Plotting PySamba scan data with Gnuplot

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1 How to start gnuplot

Open a terminal. You could simply right click on the desktop and choose “Open Terminal”. Alternatively, you can press Alt-F2 and then type “gnome-terminal”. A terminal window will open. Move to the right folder, that where your data are. It is not strictly necessary, but it will simplify file names. To change folder use cd:

```
cd ExperimentalData/2010/20100721_myDataFolder
```

to start gnuplot type `gnuplot`

Gnuplot will start and a gnuplot prompt will appear.
```
gnuplot>
```

2 Plotting data from a plain ASCII file

2.1 Plotting

Gnuplot accepts multicolumn ASCII files. It can skip comments automatically, but it is preferable that comment lines start with a `#` character.

Each column is identified by a number starting from 1. To plot a single column file type:

```
plot "filename"
```

To select the column 1 to be used as X-axis and column 2 as Y-axis, type:

```
plot "filename" using 1:2
```

For short you can type:

```
p "filename" u 1:2
```

To plot several files over the same graph:

```
p "filename1" u 1:2,"filename2" u 1:2
```

You can also compare several columns of the same file without typing the name of the file:

```
p "filename1" u 1:2,"" u 1:3,"" u 1:4
```

You can combine the two:

```
p "filename1" u 1:2,"" u 1:3,"" u 1:4,"filename2" u 1:2
```
2.2 Select line styles

Plots are drawn as big points by default. You can change the default behaviour with the following commands:

- `set style data lines`
- `set style data points`
- `set style data linespoints`

Data will be plot all by default with the specified styles.

Alternatively, you can plot data in different styles by specifying it in the plot command:

- `plot "filename" using 1:2 with lines`
- or in the short form:
  - `p "filename" u 1:2 w l, "filename2" w p, "filename3" w lp`

To change the color of a curve (all curve have different colors):

- `p "filename" u 1:2 l`
  - this will plot with color 1 the file.

Example:

- `plot "filename" u 3:5 every 2 axis x1y1 with lines 1 linewidth 2,"filename2" u 1:3 every 5 axis x1y2 with points 3 pointsize 2`

The new cards will plot every 2 points on the axis x1y1, x1y2, x2y1 ... et cetera.

You can mix functions and files:

- `p "filename" u 1:2 w p, sin(x) w l`

Try to do it, “w p” means “with points” and “w l” means “with lines”.

2.3 Simple formulas

The following example will plot the third column of the file with name filename multiplied by 2 and versus the first column.

- `p "filename" u 1:($3*2)`

When you want to use a formula you must:

1. Use the using command, even for a single column;

2. put the formula in brackets;

3. the name of the \textit{n}^{th}-column is $n$.

Another example:

- `p "filename" u ($3^2-2*2):((\ln(\$1))^{\exp(\$10)-5})`

You can mix in the formula different columns to obtain a vector to plot over x- or y-axis.
3 Plotting a PySamba scan file

3.1 Files produced by escan

An escan file is a file with a variable and quite large number of columns. Despite this fact, the most important columns are a few and easily accessible:

1: energy (eV);
2: angle (°);
3: calculated absorption, total fluorescence in sexafs or fluo modes or electron yield in tey mode;
4: standard in absorption mode or normalized total electron yield in sexafs mode;
5: \( I_0 \)
6: \( I_1 \)
7: \( I_2 \)

So it is quite simple to draw \( \mu_x \) versus energy, where \( \mu_x = \ln \left( \frac{I_0}{I} \right) \):

\[
p \text{ "filename}_0001\text{.dat" u 1:3 }
\]

or

\[
p \text{ "filename}_0001\text{.dat" u 1:ln($5/$6))}
\]

Fluorescence counts of single detectors are in separate columns and should be found in the file header by opening it with a text editor.

3.2 Files produced by ascan or dscan

These files are multicolourn and contain the value of the motor in the first column. All other columns represent the counter values of the pseudocounter. There is no way to know a priori the content of the file, but usually the counter start with \( I_0 \) and goes on with \( I_1, I_2 \) and so on. There is no reason that a file must be significantly different from another if you do not change the number of ROIs of the MCA.

Example: to plot absorption coefficient measured between the first two ionisation chambers versus the position of the motor, you have to type

\[
\text{plot "filename" u 1:(ln($2/$3)) w l}
\]

4 Using the mouse

Move the mouse to the graphic window, if there is one. Type the letter “h” and you will appear an help list in the console.

Here below, only the most important keys are listed.

\(<\text{Button1}>\) print coordinates to clipboard using ‘clipboardformat’ (see keys ‘3’, ‘4’)

\(<\text{Button3}>\) mark zoom region (only for 2d-plots and maps).

\(<\text{Space}>\) raise gnuplot console window

\(<\text{q}>\) close this X11 plot window
a autoscale (equivalent to: set autoscale keepfix; replot)
...
e replot
g toggle-grid
h help
l toggle-log scale
y logscale for plots
...
L nearest-log: toggle logscale of axis nearest cursor
m toggle-mouse
r toggle-ruler
...
n go to next zoom in the zoom stack
p go to previous zoom in the zoom stack
u unzoom
...
* indicates this key is active from all plot windows.