Computer Tools for Nuclear Physics

Introduction to SRIM/TRIM

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Introduction to SRIM / TRIM

SRIM is the package aiming to estimate the:

- Losses of energy of a beam of particles passing through an absorber, and the spread after a given length.
- range of ions penetrating the material
- Radiation losses in the material

It consists of:

- Tables of measured and interpolated energy losses: www.srim.org/SRIM/SRIMPICS/STOPPLOTS.htm
- SRIM: calculator of energy losses of a given ion passing through a (thin layer of a) given absorber
- TRIM: simulation of a passage of ions through a given (set of) absorber(s)

How to install

Windows

- Create folder `SRIM-2013` and go there.
- Download `www.srim.org/SRIM/SRIM-2013-Std.e`
- Add `xe` to the end of the name `SRIM-2013-Std.e`
- Run the executable to unpack stuff
- In the folder `SRIM-Setup` run `MSVBvm50.exe`
- Copy `*.ocx` to the main folder `SRIM-2013`
- Run `SRIM.exe`

Linux + Wine

- `mkdir SRIM-2013 ; cd SRIM-2013`
- `wget www.srim.org/SRIM/SRIM-2013-Std.e`
- `mv SRIM-2013-Std.e{,xe}`
- `nice wine SRIM-2013-Std.exe`
- `cd SRIM-Setup ; wine MSVBvm50.exe`
- `cp *.ocx .. ; cd ..`
- `nice wine SRIM.exe`

Troubleshooting

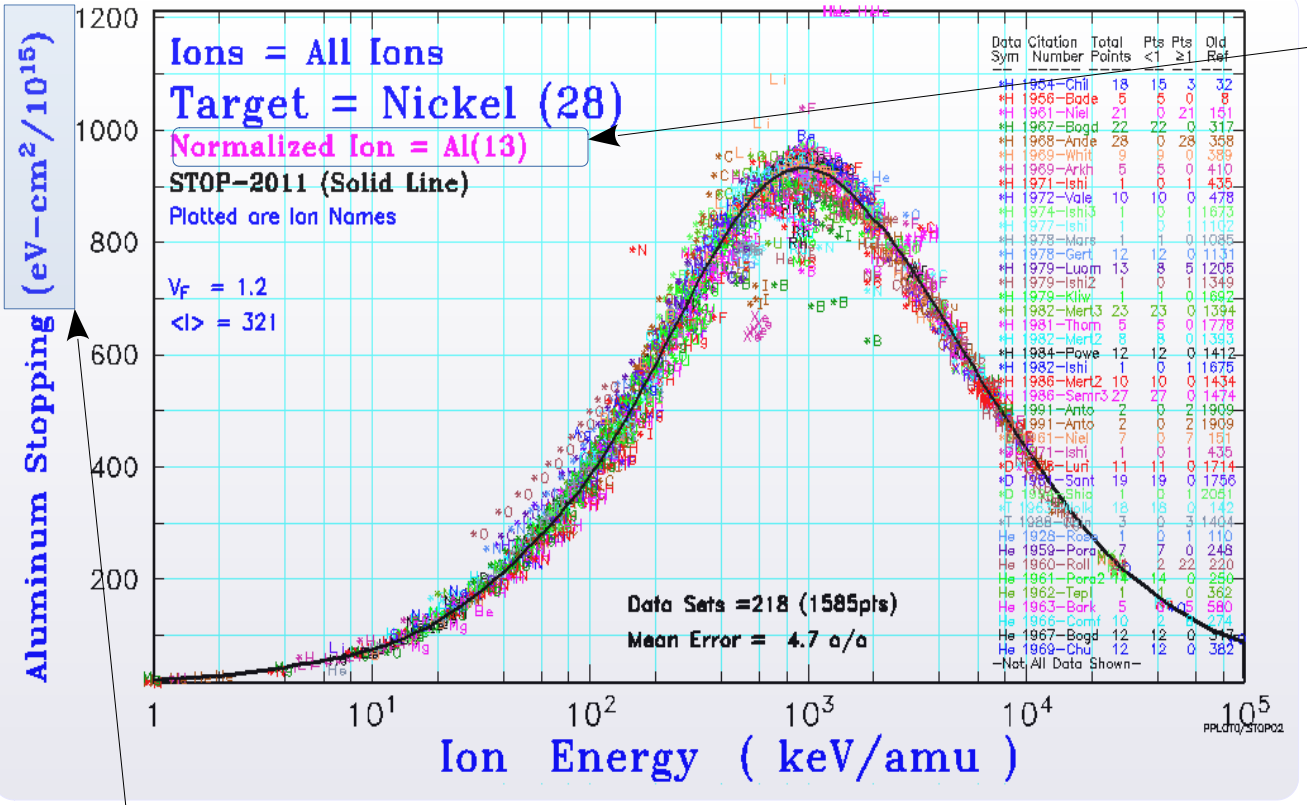
– [Windows] TRIM crashes or freezes → Change date format to "English (US)" and time to dd-MMM-yy (Win 10 / Win 11)
– [Linux] TRIM crashes or freezes → in file `~/.wine/user.reg` change the variable `sDecimal` from "," to "."
– Some OCX component not found → find this file in `SRIM-Setup` folder ⊕ do `cmd` as admin ⊕ register it.
– [Compound Dictionary] unreadable → add font `SRIM-2013/Linedraw.ttf` (and activate it)

- Help: `SRIM ReadMe (English-2011).rtf` file

Energy loss database on-line

- www.srim.org/SRIM/SRIMPICS/STOPPLOTS.htm

  → shows the plots of *specific energy loss* (= loss of energy per unit path)
  of [ion X] in [any target] or of [any ion] in [target X] .



Values of d*E*/d*x* for every specie of beam ion were normalized to the value for ^{13}Al beam ion, basing on the Bethe-Bloch approximation:

$$-\frac{dE}{dx} \sim \left.\frac{M\,Z^2}{E_{Kin}}\right|_{Ion} \sim \left.\frac{Z^2}{E_{Kin}/A}\right|_{Ion}$$

In order to retrieve the d*E*/d*x* for your ion specie, you need to rescale:

$$\left.-\frac{dE}{dx}\right|_{Ion\,X} = \left.-\frac{dE}{dx}\right|_{^{13}Al} \times \left(\frac{Z_{Ion\,X}}{Z_{Al}}\right)^2$$

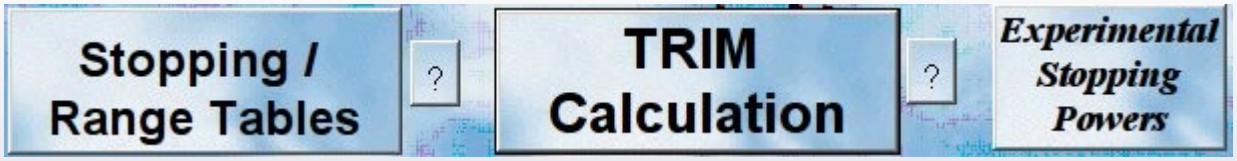
- The unit of d*E*/d*x* is unusual: [eV · cm² / 10¹⁵] .
  That's because the value of d*E*/d*x* is given for a target of 1 cm² section which contains 1 atom.
- Let's call N_{S1} the number of such atoms in *your* target. How to calculate N_{S1} ?

  ① For a target of given *A* and ρ, the concentration *n* is : $\frac{n}{N_A} = \frac{\rho}{\mu}$

  ② Number N_{S1} of atoms in a target of thickness *x* and section S_1 = 1 cm² : $N_{S1}(x) = n \cdot x$

Main menue

SRIM, i.e. energy loss calculator



(database available in the "pro" version only)

SRIM Menue

To admix a new species of atoms to the absorber

E_{Kin} of beam ion [keV]

Caution: not E_{Kin}/A

Limit: $E_{kin}/A \leq 10$ GeV

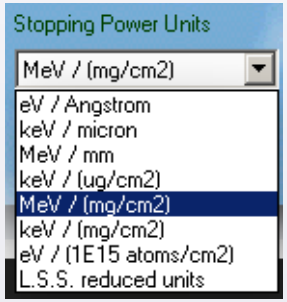
If the target is gaseous

List of various chemical compounds

Stoichiometric composition,
e.g. $H_2 \rightarrow$ Stoich = 2

Show results

Choice of units



$[\rho x] = g/cm^2$

$$P_{\text{int}} = \sigma_R \frac{(\rho x)_T}{A_T} N_A$$

$$N(x) = N_0 \exp\left(-n_T \sigma x_T\right)$$

For the compound: corrections wrt. Bragg Rule

SRIM – results

d*E*/d*x* from **electromagnetic** interactions

d*E*/d*x* from **nuclear** interactions

Range of beam ion in an absorber

Straggling

(positional dispersion of beam ions after their stopping)

Stopping Units = eV / (1E15 atoms/cm2)
See bottom of Table for other Stopping units

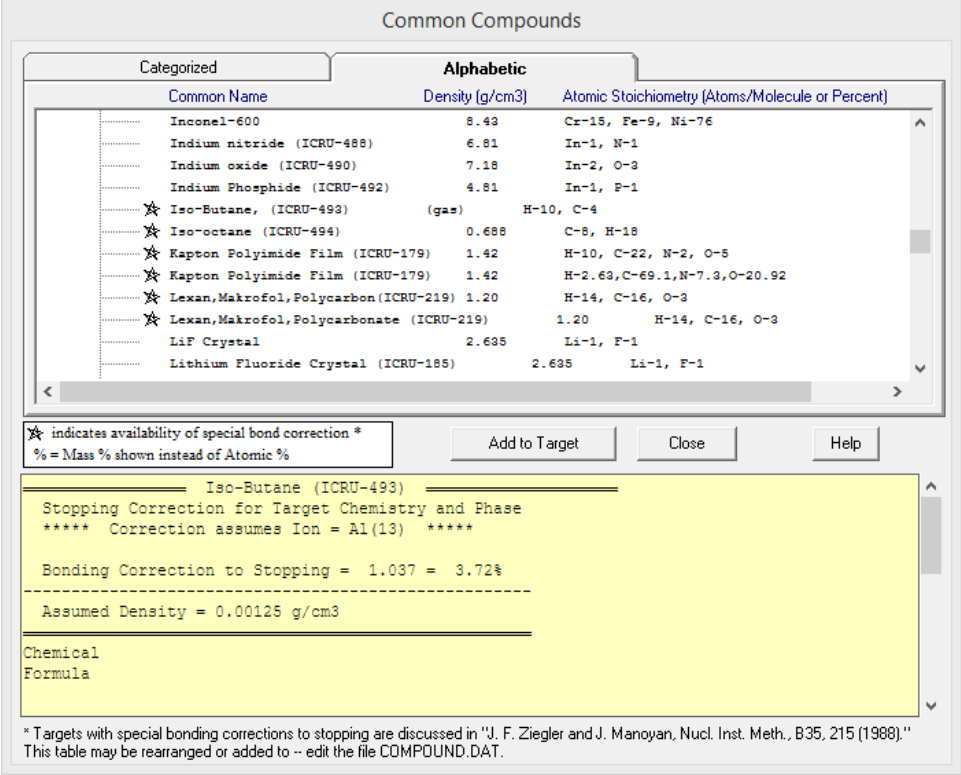
Ion Energy	dE/dx Elec.	dE/dx Nuclear	Projected Range	Longitudinal Straggling	Lateral Straggling
10.00 MeV	7.795E+02	4.045E+00	2.42 um	2428 A	3020 A

Factors for **conversions** between d*E*/d*x* units

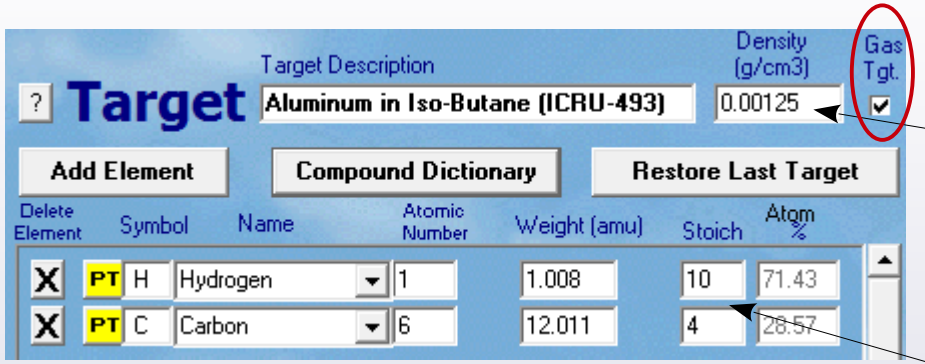
Multiply Stopping by	for Stopping Units
9.1274E-01	eV / Angstrom
9.1274E+00	keV / micron
9.1274E+00	MeV / mm
1.0261E-02	keV / (ug/cm2)
1.0261E-02	MeV / (mg/cm2)
1.0261E+01	keV / (mg/cm2)
1.0000E+00	eV / (1E15 atoms/cm2)
3.9592E-03	L.S.S. reduced units

Selection of compounds

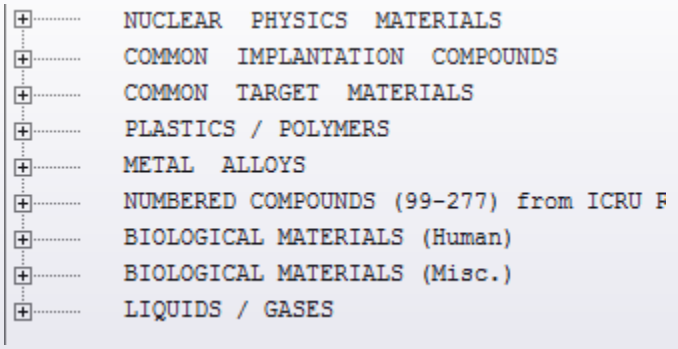
[Link]



- Example: Al ion penetrating the Iso-Butane gas



- **List of categories:**



- **Bragg Rule:**

For a compound made of atoms of type A ⊕ B,

$$\frac{dE}{dx} = \left.\frac{dE}{dx}\right|_A + \left.\frac{dE}{dx}\right|_B$$

→ It's an approximation that has corrections

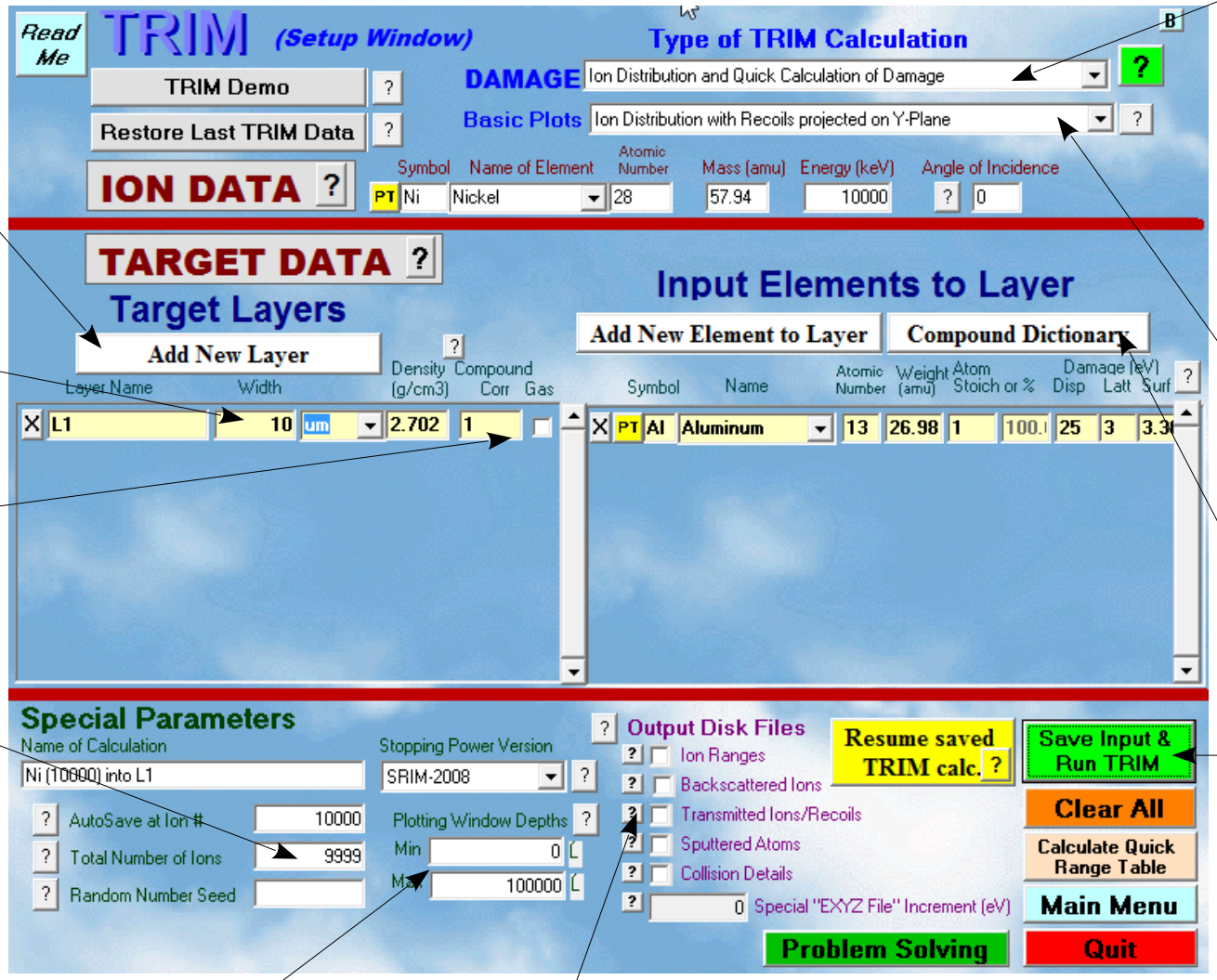
[☆] for substances marked in this way, SRIM includes corrections based on CAB model

Density for pressure p = 1 atm.
If p is different, the density should be rescaled.

Caution: value for Iso-Butane @ p = 1 atm is erroneous. Should be: ρ = 0,00251 g/cm^3

Stoichiometry for C_4H_{10}

TRIM – Dialog box



If the absorber has more layers

thickness of the absorber

Click if the target is gaseous

No. of ions to propagate

Simulation type:

1. Neglect damage of target and emission of atoms from target.
2. Full simulation
3. Allow for emission of atoms from the target

Plots to be visualized during the simulation (in-flight)

Selection of compound substances

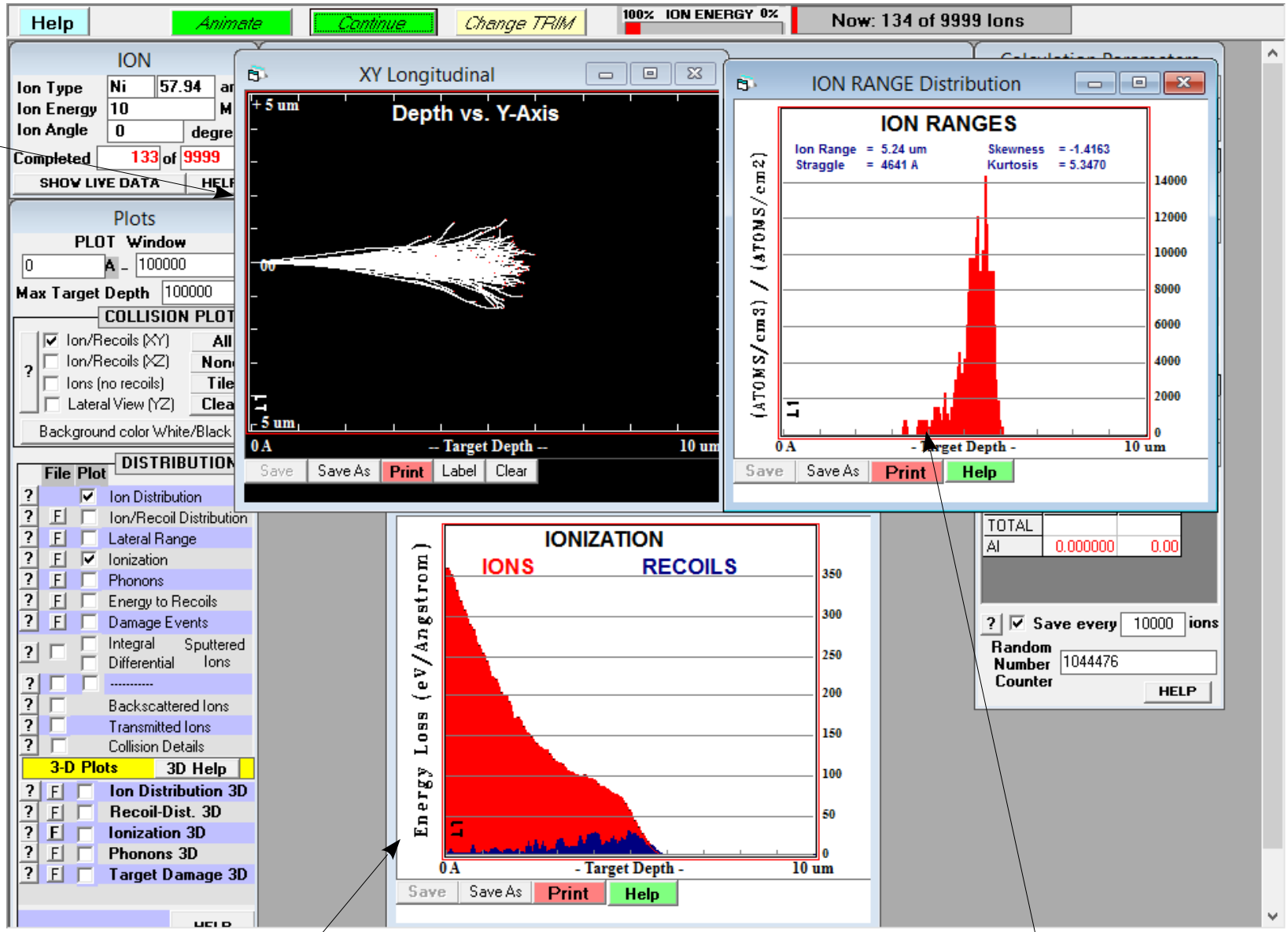
Go simulate!

Range of beam axis ("X") on the plot

Choice of output files (that TRIM will generate)

Important option: "Transmitted Ions/Recoils" → file `transmit.txt`

TRIM – simulation window



Tracing of passage of the beam ions

Choice of:

– plots

– output files

Profile of $\langle dE/dx \rangle$ as function of x

It changes along x, since particle's energy drops during passage

Distribution of ion ranges

TRIM – beam straggling

Straggling: spread of energy and/or position of the beam ions after passage the absorber of a given thickness (e.g. a beam through a target/degrader or through the detector window)

0. We assume here that at least some beam ions would reach the end of the absorber.

In the TRIM dialog box:

1. Switch on [Output Disk Files] → [Transmitted Ions/Recoils] → ☑ , and then select "1"
2. After the simulation: check for the `transmit.txt` file in the `SRIM Outputs` folder.

TRANSMIT.txt

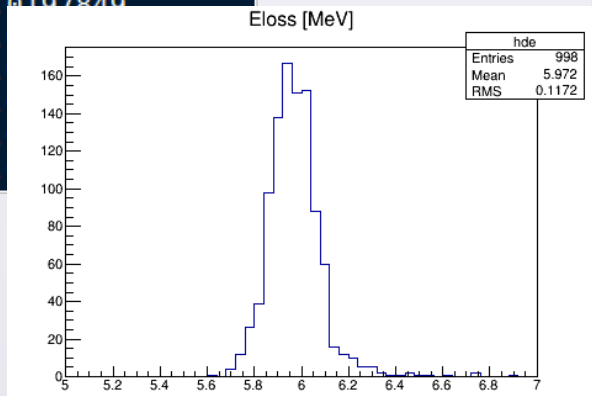
```
============================== SRIM-2013.00 ================================
================================================================================
=================  TRANSMIT.txt : File of Transmitted Ions  ==================
=  This file tabulates the kinetics of ions or atoms leaving the target.      =
=  Column #1: S= Sputtered Atom, B= Backscattered Ion, T= Transmitted Ion.    =
=  Col.#2: Ion Number, Col.#3: Z of atom leaving, Col.#4: Atom energy (eV).   =
=  Col.#5-7: Last location:  X= Depth into target, Y,Z= Transverse axes.      =
=  Col.#8-10: Cosines of final trajectory.                                    =
= *** This data file is in the same format as TRIM.DAT (see manual for uses).=
====== TRIM Calc.= Al(10 MeV) ==> Layer 1(  1 um) ============================
 Ion  Atom   Energy        Depth       Lateral-Position        Atom Direction
 Numb Numb    (eV)          X(A)         Y(A)       Z(A)      Cos(X)  Cos(Y) Cos(Z)
T    1 13 .3983746E+07   1000064E-02  .2971E+03  .4864E+03   .9767120  .1769064  .1213995
T    2 13 .4071823E+07   1000190E-02 -.1117E+03  .3788E+03   .9963755  .0134767  .0839890
T    3 13 .4099861E+07   1000121E-02 -.5497E+01 -.1227E+03   .9991514 -.0411854  .0005086
T    4 13 .4098159E+07   1000217E-02 -.3030E+03  .8463E+02   .9986100 -.0427266  .0308636
T    5 13 .3947297E+07   1000098E-02  .2790E+03 -.7825E+02   .9653103 -.1829261 -.1863174
T    6 13 .3987888E+07   1000197E-02 -.1563E+02 -.8668E+01   .9989632 -.0410004  .0197849
T    7 13 .4131337E+07   1000161E-02  .1038E+03 -.3660E+03   .9990785  .0113496 -.
T    8 13 .4141843E+07   1000133E-02  .4241E+02 -.2878E+03   .9992457  .0294721 -.
T    9 13 .4048078E+07   1000050E-02 -.1080E+03  .8655E+02   .9978623 -.0515206  .
T   10 13 .3798280E+07   1000108E-02  .1461E+04  .5658E+03   .9552314  .2949221  .
T   11 13 .4052493E+07   1000137E-02  .1921E+03  .4439E+03   .9943126  .0437691  .
```

After passage through the absorber

E_{Kin} of ion [eV]

⊥ position [Å]

deviation of direction



TRIM – tracing the energy loss on the way

TRIM can print out all the subsequent acts of interaction in the medium, giving per interaction:
position of this interaction, ion energy and the local value of the specific energy loss (loss of *E* per unit of path).

In the TRIM dialog box:

1. Switch on [Output Disk Files] → [Collision Details] → ☑
2. After the simulation: check for the `collison.txt` file (typo is intended) in the `SRIM Outputs` folder.

Example for 1 given ion. Lines reporting the subsequent interactions appear in the raw output like this:

```
...
  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
-------------------------------------------------------------------------------------------------------------
300001319.97E+03337875.E-033-4930.E-063 5782.E-0630772.053   C 333617.E-033000000001.0003      3      3
300001319.93E+03364043.E-033-2281.E-053 1614.E-0530771.363   O 318512.E-023000000002.0913      3      3
300001319.90E+03311632.E-023-1204.E-043-1444.E-0530770.633   C 310026.E-023000000001.1613      3      3
300001319.81E+03322070.E-023-2379.E-043-4559.E-0530768.883   C 313711.E-023000000001.5683      3      3
300001319.77E+03327281.E-023-3026.E-043-9741.E-0630768.123   C 339293.E-033000000001.0003      3      3
...
```

The raw output file is misformatted (redundant “3” ‘s appear) .
After correction, the upper printout should look like much cleaner:

```
  Ion     Energy     Depth      Lateral Distance (A)    Se     Atom
  Numb    (keV)       (A)        Y Axis     Z Axis     (eV/A)  Hit
-------------------------------------------------------------------
   1  19.97E+03  7875.E-03  -4930.E-06  5782.E-06 772.05   C
   1  19.93E+03 64043.E-03  -2281.E-05  1614.E-05 771.36   O
   1  19.90E+03 11632.E-02  -1204.E-04 -1444.E-05 770.63   C
   1  19.81E+03 22070.E-02  -2379.E-04 -4559.E-05 768.88   C
   1  19.77E+03 27281.E-02  -3026.E-04 -9741.E-06 768.12   C
...
```