

# Working with Origin 7.5.

## Step1. Importing data

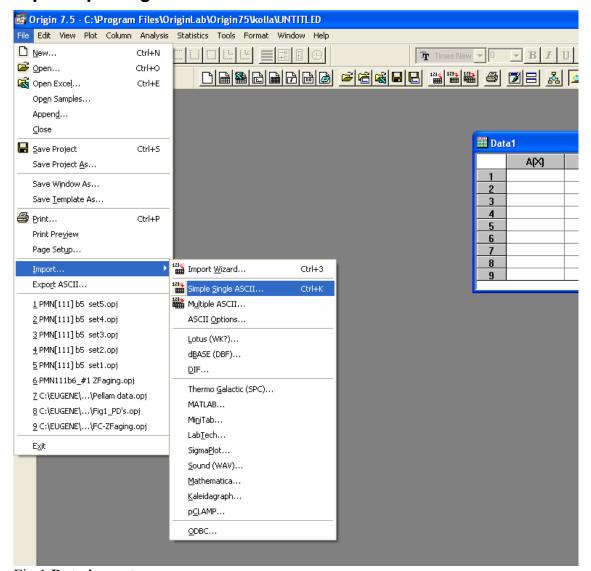


Fig.1 Data import menu

Go to *File* menu, *Import*, choose what kind of data are you going to import. In the Fig 1 is the example of importing of the *Simple Single ASCII* data set. Your data will go to the current active worksheet (Data 1 in Fig1). After you have finished with the first data set you can import

any more data sets if it is necessary. Before importing a next data set you have to prepare a new worksheet. To do this - go to *File* menu then to *New* and you will see a new window (Fig.2).



Fig.2. Opening a new worksheet

you can import all data sets in the same one worksheet adding new columns to it, or (iii) you can import all data files in the same worksheet, but in new roes. Fig.3 shows the first option. After all files appeared in bottom window push OK and all data files will be downloaded in to the Origin worksheet(s). In case of *Multiple ASCII* data import you do not need to prepare worksheets for the new data sets – they will be

After a new worksheet is ready you can import a new data set. There is another option how to import several data files in one step. You have to choose a **Multiple ASCII** option (Fig.1). This will result in appearance a new window (Fig.3.). Here you can find a proper place on your computer containing data files, then mark them and add to the list of the imported files (push *Add file(s)* button. Import could be done in three different ways: (i) you can load each file in a separated worksheet, (ii)

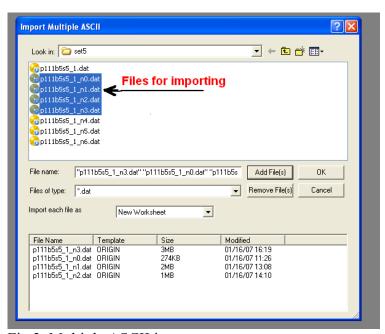


Fig.3. Multiple ASCII import

created automatically. At this point all data files are downloaded into the Origin project and you can start plotting the graphs and data analysis.

# 2. Creating and editing the data plots.

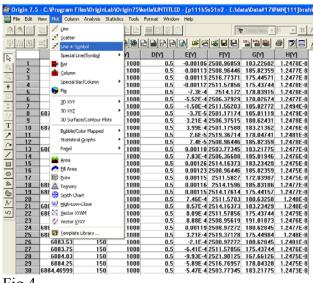


Fig.4.

First open the worksheet which contains the data for plotting. Go to *Plot* menu and choose the kind of plot you like to create. In Fig.4 the *Line and Symbol* plot option is marked. It will be also possible latter to change this while editing the plot. It will be also possible to add more plots to the graph. After choosing the plot stile the Plot Setup window will invite to data selection dialog (Fig.5.). Here in the top window is the list of all available data worksheets. Middle part of the Plot Setup window is dedicated

to make links between X and Y axes and the columns in the worksheet. vEr checkbox is to

make a link to the column (if you have this data) containing Y axis error bars, L – the same for labels. To use any column as label column it should by initially assigned as Label column (right click on the column name and go Set as Label). It is possible also to add X axis error bars on the plot. When you assigning the columns for X and Y axes you can mark several checkboxes for Y axis if it is necessary. After X and Y axes are chosen push Add and different information about the plot will appear in bottom window. While this dialog you can add as many plots to the graph as you need

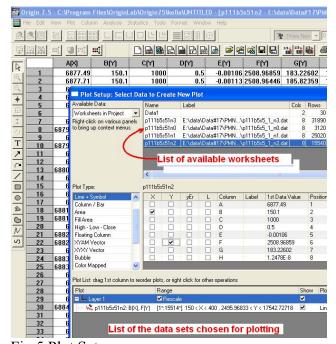


Fig.5 Plot Setup.

- check another worksheet and mark new columns as X,Y axes (yErr, xErr etc.). After the

dialog is done – push OK (not visible in Fig.5.) and all chosen data sets will appear in the same graph. The graph which will open in the graph window will be very simple and have to work on it a lot to bring to the level required for report or publication. To make a nicer design of the graph let we start to work on axes. Click on X or Y axis and corresponding pop-up menu will appear (Fig.6.). Here you can change a lot related to graph design: type of the axis (linear, log10,

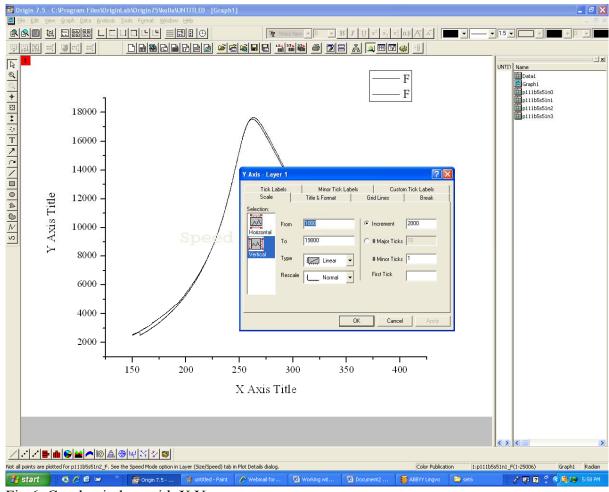


Fig.6. Graph window with X Y axes menu.

In etc.), scales, grids, tick labels, axes titles etc. You can easy switch from Y axis to X axis using selection window. The next what you can do with the graph is to work on plot design – line style, colors, etc. Click on the plotted line or go to the main menu  $Format \rightarrow Plot$  and a new pop-up menu will appear on the graph (Fig.7). At this point you can redesign each plot depicted in the active graph. You can do it separately with each plot or you can use the Group (see Origin manual how to use the Group option) option and do all changes in all presented plots in the same time. This could be very helpful if you work with a large number of plots in the graph. In Fig.7 is

shown the case of the "*Line*" *Plot Type* but if you will change it to "*Line* + *Symbol*" there will two more submenus for *Symbol* style and *Drop Lines* editing.

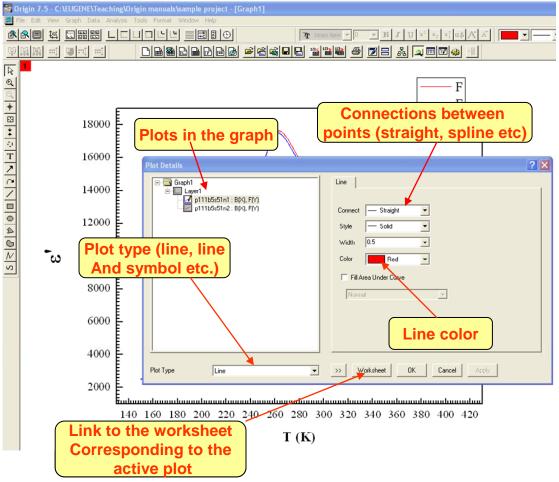


Fig.7. Plot Details menu.

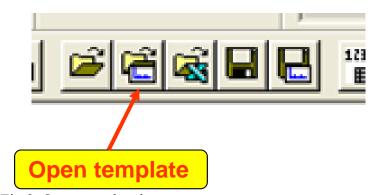


Fig.8. Open template button

After the graph design has been done you can save it as graph template for future use. Go to the main menu  $File \rightarrow Save\ Template$ As. It will save your Graph without plots and you can use this template in this or in future project and it will save you a lot of time. To open a previously designed

template or template from OriginLab collection (C:\Program Files\OriginLab\Origin75\\*.OTP)

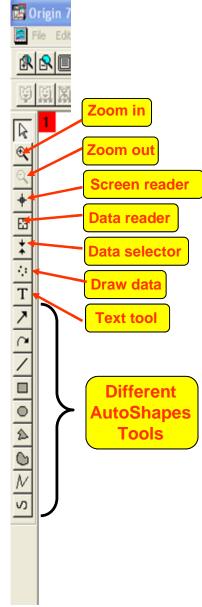
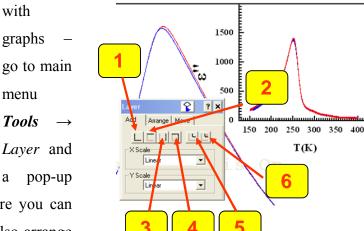


Fig.9. Tools toolbar.

you can use a special toolbar button (see Fig.8.). One more toolbar is very useful while working with graphs. Usually\* (\*the positions of all toolbars is not fixed on the screen) it is located on the left side of the main window. **Zoom in** makes enlarging of the particular selected area by re plotting of the data included in this area but not as a simple zooming of the graphical image. Screen reader shows X, Y coordinates of the screen in respect to scales of the axes. *Data reader* shows X, Y coordinates of the selected data point in the graph. Data selector puts the limits for data in the graph which will be used in further data analysis (fitting, regressions etc.). *Draw data* is for manual creating of the plot in the graph; corresponding data will go to a new worksheet. *Text tool* is for writing text in any place of the graphical page. AutoShapes tools are for adding to the Graph page some lines arrows etc. All these graphical elements will be saved when saving this graph as a template. One more useful tool set for working



menu Layer (Fig.10) will appear. Here you can add a plot to the graph ("Add") and also arrange the plots on the page ("Arrange") or change the

Fig10. Layer tools

positions of the plots on the page ("*Move*"). In Fig.10 the Add submenu is shown. Here you can: (1) add a full scale plot with new left X and bottom new Y axes, (2) add a full scale plot with a

new X axis on the top of the graph with a common Y axis, (3) add a full scale plot with a new Y



Fig.11. Plot tags.

axis on the right side and common X axis, (4) add a full scale graph with a new top X axis and a new right Y axis, (5) add a small insert plot in the right top corner (shown in Fig.10.), (6) the same as (5) but a new plot will contain the data from the original plot. Except (6) the new plot will be created as a blank and you will need to attach the data by clicking on the corresponding tag (Fig. 11.) and choosing the data for plotting (similar as shown in Fig. 5.).

### 3. Data analysis and data fitting

### Linear fitting

Origin provides some very powerful and convenient tools for data analysis and data fitting. To perform the polynomial fitting go  $Analysis \rightarrow Fit Polynomial$ . The polynomial fit pop-up menu

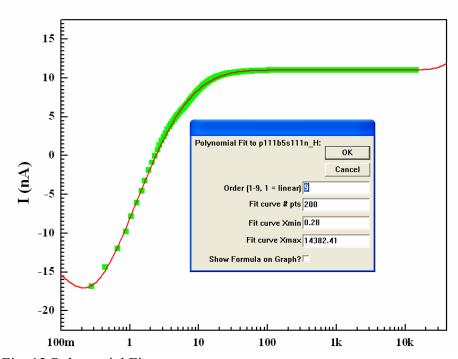


Fig. 12.Polynomial Fit menu.

will appear (Fig.12). This procedure works with graphical window and if you have several plots on the same graph go first to main menu Data and click on the data set you wont to work on. The next step is very simple you have choose

*Order* of polynomial, *Xmin* and *Xmax* for fit curve and number of points for fit curve. To display the polynomial coefficients on the graph you have to check *Show formula on Graph*.

The choice of Xmin and Xmax will not effect the fitting result – the entire data set will be used for fitting. To restrict the range of the data points involved in fitting you can use Data selector tool (see Fig.9). The maximum polynomial order number is 9. For fitting with linear function (polynomial order =1) you can use option  $Analysis \rightarrow Fit \ Linear$ . It will do the same as Fit Polynomial with order =1.

### **Nonlinear fitting**

To perform the nonlinear fitting procedure go to main menu Analysis o Non-Linear Curve Fit o Advanced Fitting Toll... The multilayer pop-up Nonlinear Fitting menu is shown in Fig. 13. Firs step – you have to choose from the library the fitting function or write your own function. The library Functions are grouped in several Categories. For each library Function you can the Equation, Sample Curve or Function File information (Sample Curve option in Fig. 13). To

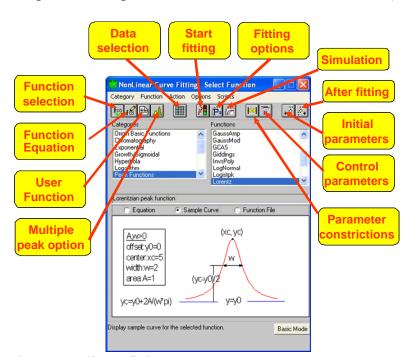


Fig.13. Nonlinear fitting menu.

write a new function - push User Function button and follow the instructions. There is a Replicas option for some (Multiple functions peak option in Fig.13.). It is very convenient tool for multiple peak fitting – you do not need to write equation for each peak but will need to do the some settings arrangement in submenu Replicas. Data **Selection** submenu is for choosing of the data set or

segment of data set for fitting. Start fitting (see below) will start the Fitting Session. Using the Simulation submenu you can plot the fitting curve or to play with initial parameters to manually optimize they. Parameter constrictions submenu will set the constriction to the parameters during the fitting session. In Control parameters submenu you can adjust some fitting parameters such as tolerance factor, number of significant digits of the fitting parameters etc. Initial parameters submenu is for enter that initial parameters, but the same you can do in

Fitting session submenu. After fitting submenu gives some options how to plot final fitting curve. In Fig. 14 the Fitting session window is shown. The most important for successful fitting is the choice of the initial parameters. They can be entered in corresponding boxes (Value) here or in Initial parameters submenu. To start fitting push one of three buttons: "1 iter.", "200 iter." or "200 Simplex iter." Pushing "1 iter." will results in singe iteration using Levenberg-

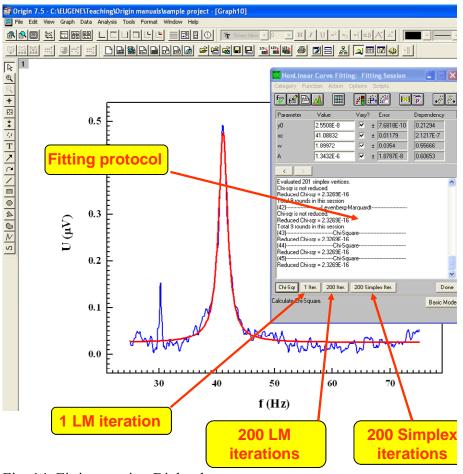


Fig. 14. Fitting session Dialog box.

Marquardt (LM) algorithm, "200 iter." - 200 LM iterations *"200* **Simplex** and - 200 Simplex iter." iterations. Number could "200" be changed to 10, 30, 50 or 100 in Control parameters submenu. Normally, you will not use need to the Simplex method because it is much less robust and reliable than the LM method. However, if the LM method for a set of data behaves poorly,

try the Simplex method. Some general recommendation of fitting procedure: (i) do not start with a big number of iteration until you are not sure that the process goes in the proper direction, (ii) in some cases helps to fix one or several parameters (uncheck corresponding checkboxes), (iii) try to change the value of some initial parameters if the fitting does not go well and start fitting again. After each iteration step or steps the fitting curve will be displayed in graphical window (red curve in the example shown in Fig.14). The criteria of end of fitting is if the *Reduced Chi*-

*sqr* (see fitting protocol window) does not decrease more. Push *Done* and all fitting parameters and some complimentary information will be displayed in Graph.

### 4. Worksheets

To perform some operations with worksheet first you have to open it. Next right click on the column header. Column becomes highlighted and a pop-up window appears. Here you can

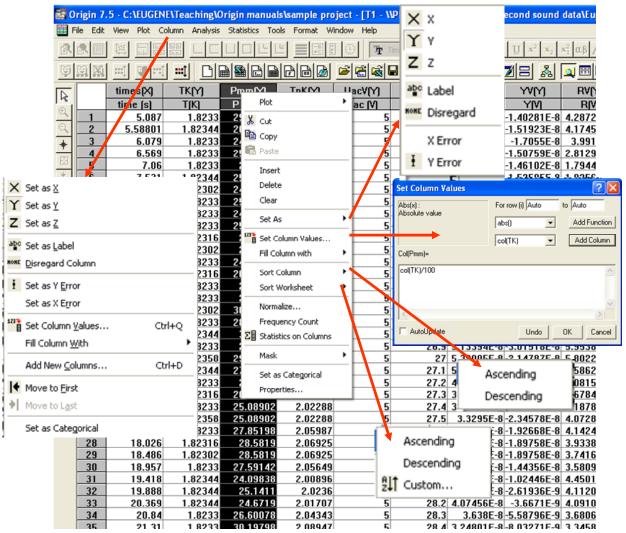


Fig. 15. Working with worksheet.

perform several useful operations on the worksheet. **Set As** will assign a column **X**, **Y** or **Z** (for 3D graphs) axes data. **Set Column Values** option will perform some mathematical operation on the data from one or several columns. **Sort Column** and **Sort Worksheet** will perform sorting of the column or worksheet respectively. **Statistics on Column** will open a new worksheet containing all statistical information (**Min, Max, Sum**, etc.) on data set in the column. **Properties** will open a new pop-up window (not shown in Fig.15) and here you can change the **Column** 

*Name, Column Label, Column Width*, etc. You can also plot the data from the highlighted column (as Y axis data) in respect of previously assigned X column, but this way of creating a plot is less convenient and less flexible as discussed above and shown in Fig.5. Some listed here operations you can do through the main menu  $\rightarrow$  *Column* (see Fig.15).

#### 5. Final Comments

Origin 7.5 provides much more features and opportunities to work with data and graphs than we discussed above. It has a powerful engine for 3D graphics, tolls for smoothing the data depicted in plots. You can apply (main menu Analysis) on the plotted data the Fast Fourier Transform (FFT), perform some math ( $Subtract \rightarrow Strait\ Line$  or  $Reference\ Data$ ) and Calculus (Differentiate, Integrate) operation on data in plots. Fitting to some typical ( $Exponential\ Growth$ .  $Exponential\ Decay\ etc.$ ) functions can be performed very simple without opening  $Nonlinear\ Curve\ Fitting\ window\ (Fig.14)$  – go to mane menu  $Analysis\$ and click on the listed function.

### References

Here is the link to the official OriginLab WEB site:

http://www.originlab.com

For Tutorials go to:

http://www.originlab.com/index.aspx?s=9&lm=72

Manuals and other documentation:

http://www.originlab.com/index.aspx?s=12&lm=66

File Exchange page:

http://www.originlab.com/fileexchange/index.aspx