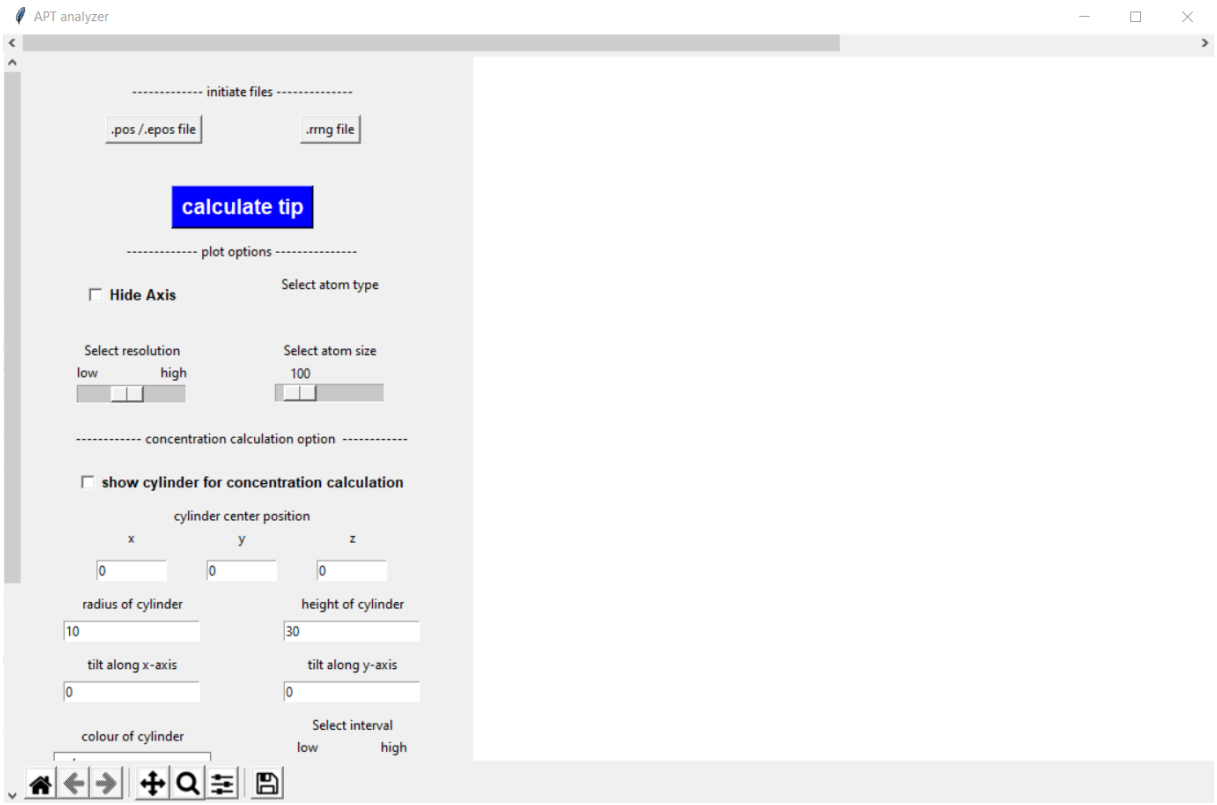
APT- analyzer

The APT-analyzer is a python based tool for visualizing and analysing atom probe tomography data, with a focus on calculating concentration and excess profiles of elements.

Getting started:

Run the APT-analyzer code with the python software of your choice. If successful following window should appear:



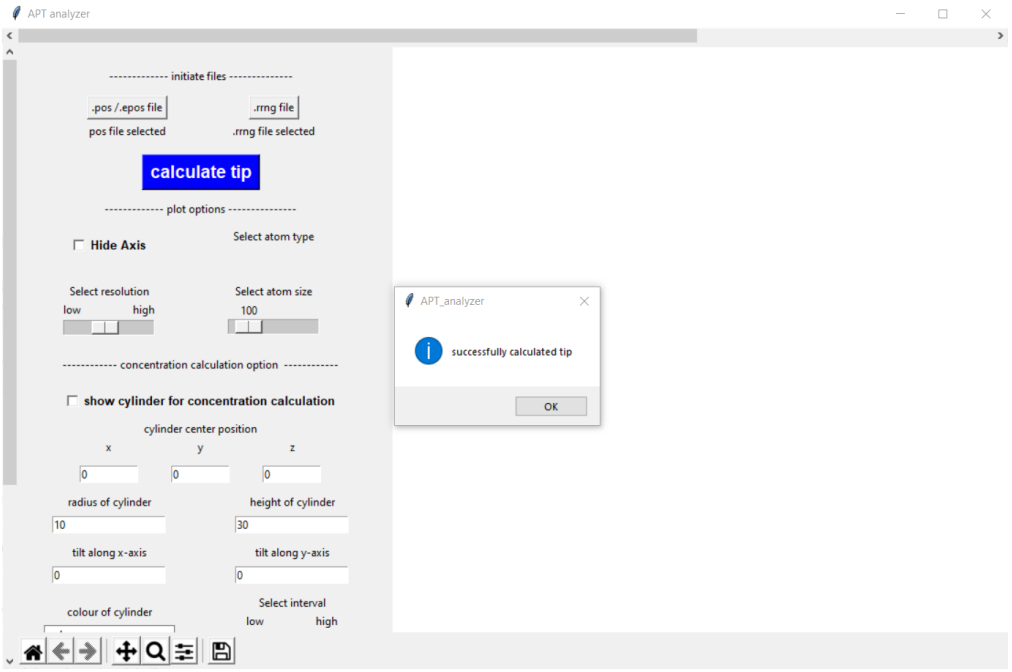
In order to visualize a APT tip, two files are necessary:

- .pos file (instead of a .pos file also a .epos file can be used)
- .rrng file.

So the first step is to load in a .pos/.epos file and a .rrng file from your directory. (Note that the APT-analyzer will only recognize the file as such if .pos/.epos or .rrng is written in them, also .POS/.EPOS and .RRNG are valid, everything else will result in the program not recognizing the file).

After you successfully selected the files and a label saying “pos file selected” /”rrng file selected” can be seen underneath the search button, the blue button **calculate tip** may be pressed.

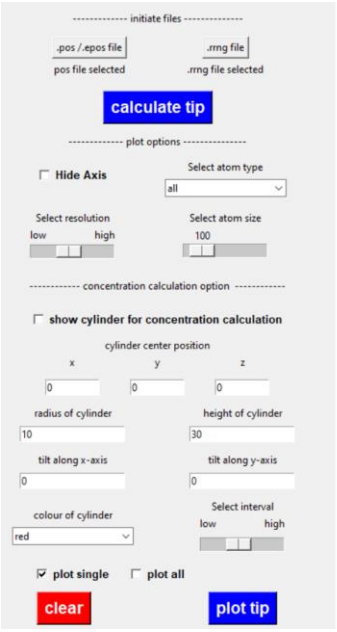
For calculating the tip the program may need a few seconds. When compete a message box with the message “successfully calculated tip” will appear.

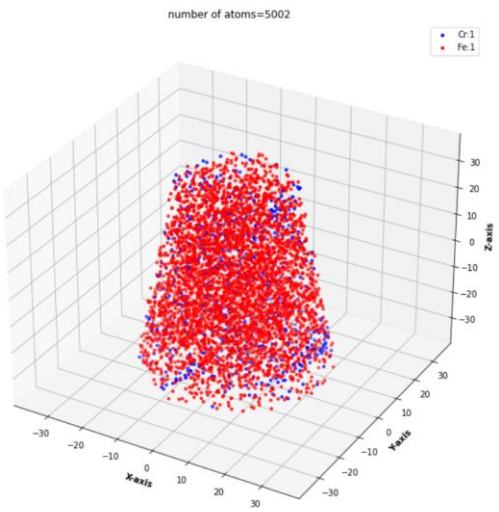


Now the tip can be plotted. In the section “plot options” the plot can be adjusted.

- Hide Axis — hides the axis and title of the 3d plot of the tip
- Select atom type — single element types can be seen, to see whole tip select ‘all’
- Select resolution — the number of atoms plotted
- Select atom size — the size of the displayed atoms

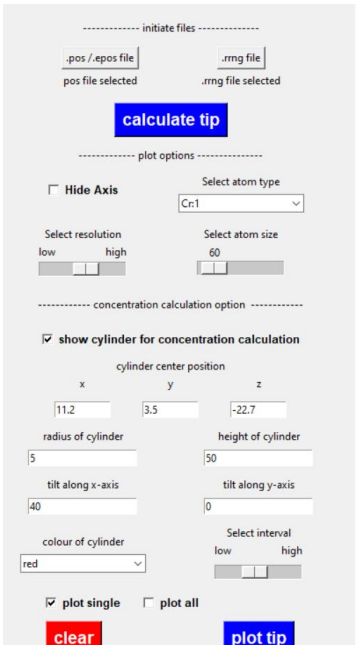
If you want to plot the tip now you may scroll down until you see the blue button **plot tip**. When you press it without changing any setting the window may appear in the following settings:

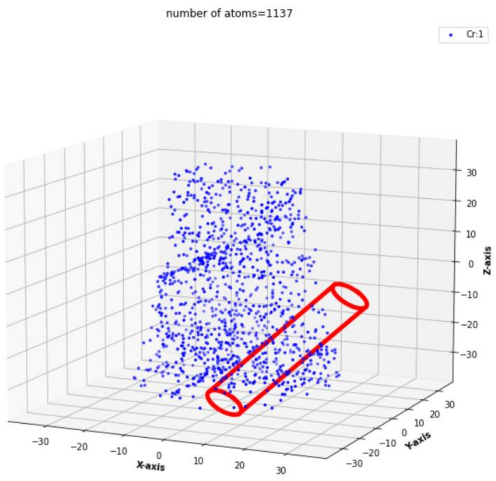




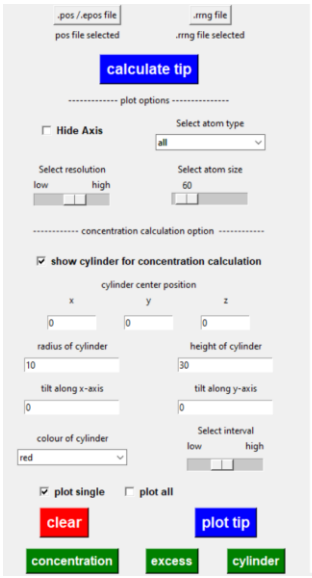
By holding the left mouse button you can view the 3 plot from different angles and by holding the **right mouse button** and moving your mouse up and down you can zoom in and out of the image.

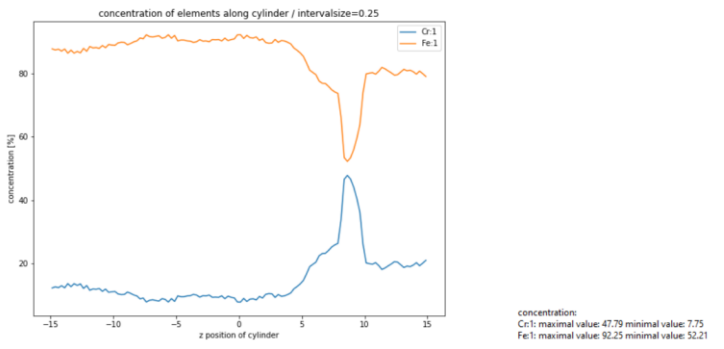
In order to analyse the chemical composition of the tip a volume (cylinder) in which it is evaluated can be selected. A default setting is already set and by selecting "**show cylinder for concentration calculation**" it can be seen. The x, y and z position of the middle of the cylinder can be adjusted as well as the radius and height. Also the angles along the x and y axis can be changed to tilt the cylinder. The cylinder will then look something like this:



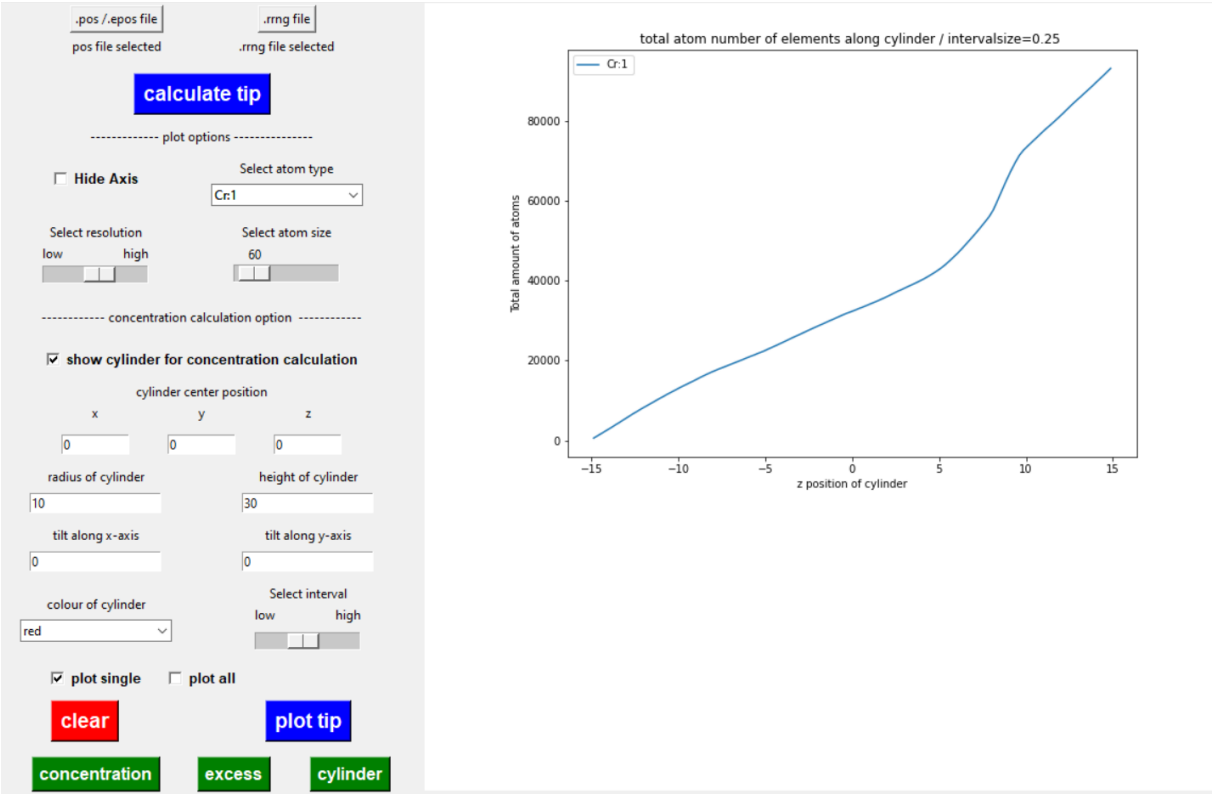


Along this cylinder, from bottom to top in a set interval the concentration of each element in relation to each other can be calculated by pressing the green **concentration** button. After pressing the button a concentration profile can be seen, as well as a text describing the maximal and minimal values of each concentration curve.

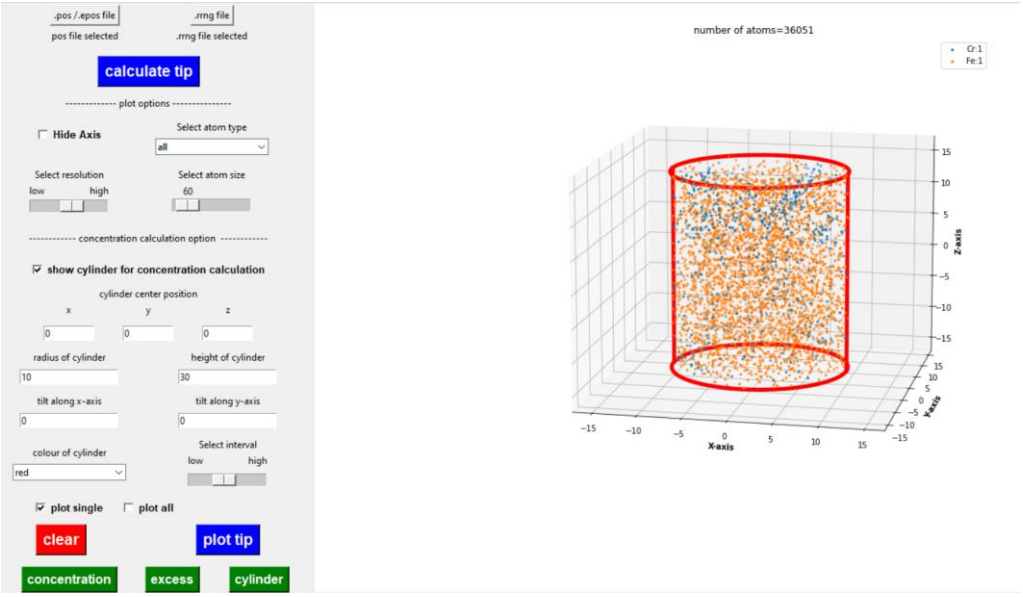




If in the plot options only 1 element was selected, also the concentration data of only 1 element will be shown. The concentration is always calculated in regards to the % of the total amount of all atoms. Similar to the concentration, the integral of the concentration (or total amount of atoms) can be plotted by pressing the green **excess** button.

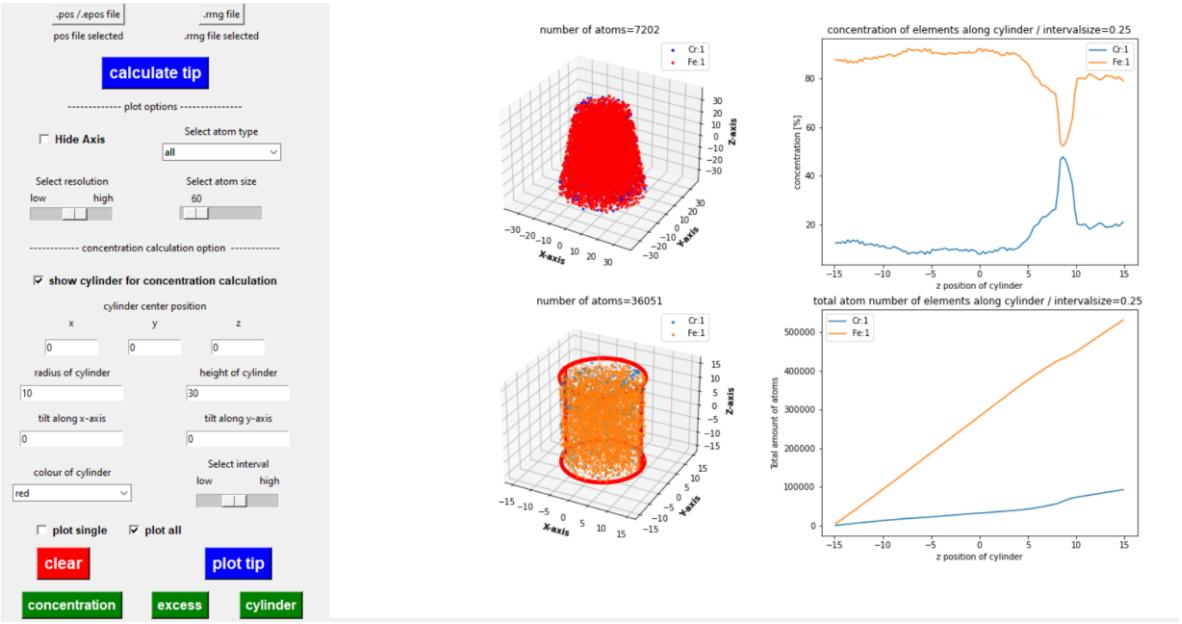


For this plot only showing one element is preferable since the slope of the curve can be analysed better and therefore so can the excess.
In addition, you want to look at the selected atoms inside the cylinder a little closer a zoomed 3d image can be seen by pressing the green **cylinder** button.



If you want to look at the plotted tip, the concentration and the total amount of atoms inside the cylinder at the same time you may select **plot all**.

Warning: **plot all** option makes it, that by plotting you do not clear the previous plot anymore. Therefore, to clear the red **clear** button shell be pressed.



So enjoy using the APT analyzer.

If you find any bugs or have any suggestions how to improve the APT analyzer, please contact me: alexander.reichmann@unileoben.ac.at

The example files used here have been copied from the APT-GB toolset:
[GitHub - RhettZhou/APT_GB: Help identify grain boundaries from atom probe datasets for mapping interfacial excesses and concentrations.]