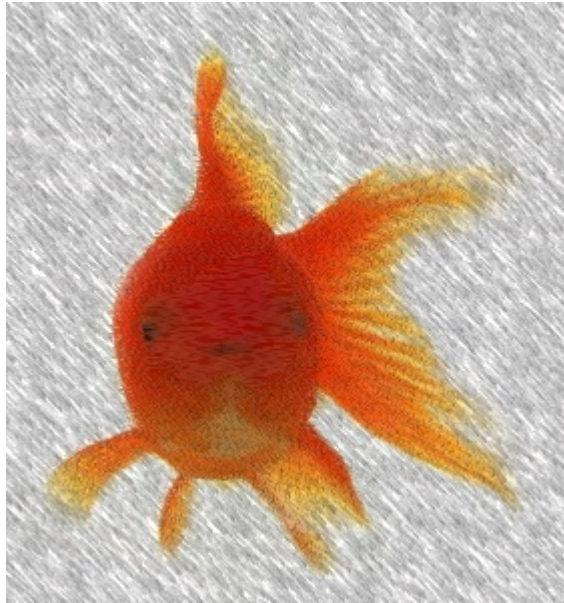


A Rough Guide to FISH



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Downloading the program:

Download FISH from the following web address:

<http://www.small-angle.ac.uk/small-angle/Software.html>

There are both PC and linux versions available.

You will be asked to provide your name, institution and e-mail address (this is so we can tell you about updates as required and so we can tell our management about how popular our software is).

Click the 'Submit Download Request' and you will then receive an e-mail containing a single use weblink which you can follow to download FISH to your computer.

The following instructions are for the PC version:

Save the zip file on your computer and then extract the contents to an appropriate folder which, from now on, will be referred to as the FISH folder and the example used here is:

C:\FISH

Once extracted your FISH folder should contain four folders (bin, doc, lib, work) and two files (fish.exe and lsinp.dat). In the doc folder you will find the FISH manual in pdf format and also some release notes (which tell you what system requirements and software you need to run FISH). Contained in the work folder are some sample data files in various formats (you don't need to worry about the other two folders, but make sure they are there!). The file lsinp.dat contains many useful fitting models which are available to you when you use FISH. File fish.exe starts the program running, right click on it to make a short cut for your desk top.

Getting started:

Double click on fish.exe and two windows should appear (be patient) as pictured below in Figure 1:

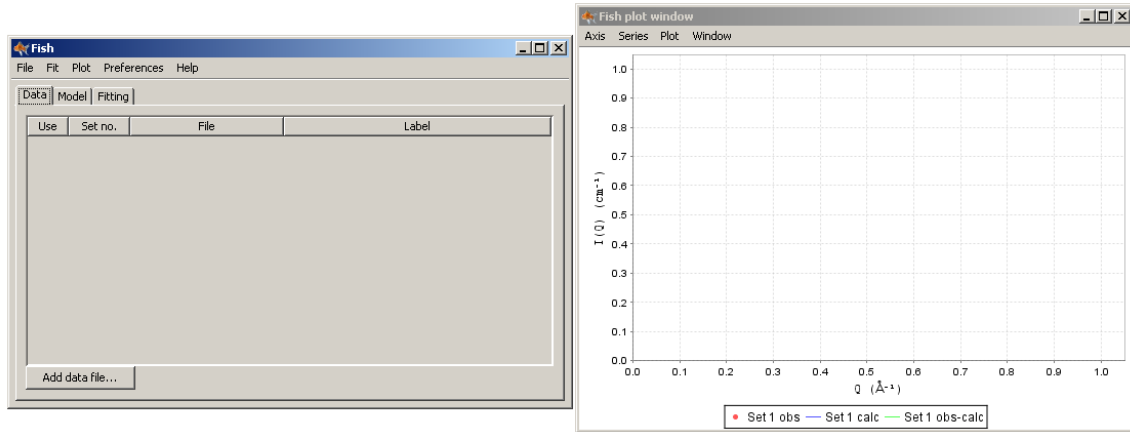


Figure 1

Click 'Preferences' and from the drop down menu chose 'Preferences...'. From here you can set your working directory (the default directory where FISH looks for data sets and saves output files too) and also your initial model file (the directory where FISH looks for model files). It is usual to set the working directory to:

C:\FISH

but you are still given the option to look for data sets and save output files elsewhere as with most programs. More importantly, set the 'Initial model file' to:

C:\FISH\lsinp.dat

so that FISH will automatically look in the correct place for the default model files.

Reading in a data set:

To read in a data set select the 'Data' tab and click the 'Add data file...' button and select your file (the default directory will be C:\FISH if you have followed the suggestions above but you can search elsewhere) and click 'Add'. The file will appear in the 'Data' tab, providing there are no errors in the file. If there is more than one data set in the file, for example if you have linear and logarithmically binned data in the same file, two lines will appear (the order in which they appear depends on the order of the data in the file). More data sets can be added if required (for example for the General Microemulsion model three sets are needed).

FISH will read ASCII data files conforming to any of the following formats: CanSAS SASXML (v1.0), 3-column CSV (comma separated variable – additional columns are ignored, column headers are permitted), or the historic ISIS COLETTE program output.

Once you've added all the files you require then select the data set which you would like to fit by ticking the box in the 'Use' column (as shown in Figure 2). Your data should appear in the plot window (red markers), along with a blue line which represents a calculated $I(Q)$ for a selected model, a green line which represents the difference between the calculated $I(Q)$ and the actual data i.e. the difference between the data and the fit to the data and a yellow line which is a constant and helps the user to see how the Obs – Calc parameter is changing as the fitting of the data progresses.

Figure 2 shows six sets of data (from three files) displayed in the 'Data' tab. In this example logarithmically binned data from the first data file has been selected for analysis with FISH (2nd row down) and has been given the label 'Set 1'.

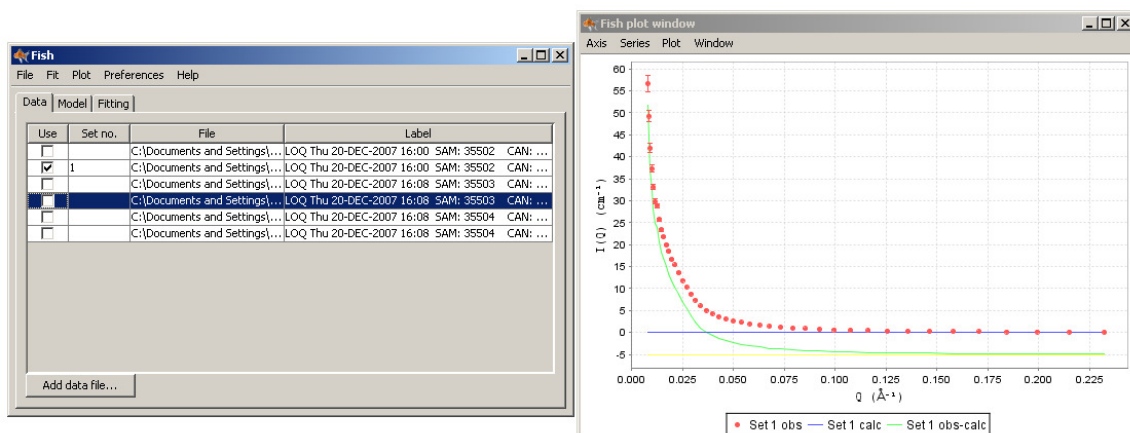


Figure 2

Choosing a model:

A model can now be chosen. This is done by selecting the 'Model' tab and then clicking the left mouse button once on the model of choice. When you click a model the blue in the plot window will change to the appropriate calculated $I(Q)$ vs. Q for that model with standard values as parameters (the green line will obviously alter too as the Obs – Calc value is also changing). 'Hovering' the mouse pointer over a model will allow a brief description of the model file to be viewed as shown in Figure 3 (for more detail see the manual and the `lsinp.dat` file).

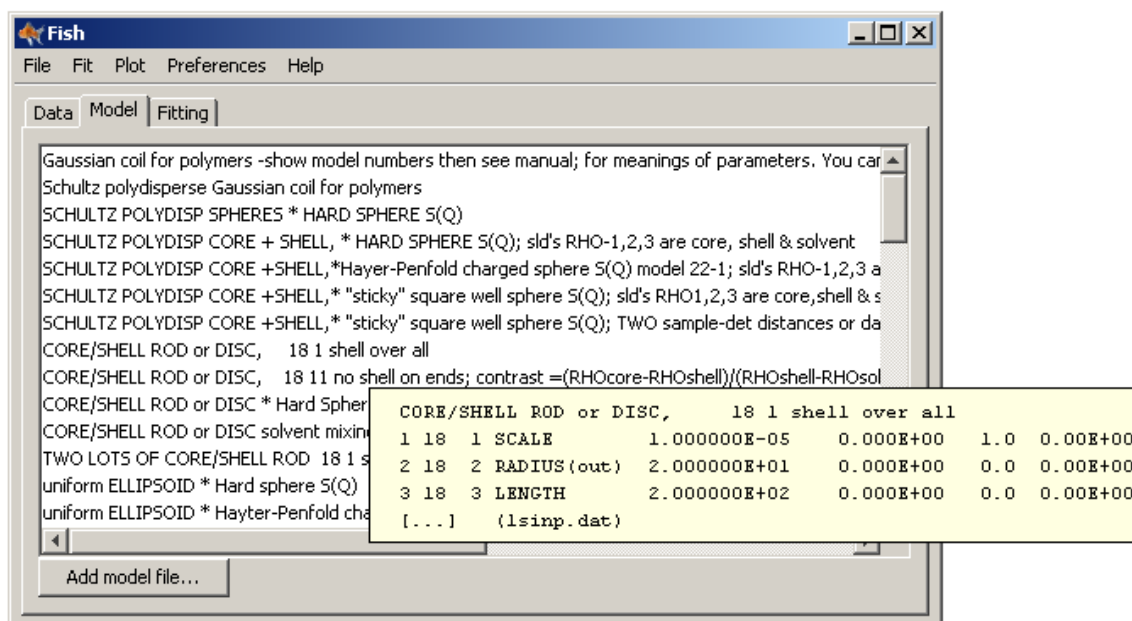


Figure 3

Fitting the data:

Parameters within a model file can be altered using the 'Fitting' tab. Once this tab has been selected a list of the parameters (column 1) with values from the LSINP.DAT file (column 2) will be displayed (as shown in Figure 4, for the case of a core/shell cylinder model). Change the values as required by double clicking on the actual value in column 2 and typing in a new number.

As you change parameter values, the blue line will change to the new calculated $I(Q)$ generated from the values being input into the system. Parameters can either be allowed to float or remain fixed whilst fitting by selecting (or not selecting) the values in the 'Fit' column (column 4) (it is best not to let too many parameters float all in one go!). In Figure 4 the SCALE, RADIUS(out), LENGTH and Flat Bkg parameters are all being allowed to adjust as the fit is progressed, but the other parameters are all held constant. Pressing the 'Run' button starts one cycle of the fit routine.

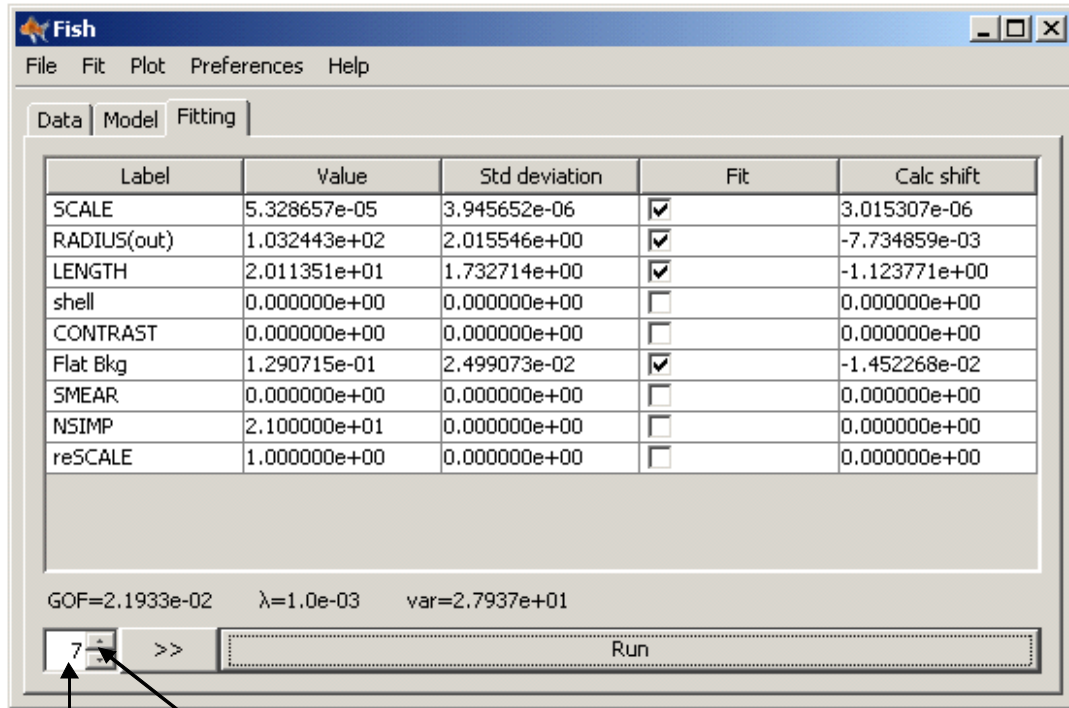
The default fit type used is determined by the control parameters in the model file, but is usually a Marquardt 'steepest descent'. This is guaranteed to find a better fit, but will not explore a large region of parameter space, so can become stuck in a local minimum (see Appendix to FISH manual). Change to normal "least squares" by clicking 'Fit', choosing 'Constants and Flags...' from the drop down menu and then selecting the different fit type. The same menu enables you to re-set the Marquardt λ parameter to its starting value of 1.0.

The 'Run' button can be pressed several times to continue cycling through the fitting routine and the calculated $I(Q)$ will be updated with each cycle and displayed on the plot. It is possible to go back a cycle by pressing the down arrow next to the cycle number (see Figure 4) or you can 'turn back' the fit cycle further by selecting a much lower cycle number. However, the more recent fits will be lost.

The default statistical information shown on the 'Fitting' tab is the GOF (goodness of fit or χ^2), λ (for the Marquardt algorithm) and the variance. The actual values of XDWE and SWSE can be displayed by selecting 'Show SWSE and XDWE' from the 'Preferences' tab.

For full information on the models please see the appropriate section in the FISH manual (it is worth noting that in FISH the units for length, radius etc is always Å and for scattering length density is 10^{10} cm^{-2} - so D_2O has a value of 6.35). To find the "model number" that is referenced in the manual you may need to use the "preferences" drop down and check "show model numbers".

For more information on the statistics used in FISH please see Appendix E in the manual.



You can go forward/backward cycles by using these arrows

Number of cycles

Figure 4

Plotting:

The plot of the fit automatically updates as cycles of the calculation are performed. However, certain aspects of the plot can be altered as required:

Zooming in or out of a plot. Pressing the right mouse button anywhere on the plot will give a display as shown in Figure 5. Using this box allows the user to zoom in or out of both axis or just the Domain Axis (X-axis) or Range Axis (Y-axis). Selecting 'Auto Range' will bring back the original display.

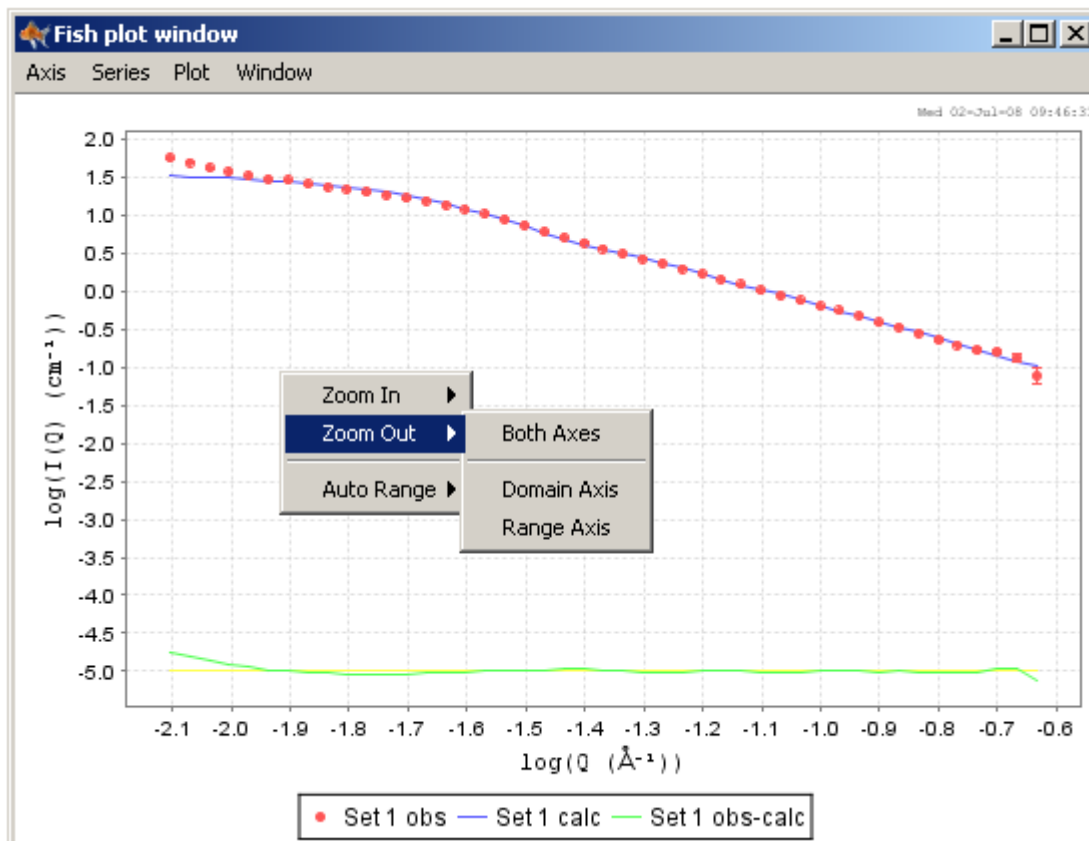


Figure 5

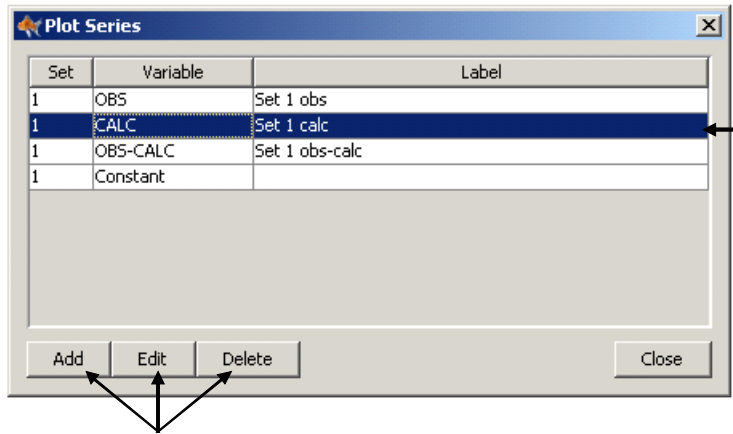
The data can be displayed on either linear (the default) or logarithmic axis by clicking the 'Axis' tab, choosing X-Axis or Y-axis and selecting either 'Linear' or 'Logarithmic'. Once the new axis type has been chosen this can then be selected as the default display by once again clicking the 'Axis' tab and then selecting 'Save As Defaults'.

Extra variables can be displayed. The default settings are to have Set 1 Obs (data for set 1), Set 1 calc (the calculated fit to the data for set 1), Set 1 obs – calc (the difference between the data and fit) and a constant (which makes it

clearer to see how the difference changes) displayed. However, these can be deleted from the plot and/or extra variables can be displayed, for example:

- P(Q) (the form factor contribution to the fit)
- S(Q) rescaled (the structure factor contribution to the fit)
- beta(Q) rescaled (a ratio by which the structure factor has to be corrected when models for polydisperse or asymmetric particles are used)

These can be displayed by clicking the 'Series' tab from the plot window and then selecting 'Edit Series...'. A box will pop up and from here variables can be added, edited or deleted (see Figure 6):



To edit or delete a variable the row must be selected (click left mouse button once on column) as shown here

Variables can be added, edited or deleted using these buttons

Figure 6

To add a variable click 'Add' and another box will appear (Figure 7). Choose the required variable from the drop down menu and click 'Ok' to accept the changes.

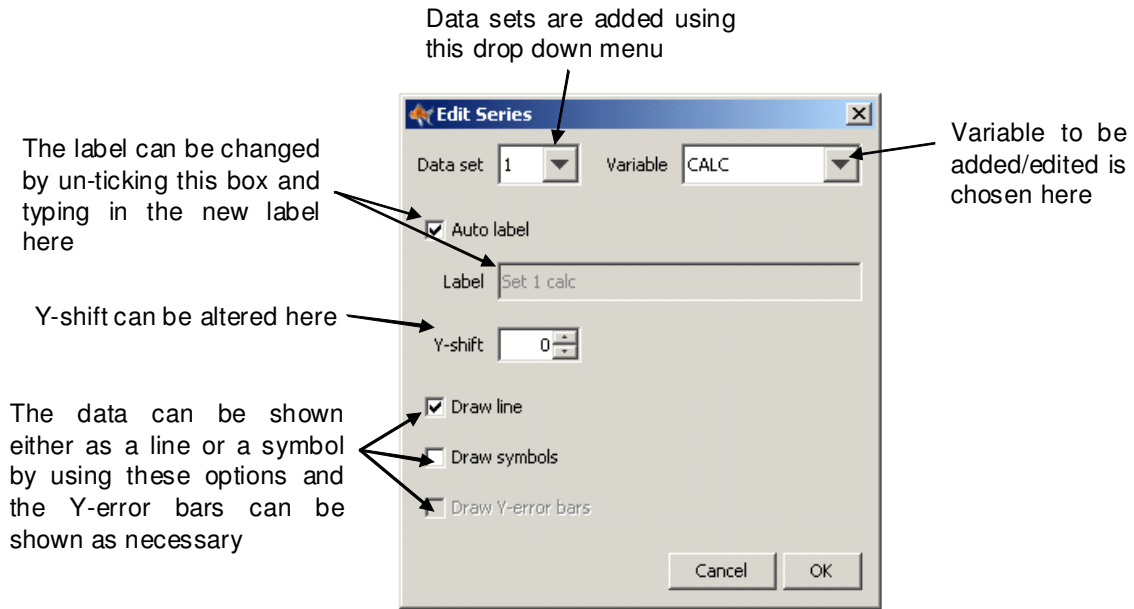


Figure 7

To edit a variable highlight the variable which requires altering (as shown in Figure 6). Then press 'Edit'. The box shown in Figure 7 will appear and the desired alterations can be made. Again, click 'Ok' to accept changes.

To delete a variable select the appropriate variable (again as in Figure 6) and press 'Delete'. Variables can be re-added if required!

A plot title can be added and axis labels and ranges can be altered. Select the 'Plot' tab and then choose 'Properties...'. A box will appear as shown in Figure 8.

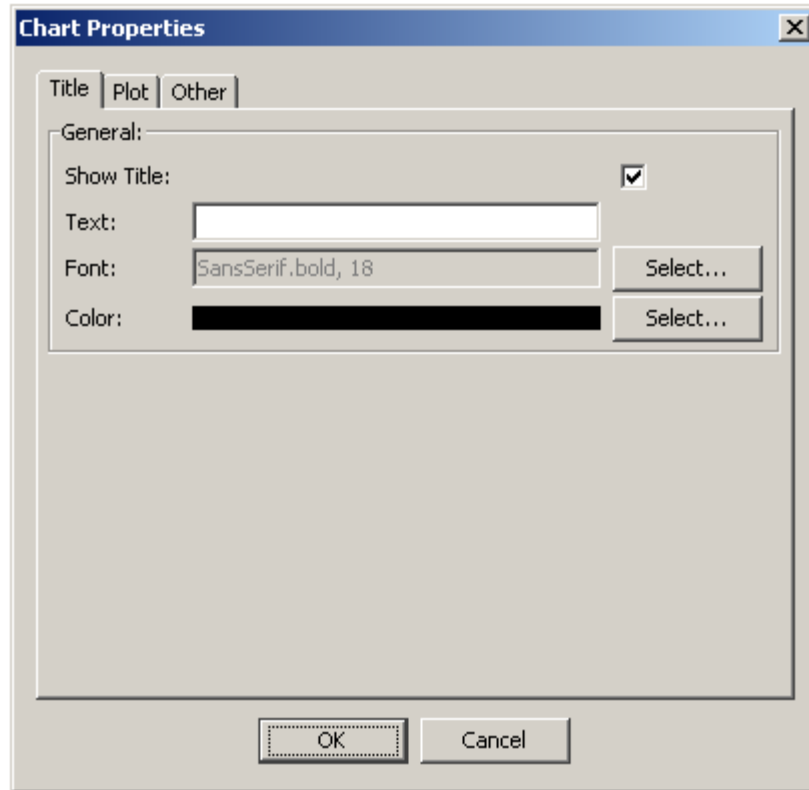


Figure 8

Type the title in the 'Text:' line and make sure the 'Show Title:' box is ticked. The font and colour of the text can also be changed from here.

Clicking on the 'Plot' tab shown in Figure 8 brings up the options as shown in Figure 9. The label and range of both axes can be changed from this tab along with the appearance (font, colour, weight).

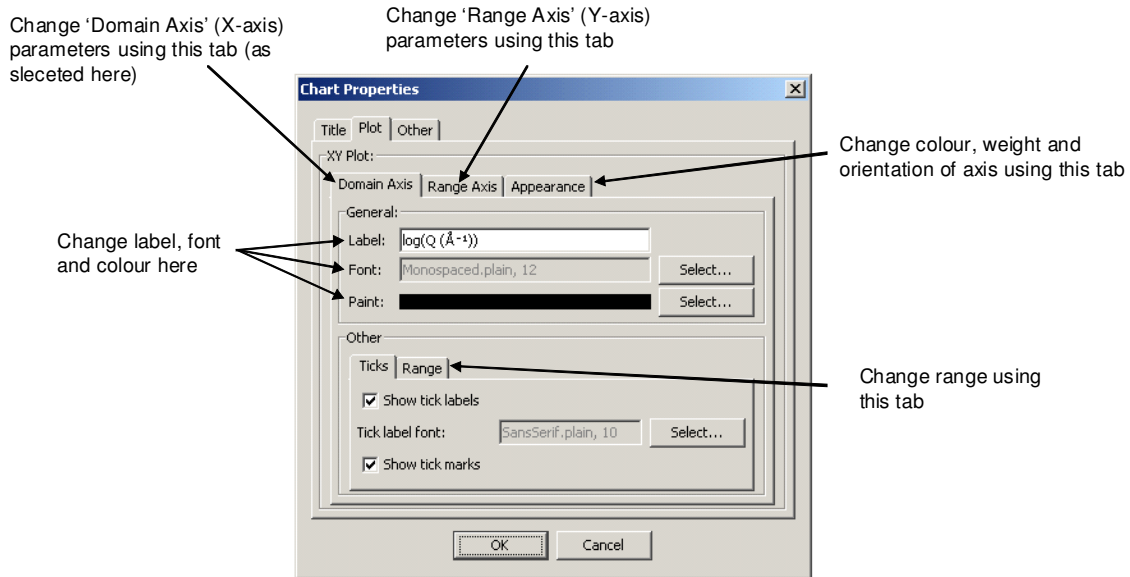


Figure 9

Selecting the 'Other' tab shown in Figures 8 and 9 allows the background colour of the chart to be altered.

The plot can be saved (as a picture not the data) and printed by clicking the 'Plot' tab and then selecting either 'Save as...' or 'Print', then follow the instructions, this can be quite slow to respond.

Parameter table, time, date and legend can be added or removed from the plot window. All these functions can be found by clicking the 'Window' tab. Choosing 'Show Parameter Table' will display the fit parameters on the top left hand side of the plot. Opting for 'Show Full Model Definition' will display the fit parameters, standard deviation, whether or not a parameter was 'switched on' whilst fitting was taking place and the calculated shift on the top left hand side of the plot. Selecting 'No Parameter Table' will remove both of these options. 'Show Time and Date' will display the time and date on the top right hand side of the fit and 'Show Legend' displays the legend. Once alterations to the window have been made then these settings can be saved as the default by choosing 'Save As Defaults' from the 'Window' tab.

The plot routines make use of "jfreechart" from <http://www.jfree.org/jfreechart/>

Saving data:

Both the current fit and parameters (in model file format) can be saved. To do this go to 'File' then either 'Save data as...' or 'Save parameters as...' to save either the fit or parameters as new files. To append new data or parameters to an existing file then opt for 'Save data' or 'Save parameters'. Once 'Save data as...' has been selected you will be given the option to save a number of data sets (1 – 8 depending on how many sets you have been fitting) and also to save various data types:

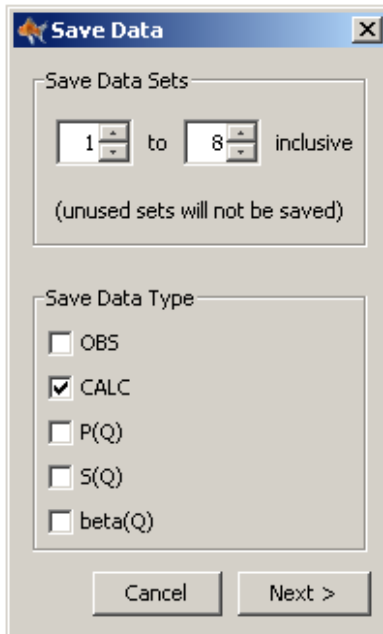


Figure 10

If sets are unused then using the default settings (as shown in Figure 10) will only save sets which actually contain data.

The five data types are:

- OBS (the observed scattering i.e. your data)
- CALC (the calculated fit)
- P(Q) (the form factor contribution to the fit)
- S(Q) (the structure factor contribution to the fit)
- beta(Q) (a ratio used in a correction to S(Q) for polydisperse or asymmetric particles – see manual)

The default settings will only save the calculated data type (as in Figure 10).

Currently, the data files are written out in the original ISIS Colette program output format (a 3 column space separated variable format with header). These are easy to import into graphing packages.

Advanced stuff and helpful tips:

If a model is expecting more than one data set, the order in which the check boxes in the “use” column of the data tab are checked is the order in which the FISH model expects them. e.g. for core, shell & drop contrasts, first un-check any checked boxes, then check the data set you need for the core, followed by the shell and then the drop contrast.

To start a plot for the second and third data sets use the “plot” menu and select “new window”. The same command will also allow say both linear and log plots of a single data set on the screen simultaneously.

Add “-console” to the short-cut you use to start FISH to see the Fortran output screen which contains useful diagnostics, especially if something is not working. (e.g. in the “target” box, “C:\fish\fish.exe -console”, note the minus sign!)

The present version of the new FISH does not allow constraints to be turned on or off. To get around this you have to copy and paste a separate model in LSINP.DAT with the alteration made.

The default LSINP.DAT contains many useful models, however some more obscure models or particular combinations of model that you may need may not be there. It is quite easy, with help from the full reference manual, to edit the LSINP.DAT file to introduce them, but if you are unsure, please contact Richard Heenan for help.

Note you can edit your own saved models back into LSINP.DAT or simply use a previously saved model file as a starting point for the next session. Opening a further model file with “add model file” appends the models in the new file to the *end* of the list in the models tab, so you may have to scroll down to find them.

Models that require two or three dimensional numerical integration, such as core/shell cylinders oriented in shear flow are currently still only available in the old line-mode Fortran version of FISH.