Simulation – Quenching Factor Assessment

F. DI GIAMBATTISTA, A.F.V. CORTEZ, D. PINCI, E. BARACCHINI

GRAN SASSO SCIENCE INSTITUTE & INFN

OUTLINE

- Objectives
- Simulation Results – SRIM
- SRIM with Python -PySRIM
- Conclusions and Future work

Objectives

- Perform the simulation to cross check Emanuele Marconato's results.
- Using SRIM, we will…

- Study Protons, Heliums, Carbons and Fluorines in He/CF4 (60/40) gas mixtures;
- Starting with the evaluation of Quenching Factor for energies of
  1,2,3..10,20,30..1000 keV;
- Study the Ionization Profile for the same ions by producing samples of 1000 events of for energies of 1,3,6,10,30,60,100 keV.

For each event use the combination of info provided by Collision.txt and Ionization.txt and save data in text file as the one in the upper left of next slide ;

Objectives

COLLISION.txt

```
========================== SRIM-2013.00 ============================
================================================================================
--------------------------------------------------------------------------------
====== TRIM Calc.= He(1 keV) ==> Layer 1(  100 mm) ==========================
--------------------------------------------------------------------------------
============================================================
∫     Ion Name   =     He                                  ∫
∫     Ion Mass   =    004,003 amu                          ∫
∫     Ion Energy =000000001,0 keV                          ∫
============================================================
>     He  Displacement Energy of He = 0005,00000 eV
  Latt.Binding Energy of He = 0001,00000 eV
  SurfaceBind. Energy of He = 0002,00000 eV
>      C  Displacement Energy of  C = 0028,00000 eV
  Latt.Binding Energy of  C = 0003,00000 eV
  SurfaceBind. Energy of  C = 0007,41000 eV
>      F  Displacement Energy of  F = 0025,00000 eV
  Latt.Binding Energy of  F = 0003,00000 eV
  SurfaceBind. Energy of  F = 0002,00000 eV
============================================================
================================================================================
≥=> Recoils Calculated with Kinchin-Pease Theory (Only Vacancies Calc) <=≥
================================================================================

=========================  COLLISION HISTORY  ==================================
  NOTES: Only Ion Collisions which produce Displacements are tabulated.
         Atom Sums and Averages are Incomplete if Recoil Cascades Leave Target.
         Target DISPlacements = VACancies + REPLACement Collisions.
         Target VACancies = INTERstitials + Sputtered + Transmitted Atoms.
                            Recoil Atoms which end at the surface, are not counted (see manual).
================================================================================================
  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
------------------------------------------------------------------------------------------------
≥00001≥84,24E-02≥55070,E+00≥-1011,E+01≥ 8428,E+00≥0000,00≥  F ≥77462,E-03≥000000001,034≥      ≥      ≥
≥00001≥69,91E-02≥76086,E+00≥-4502,E+01≥-3533,E+00≥0000,00≥  F ≥54113,E-03≥000000001,000≥      ≥      ≥
≥00001≥52,76E-02≥14405,E+01≥-7826,E+01≥-1484,E+01≥0000,00≥  F ≥62792,E-03≥000000001,000≥      ≥      ≥
≥00001≥40,61E-02≥18021,E+01≥-1059,E+02≥ 3636,E+00≥0000,00≥  F ≥97229,E-03≥000000001,289≥      ≥      ≥
≥00001≥21,07E-02≥19184,E+01≥-1294,E+02≥-6842,E+01≥0000,00≥  F ≥63375,E-03≥000000001,000≥      ≥      ≥
≥00001≥40,86E-03≥13007,E+01≥-1007,E+02≥-9480,E+01≥0000,00≥ He ≥97288,E-04≥000000001,000≥      ≥      ≥
================================================================================================
```

Provides the energy of the incident particle and the one passed to recoils.

QF = (Eion+Erecoils)/Einitial

Provides the track information and energy deposited.

IONIZ.txt

Table 9-14 - Datafile of Ionization Energy Loss in Target

---- Header Information omitted from Table ----

```
============================================================
Total Ions calculated =003859.69
Ionization Units are  >>>>  eV / Angstrom / Ion  <<<<
============================================================
  TARGET       IONIZ.       IONIZ.
  DEPTH         by           by
  (Ang)        IONS         RECOILS
----------  ----------  ----------
700100.E-04  7770.18E-02  2116.60E-03
140010.E-03  7837.15E-02  2705.78E-03
210010.E-03  8014.79E-02  2966.79E-03
280010.E-03  8144.14E-02  2875.40E-03
350010.E-03  8216.98E-02  3197.69E-03
420010.E-03  8345.11E-02  3316.41E-03
490010.E-03  8418.28E-02  3501.37E-03
560010.E-03  8565.63E-02  3741.85E-03
630010.E-03  8562.24E-02  3874.91E-03
700010.E-03  8581.36E-02  4178.15E-03
```

---- Data Omitted from Table ----

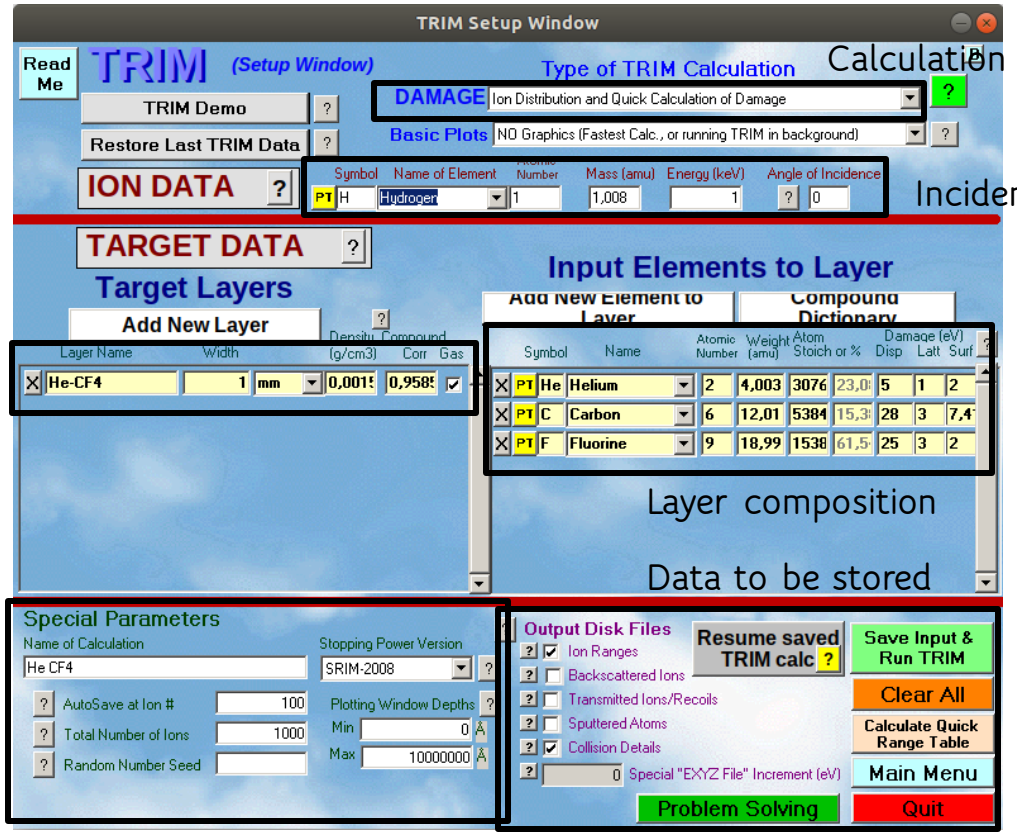
Format file needed for the analysis.

1	1	0.005507	-0.001011	0.000843	0.157600
1	2	0.007609	-0.004502	-0.000353	0.143300
1	3	0.014405	-0.007826	-0.001484	0.171500
1	4	0.018021	-0.010590	0.000364	0.121500
1	5	0.019184	-0.012940	-0.006842	0.195400
1	6	0.013007	-0.010070	-0.009480	0.169840

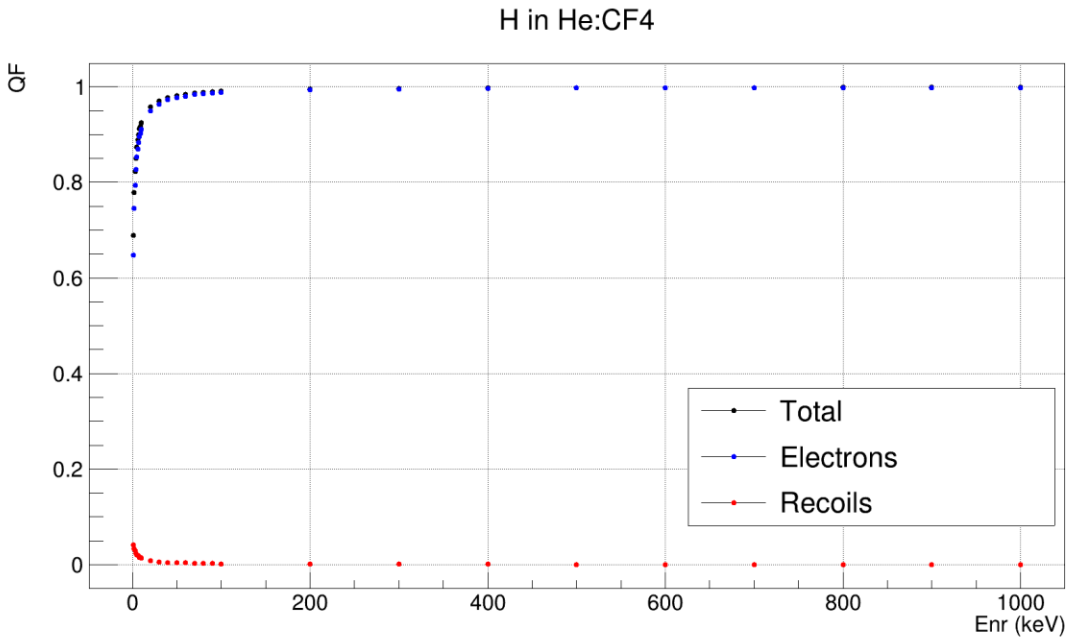
SRIM
Preliminary Results

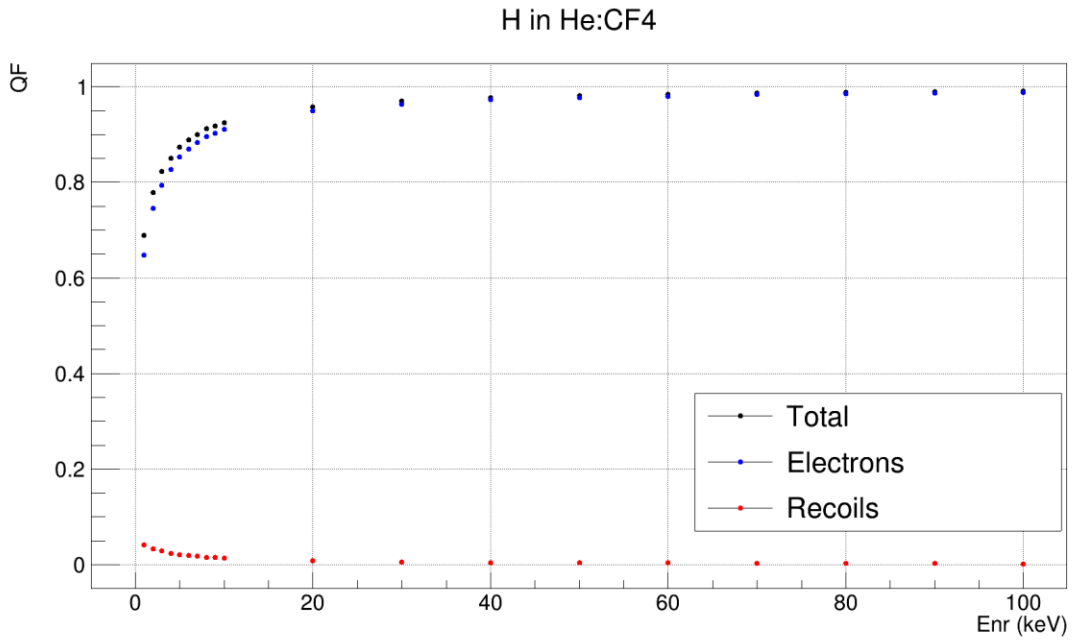
Quenching Factor assessment

- Simplified approach to QF analysis already performed for H, He, C, F for different energies (from 1 keV up to 1 MeV);
- In this approach we used the "quick calculation" of SRIM;
- Parameters used:
  - Gas density: 0.00156 g/cm3;
  - Atomic percent (He-23.1%, C-15.4% and F-61,5%);
  - Target width (depends on the energy and was conceived to optimize the bin to particle range);
  - Number of ions simulated: 1000 per run;

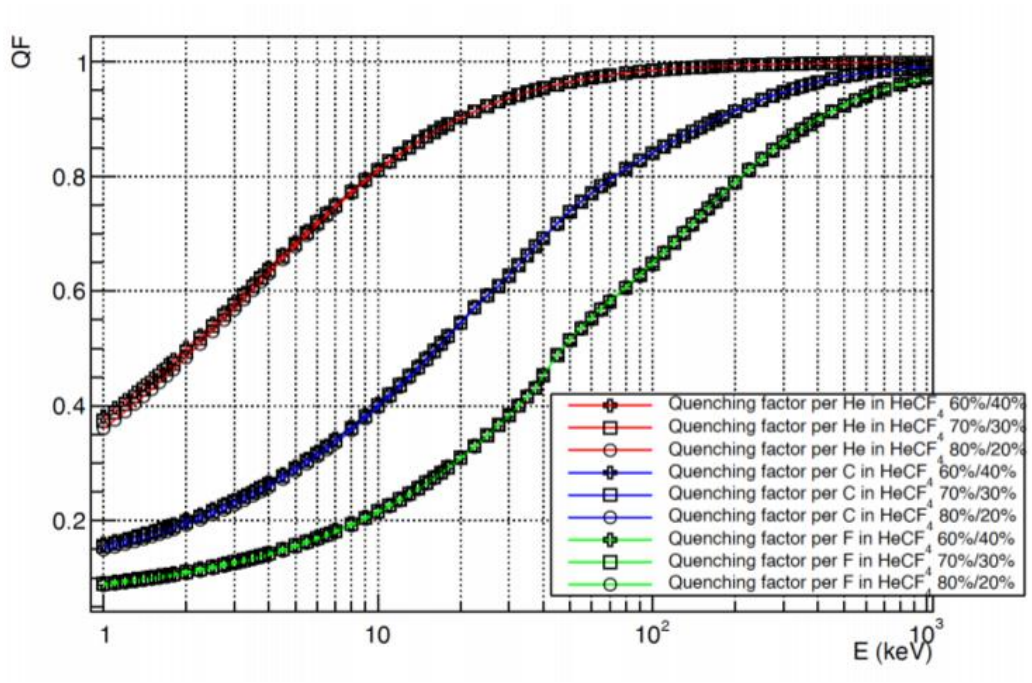


Quenching Factor assessment

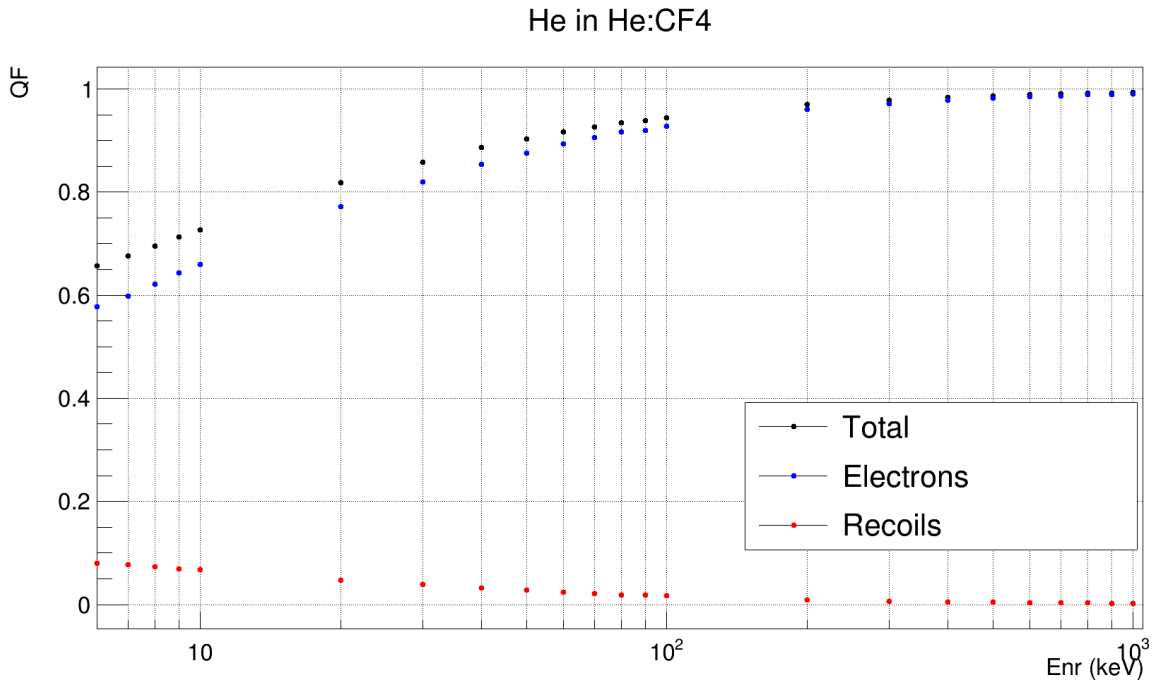




Quenching Factor assessment

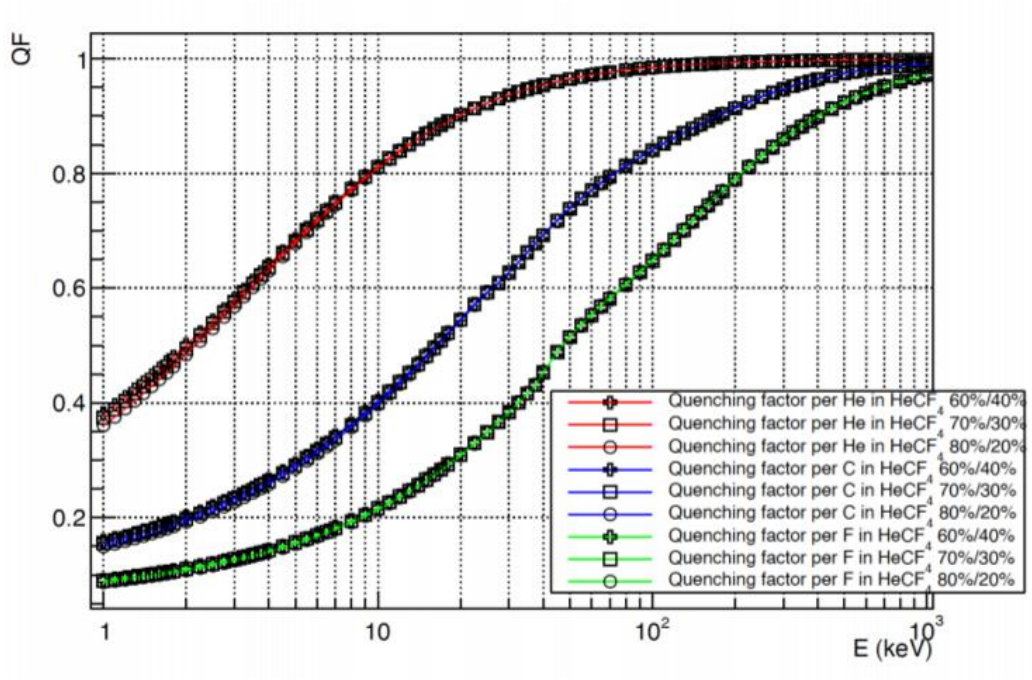


QF = 0.8 for 10 keV
(Emanuele Marconato)

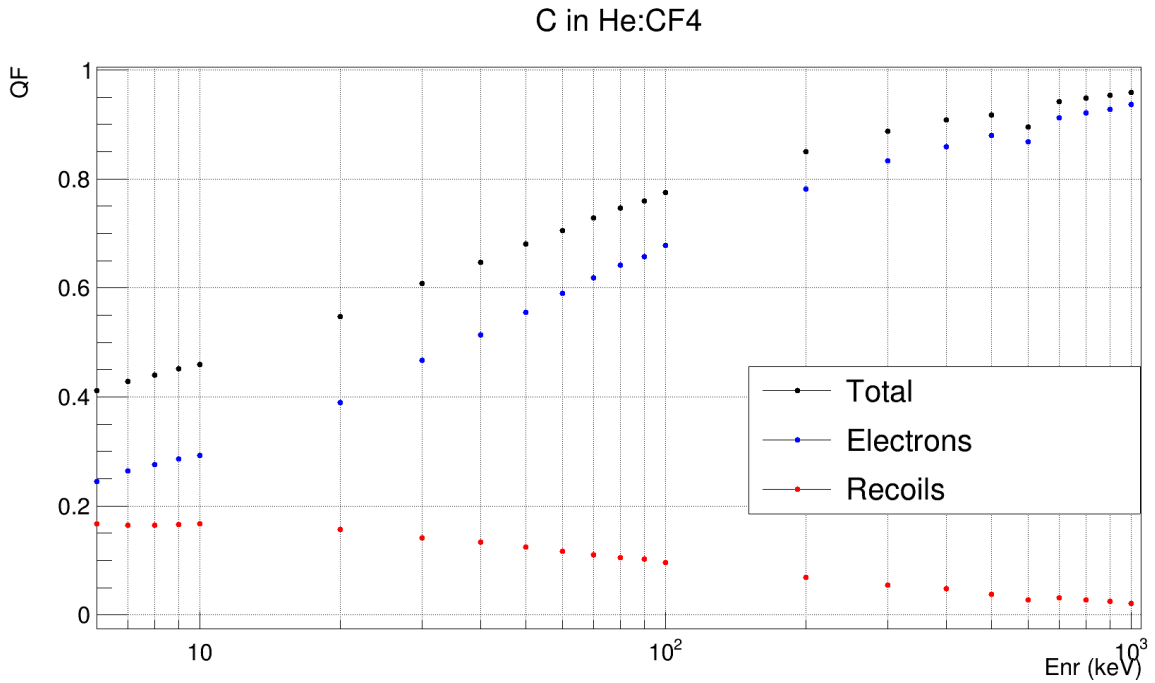


QF = 0.73 for 10 keV
(This work)

Quenching Factor assessment

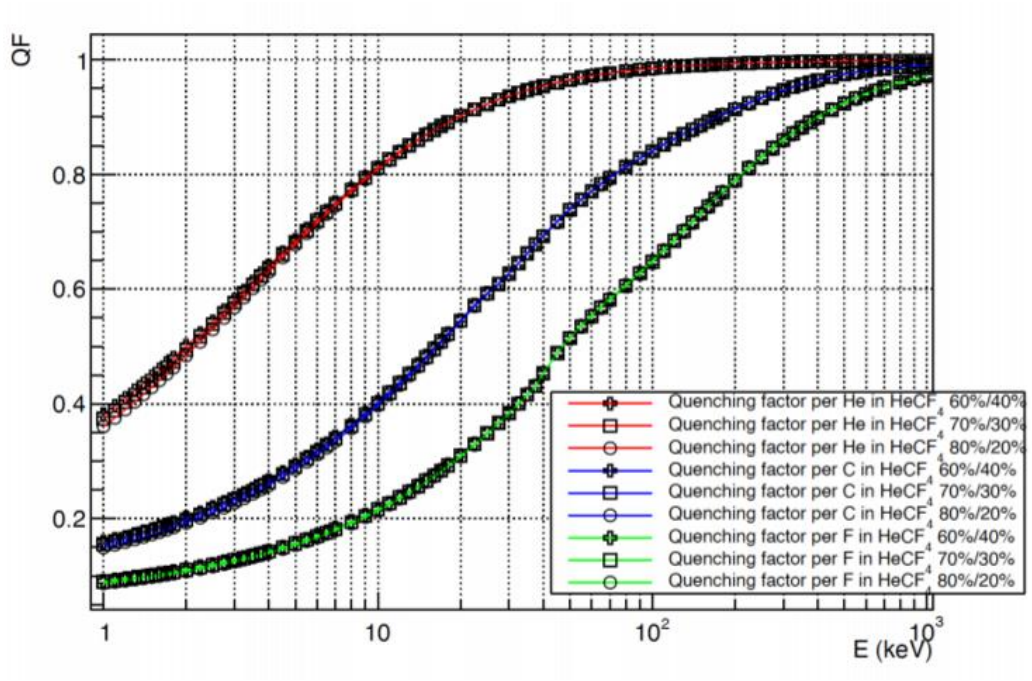


QF = 0.4 for 10 keV
(Emanuele Marconato)

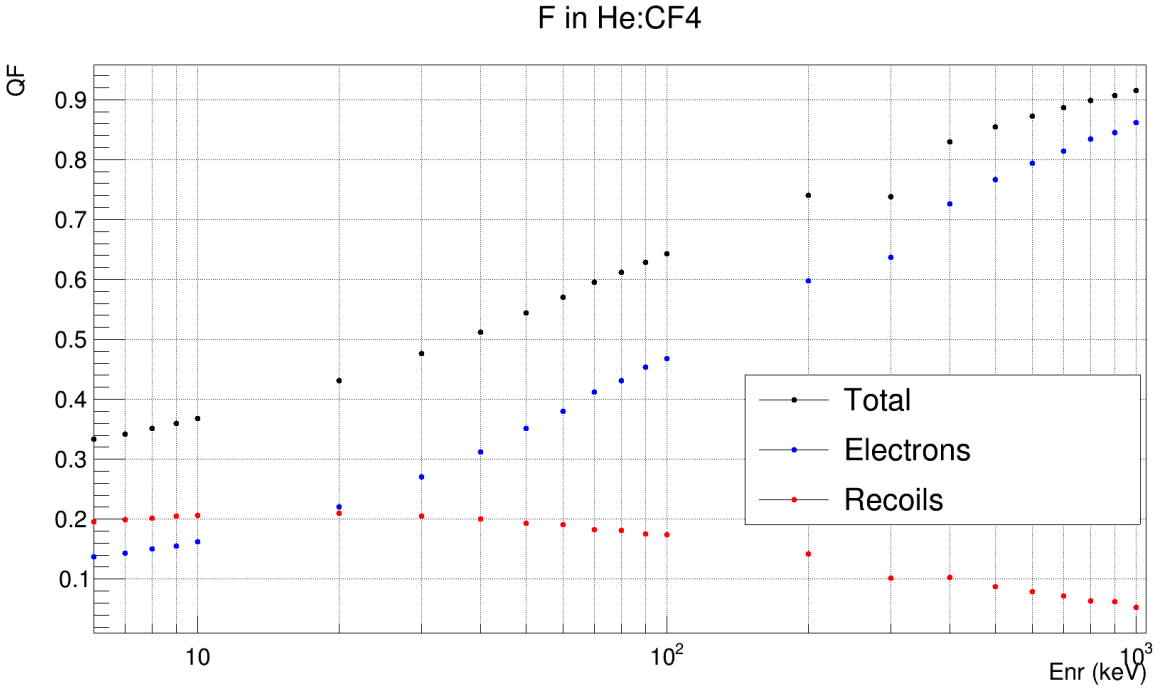


QF = 0.46 for 10 keV
(This work)

Quenching Factor assessment



QF = 0.2 for 10 keV
(Emanuele Marconato)



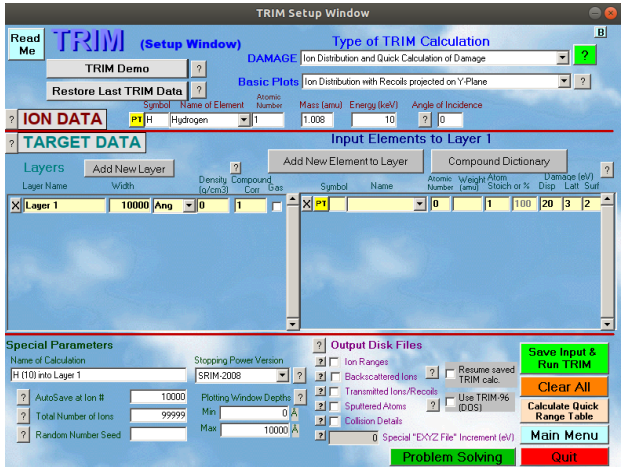
QF = 0.37 for 10 keV
(This work)

Quenching Factor assessment

- Simplified approach to QF analysis already performed for H, He, C, F for different energies (from 1 keV up to 1 MeV);
- In this approach we used the "quick calculation" of SRIM;
- Parameters used:
  - Gas density: 0.00156 g/cm3;
  - Atomic percent (He-23.1%, C-15.4% and F-61,5%);
  - Target width (depends on the energy and was conceived to optimize the bin to particle range);
  - Number of ions simulated: 1000 per run;

SRIM with Python - PySRIM

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



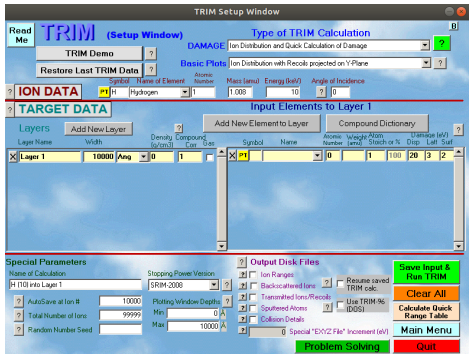
- Has several limitations, but probably the main one is that is not very practical for longer simulations or when you need to study event by event.

- Luckily we will always have python

- PySRIM which combines the advantages of running SRIM with python.

SRIM with Python - PySRIM

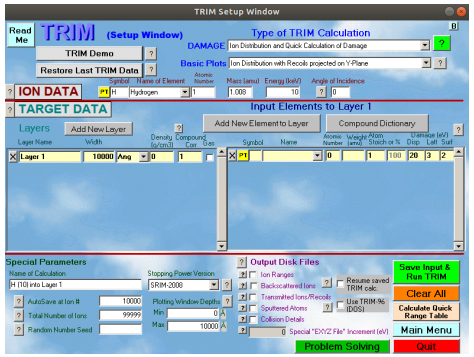
- Python script




```
from srim import Ion, Layer, Target, TRIM

for j in ['H','He','C','F']:
for k in [1e3,3e3,5e3,8e3,1e4]:
for i in range(1,1000):
# Construct a 3MeV Nickel ion
ion = Ion(j, energy=k)

# Construct a layer of nick 200um thick with a displacement energy of 30 eV
layer = Layer({
        'He': {
            'stoich': 3.0,
            'E_d': 5.0,
            'lattice': 1.0,
            'surface': 2.0}
        'C': {
            'stoich': 2.0,
            'E_d': 28.0,
            'lattice': 3.0,
            'surface': 7.41}
        'F': {
            'stoich': 8.0,
            'E_d': 25.0,
            'lattice': 2.0,
            'surface': 3.0}
        }, density=0.000156, width=200000.0*k/1e3)

# Construct a target of a single layer of Nickel
        target = Target([layer])

    # Initialize a TRIM calculation with given target and ion for 1000 ions, quick calculation
        trim = TRIM(target, ion, number_ions=1, calculation=1)

    # Specify the directory of SRIM.exe
    # For windows users the path will include C://...
        srim_executable_directory = '/home/cortez/Products/SRIM2008'

    # takes about 10 seconds on my laptop
        results = trim.run(srim_executable_directory)
    # If all went successfull you should have seen a TRIM window popup and run 1 ion each time!
    # results is `srim.output.Results` and contains all output files parsed
    from srim import TRIM

    TRIM.copy_output_files('/home/cortez/Products/SRIM2008','/home/cortez/Producrs/SRIM/Results')
os.rename (r'/home/cortez/Producrs/SRIM/Results/LATERAL.txt', r'/home/cortez/Producrs/SRIM/Results/LATERAL'+j+'run'+str(i)+'Energy'+str(k/1000)+'keV.txt')
...
os.rename (r'/home/cortez/Producrs/SRIM/Results/TDATA.txt', r'/home/cortez/Producrs/SRIM/Results/TDATA'+j+'run'+str(i)+'Energy'+str(k/1000)+'keV.txt')
os.rename (r'/home/cortez/Producrs/SRIM/Results/VACANCY.txt', r'/home/cortez/Producrs/SRIM/Results/VACANCY'+j+'run'+str(i)+'Energy'+str(k/1000)+'keV.txt')
print ('Running event from ' + j + ' of ion '+str(i)+ ' out of 1000, for the energy ' + str(k/1000) + ' keV.')
```

SRIM with Python - PySRIM

- Python script



Defines the elements to be used in the simulation

Defines the energy of the incident particles

Allows for the simulation of event by event to better estimate the effects of the incident particles

Stores the files with different names

To be done:

- Need to solve the issue for single event (program crashes)
- Solve the issue for the width for different materials to maintain aprox. number of bins/distance (for the same element there's no issue).

Conclusions and Future work

- First results on the QF were obtained.
- Need to be cross-checked
- H and He QF in He-CF4 (60-40) seems to be worse than the results from Emanuele;
- C and F QF on He-CF4 seems to be better than Emanuele's results;
- We can now control SRIM using python, that allows to optimize the time needed to run event by event calculation.

- We will now proceed with the ionization profile analysis;
- Solve the issues observed with the python code (error observed in single event);
- Once finished, we intend to make better estimate of the QF;

Thank you!