**Pit\_Graph Manual**

Pit\_Graph is a software designed to work with XY plots. It can draw several plots in one frame of reference and perform different mathematical operations.

0) Software content.

No installation is needed, just copy all necessary files into any folder and execute *Pit\_Graph.exe*. The software works at Windows OS. No registry entries or other traces in the OS are created.

Additional necessary files:

*corona.dll* – a library required to open image files for subsequent conversion into arrays of numbers.

*formats.txt* – contains description of formats for graphs loading. It is loaded when the application starts. Can be edited manually.

*settings.txt* – contains all information set up in “File→Settings…” menu item, and information about custom colormap. It is loaded when the application starts and it is rewritten when the application is closed to save your preferences.

*/undo* – this folder will contain data necessary to perform “undo” operation.

1) Importing data.

1.1. Direct import from the data file is available using “File→Add Graph...” menu item. The file is scanned for the numerical values. The first encountered number goes to X array, the second goes to Y array and the process starts over again. Everything but numbers will be ignored. The first string is scanned for the axis names. The axis names are considered to be found if a proper separator is present in the string and the string does not start with a number. Otherwise, the numbers scanning starts from the file beginning. The recognized separators are '|', 'TAB', ';', '/', ',' and 'SPACE'. If a certain separator symbol presents multiple times, it is ignored. The example of the input file is given below:

T (K) / R1 (Ohm)

300; 100

400 a300

500 450zzz

Axis names will be 'T (K)' for OX and 'R1 (Ohm)' for OY. X array will be {300, 400, 500} and Y array will be {100, 300, 450}.

It is possible to load multiple graphs with the same X array. Use 'xy1y2' or 'xy1y2y3' filters to load numbers in the sequence X–Y1–Y2 or X–Y1–Y2-Y3, respectively. The example of the input file is given below ('xy1y2' filter):

100 150 300

200 250 400

300 350 550

400 500 800

Axis names will not be found and remain unchanged. The first graph will contain X array of {100, 200, 300, 400} and Y array of {150, 250, 350, 500}. The second graph will contain X array of {100, 200, 300, 400} and Y array of {300, 400, 550, 800}.

The available filters are contained in “formats.txt” file, which can be edited to adjust the reading algorithm to the specific file type. The file is loaded at the program startup, so if you edit it, you should restart the program to see changes.

The example of the format is given below:

I-V curve|\*.\* :: s1 i x\_1 e y\_1 e

The format starts with the name describing loaded file types (text before ‘|’). It is only shown in CFileDialog filter field and has no effect on the loaded data. Between ‘|’ and ‘::’ there is a standard C++ filter rule, where ‘\*’ means any string. For instance, if you want to see only .txt files, write ‘\*.txt’.

Format description starts with optional ‘s’ rule, which means that you want to skip a number of string in the beginning of the file. For instance, write ‘s57’ if you want to skip 57 strings.

The remaining part of the format is executed in an infinite loop ending at the end of file. The file is scanned, and when the number is found, it can either be ignored (‘i’ rule) or go to X (‘x’ rule) or Y (‘y’ rule) array. ‘x’ or ‘y’ rule require explicit indication of the graph number. Numbering starts from index ‘1’. The amount of x and y indices must be the same, increment = 1, and there must be no index skips. For instance, you can write “x\_1 x\_2 y\_1 y\_2 x\_3 y\_3”. If one number belongs to several different graphs, list all corresponding indices. For instance, ‘xy1y2y3’ filter discussed above is described as “x\_1\_2\_3 y\_1 y\_2 y\_3”.

After each ‘x’ or ‘y’ you can add an optional ‘e’ rule. It means that a multiplier will be looked for after a number. The recognized multipliers are: 'd' (1e-1), 'c' (1e-2), 'm' (1e-3), 'u' (1e-6), 'n' (1e-9), 'p' (1e-12), 'f' (1e-15), 'a' (1e-18), 'z' (1e-21), 'y' (1e-24), 'h' (1e2), 'k' (1e3), 'M' (1e6), 'G' (1e9), 'T' (1e12), 'P' (1e15), 'E' (1e18), 'Z' (1e21), 'Y' (1e24). For instance, let us load the following file using the format “I-V curve|\*.\* :: s1 i x\_1 e y\_1 e”:

Index V1 I1

1 -50.00 mV -87.1340 mA

2 -49.75 mV -86.7120 mA

3 -49.50 mV -86.2720 mA

The first string is ignored (‘s1’ rule), the reading starts with a number, so axis names will be unchanged. Index column is ignored (‘i’ rule), voltage goes to X array, current goes to Y array. All values will be multiplied by 0.001 (‘e’ rule applied to the letter ‘m’. The result is: X array of {-0.05, -0.04975, -0.0495} and Y array of {-0.087134, -0.086712, -0.086272}.

1.2. Generating a graph from the explicit analytical function is available using “File→Add Function...” menu item. Set the function range (x1 and x2), number of points (N) and the expression in the dialog box.

Expression recognizes the following operators: '+', '-', '\*', '/', '^' (for power) and '%' (for mod) and the following functions: 'abs', 'acos', 'asin', 'atan', 'atan2', 'ceil', 'cos', 'cosh', 'exp', 'fac', 'floor', 'ln', 'log10', 'ncr', 'pcr', 'pow', 'sin', 'sinh', 'sqrt', 'tan', 'tanh'. Use 'e' and 'pi' for Euler and pi numbers. Use 'x' for the argument. The functions are named according to the C++ standard.

1.3. Generating a graph from the image file (bmp, jpg, png, pcx, tga and gif formats are acceptable) is available using “File→Image to data...” menu item. The image must be a continuous line extending from the left-most to the right-most pixel of the image. One image may contain several lines, which will be treated as separate graphs. In the dialog box, set the graph range (x1, x2, y1 and y2). Sensitivity threshold allows ignoring the image pixel if a sum of its red, blue and green channels is bigger than the threshold value (each channel has a value between 0 and 255).

2) Exporting data.

2.1. Use “File→Export all Data” to write all data into the text file. This file will contain coordinates of all points, names of the axis, colors, sizes, etc. Opening such file using File→Add Graph... menu item will completely restore the appearance of the workspace at the moment of export.

2.2. Use “File→Export Current” to write the data of the currently selected graph into the text file in a form of two columns containing numbers (the first one contains X values, the second one – Y values). It is a basic format compatible with any other software, but it will not save any information about graph appearance.

2.3. “Edit→Сopy” menu item (or the corresponding toolbar button) puts everything drawn in the client area of the application into the clipboard. The image is in a raster format and can be inserted into any software working with images.

2.4. Use “File→Save as EPS…” to save everything drawn in the client area of the application into the Encapsulated Postscript (\*.eps) file containing vector graphics.

3) Zooming.

3.1. Explicit assignment of the graph range is available through “View→Size...” menu item. Just set the desired values in the dialog box.

3.2. Zooming is possible using a mouse. The left-click determines the top-left vertex of the new field of view. Drag a mouse to the position where the bottom-right vertex of the new field of view should be located and click the right mouse button. If vertical or horizontal position of these vertexes are identical, then (instead of zooming) a line indicating a distance between points will be drawn. Single right click anywhere in the field of view will indicate a corresponding point and output its coordinates.

3.3. Use 'Default size' toolbar button to fit all loaded graphs into the field of view. Use 'Default Y size' toolbar button to fit all loaded graphs into the field of view without changing X range.

4) Workspace appearance.

4.1. Use “View→Axis...” menu item to change the appearance of axis. Using the DialogBox you can modify axis names, size of the fonts for names and numbers. Margins are the spacers between the borders of the client screen and the area where graphs are drawn (values are in pixels). 'Y name shift' allows to shift the name of OY in vertical direction (value is in pixels). Numbers near OY may be hidden if a corresponding check is set. Selector is a line at the top-right corner of the window, which allows selecting different graphs as active. “Hide dashed net” hides all lines forming a coordinate net of a graph. 'N X' (and 'N Y') in 'Markers' field set a number of vertical (horizontal) lines dividing the graph area into equal parts. 'Tolerance' sets the number of signs after the decimal point. Numbers may be presented in exponential form (i.e. 321 = 3.21e2).

4.2. Use “View→Graph...” menu item to modify the appearance of graphs. Color and width of the line connecting neighboring points may be changed. Each point may be presented as a circle, cross or square (“Marker” RadioButton control). Also, you can draw the graph as a dashed line. Use ListBox or '+' and '-' buttons to switch between different graphs. Use ‘↑’ and ‘↓’ buttons to change the order of the graphs. The name of each graph can also be changed.

4.3. Use “View→Window Size...” menu item to set the exact extension of the client area (the values are in pixels).

4.4. Use “View→Polar” menu item to present all graphs in the polar coordinates.

4.5. Use “View→Approximation...” menu item to change color and width of the approximation graphs. Use '+' and '-' buttons to switch between different graphs: each graph can have its own style of approximation line (only “Custom” and “Polynomial”; “Voight” approximation is a single graph).

4.6. Use “View→Recolor Graphs…” to set the color of all graph in accordance with a certain colormap. There are four predefined colormaps, and you can also define your own by setting the colors and positions of up to 5 reference points. Between the reference points, color changes linearly.

5) Working with graphs.

5.1. To select a certain graph as the active one, use a selector in the top-right corner of the application (‘+’ and ‘–’ buttons). Alternatively, it can be done using “View→Graph...” menu item.

5.2. A general transformation of the active graph can be done using “Edit→Transform...” menu item. Any expression similar to one described in 1.2. may be used. Use 'x' and 'y' for the arguments.

5.3. A small shift of the active graph can be applied via toolbar buttons “Move up”, “Move down”, “Move left” or “Move right”. The amount of shift is set up using “File→Settings…” menu item by editing “Move scale” value. For instance, the value of ‘0.01’ corresponds to the shift by 1% of the current scale after every pressing of the button.

5.4. Manual correction of Y coordinates can be done using the toolbar button “Point correction”. When the button is pressed, it changes the functionality of the right mouse button. Press the right mouse button, drag the mouse to the new position and release the mouse button. Any points, which have X coordinates between the path’s starting and ending points, will be shifted to the Y coordinate of the mouse path.

5.5. Unnecessary parts of the graph can be removed using “Edit→Crop…” menu item. All points outside the intervals X (x\_min, x\_max), Y (y\_min, y\_max) will be removed. If interval’s min and max values are equal, the rule does not apply (so you can choose to affect only X or only Y axis).

5.6. The graph can be divided into independent parts using “Edit→Split…” menu item. All points with X coordinate less than that set up in the Dialog will go to one graph, the remaining will go to another graph.

5.7. Different graphs can be merged into a single one using “Edit→Merge…” menu item. In DialogBox, specify indices of the graphs that should be merged. Indexing starts from ‘1’. Write ‘0’ if you want to merge all graphs into one.

5.8. Different graphs can be mathematically combined into a single one using “Edit→Combine…” menu item. Any expression similar to one described in 1.2. may be used. Use 'y1', 'y2', ‘y3’ … for the arguments (index is the number of the graph). Indexing starts from ‘1’. Maximum index is ‘7’. Old graphs will be kept after the function execution, and the new one will appear. X limits of the combined graph will correspond to the interval where each of the graphs from the expression is defined. The number of points and value of X coordinates of the combined graph will be the same as for the graph with the lowest index.

5.9. Graph smoothing is available using “Edit→Smoothing” menu items. There are two smoothing algorithms.

5.9.1. “Moving average…”. In the Dialog, ‘Order’ is a number of points near the central one used to calculate the average value. First, all average values are calculated. Second, Y coordinate of each point is replaced by an average value. Use ‘Iterations’ number to repeat the algorithm several times.

5.9.2. “Step cross-correlation…”. Procedure calculates cross-correlation between an active graph and a rectangular step function. The step function has a width specified in the dialog box and is centered at 0. ‘N points’ is the number of points of the smoothed graph. Use ‘Iterations’ number to repeat the algorithm several times. Smoothed graph has the same total integral as an initial one.

5.10. “Edit→Background correction” menu item can be used to subtract a baseline. Three different algorithms are available:

5.10.1. “Polynomial”. The baseline is modeled by a single polynom. The polynom is fitted to the active graph by the least squares method under the condition that it is located strictly below the graph. Polynom order is limited to 9 (N = 0 … 9). Choose an order and press the button “Fit”. The resulting baseline is drawn below the graph. To fix the result, press “OK” button. The baseline will be subtracted from the graph.

5.10.2. “Shirley”. The baseline is modeled according to the Shirley model (used for analysis of XPS data).

5.10.3. “Shape”. In this method, a set of ellipses is placed under the graph. Each ellipse has dimensions set up in the Dialog (‘dX’ and ‘dY’). X coordinate of each ellipse center equals to the X coordinate of the graph (there are also additional ellipses to the left and to the right of the graph to avoid unexpected edge effects). Each ellipse is located strictly below the graph, but as close to it as possible. The baseline is built as an envelope of these ellipses. Use ‘Iterations’ number to repeat the algorithm several times. If “Show BG” button is checked, the initial graph will be kept, the baseline will be drawn as an additional graph, and the modified graph (without the baseline) will be drawn as well. If the button is not checked, only the modified graph will be drawn.

5.11. To remove an active graph, use “Edit→Remove→Remove Current” menu item. To remove all graphs, use “Edit→Remove→Remove All” menu item. Alternatively, you can use “New” button on the toolbar. To remove all graphs except an active one, use “Edit→Remove→Remove All but Current” menu item.

5.12. Use “Edit→Remove→Points…” if you want to reduce the number of points in the active graph. For instance, type 75% if you want to remove ¾ of points (i.e. the first point is kept, three next are removed, the fifth is kept, three next are removed etc.). It can be useful for optimization (i.e. if you have many heavy graphs to draw or need to make a heavy approximation).

5.13. Check “Integral” button on the toolbar if you want to integrate the active graph. Press the left mouse button at the starting point of integration. Drag the mouse to the finishing point of integration. Press the right mouse button. Integral of the active graph in the chosen interval is displayed.

5.14. If something went wrong, you can undo the last procedure using “Edit→Undo” menu item. Use “Edit→Restore” menu item if you want to return to the graph range assigned through “View→Size...” after mouse zooming.

6) Approximation

6.1. “Edit→Approximation→Polynomial…” makes approximation of the current graph with polynomial function (up to 9th power). Just set the desired order of polynom (N) and press the button “Clac” to see the result.

6.2. “Edit→Approximation→Custom…” makes approximation of the current graph with any function defined similarly to 1.2. Here you can use up to 5 parameters (A, B, C, D, E) in the formula. You should specify the range of every parameter (i.e. Amin, Amax) and the number of steps for every parameter (i.e. A N). Fit button looks for the best approximation in the specified ranges searching through the parameters with specified steps. Finding the best solution may require more than one search, and you can automatically initialize few consequential searches using “iterations” box.

6.3. “Edit→Approximation→Voight…” makes approximation of the current graph with pseudo-Voight function defined as:

The function can have up to 7 summands with parameters specified in the DialogBox. “Integral” field displays the total integral of each summand. To make automatic approximation, you should specify the initial values of each parameters, and limits where the software will look for the best fit. Limits can be quickly adjusted by clicking “default” button. See section 9 for adjustment details. Radio buttons are used to select a certain summand to display the limits corresponding to this summand. Once the initial values and limits are properly set, press “Fit” button to look for the best parameters of a certain summand. Finding the best fit may require several iterations. To perform all these iterations for all summands automatically, set the maximum number of iterations in “N iterations” field and press “Fit All” button. The current fit can be exported to a file using “Export…” button. You can later import it using “Import…” button.

6.4. You can hide all approximation curves by checking “Edit→Approximation→Hide” menu item.

7) Adding text notes.

7.1. To add the text, press “Add/Edit Text” toolbar button. Click the left mouse button where the new text should appear, type it and press OK. You can specify text color, size and orientation (text angle – “alpha”). Check “Outline” box if you need a white outer glow around the text.

7.2. To edit the existing text note, left click on it with the checked “Add/Edit Text” toolbar button.

7.3. To move the existing text note, press “Move Text” toolbar button. Press the left mouse button on the existing note, drag it to the new position and release the mouse button. Precise shift of the note can be done using keyboard keys (left, right, up and down). Note that the keys affect the note, which was last moved or modified.

7.4. Use “Edit→Remove→Texts” menu item to delete all text notes. “New” button on a toolbar also removes all text notes.

7.5. Note that all text notes are bound to the client area. It means that changing the graph scale will not affect their positions.

8) Batch operations.

8.1. Use “Edit→Batch Operation→Average” menu item to make a single graph from several different files. First, select a folder where all necessary files are located. Each file in the folder will be converted into a graph using a filter selected as a default one in “File→Settings…” menu. A single graph will be created by averaging all loaded data. When averaging is performed, some Y values may be considered as bad and not taken into account. Let at certain X there is an array of Y values [y1, … yn], yave is an average value and ystd is a standard deviation for the average. yk is considered as bad if |yave – yk| > Nsigma \* ystd, where Nsigma is a parameter defined in the “Average – parameters” dialog box. After averaging, the single graph is displayed.

8.2. Use “Edit→Batch Operation→Transform” menu item to apply a certain operation to all files from a selected folder. First, select an operation: crop (see 5.5), transform (see 5.2), background correction (see 5.10), or smoothing (5.9). Use “Set…” button to specify parameters of the operation. Then, press “OK” and select a folder. Each file in the folder will be converted into a graph using a filter selected as a default one in “File→Settings…” menu. Then, the selected operation will be applied to the graph, and the new graph will be saved in a separate file with the same name as the initial one, but with prefix “ed\_”.

8.3. Use “Edit→Batch Operation→Analyze” menu item to obtain certain data from all files from a selected folder. First, select an operation: integral; polynomial approximation (see 6.1); custom approximation (see 6.2); or Voight approximation (see 6.3). Use “Set…” button to specify parameters of the operation. Then, press “OK” and select a folder. Each file in the folder will be converted into a graph using a filter selected as a default one in “File→Settings…” menu. Then, the selected analysis operation will be applied to the graph, and the result of this operation will be recorded in a separate file “result.txt”. This file will contain number of strings equal to the number of graphs in the selected folder. Each string will start from the file name (without extension). After the file name, the total integral in the specified range; the coefficients of polynomial, custom or Voight approximation of the graph will be recorded.

9) General settings

Use “File→Settings…” menu item to adjust some general settings:

• “Default File mode” is a number of file filter used by default when the graph is imported. Indexing starts from 1.

• “Decimal separator” is a symbol treated as a decimal separator when the graph is imported from a text file.

• When “View→Polar” is active, X arrays of all graphs are converted into polar angle assuming that they contain either degrees or radians. Use the preferred option in “Polar units” field.

• “View mode” chooses the way to plot all lines. “Default” uses only standard C++ MFC functions. “DirectX” uses “CDXSurfaceManager” external library; this way works somewhat faster and it can be useful if you plot many graphs with thousands of points. However, there are some memory leaks in the library, and it causes the freezing of the software after several hours of work.

• “EPS font scale” is a scale factor for all text notes used when you save everything in \*.eps file.

• “Move scale” is the amount of shift applied by toolbar buttons. See section 5.3.

• “Colors” button opens another dialog, where sizes and colors of lines and text displayed on measurements (see 3.2 and 5.13) can be changed.

• “Voight” button opens another dialog, where the behavior of “default” button for limits setting (see 6.3) can be adjusted. “H0 +/-” and “H step” define the limits for H. For instance, if “H0 +/-” = 20%, “H step” = 1% and the current value H = 5000, then the limits will be set to [4000 – 6000] with a step of 50. “FWHM +/-” and “FWHM step” define the limits for FWHM. For instance, if “FWHM +/-” = 5, “FWHM step” = 0.01 and the current value FWHM = 20, then the limits will be set to [15 – 25] with a step of 0.01. “<x> +/-” and “<x> step” define the limits for <x> and work similarly to FWHM parameters. “n min”, “n max” and “n step” explicitly define the limits for n.