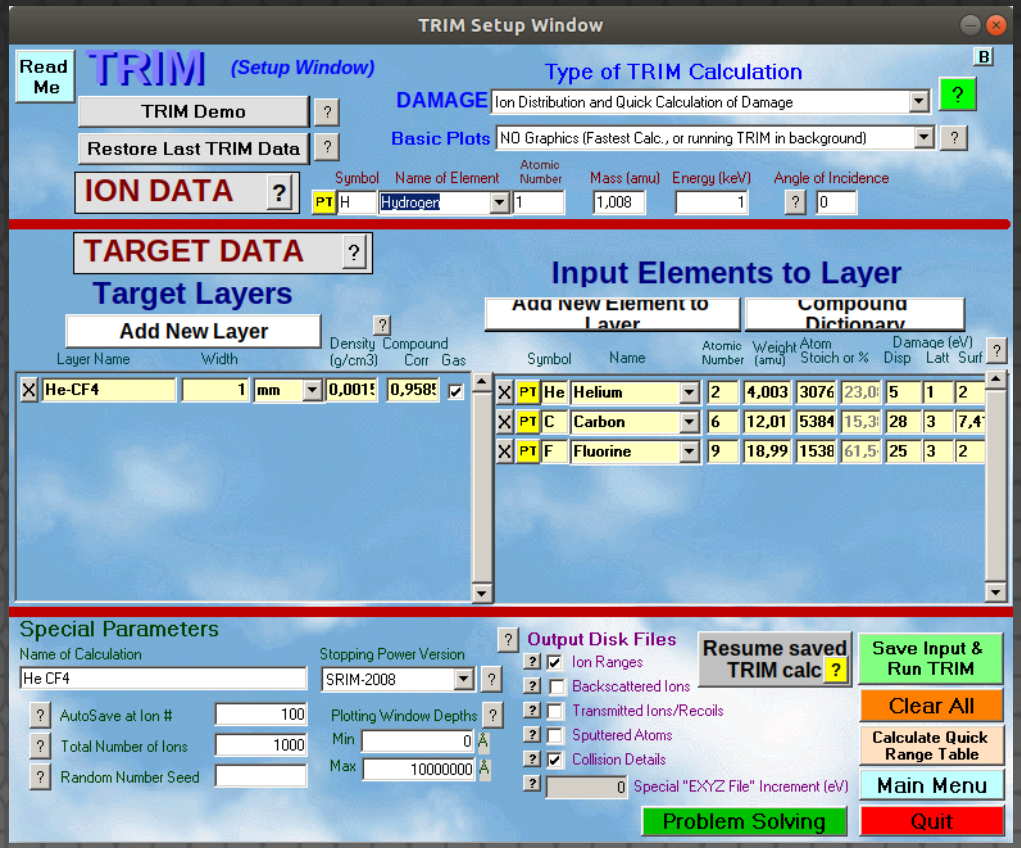
SRIM

- SRIM is a collection of software packages which calculate many features of the transport of ions in matter



- *Target*: density, width, layer composition (atomic percentages)
- *Ion*: element, energy, angle
- *Output*: n° of ions, plotting window, random number seed, output files
- *Type of calculation*:
  - **Quick**: "if you don't care about details of target damage"
  - **Full Cascade**: follows every recoil until its energy drops below the lowest displacement energy
  - **Monolayer collision steps**: every collision is calculated without any approximation

Quenching factor

- Quick calculation mode, 1000 ions per run
- IONIZ.TXT: primary and secondary ionization energy loss
  - Integrating over whole range results in the total ionization energy loss
  - $QF=(E_{ioniz,e}+E_{ioniz,recoil})/E$

Energy (keV)	(E)e (eV/ion)	(QF)e	(E)r (eV/ion)	(QF)r	(E)tot (eV/ion)	(QF)tot
1	647.477	0.647477	41.4202	0.0414202	688.897	0.688897
2	1491.7	0.745849	66.214	0.033107	1557.91	0.778956
3	2381.24	0.793747	84.8442	0.0282814	2466.08	0.822028
4	3307.53	0.826883	95.4481	0.023862	3402.98	0.850745
5	4263.85	0.85277	105.601	0.0211201	4369.45	0.87389
6	5216.2	0.869366	116.483	0.0194138	5332.68	0.88878
7	6179.19	0.882741	122.845	0.0175492	6302.03	0.90029
8	7168.58	0.896072	124.298	0.0155373	7292.87	0.911609
9	8124.42	0.902713	130.208	0.0144676	8254.63	0.917181
10	9103.29	0.910329	135.636	0.0135636	9238.92	0.923892

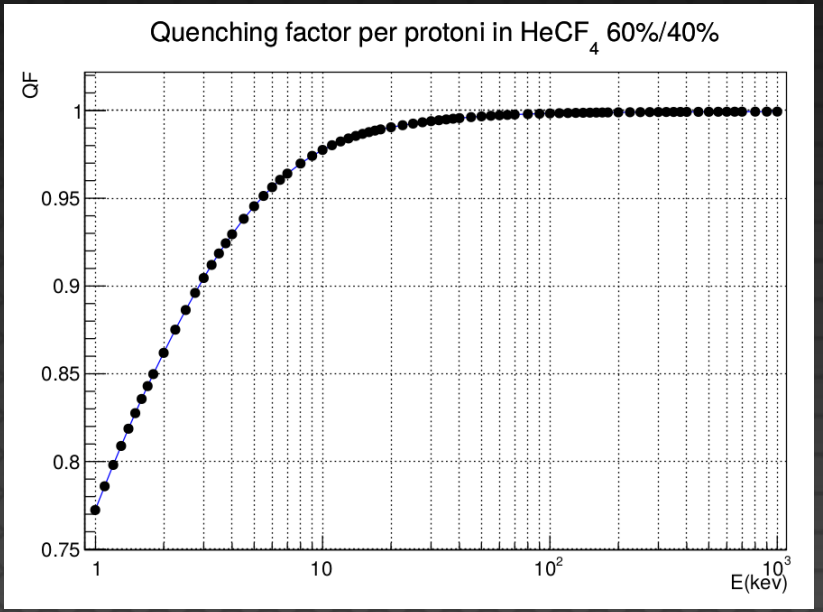
```
====== H (191) into Helium                          =======
        SRIM-2013.00
========================================
      Ion and Recoil IONIZATION
 See SRIM Outputs\TDATA.txt for details
========================================
====== TRIM Calc.=  H(10 keV) ==> He-CF4(  700 um) ============================
--------------------------------------------------------------------------------
-----------------------------------------------------------------
    Recoil/Damage Calculations made with Kinchin-Pease Estimates
-----------------------------------------------------------------
 See file :  SRIM Outputs\TDATA.txt   for calculation data
 Ion    =  H   Energy = 10 keV
============= TARGET MATERIAL ======================================
Layer 1 : He-CF4
Layer Width = 70000.E+02 A ;
  Layer # 1- Density = 6.511E19 atoms/cm3 = .0015 g/cm3
  Layer # 1- He = 23.0 Atomic Percent = 6.38 Mass Percent
  Layer # 1-  C = 15.3 Atomic Percent = 12.7 Mass Percent
  Layer # 1-  F = 61.5 Atomic Percent = 80.8 Mass Percent
=================================================================
 Total Ions calculated =001000.00
=============================================================
  Ionization Energy Units are  >>>>  eV /(Angstrom-Ion)  <<<<
=============================================================

  TARGET       IONIZ.       IONIZ.
  DEPTH         by           by
  (Ang)        IONS        RECOILS
-----------  -----------  -----------
700000.E-01  3320.13E-06  1257.07E-09
140000.E+00  3239.37E-06  4406.93E-09
210000.E+00  3203.42E-06  3517.30E-09
280000.E+00  3164.92E-06  7391.93E-09
350000.E+00  3206.12E-06  1270.25E-08
420000.E+00  3218.09E-06  2243.15E-08
490000.E+00  3127.07E-06  1798.85E-08
560000.E+00  3125.33E-06  9444.00E-09
630000.E+00  3107.91E-06  2000.71E-08
```

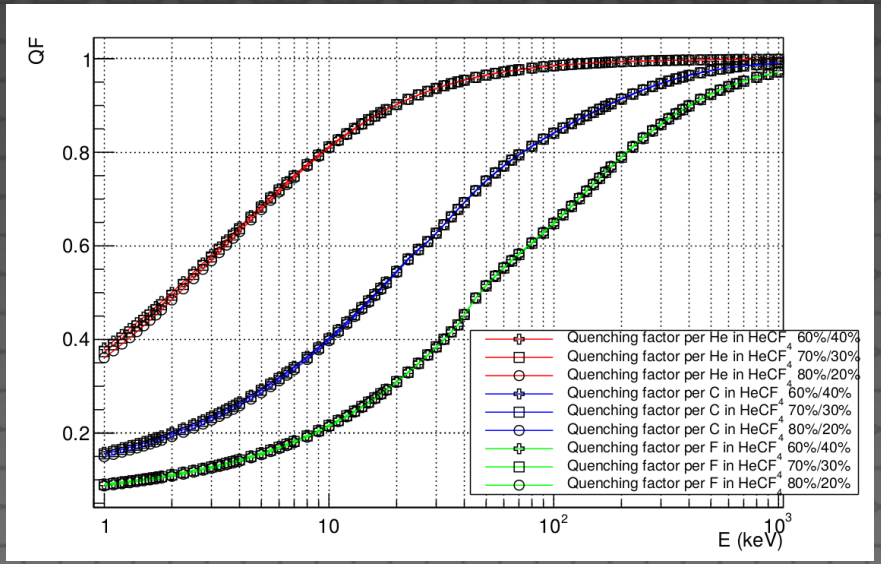
Quenching factor

- E.Marconato used the *Tables of Stopping Powers and Ion Ranges*

$$QF=(dE/dx)_{elec}/[(dE/dx)_{elec}+(dE/dx)_{nuclear}]$$

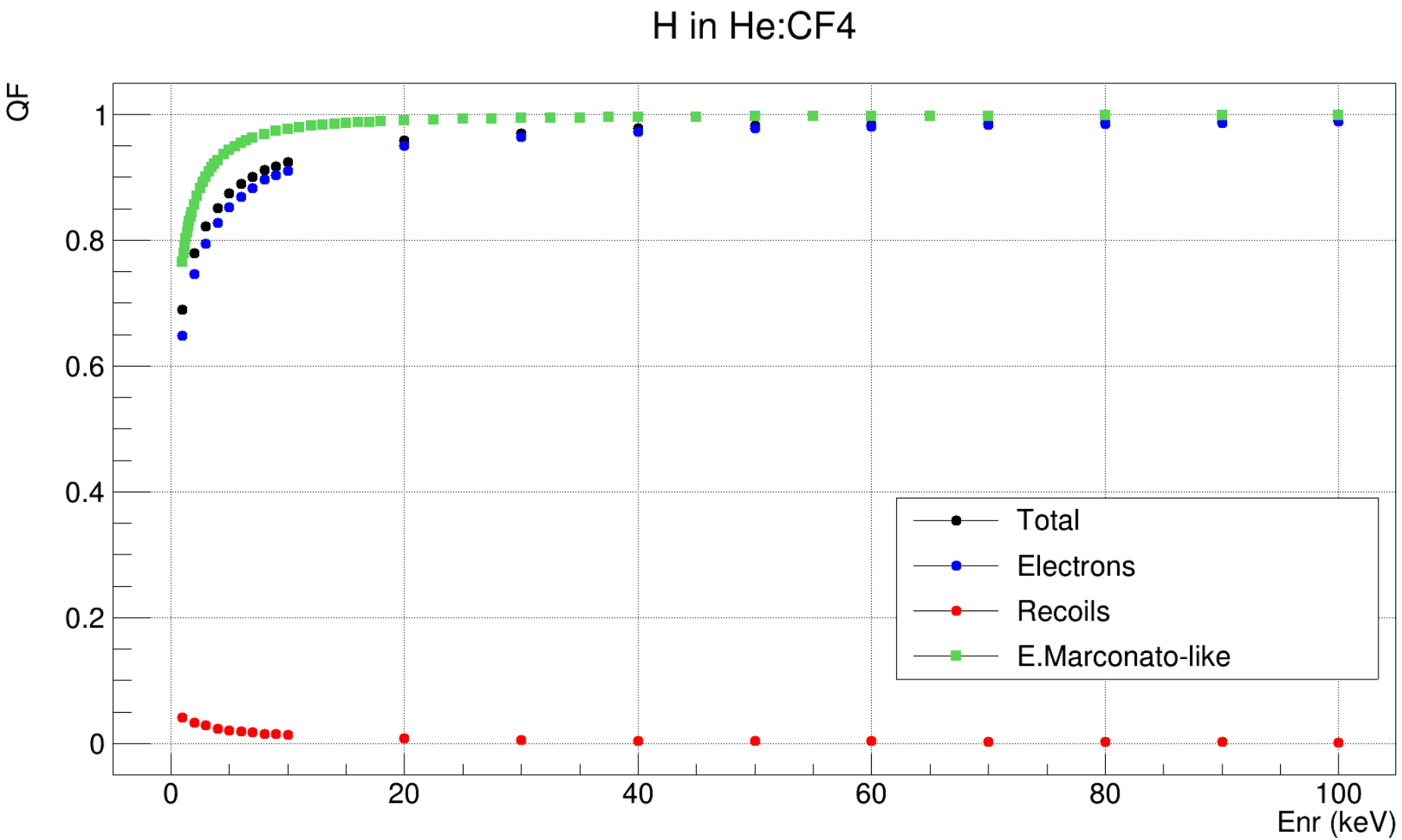
$$(dE/dx)_{elec}=(dE/dx)_{ioniz,e}+(dE/dx)_{other,e}$$



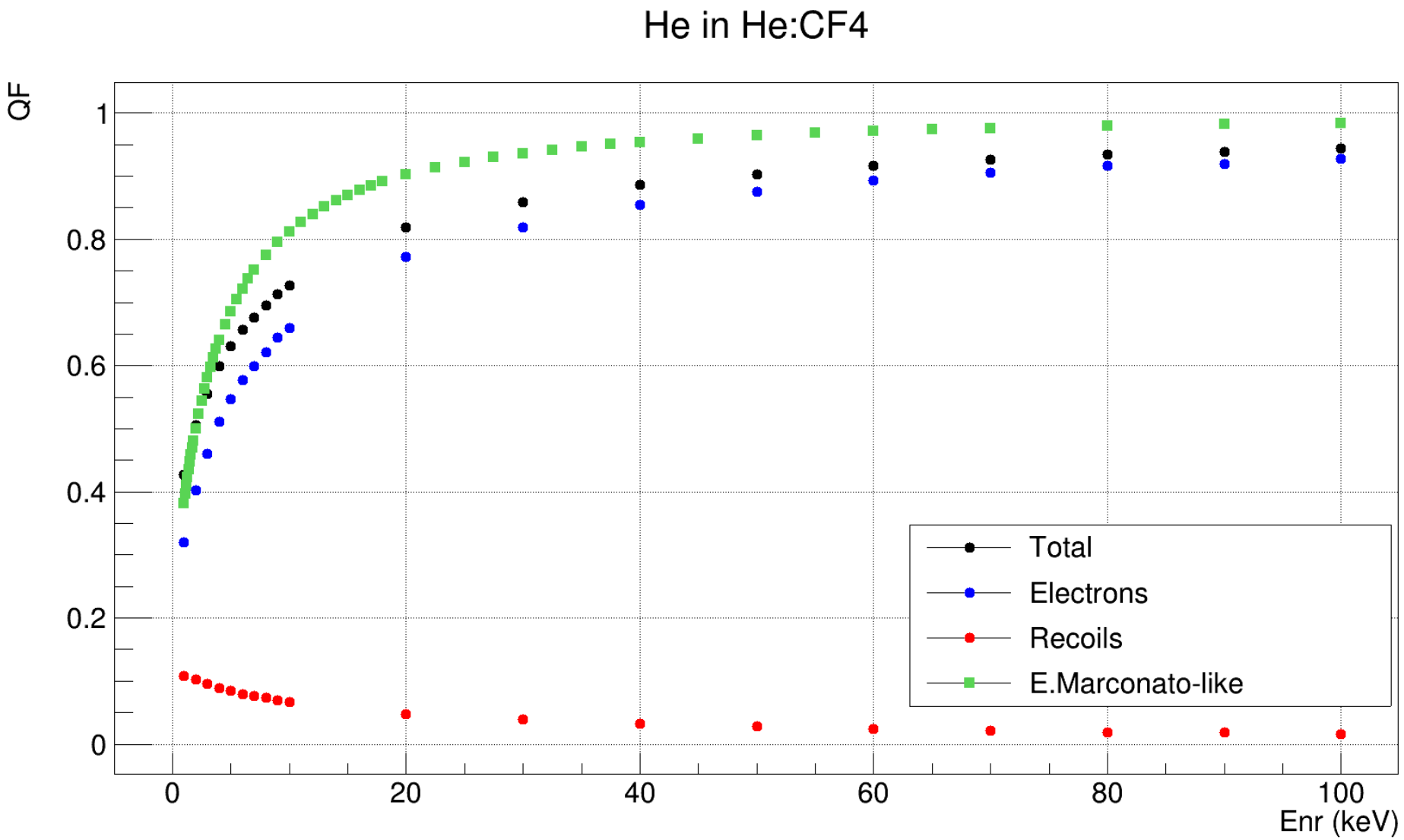



```
 ================================================================
              SRIM version ---> SRIM-2013.00
              Calc. date   ---> ottobre 14. 2020
 ================================================================

 Disk File Name = SRIM Outputs\H_HeCF4.txt

 Ion = Hydrogen [1] . Mass = 1.008 amu

 Target Density =  1.5630E-03 g/cm3 = 6.5081E+19 atoms/cm3
 Target is a GAS
 ======= Target  Composition ========
    Atom   Atom   Atomic    Mass
    Name   Numb   Percent   Percent
    ----   ----   -------   -------
     He      2    023.08    006.39
      C      6    015.38    012.77
      F      9    061.54    080.84
 ====================================
 Bragg Correction = -4.14%
 Stopping Units =   eV / Angstrom
 See bottom of Table for other Stopping units

       Ion         dE/dx       dE/dx      Projected   Longitudinal   Lateral
      Energy       Elec.       Nuclear      Range      Straggling   Straggling
  -------------  ----------  ----------  ----------  -----------  -----------
0.999999 keV     8.119E-04   2.495E-04    33.59 um     34.05 um     26.22 um
   1.10 keV      8.515E-04   2.419E-04    37.13 um     36.60 um     28.30 um
   1.20 keV      8.894E-04   2.348E-04    40.68 um     39.07 um     30.33 um
   1.30 keV      9.257E-04   2.282E-04    44.26 um     41.47 um     32.32 um
   1.40 keV      9.606E-04   2.220E-04    47.85 um     43.80 um     34.27 um
   1.50 keV      9.944E-04   2.162E-04    51.46 um     46.06 um     36.18 um
   1.60 keV      1.027E-03   2.107E-04    55.07 um     48.26 um     38.05 um
   1.70 keV      1.059E-03   2.056E-04    58.70 um     50.39 um     39.89 um
```

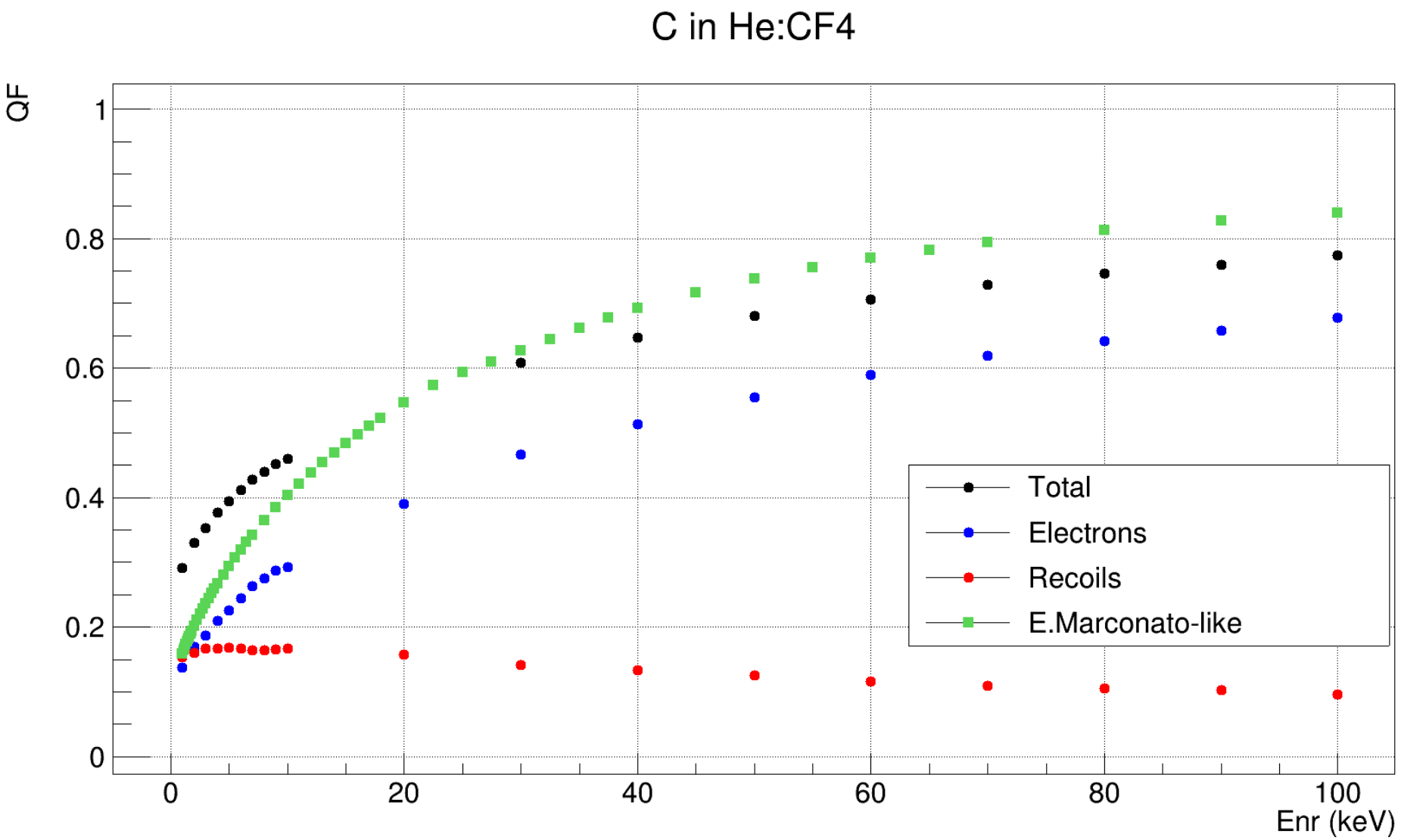
Quenching factor (protons)



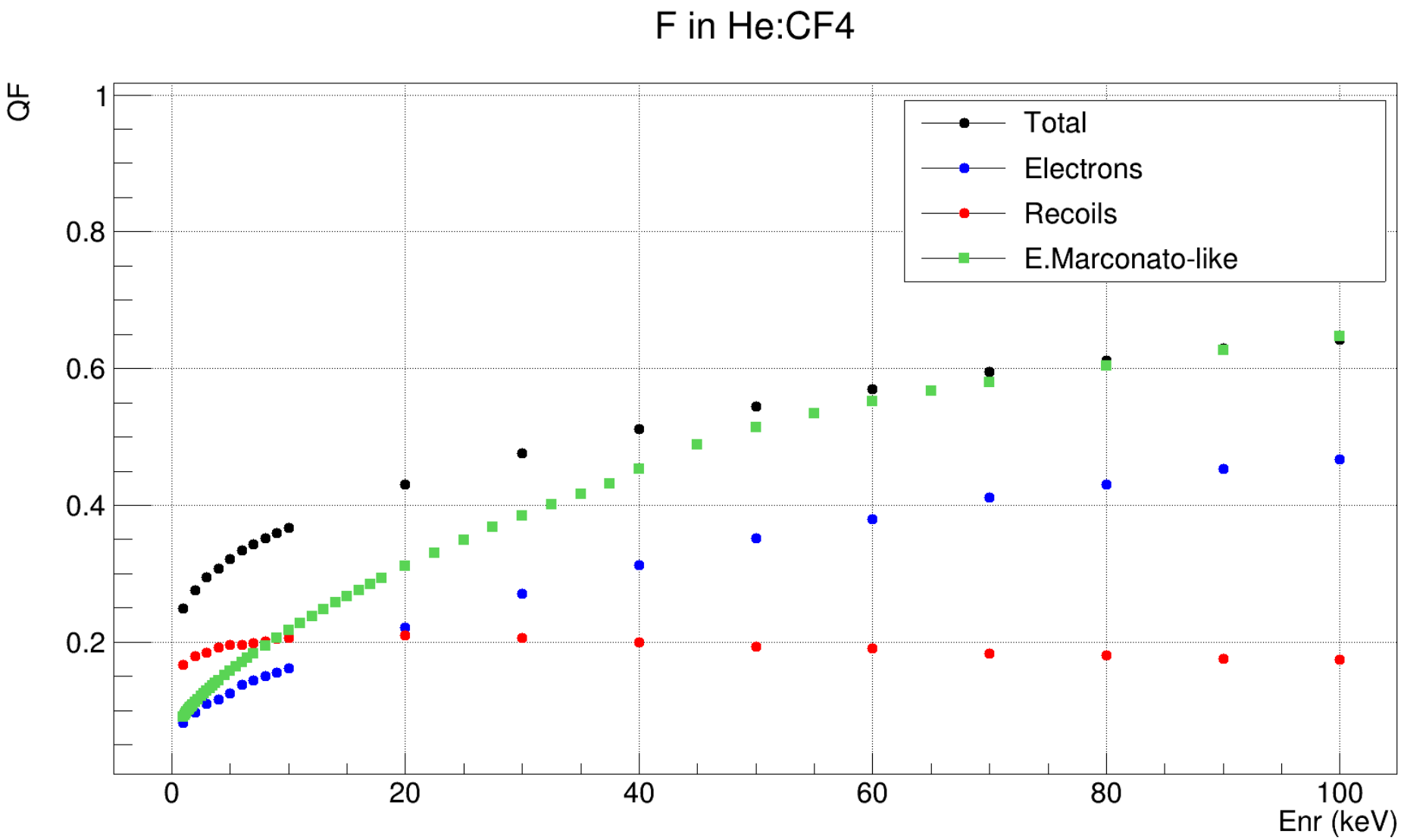
Quenching factor (He)



Quenching factor (C)



Quenching factor (F)



Pysrim

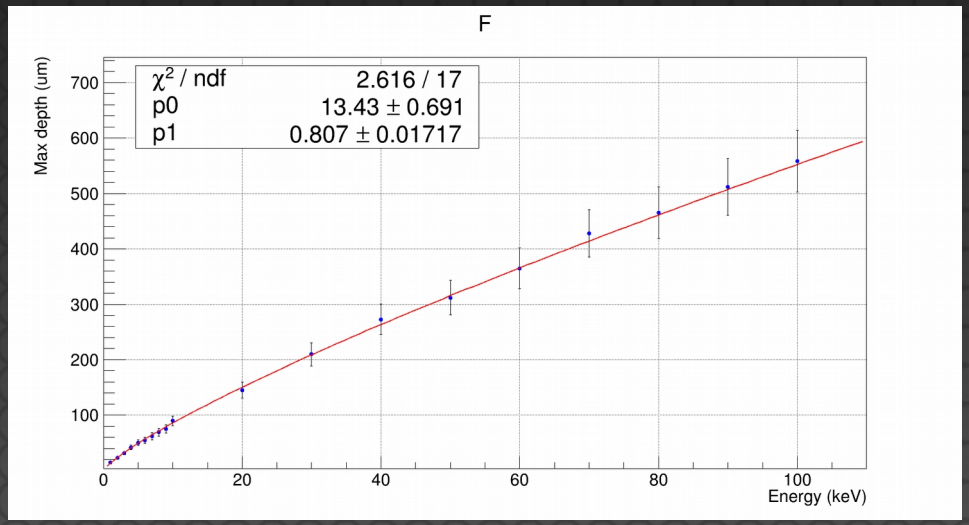
Module for automating SRIM calculations

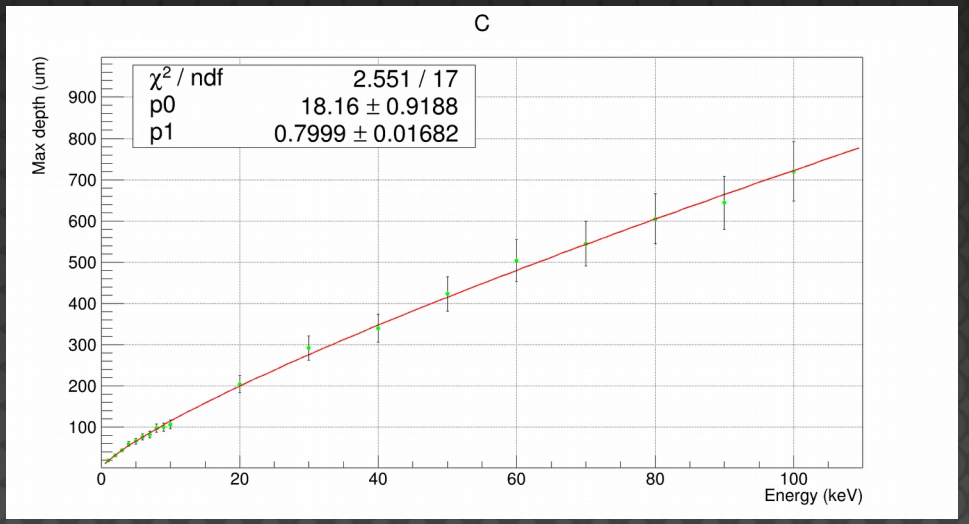
- Defines ion type and energy
- Defines target properties (atomic composition, density, width)
  - Adjust the target width according to ion type and energy
  - We found a way to fix the width of the bins in IONIZ.TXT (by default it's 1/100 of the width)
- Defines number of events and type of calculation
- Saves and renames the files of interest

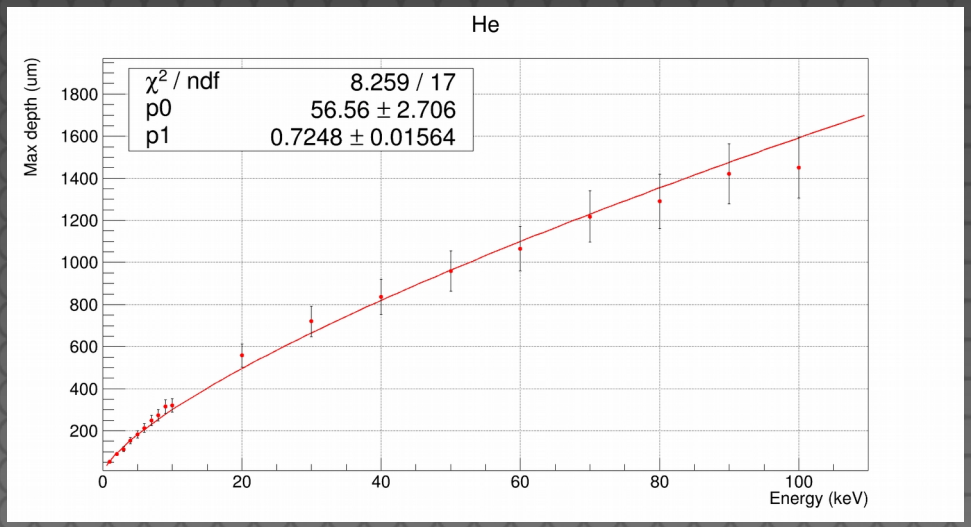
This allows us to simulate event by event in an efficient way

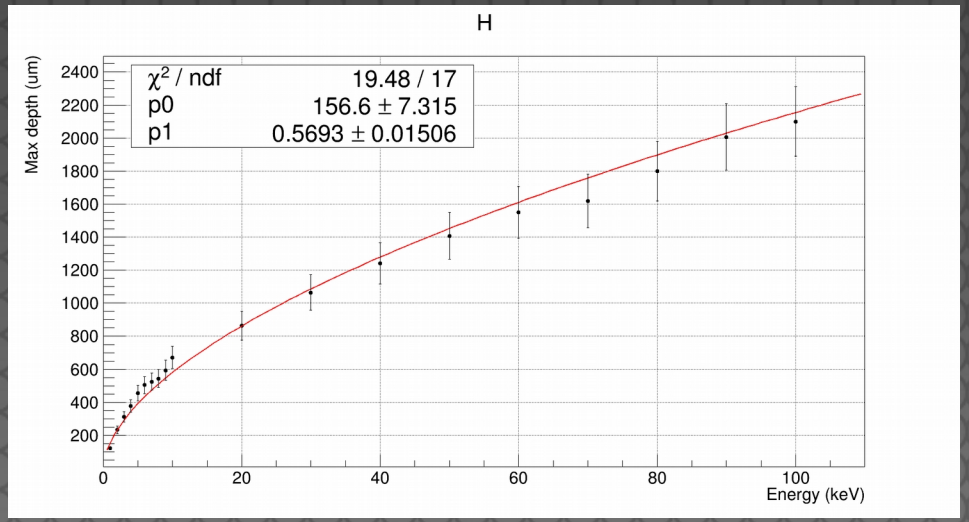
Pysrim – target width

From the data of the quick calculation we estimated the target width necessary to fully contain the events; fit function $p_0 E^{p1}$









Ionization profile

```
=================================================================================================================
  Ion    Energy    Depth     Lateral Distance (A)   Se    Atom  Recoil    Target Target Target Target
  Numb   (keV)      (A)       Y Axis    Z Axis    (eV/A)  Hit  Energy(eV) DISP.  VAC.   REPLAC INTER
-----------------------------------------------------------------------------------------------------------------
³00003³60,45E-02³85759,E+01³-6336,E+02³ 1130,E+03³0000,00³  F ³69625,E-03³ <== Start of New Cascade  ³
=================================================================================
  Recoil Atom Energy(eV)   X (A)      Y (A)      Z (A)   Vac Repl Ion Numb 00003=
Û 00001   09  69625,E-03 8576,E+02 -6336,E+02  1130,E+03  1   00 Û<ÄPrime RecoilÛ
Û 00002   02  59339,E-04 8605,E+02 -6375,E+02  1122,E+03  1   00 Û
Û 00003   02  82104,E-04 8576,E+02 -6339,E+02  1130,E+03  1   00 Û
=================================================================
³                              Summary of Above Cascade ==> ³69625,E-03³000003³000003³000000³000003³
³00003³22,55E-02³58633,E+01³-8303,E+02³ 9538,E+02³0000,00³ He ³24486,E-03³ <== Start of New Cascade  ³
=================================================================================
  Recoil Atom Energy(eV)   X (A)      Y (A)      Z (A)   Vac Repl Ion Numb 00003=
Û 00001   02  24486,E-03 5863,E+02 -8303,E+02  9538,E+02  1   00 Û<ÄPrime RecoilÛ
³00003³19,60E-02³58295,E+01³-8267,E+02³ 9411,E+02³0000,00³  F ³37140,E-03³ <== Start of New Cascade  ³
=================================================================================
```

COLLISON.TXT includes all the details of every collision with a target atom (also follows every cascade)

But

It doesn't provide the ionization energy losses

```
====== pysrim run =======
       SRIM-2013.00
=======================================
     Ion and Recoil IONIZATION
 See SRIM Outputs\TDATA.txt for details
=======================================
====== TRIM Calc.=  C(1 keV) ==> None( 18.2 um) ==============================
--------------------------------------------------------------------------------
 See file :  SRIM Outputs\TDATA.txt   for calculation data
 Ion    =  C   Energy = 1 keV
============= TARGET MATERIAL ======================================
Layer 1 : None
Layer Width = 18200.E+01 A ;
  Layer # 1- Density = 6.353E19 atoms/cm3 = .0015 g/cm3
  Layer # 1-  C = 15.3 Atomic Percent = 12.7 Mass Percent
  Layer # 1- He = 23.0 Atomic Percent = 6.38 Mass Percent
  Layer # 1-  F = 61.5 Atomic Percent = 80.8 Mass Percent
====================================================================
 Total Ions calculated =000001.00
=============================================================
  Ionization Energy Units are  >>>>  eV /(Angstrom-Ion)  <<<<
=============================================================
-------------------------------------------------------------
-  NOTE: Because of the application of straggling to the ion  -
-  energy, Ionization is not accurate for less than 20 ions!  -
-------------------------------------------------------------

  TARGET       IONIZ.       IONIZ.
  DEPTH         by           by
  (Ang)        IONS         RECOILS
-----------  -----------  -----------
182001.E-02  2253.74E-06  4290.24E-10
364001.E-02  2174.91E-06  0000.00E+00
546001.E-02  1710.33E-06  0000.00E+00
```

IONIZ.TXT gives the ionization energy losses divided in the *ions* component (leading to the primary ionization) and a *recoils* component (leading to secondary ionization)

But

It doesn't provide the 3D position

→ We need both

Ionization profile

Ioniz-3D.TXT – only included in 2013 version

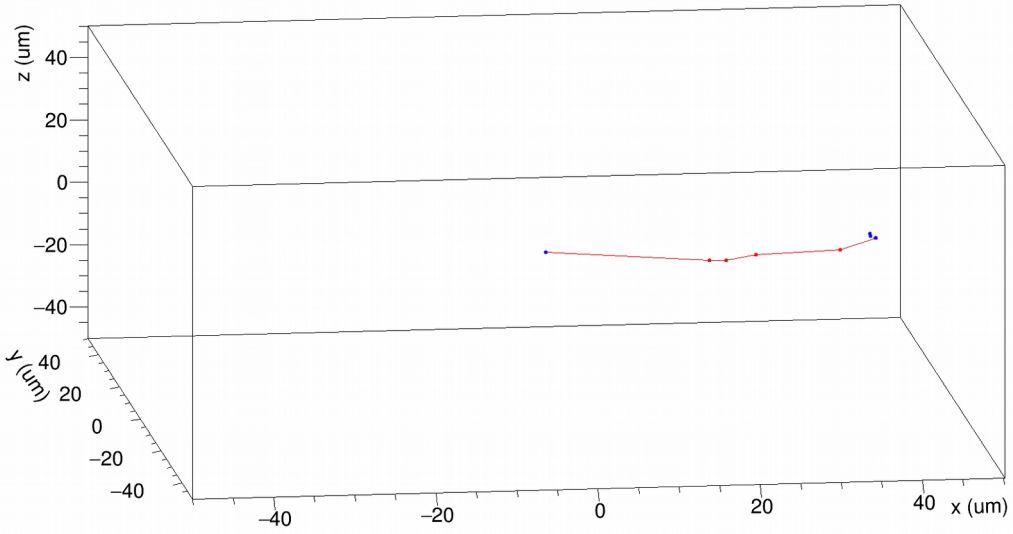
```
       SRIM-2013.00
========================================
       Ion and Recoil IONIZATION
 This is a special 3-D array of 100x100 values.
 These values can be used as input to other graphics software.
========================================
====== TRIM Calc.=  H(1 keV) ==> He-CF4(  150 um) ===========================
-------------------------------------------------------------------------------
 See file :  SRIM Outputs\TDATA.txt   for calculation data
 Ion    =  H   Energy = 1 keV
============= TARGET MATERIAL ======================================
Layer 1 : He-CF4
Layer Width = 15000,E+02 A ;
  Layer # 1- Density = 6.511E19 atoms/cm3 = .0015 g/cm3
  Layer # 1- He = 23.0 Atomic Percent = 6.38 Mass Percent
  Layer # 1-  C = 15.3 Atomic Percent = 12.7 Mass Percent
  Layer # 1-  F = 61.5 Atomic Percent = 80.8 Mass Percent
====================================================================
 Total Ions calculated =000001,00
==============================================================================
      Ionization Energy Units are  >>>>  eV /(Angstrom-Ion)  <<<<
==============================================================================
-------------------------------------------------------------
-  NOTE: Because of the application of straggling to the ion  -
-  energy, Ionization is not accurate for less than 20 ions!  -
-------------------------------------------------------------
             Below is an array of 10,000 values of target Ionization.
             It includes ionization by both the ion and all recoils.
             The values form a 100x100 spatial array.
  TARGET     The depth values are in the first column, on the left.
  DEPTH      The grid of values are spaced at intervals of >>  1500 nm <<
  (Ang)      The Beam enters the target at column #50 of the top row.
----------- ------------------------------------------------------------------
  15000E+00    0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   3681,61E-07   3959,65E-07   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00
  30000E+00    0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   5580,32E-07   2729,35E-07   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00   0000,00E+00
0000,00E+00   0000,00E+00   0000,00E+00
```

Ionization energy losses (ion+recoils) in 2D space

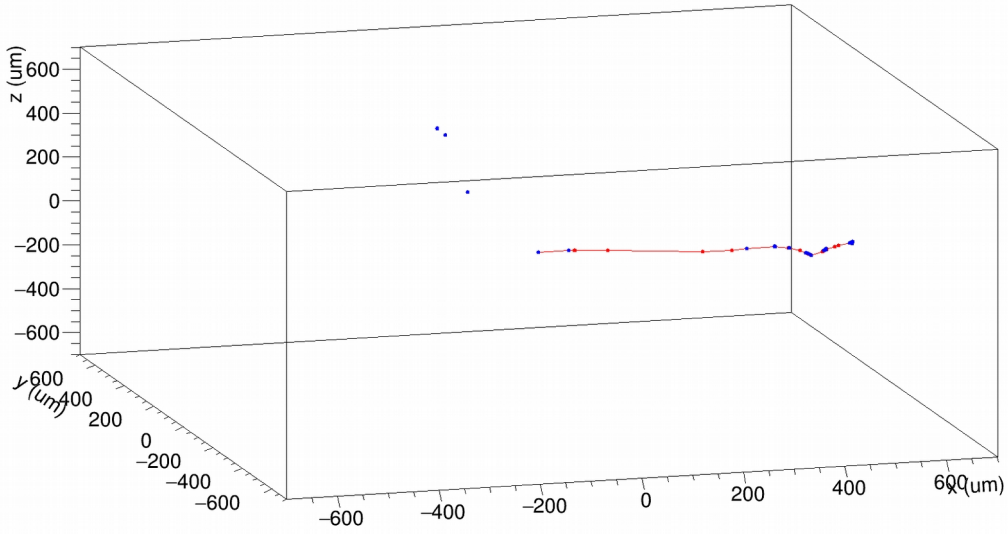
Pysrim is optimised for SRIM-2008, we’re trying to figure out how to produce this file

Track reconstruction (He)

He recoil 1 keV



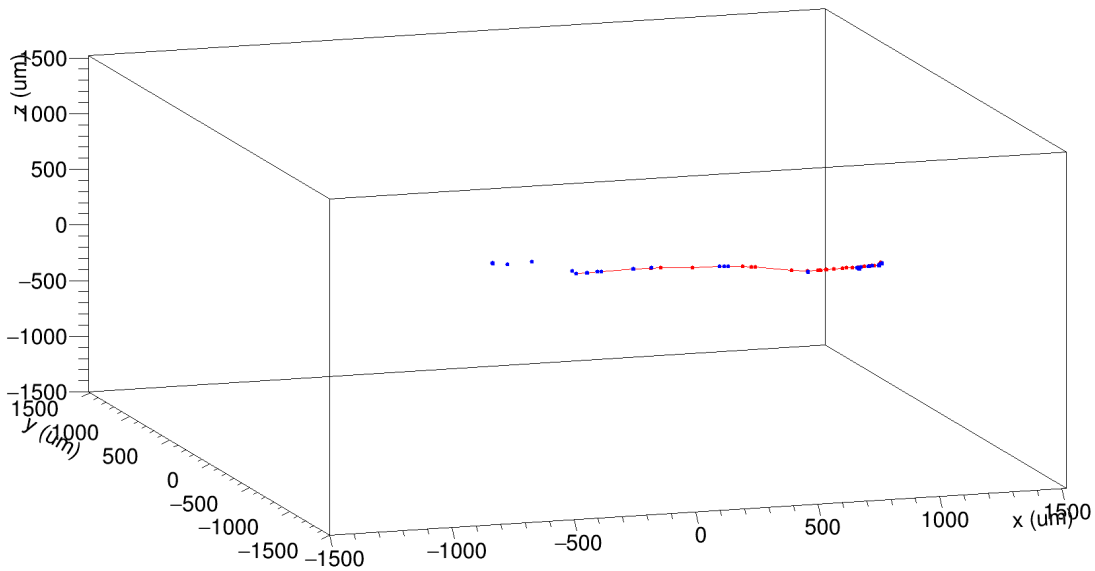
He recoil 50 keV



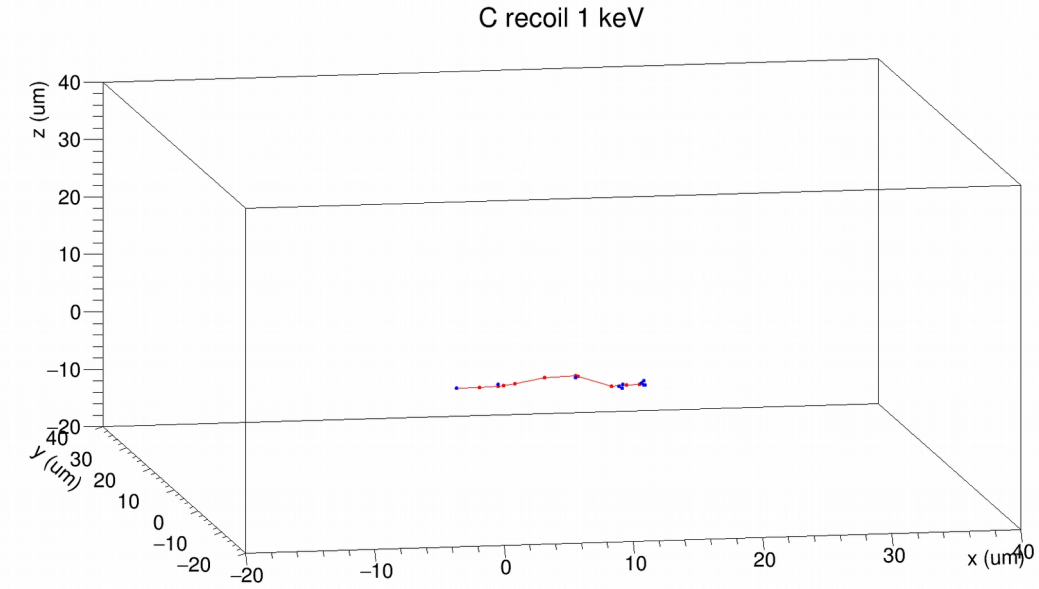
Data from COLLISON.TXT

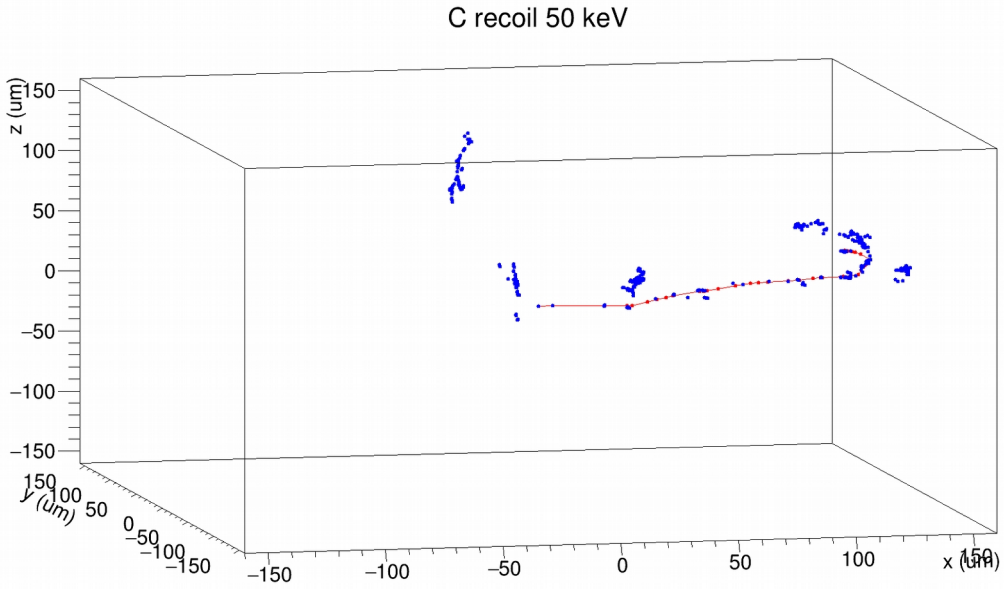
- Red dots are recoils produced by the primary ion
- Blue dots are secondary recoils, produced by primary recoils

He recoil 100 keV



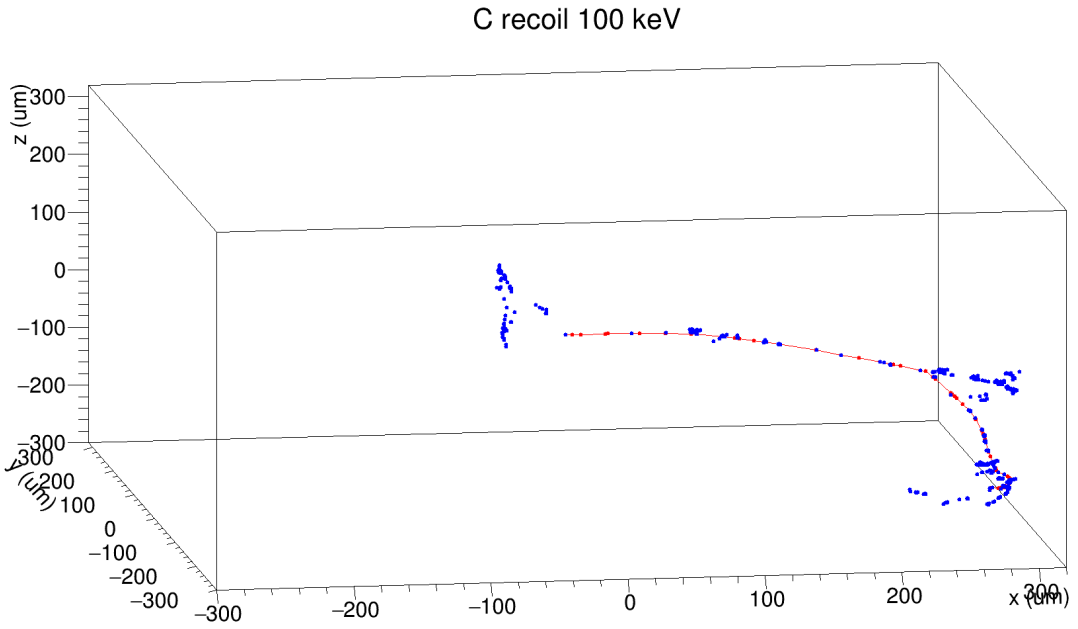
Track reconstruction (C)





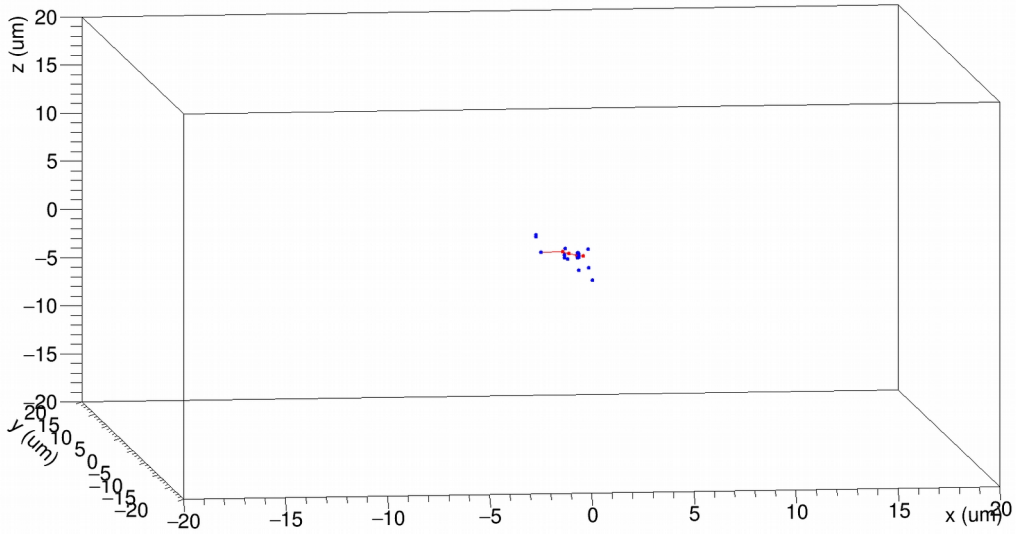
Data from COLLISON.TXT

- Red dots are recoils produced by the primary ion
- Blue dots are secondary recoils, produced by primary recoils

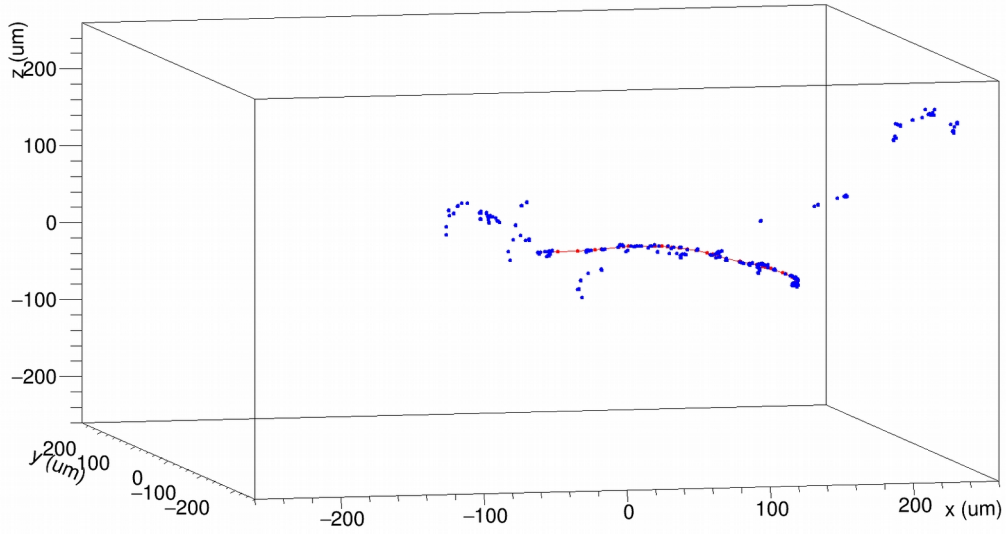


Track reconstruction (F)

F recoil 1 keV



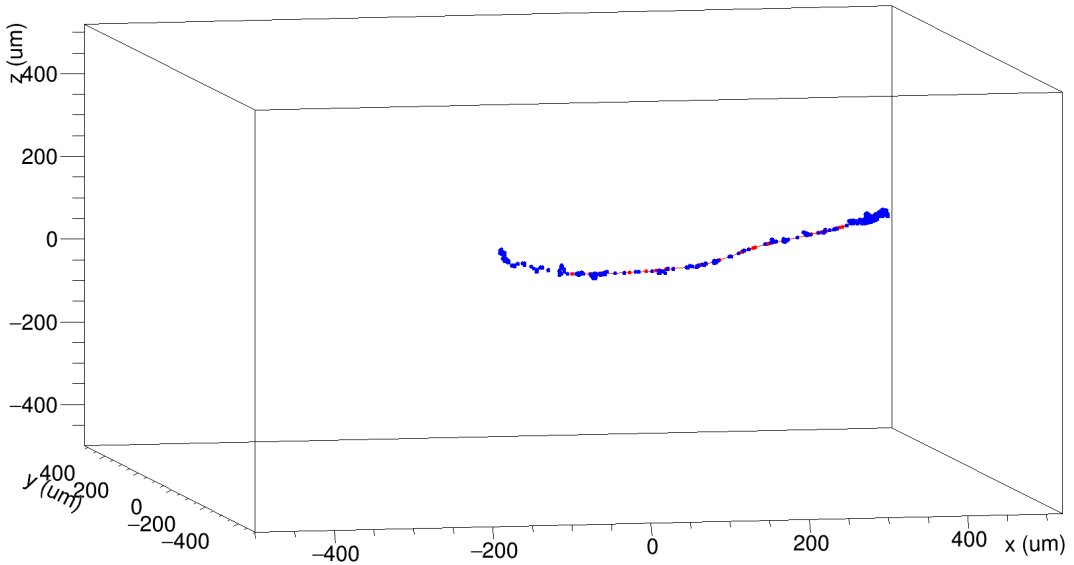
F recoil 50 keV



Data from COLLISON.TXT

- Red dots are recoils produced by the primary ion
- Blue dots are secondary recoils, produced by primary recoils

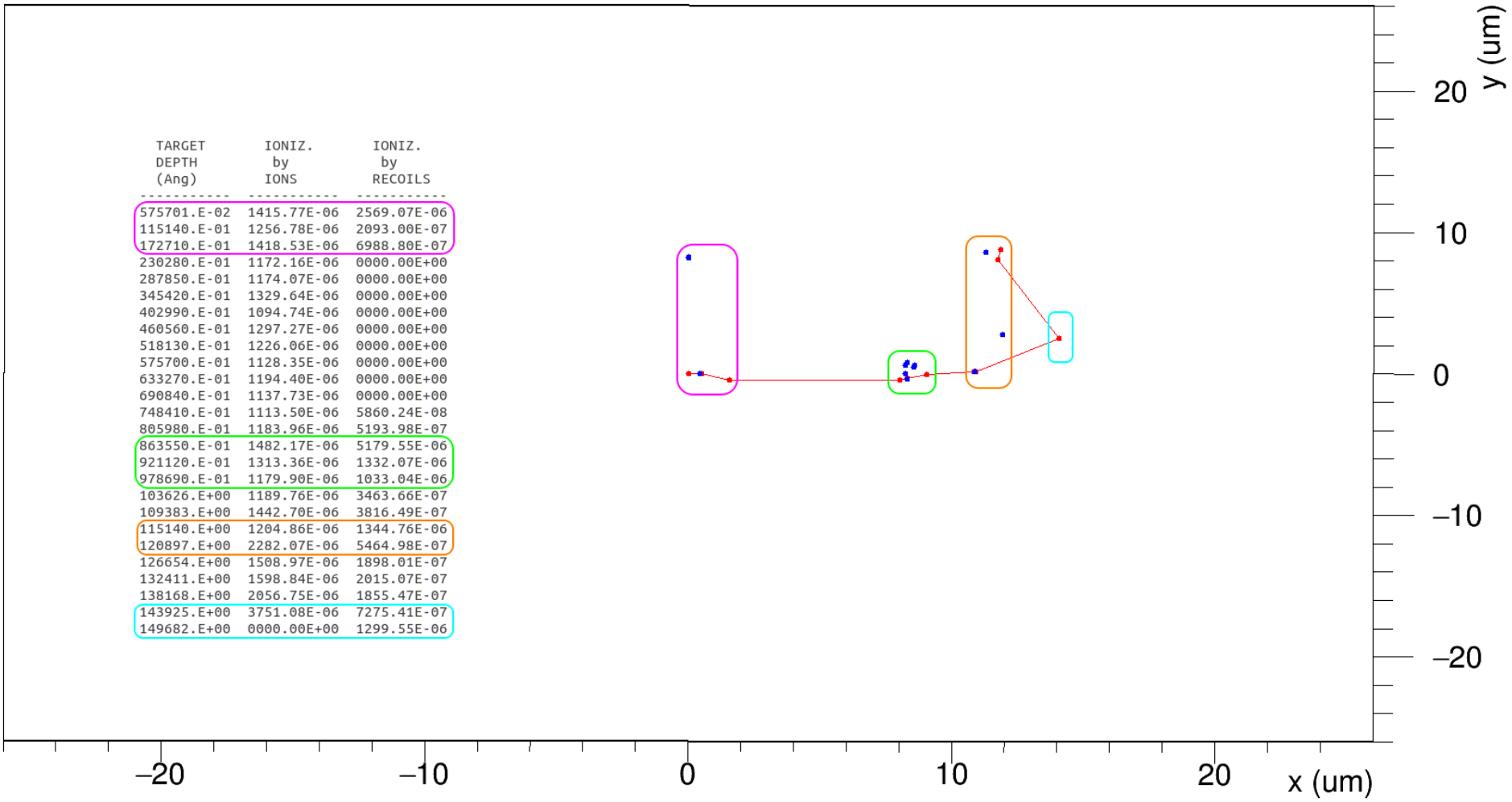
F recoil 100 keV



Ionization profile

He recoil 1 keV

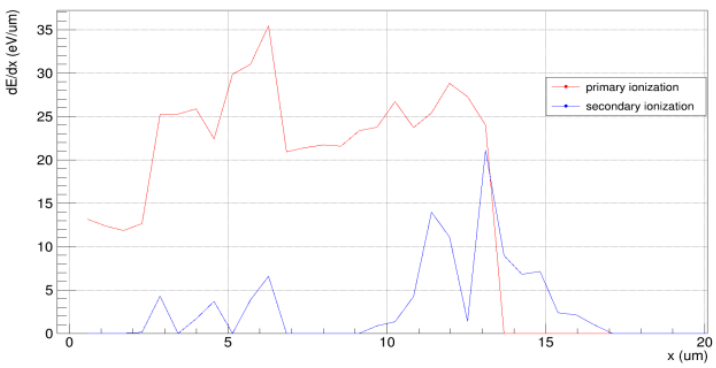
TARGET DEPTH (Ang)	IONIZ. by IONS	IONIZ. by RECOILS
575701.E-02	1415.77E-06	2569.07E-06
115140.E-01	1256.78E-06	2093.00E-07
172710.E-01	1418.53E-06	6988.80E-07
230280.E-01	1172.16E-06	0000.00E+00
287850.E-01	1174.07E-06	0000.00E+00
345420.E-01	1329.64E-06	0000.00E+00
402990.E-01	1094.74E-06	0000.00E+00
460560.E-01	1297.27E-06	0000.00E+00
518130.E-01	1226.06E-06	0000.00E+00
575700.E-01	1128.35E-06	0000.00E+00
633270.E-01	1194.40E-06	0000.00E+00
690840.E-01	1137.73E-06	0000.00E+00
748410.E-01	1113.50E-06	5860.24E-08
805980.E-01	1183.96E-06	5193.98E-07
863550.E-01	1482.17E-06	5179.55E-06
921120.E-01	1313.36E-06	1332.07E-06
978690.E-01	1179.90E-06	1033.04E-06
103626.E+00	1189.76E-06	3463.66E-07
109383.E+00	1442.70E-06	3816.49E-07
115140.E+00	1204.86E-06	1344.76E-06
120897.E+00	2282.07E-06	5464.98E-07
126654.E+00	1508.97E-06	1898.01E-07
132411.E+00	1598.84E-06	2015.07E-07
138168.E+00	2056.75E-06	1855.47E-07
143925.E+00	3751.08E-06	7275.41E-07
149682.E+00	0000.00E+00	1299.55E-06

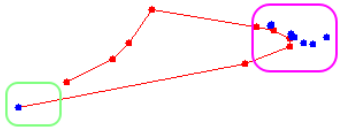


Ionization profile

He recoil 1 keV

We want to relate the tracks to the ionization losses (but we only know the x position)





TARGET DEPTH (Ang)	IONIZ. by IONS	IONIZ. by RECOILS
570001.E-02	1314.61E-06	1238.30E-10
114000.E-01	1236.84E-06	0000.00E+00
171000.E-01	1183.89E-06	0000.00E+00
228000.E-01	1263.34E-06	1327.61E-08
285000.E-01	2521.13E-06	4282.66E-07
342000.E-01	2526.41E-06	1208.92E-10
399000.E-01	2587.08E-06	1685.54E-07
456000.E-01	2242.79E-06	3696.75E-07
513000.E-01	2985.89E-06	7063.96E-10
570000.E-01	3100.25E-06	3881.43E-07
627000.E-01	3544.56E-06	6584.11E-07
684000.E-01	2089.86E-06	1193.07E-10
741000.E-01	2138.90E-06	0000.00E+00
798000.E-01	2169.79E-06	3489.71E-10
855000.E-01	2158.50E-06	0000.00E+00
912000.E-01	2334.87E-06	1156.94E-10
969000.E-01	2377.02E-06	8933.54E-08
102600.E+00	2670.88E-06	1346.49E-07
108300.E+00	2371.19E-06	4237.59E-07
114000.E+00	2538.67E-06	1394.98E-06
119700.E+00	2883.29E-06	1111.72E-06
125400.E+00	2726.51E-06	1419.05E-07
131100.E+00	2400.20E-06	2111.57E-06
136800.E+00	0000.00E+00	8947.64E-07
142500.E+00	0000.00E+00	6831.44E-07
148200.E+00	0000.00E+00	7160.37E-07
153900.E+00	0000.00E+00	2382.91E-07
159600.E+00	0000.00E+00	2137.11E-07
165300.E+00	0000.00E+00	9666.29E-08

Conclusions and future work

- Solve pysrim minor issues
- Run for several ions
- Better estimate the quenching factor
- Merge information of COLLISON.TXT, IONIZ.TXT
  - With the help of Ioniz-3D.TXT and/or EXYZ.TXT?

```
Calc. Date= 10-15-2020, Time= 15:54:08
============================== SRIM-2013.00 ==============================
 ======================================================================
 =                    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  1keV    10eV
 ======================================================================
Ion       Energy     Depth (X)     Y           Z       Electronic   Energy Lost to
Number    (keV)    (Angstrom)  (Angstrom)  (Angstrom)  Stop.(eV/A)  Last Recoil(eV)
------- ---------- ---------- ---------- ---------- ----------  ---------------
0000001 1,0000E+00  0,0000E+00  0,0000E+00  0,0000E+00  8,1236E-04  0,0000E+00
0000001 9,8998E-01  1,3074E+04  3,2194E+01  5,9332E+01  8,0828E-04  1,1696E-11
0000001 9,7999E-01  2,5249E+04  2,9753E+01  3,9592E+02  8,0420E-04  4,3015E-04
0000001 9,6988E-01  3,8091E+04  6,2757E+01  8,6065E+02  8,0004E-04  1,4780E-01
0000001 9,5996E-01  4,8696E+04  9,6398E+02  8,1966E+02  7,9594E-04  0,0000E+00
0000001 9,4997E-01  6,0790E+04  2,4714E+03 -4,4660E+02  7,9178E-04  0,0000E+00
0000001 9,3997E-01  7,1956E+04  3,5989E+03 -1,2547E+03  7,8760E-04  2,3168E-12
0000001 9,2926E-01  8,3685E+04  5,2339E+03 -2,2230E+03  7,8310E-04  1,0239E+00
0000001 9,1999E-01  9,3980E+04  8,2779E+03 -2,0528E+03  7,7919E-04  2,4458E-09
0000001 9,0989E-01  1,0632E+05  1,2290E+04 -2,0175E+03  7,7490E-04  4,8194E-01
0000001 8,9996E-01  1,1873E+05  1,6538E+04 -3,2314E+03  7,7066E-04  3,8945E-10
```