



- User's Guide - (for version 1703)

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d1Dplot is programmed with Java™

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1. Installation and use of *d1Dplot*

No installation of the program is required. Only extract the files and folders of the zip file into the desired folder in your hard drive and run the executable file (`d1Dplot.exe` in Windows and `d1Dplot` in Linux). In most of the recent Linux distributions, the executable files can be executed by double click from the file explorer but alternatively you can also run it from the command line with `./d1Dplot`. If the execute flag of the file is turned off, turn it on with: `chmod +x d1Dplot`

Tip: Running it from the command line has the advantage that you can give a pattern file as the argument and it will be automatically opened.

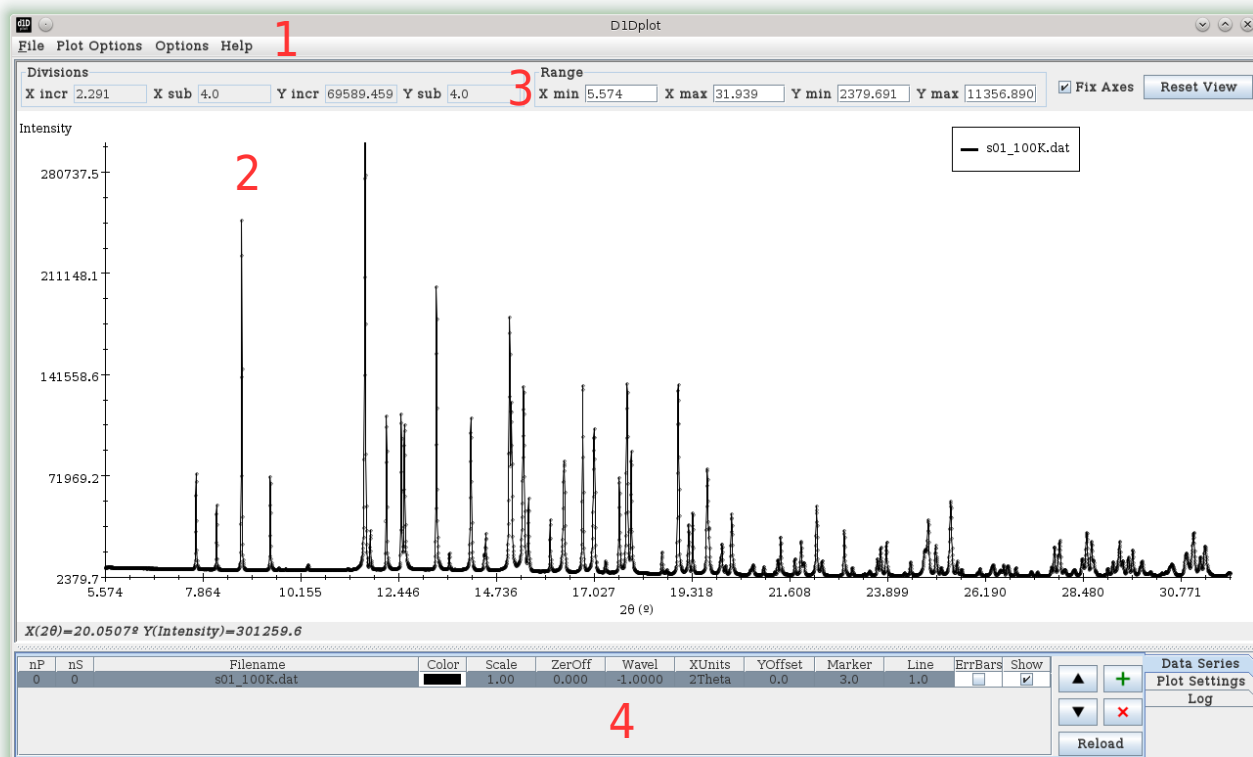
Note: JAVA is required (version 1.6.0_18 or higher).

Configuration file

The first run, the program generates a plain text configuration file (`d1dconfig.cfg`) at the same folder where the program is installed. However, in some systems it can be created inside the user folder or somewhere else (the program will display the location of the file on the output panel located at the bottom part of the main window). Usually there is no need to change anything of this file but, if desired, the parameters are self-explanatory and their value can be modified.

2. Main Window

This is the aspect of the main window after loading a pattern (via menu File-Open, or by clicking the button +, or from command line).



The main parts are the menu bar (1), the plotting area (2), the plot control panel (3) and the bottom tab panel (4). Next sections of the guide will explain each part in detail.

1. Menu bar. To access all the program modules and options. It contains:

- **File**
 - **Open.** Opens a pattern file.
 - **Save As.** Save the (selected) pattern file to any of the supported formats.
 - **Export as PNG.** Export plot area as a PNG image. It asks for a (optional) factor to create a bigger image.
 - **Export as SVG.** Export plot area as Scalable Vector Graphics file.
 - **Close.** Close selected pattern

- **Close all.** Close all opened patterns.
- **Quit.** Exit the program
- **Plot Options**
 - **2D plot.** Bidimensional plot of the selected patterns.
 - **Sequential Y offset.** Apply a Y offset (vertical) to the selected patterns sequentially so that they end in a “stacked” position.
- **Processing**
 - **Find peaks.** Search for peaks (list of peaks can be saved later).
 - **Calc Background.** Estimation of the background.
 - **Subtract patterns.** Subtract patterns (with an optional factor).
 - **Convert to wavelength.** “Convert” the selected pattern to a new wavelength, for comparison purposes in 2theta units.
 - **Change X units.** Change the X units of the selected pattern (to/from 2theta, d-spacing, Q, ...)
 - **Sum selected patterns.** To sum the selected patterns.
- **Help**
 - **About.** Some information about the program.
 - **Manual.** Link to this user's guide.

2. Plot Area. Where the patterns are shown. The general interaction is:

- Left mouse button: Zone selection for zoom in X. Add peaks (peak search module)
- Middle mouse button: Press and drag to navigate the pattern in X and Y. Click to reset zoom and fit view.
- Mouse wheel: Zoom on Y.
- Right mouse button: Press and drag (UP and DOWN) for zoom on X. Press and drag (LEFT and RIGHT) to navigate the pattern along X. Remove peaks (peak search module)

These default mouse button assignments can be changed in the options file.

3. Plot control panel. From here the plotted range (X min, X max, Y min, Y max) can be controlled as well as the divisions of each of the axes:

- *X incr, Y incr*: X and Y major tick increments (with value labels).
- *X sub, Y sub*: X and Y subdivisions between major tick increments (no value labels)

Changing a value and pressing enter applies the value. Reset the view with the corresponding button. Fix Axes, when activated it keeps the ticks and separations of the axes fixed, only the values of the labels are changing according to how the pattern is moved or zoomed. If Fix Axes is disabled, the axis will “move” with the pattern (keeping the X incr, Y incr, X sub and Y sub values fixed).

4. Pattern table and other tabs. Here, we three tabs:

- **Data Series:** It contain a table with all opened patterns. The columns are:
 - *nP*: Pattern number.
 - *nS*: series number.
 - *Name*: Name of the series (by default the filename).
 - *Color*: Color of the series.
 - *Scale*: Y scale of the series.
 - *ZerOff*: Offset of the series in X.
 - *Wavel*: Wavelength of the pattern. Put the correct value to perform operations that need it.
 - *Xunits*: Units of X. By default 2theta. Put the correct value to perform operations that need it.
 - *Y offset*: Offset of the series in Y.
 - *Marker*: Marker size.
 - *Line*: Line width.
 - *ErrBars*: To show the error bars on Y.
 - *Show*: To show or hide the current series on the plot area.

Most of the values can be edited and assigned by clicking directly on the table.

Buttons to move the patterns up/down and to remove/add and reload are available.

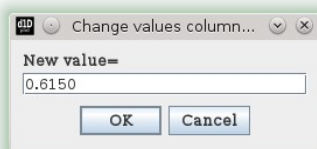
Right click button on the table opens a contextual menu with several options, such as changing values of all selected cells:

nP	nS	Filename	Color	Scale	ZerOff	Wavel	XUnits	YOffset	Marker	Line	ErrBars	Show
0	0	s01_100K.dat		1.00	0.000	-1.0			3.0	1.0		<input checked="" type="checkbox"/>
1	0	s01_109K.dat		1.00	0.000	-1.0			3.0	1.0		<input checked="" type="checkbox"/>
2	0	s01_114K.dat		1.00	0.000	-1.0			3.0	1.0		<input checked="" type="checkbox"/>
3	0	s01_119K.dat		1.00	0.000	-1.0			3.0	1.0		<input checked="" type="checkbox"/>
4	0	s01_123K.dat		1.00	0.000	-1.0			3.0	1.0		<input checked="" type="checkbox"/>

Edit Selected Values
 Convert to WL
 Change X units
 Sum selected patterns

▲ +
 ▼ -
 ✖
 Reload

Data Series
 Plot Settings
 Log
 Help



nP	nS	Filename	Color	Scale	ZerOff	Wavel	XUnits	YOffset	Marker	Line	ErrBars	Show
0	0	s01_100K.dat	Black	1.00	0.000	0.6150	2Theta	0.0	3.0	1.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>
1	0	s01_109K.dat	Blue	1.00	0.000	0.6150	2Theta	0.0	3.0	1.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>
2	0	s01_114K.dat	Red	1.00	0.000	0.6150	2Theta	0.0	3.0	1.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>
3	0	s01_119K.dat	Green	1.00	0.000	0.6150	2Theta	0.0	3.0	1.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>
4	0	s01_123K.dat	Magenta	1.00	0.000	0.6150	2Theta	0.0	3.0	1.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>

- **Plot settings:** Here several general options concerning the plot can be edited, such as the axes titles, color theme, legend, grid, show or not negative Y axis labels and PRF (FullProf profile file output after refinement; Rodríguez-Carvajal, 1993) plot settings.

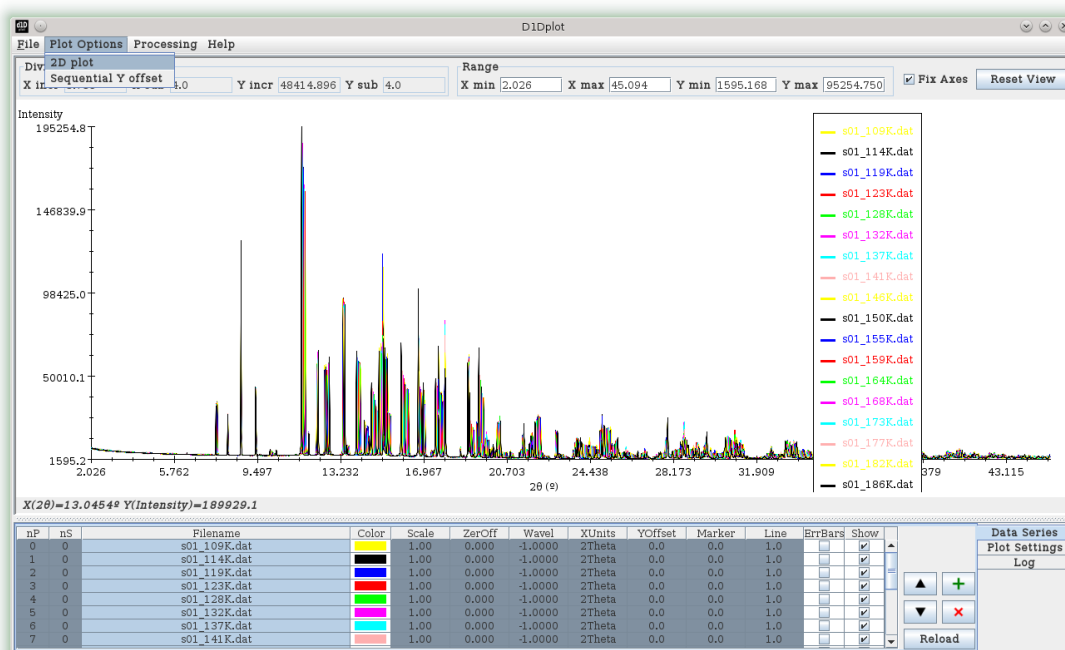
X title	2θ (°)	<input checked="" type="checkbox"/> Legend	HKL tick size (PRF)	6	<input type="checkbox"/> Grid lines
Y title	Intensity	<input checked="" type="checkbox"/> autoPos	<input type="checkbox"/> Bkg Inten (PRF)		<input type="checkbox"/> Negative Yaxis labels
Theme	Light	legendX	legendY	<input checked="" type="checkbox"/> HKL labels on mouse	<input type="checkbox"/> Vertical Y label

- **Log.** Messages of the program are shown here.

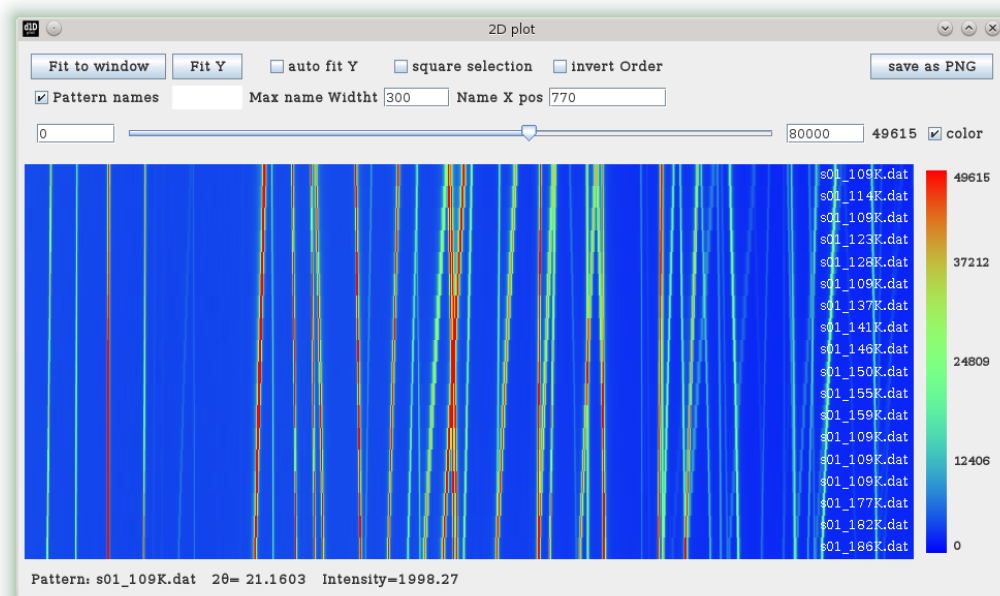
3. Plot Options

2D plot

To plot several patterns in 2D, select them on the table and click on Plot Options -> 2D plot.



A new window will open with the 2D plot:

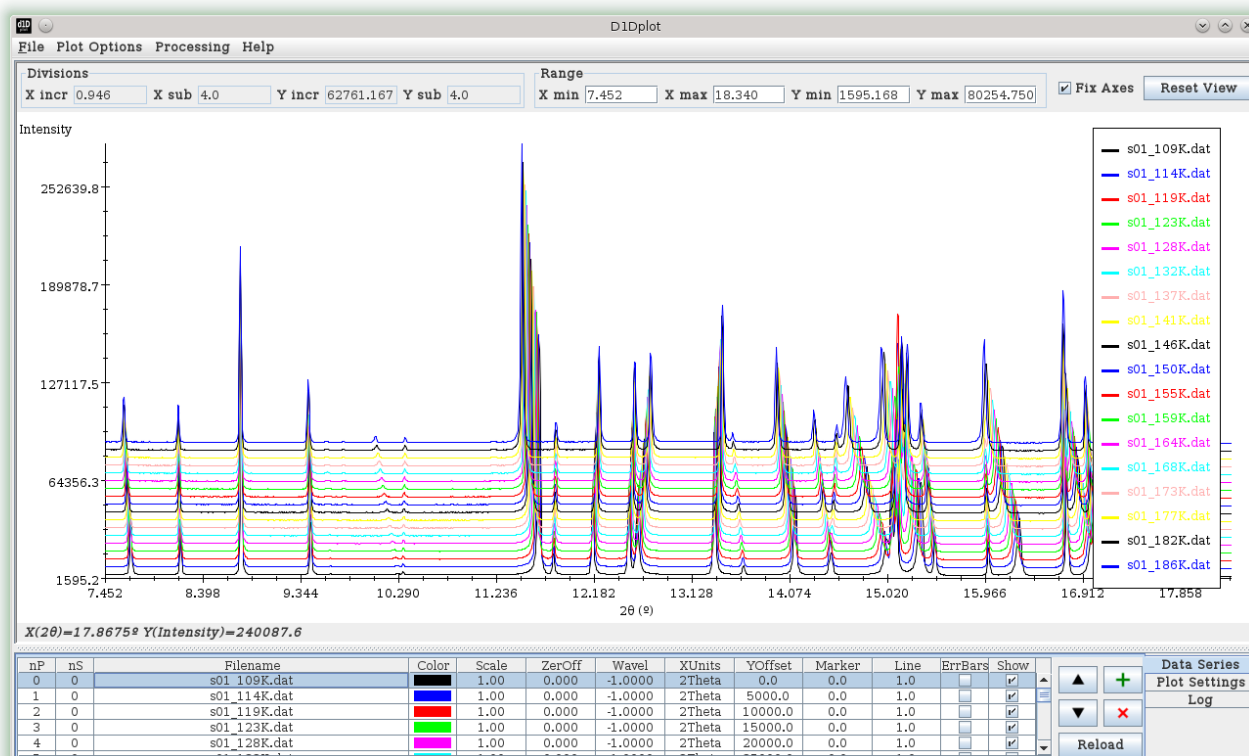


On the 2D plot window you can control the contrast with the slider bar on the top of the plot area. The limits of the contrast bar can be changed on the surrounding textboxes (and pressing enter to confirm). On the plot area, zones can be zoomed in by using the mouse (left click + drag). By default the zoom is only on the X dimension but there is the option of square selection that allows to select square-shaped areas. In that case, it is useful to enable auto fit Y to fit always the zoomed area to the height of the plot area (the button Fit Y allows to do it once only). Use fit to window to return to the initial (full) view.

There is the option to show the pattern names on the image (e.g. for showing temperatures, pressures,...), and choosing the text color and position. Also the image can be saved as PNG.

Sequential Y offset

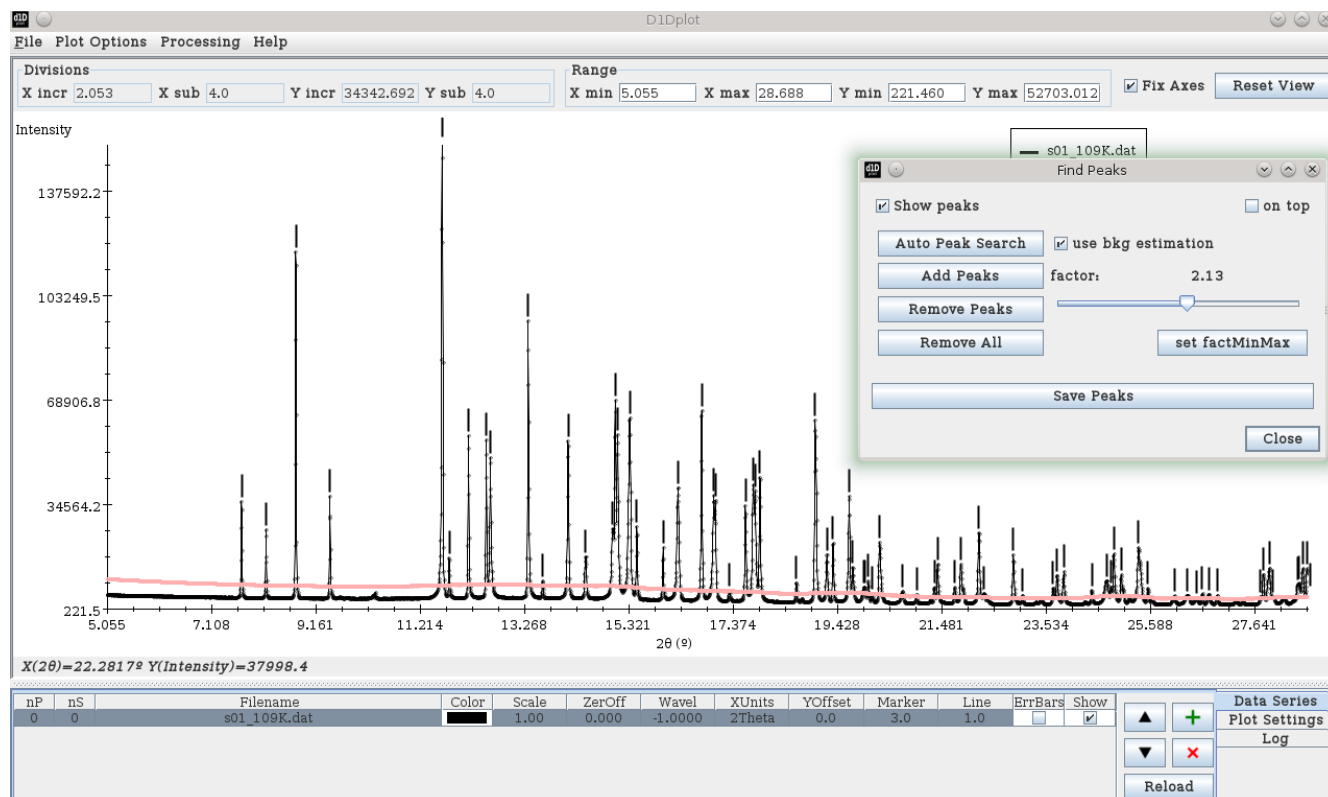
This option can be used to “pile up” diffraction patterns to compare them or check parameter evolutions, phase transitions, etc... Select the patterns you want to stack and a Y offset value between them.



4. Processing

Find Peaks

To select the peaks of the pattern.



The options are:

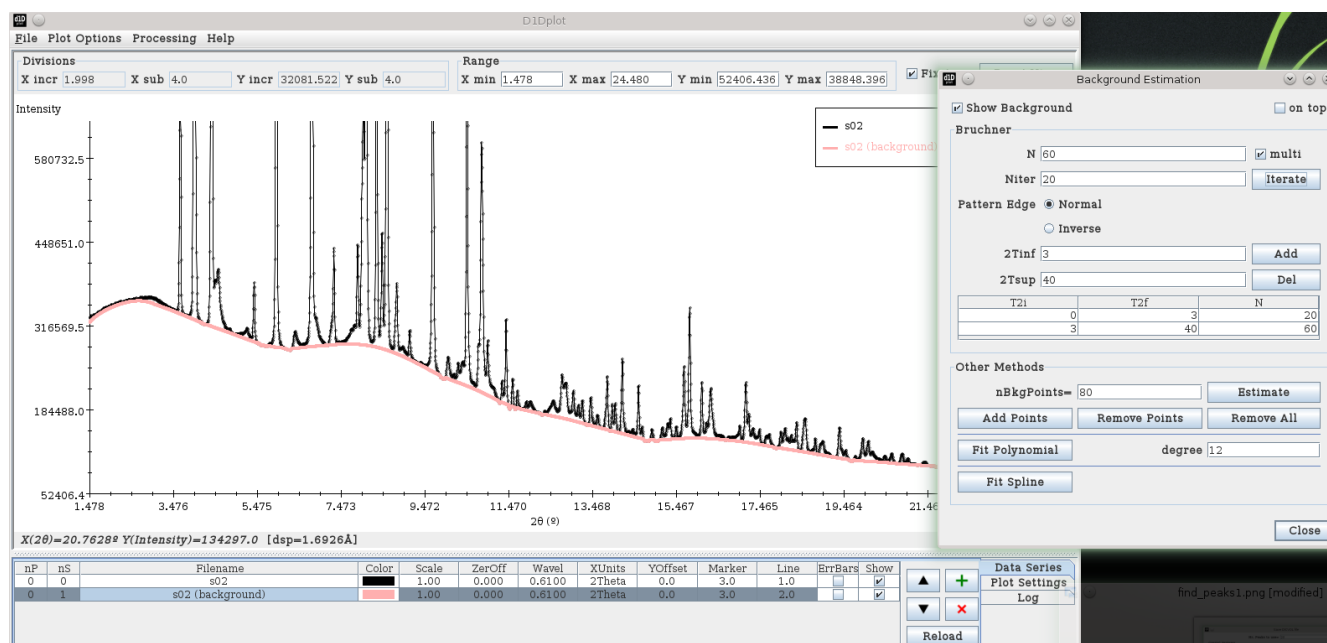
To perform an Auto Peak Search by using or not a background estimation and a slider to set the threshold. If the slider range is not enough it can be changed by clicking the button set factMinMax.

Single peaks can be added by clicking to Add Peaks, then selecting the peaks by left-button click and click again to the same button (which will show Finish). To remove peaks it is the same procedure but with the Remove Peaks button. Clear all the peaks with the Remove All button.

Click on save peaks to save the list of peaks as a text file. Two formats available: simple text file with the peak list or DICVOL (Boultif & Louër, 2004) file (an additional option dialog will be shown).

Calc Background

To estimate the background.

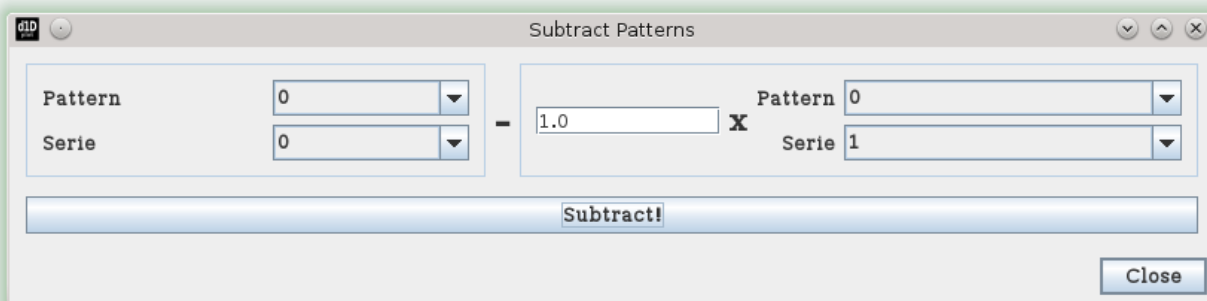


Here an estimation of the background can be calculated. It is created as a new series (can be subtracted later if desired or exported as a list of points with `save as...`). There are three methods:

- Bruchner smoothing procedure (Brüchner, 2000) allowing to use different conditions in function of 2-theta.
- N-Polynomial Interpolation (estimation of points should be done before)
- Spline Interpolation (estimation of points should be done before)

Subtract Patterns

To subtract two patterns. Select the two patterns and the factor applied to pattern 2 in the subtract dialog and click on subtract to generate the subtracted pattern as a new data series.



Rebinning

It will ask for initial 2-theta, final 2-theta and stepsize. Then it performs a rebinning of the data (by linear interpolations). A new series is generated.

Convert to wavelength

Creates a new data series of the selected pattern converted to a new wavelength.

Change X units

To change between 2Theta, d-spacing, 1/dspacing, Q. The correct wavelength needs to be assigned before (on the corresponding table cell). A new data series is generated.

Sum selected patterns

Sum the selected patterns. The resulting pattern is created as a new data series.

5. Supported formats

Supported read extensions:

- DAT (ALBA or Free Format), XYE, XY, ASC, GSA, XRDML, PRF, GR.

Supported write extensions:

- DAT (ALBA or Free Format), XYE, ASC, GSA, XRDML, GR.

DAT (ALBA), XYE, XY, ASC

These are ASCII files. DAT (ALBA) and XYE are a 3-column (2-theta, Intensity, err) with comment lines at the beginning (they may start with #, !, / or \$). XY and ASC are 2-column files (2-theta, intensity) and ASC does not contain any header.

```
# I(2Theta) vs. 2Theta : IsMon = [3362599, 3364412, 3364882] IsPos = [-2.0004, -2.99299999, ...
# imon 3362599 ixbo_timer 0.1 ixbfe_tot 4.66493951416e-08 ixbo_tot 2.3019625e-07 ixbhp_tot ...
#      7179
2.0263000E+00  7.7488743E+03  8.7492857E+01
2.0323000E+00  7.6388975E+03  8.8594582E+01
2.0383000E+00  7.5582480E+03  8.6729464E+01
2.0443000E+00  7.5894229E+03  8.6740810E+01
2.0503000E+00  7.8062298E+03  8.9039317E+01
2.0563000E+00  7.7854571E+03  8.7692645E+01
...
```

GSA

GSAS Standard Powder Data File (Larson & Von Dreele, 1994).

XRDML

Panalytical format (Degen, 2002).

PRF

FullProf (Rodríguez-Carvajal, 1993) file “profile” generated after a refinement containing the observed, calculated and difference profiles.

GR

G(r) output file from pdfgetx3 (Juhás, Davis, Farrow & Billinge, 2013).

6. References

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Brückner, S. (2000). Estimation of the background in powder diffraction patterns through a robust smoothing procedure. *Journal of Applied Crystallography*, 33(3), 977-979.

Degen, T. (2002). XrdML, a new way to store (and exchange) X-ray powder diffraction measurement data. *arXiv preprint physics/0210067*.

Juhás, P., Davis, T., Farrow, C. L., & Billinge, S. J. (2013). PDFgetX3: a rapid and highly automatable program for processing powder diffraction data into total scattering pair distribution functions. *Journal of Applied Crystallography*, 46(2), 560-566.

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Rodríguez-Carvajal, J. (1993). Recent advances in magnetic structure determination by neutron powder diffraction. *Physica B: Condensed Matter*, 192(1-2), 55-69.

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7. Miscellaneous

Release notes

d1Dplot started as a complement to DAjust, TALP (Vallcorba, Rius, Frontera & Miravittles, 2012) and *d2Dplot* for personal usage. Since I found it useful and easy to use and control the aspect of the patterns (e.g. for creating figures) I decided to make it decent for distribution (although I am sure it still contains lots of bugs...).

Feedback to the author would be greatly appreciated. Also, if you find interesting to add a certain functionality it can also be considered.

d1Dplot is completely programmed with Java™ (www.java.com) using jdk version 1.6. (Oracle License: <http://www.oracle.com/technetwork/java/javase/downloads/jdk-6u21-license-159167.txt>).

The following 3rd party libraries have been used:

- MigLayout. <http://www.miglayout.com>
BSD license: http://directory.fsf.org/wiki/License:BSD_4Clause
- Commons Math. <https://commons.apache.org/proper/commons-math/>
Apache License: <http://www.apache.org/licenses/LICENSE-2.0>
- Apache Batik. <https://xmlgraphics.apache.org/batik/>
Apache License: <http://www.apache.org/licenses/LICENSE-2.0>

(No changes on the source codes of these libraries have been made, you can download the source codes for these libraries at their respective websites).

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