

# The EXAFS FT Program

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## I. Program function and purpose

This program performs the Fourier transformation, filtering, and back-transforming steps required for EXAFS analysis using shell models. It allows the user to select a filter range or re-use a filter function from a previous application of this program or some other source. The input is an unfiltered 'wiggly-part' file (.b), and the possible outputs are:

File type	Default Extension	Function of file
FT mag.	m	Magnitude of FT of $k^n\chi(k)$
Real part	x	$\text{Re}(\text{FT}\{k^n\chi(k)\})$
Imag. part	y	$\text{Im}(\text{FT}\{k^n\chi(k)\})$
Filter function	flt	FT gets multiplied by this before being back-transformed to get filtered shell
Filtered shell	f	$\text{FT}^{-1}\{(\text{filter function}) * \text{FT}\{k^n\chi(k)\}\}$
Amplitude	a	
Phase	p	$f = a \sin(p)$
Filter residuals	2b	$2b = b - f$

All files are 2-column ASCII, so may be used in any plotting program. The filter function file need not have been generated by this program as it gets interpolated onto the appropriate grid.

## II. Usage

When the program starts up, it asks for an input file. The default extension is set to .b and the path is whatever was used by the last EXAFS-analysis program. The

screen is as shown in Figure 1a. The left-hand panel shows the Fourier transform and the right shows the filtered, back-transformed data and the original unfiltered data. The cursors in the left panel define a filter window. The filter function goes to zero at the cursor positions. If the left cursor is offscreen, then the filter becomes a low-pass filter. If the right cursor is offscreen, it's a highpass, and if both cursors are offscreen, the filter function is one everywhere so the data are resampled but not filtered. The green curve is the product of the magnitude and the filter function, so shows what's getting back-transformed.

The Display Re/Im switch causes the real and imaginary parts of the FT to be plotted along with the magnitude. The default for this is off because a display with all the curves tends to get too crowded and confusing.

The right-hand panel shows the resulting filtered file and the unfiltered original data. If you flip the switch under the graph, you can see the phase. You can write the phase without seeing it plotted. These functions are interactive in that if you change the filter by moving the cursors on the left panel, the right-hand display changes.

Figure 1b shows the Input tab of the tab control to the upper left. This tab shows the file path for the current input and lets you read in a new file.

If you want to save a filter function, choose the Filter Source tab (Figure 1c) and push the Write Filter button. You can do the same thing with the Output tab. To read in a filter file, browse in the Filter Path box and flip the Filter Source switch. This will cause the filter to be read in. Any 2-column ASCII file could be read in. The abscissa should span the range of distances you're interested in and the ordinate should go to 1 where you want the filter to pass the signal.

The Output tab (Figure 1d) lets you select what files to write. Check off the ones you want to write, then push the Write Files button. Dialogs will come up for each file, with the appropriate default extension.

To quit out of the program, hit the Stop button above the right-hand graph.

### **III. Integration with other programs**

All files used by this program are simple 2-column ASCII files which can be read or produced by any of the other EXAFS analysis codes. The amplitude, phase and filtered files are the sort of thing expected by the multishell fit routine. The file dialogs will remember and use the same directory as the other EXAFS programs.

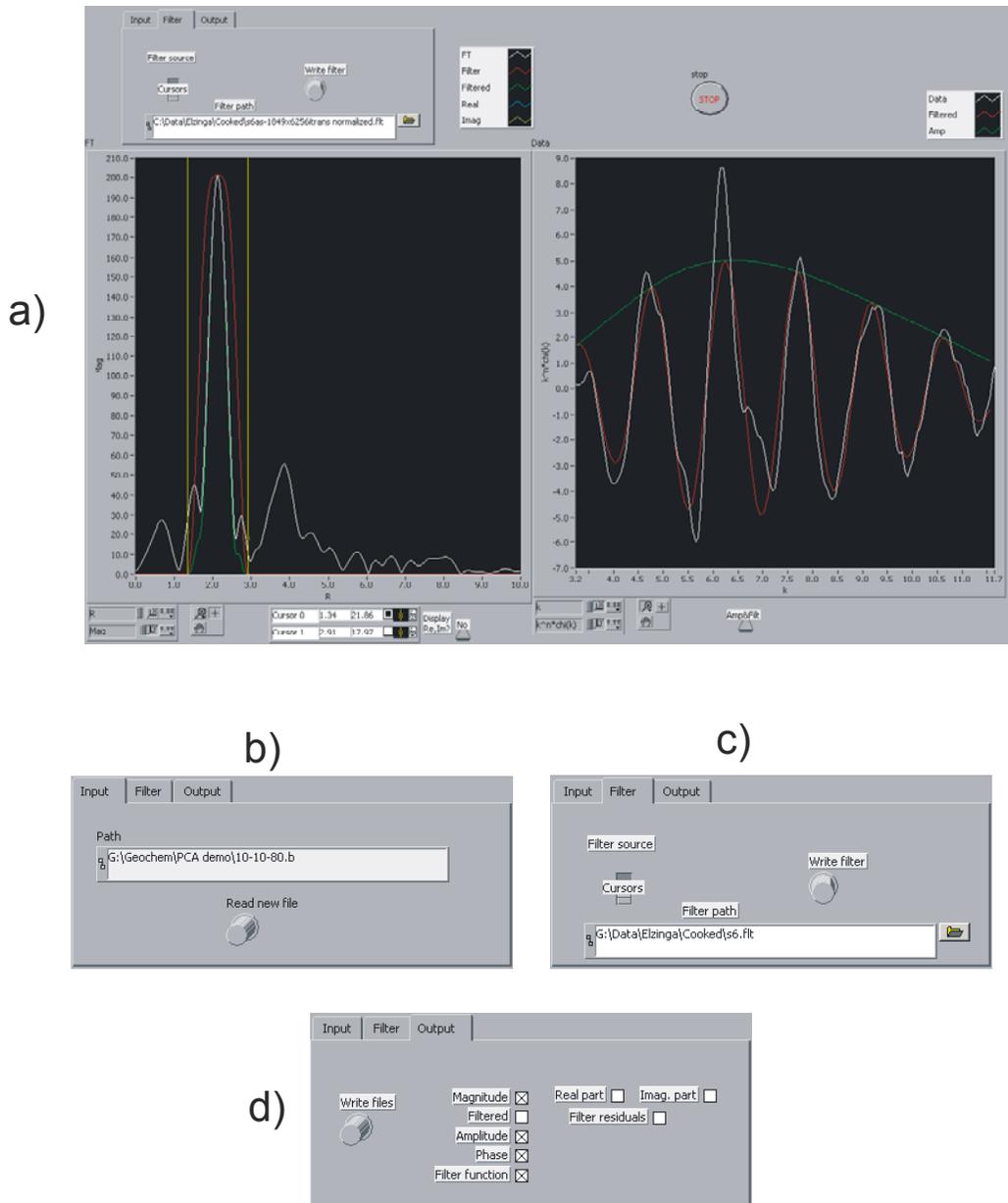


Figure 1. a) The graphics screen showing (L) the Fourier magnitude (white), the filter function (red), and the filtered magnitude (green). If the 'Display Re,Im' switch were up, this pane would also show the real and imaginary parts of the FT in blue and yellow. On the right is plotted the unfiltered (white) and filtered (red) data, and the amplitude (green). b-d) The I/O tabs showing b) the Input tab for file selection, c) the filter source tab, and d) the output tab for specifying what files to write.