



Working with Origin 8.6.

Step1. Importing data

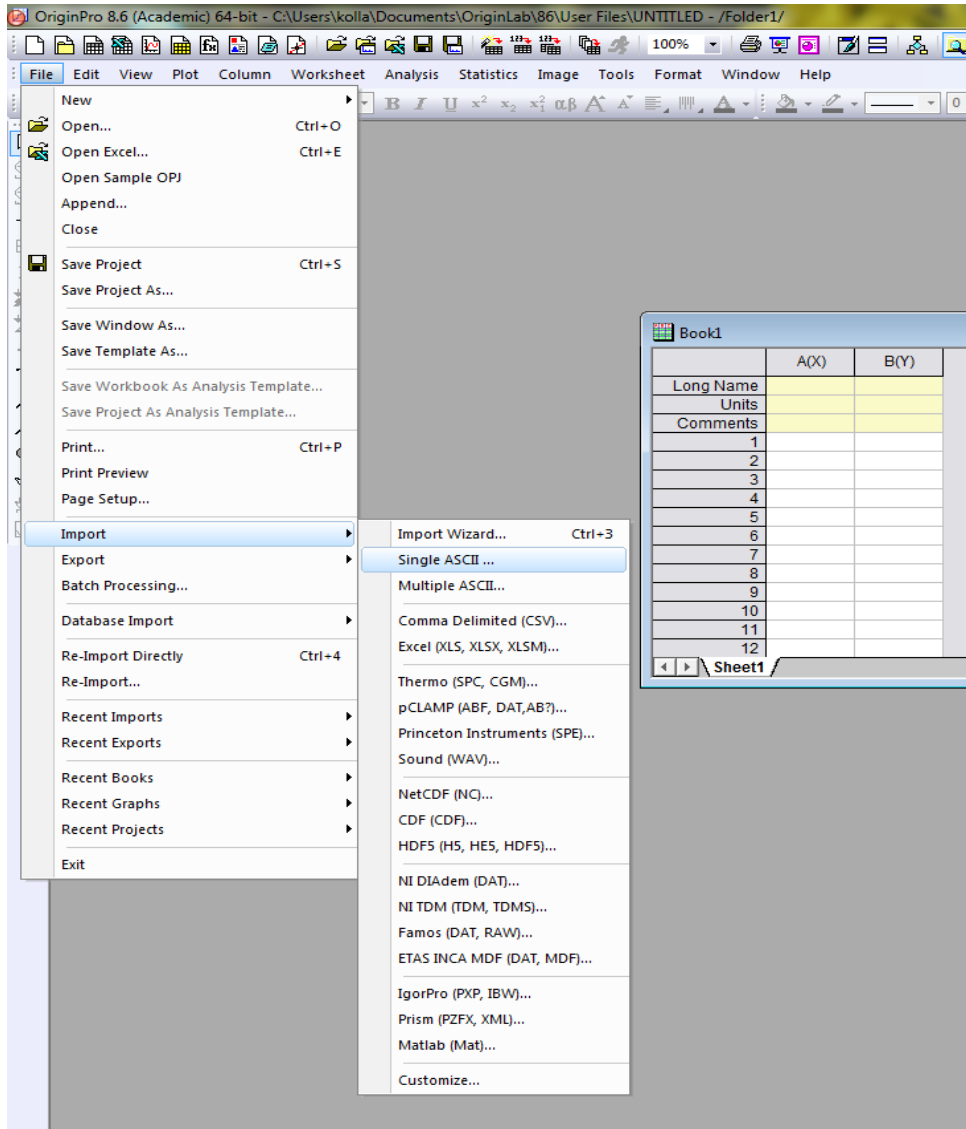


Fig.1 Data import menu

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).

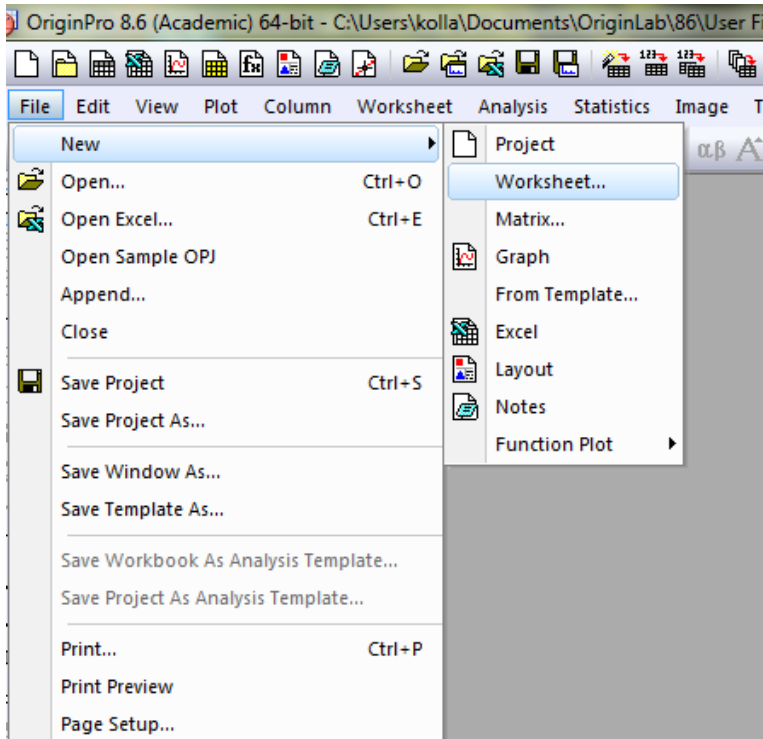


Fig.2. Opening a new worksheet

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

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)

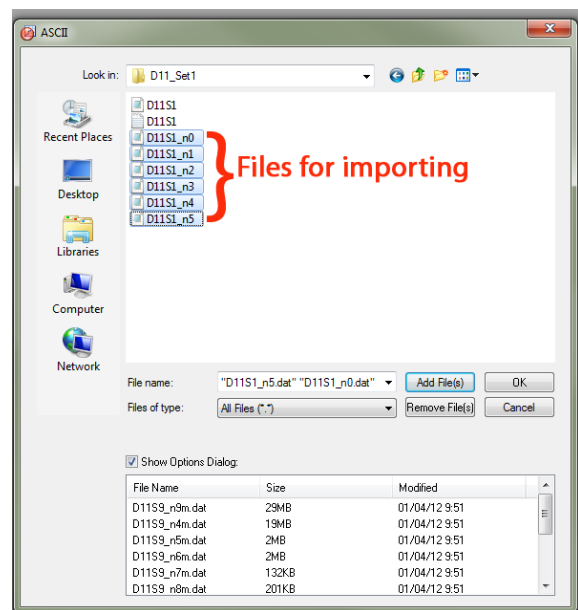


Fig.3. Multiple ASCII import

2. Creating and editing the data plots.

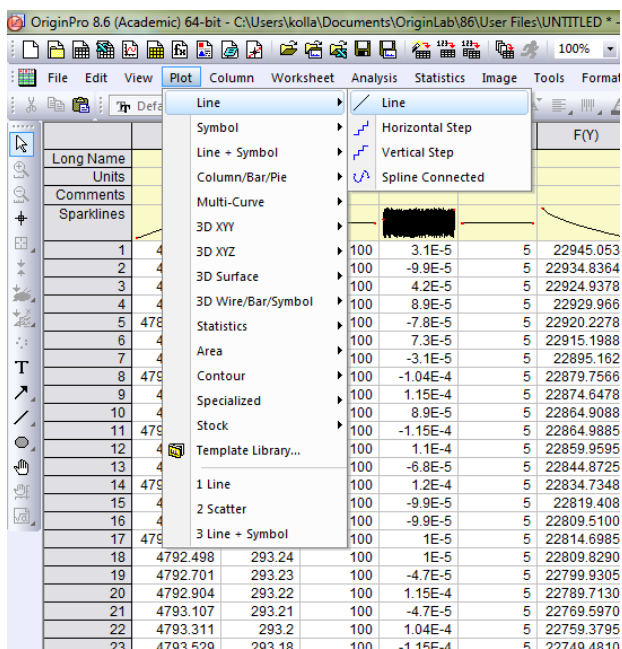


Fig.4.

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.

yEr 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

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

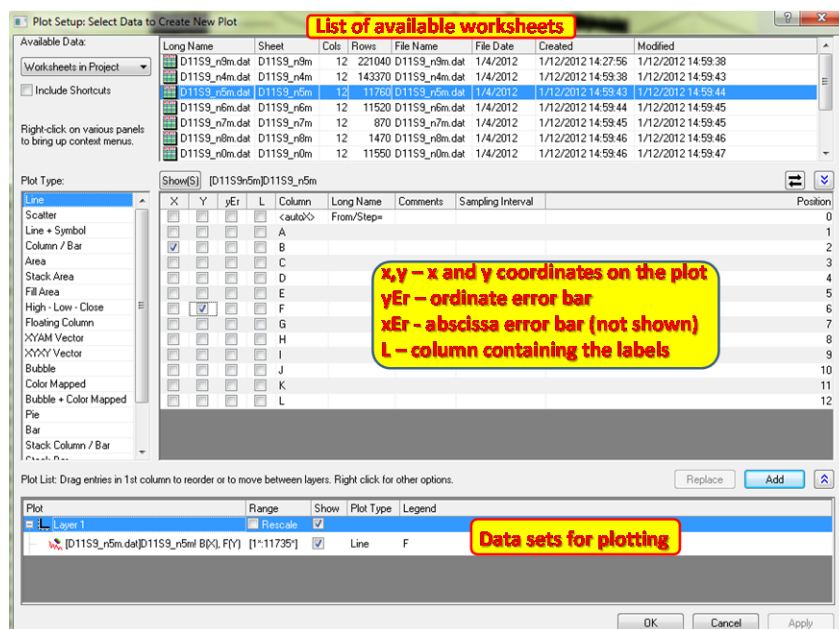


Fig.5 Plot Setup.

as many plots to the graph as you need – check another worksheet and mark new columns as X, Y axes ($yErr, xErr$ etc.). After the dialog is done – push **OK** 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 you

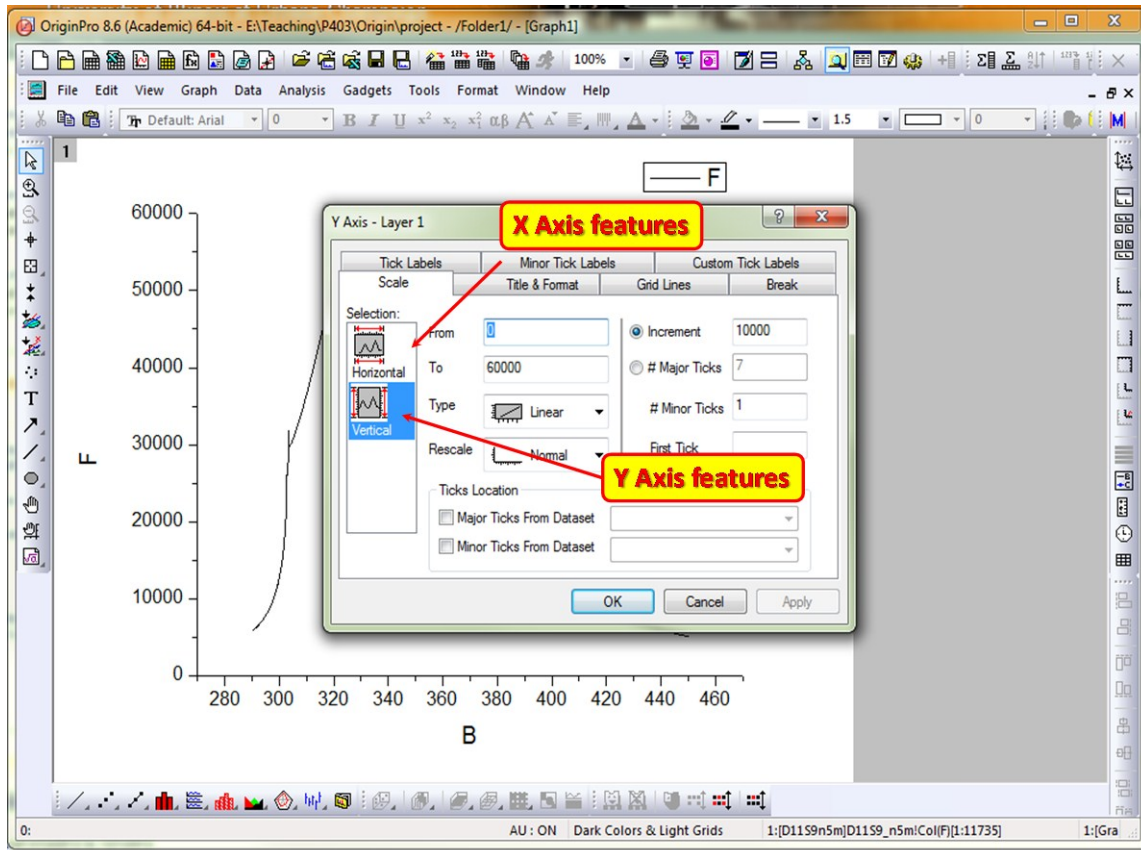


Fig.6. Graph window with X Y axes menu.

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 us 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 of related to the graph design: type of the axis (linear, log10, ln etc.), scales, grids, tick labels, axes titles etc. You can easily 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** → **Plot properties** 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.

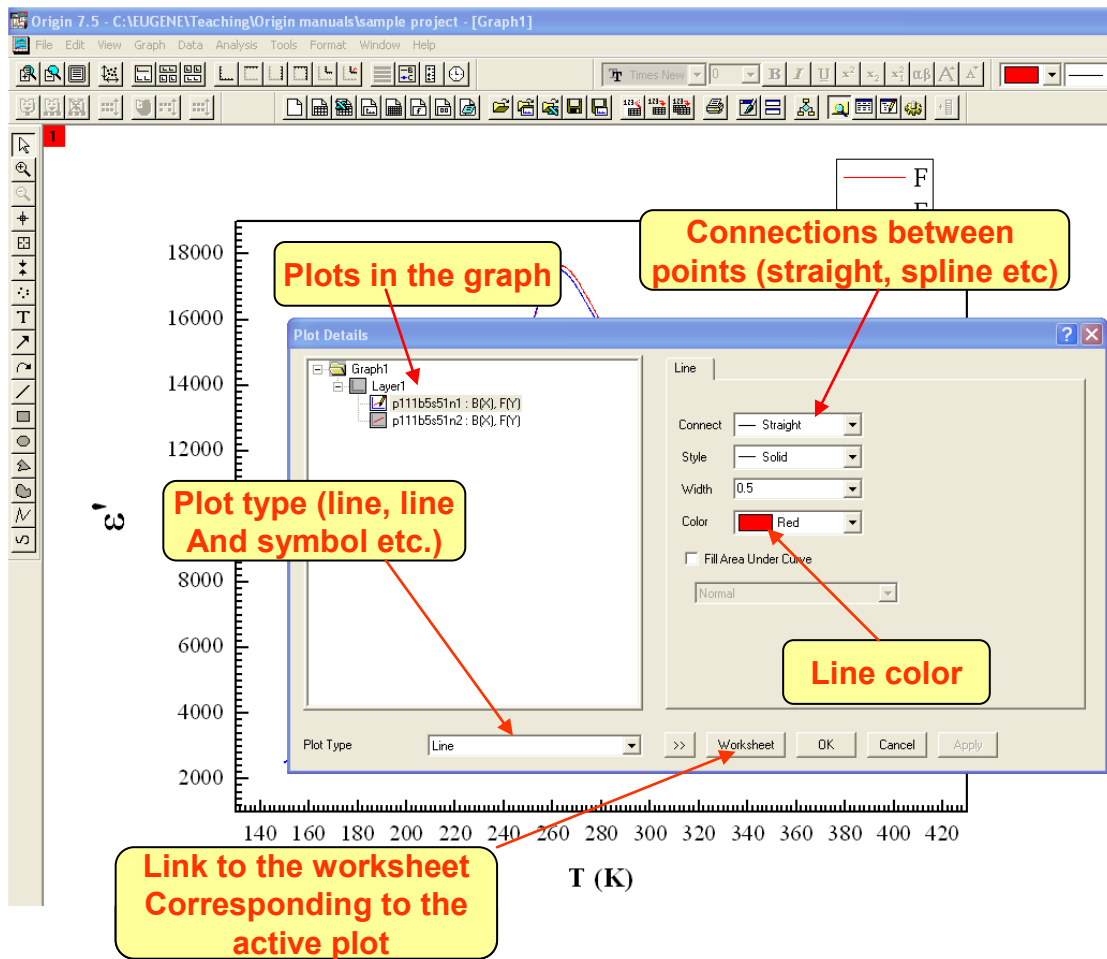


Fig.7. Plot Details menu.

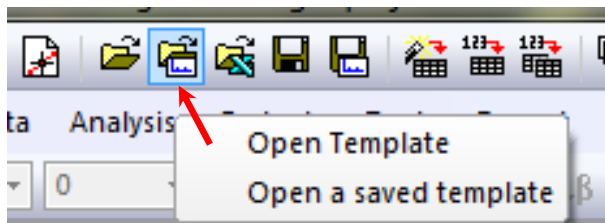


Fig.8. Open template button

After the graph design has been done you can save it as graph template for future use. Go to the main menu *File* → *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 you can

use a special toolbar button (see Fig.8.). You can also use template provided by OriginLab. Go to *Tools* → *Template Library*. There is a huge selection of different templates but they are not ready for publication and you have work on Graph design (labels, axes names etc.). One more

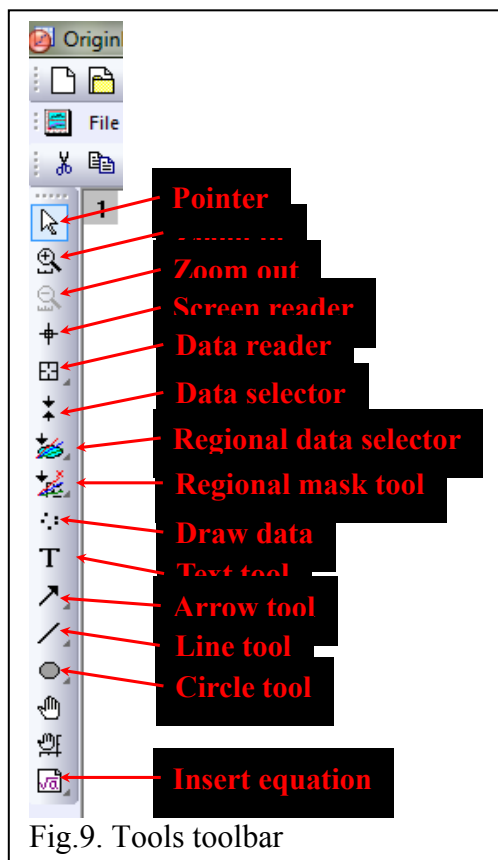


Fig.9. Tools toolbar

toolbar is very useful while working with graphs. **Zoom in** makes enlarging of the particular selected area by replotting 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.). **Regional data selector** – selects data on active plot or plots. **Regional mask tools** – selects (deselects) data on active plot or plots – these points will be excluded from analysis. **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. **Arrow, line, circle**

tools are for adding to the Graph page some lines arrows etc. **Insert equation** – is a link to MathType, MSword. MSexcel to place the equation on the active graph. All these graphical elements will be saved when saving this graph as a template. You can add more layers or inserts to the graph. Go to **Graph** → **New Layer(Axes)**. Some of those menu options are presented also in the Graph Toolbar (Fig.10). The layers on the page can be resized and rearranged by using Layer Manager (**Graph** → **Layer**

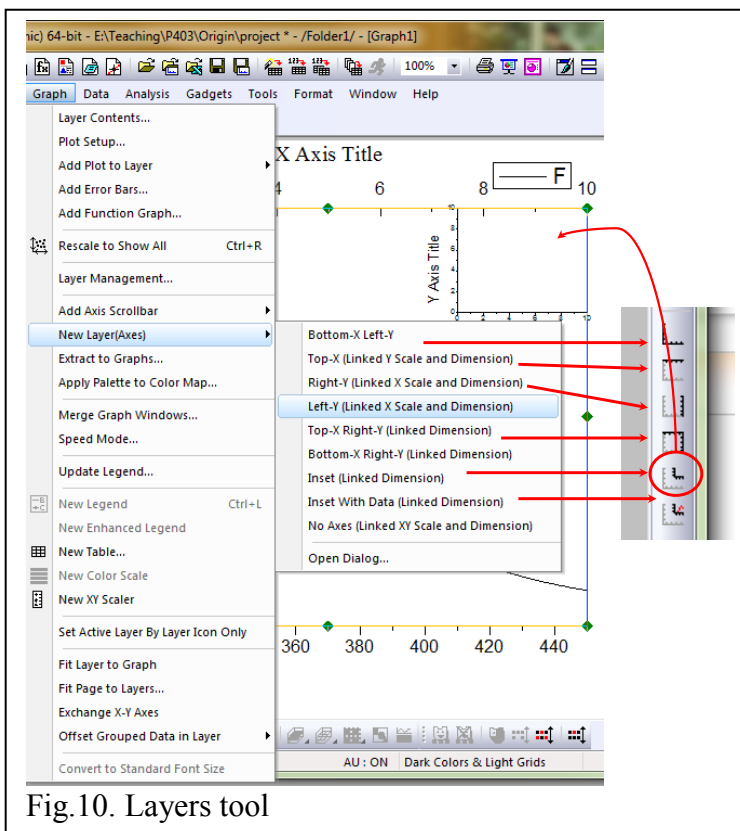


Fig.10. Layers tool

Manager).

3. Data analysis and data fitting

Linear fitting

Origin provides a set of very powerful and convenient tools for data analysis and data fitting. To perform the polynomial fitting go *Analysis* → *Fit Polynomial*. The polynomial fit pop-up menu

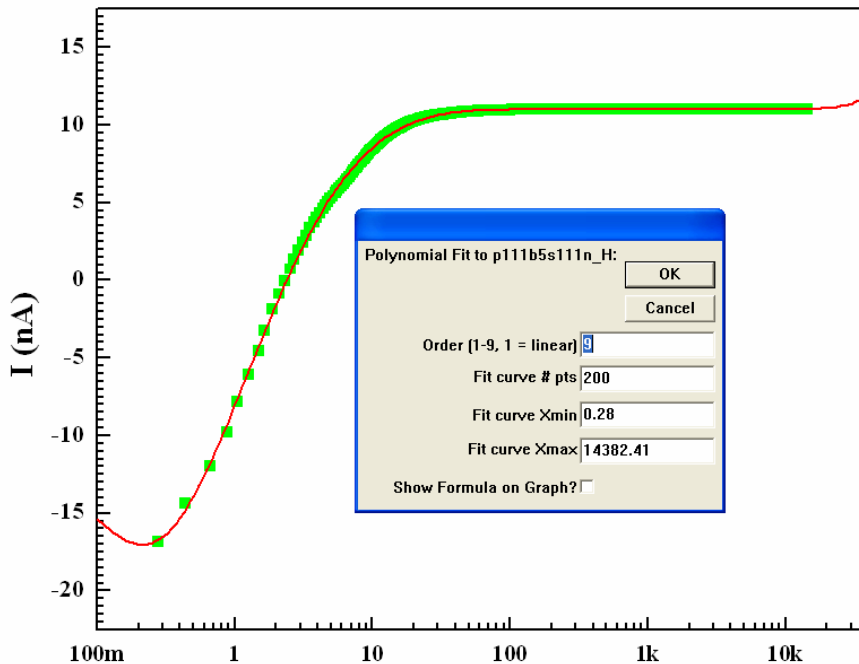


Fig. 12. Polynomial Fit menu.

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 want to work on. The next step is very simple you have to choose the

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* → *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* → *Non-Linear Curve Fit* → *Advanced Fitting Toll...* The multilayer pop-up Nonlinear Fitting menu is shown in Fig. 13. First 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 see the *Equation, Sample Curve or Function File* information (Sample Curve option in Fig.13). To write a new function - push *User Function* button and follow the instructions. There is a

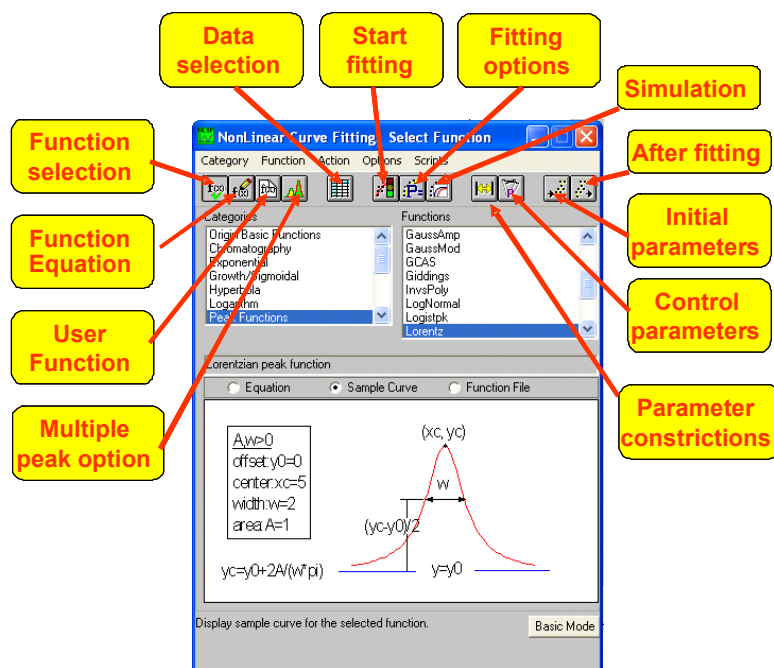


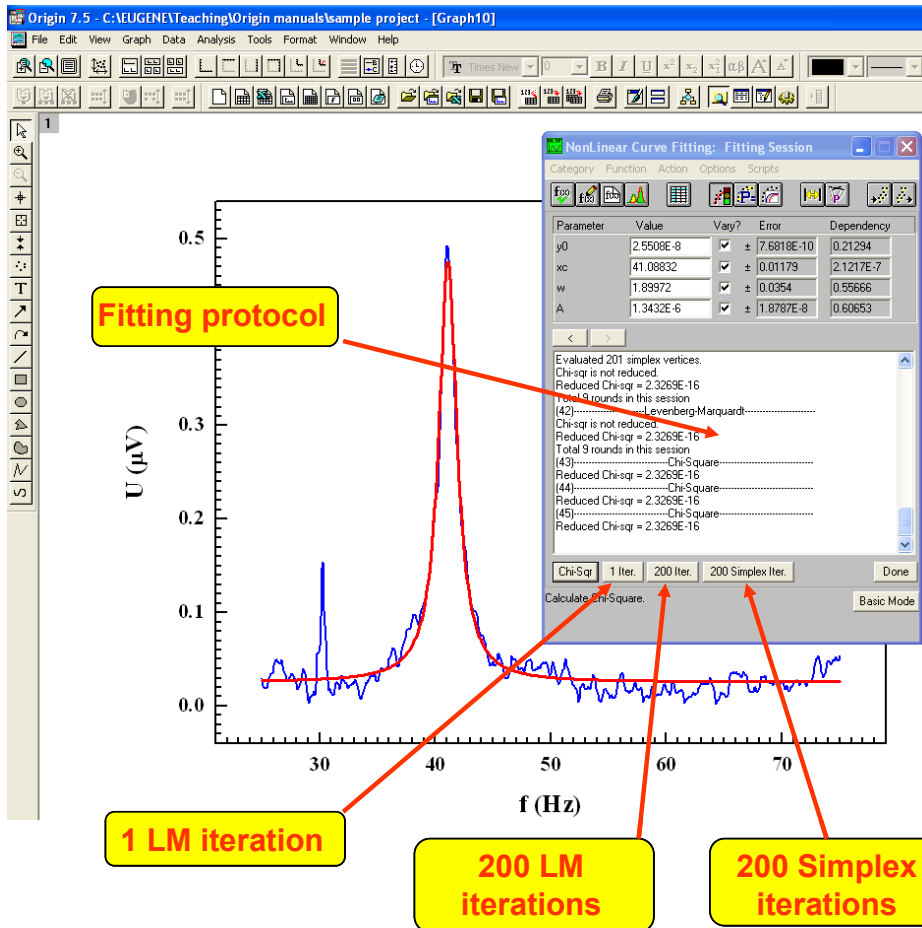
Fig.13. Nonlinear fitting menu.

start the *Fitting Session*. Using the *Simulation* submenu you can plot the fitting curve or to play with initial parameters to manually optimize them. *Parameter constraints* submenu will set the constraint 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 entering those initial parameters, but the same you can do in *Fitting session* submenu. *After fitting* submenu gives some options how to plot the 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 result in single iteration using Levenberg-Marquardt (LM) algorithm, “200 iter.” – 200 LM iterations and “200 Simplex iter.” - 200

Replicas option for some functions (*Multiple peak option* in Fig.13.). It is a very convenient tool for multiple peak fitting – you do not need to write an equation for each peak but will need to do some settings arrangement in the submenu *Replicas*. *Data Selection* submenu is for choosing of the data set or segment of data set for fitting.

Start fitting (see below) will

Simplex iterations. Number “200” could be changed to 10, 30, 50 or 100 in **Control parameters** submenu. Normally, you will not need to use 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

Fig. 14. Fitting session Dialog box.

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

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 → **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, tools 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** → **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 main 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>