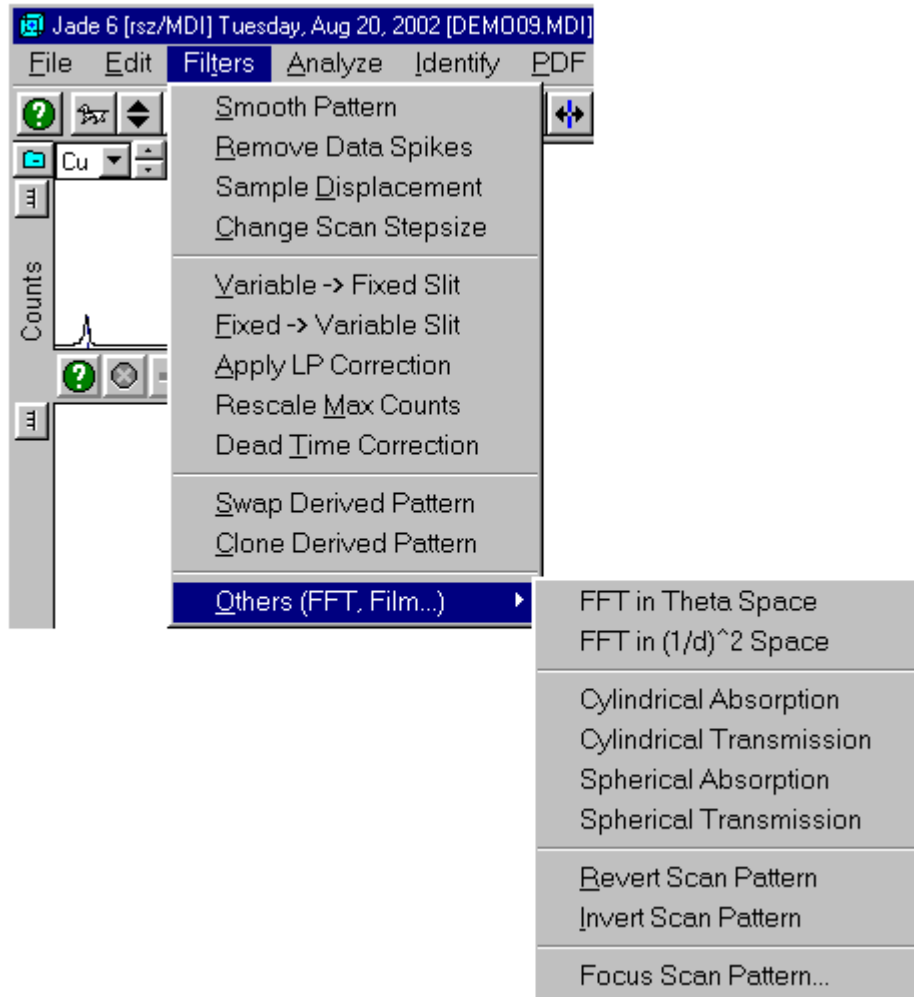


## Data Filtering Functions

The available data filters in Jade are accessible from the main 'Filters' menu:



In general, data filters that alter the intensity data (such as the Lp and the slit filters) will also be applied to the pattern overlays if any. Note that Jade does not usually prevent you from applying the same filter again to the current data. It's up to you to keep track of what you have done to the data.


**Smooth Pattern:** Jade implements MDI's proprietary variation of the Savitzky-Golay least-squares filters for pattern smoothing in the angular domain. You can bring up the following dialog from the above menu or by right-clicking the filter button on the main toolbar:



Jade carries out the smoothing immediately when you alter the parameters on the dialog, then overlays the smoothed pattern in the zoom window for comparison. You can choose a filter length from 5 to 99 points by dragging the slider left or right. The 'Quartic Filter' (4th-order polynomial) does a better job in preserving peak shoulders than the 'Parabolic Filter'. Since the dialog window is [modeless](#) (as indicated by the thumbtack icon on its title bar), you can examine the filtering results in the zoom window without having to close it down. If you left-click the filter button on the main toolbar, Jade performs the smoothing and replaces the original pattern with the smoothed one automatically without showing the above dialog.

If you choose the 'Smooth and Preserve Peaks' option, Jade will preserve the sharp peaks in the pattern when you choose longer filters to smooth the broad peaks and the background. If you choose the 'Smooth Background' option, Jade will smooth only the background regions in the pattern. Those regions are determined by the 'Peak Threshold' parameter, which you can specify on the dialog, above the newly fitted background (BG) curve. The default threshold is 3.0 sigmas, and data points above the threshold are skipped over in the smoothing. You can use the [BG editing cursor](#) to obtain a better fit of the curve if necessary by adjusting the BG tie points.

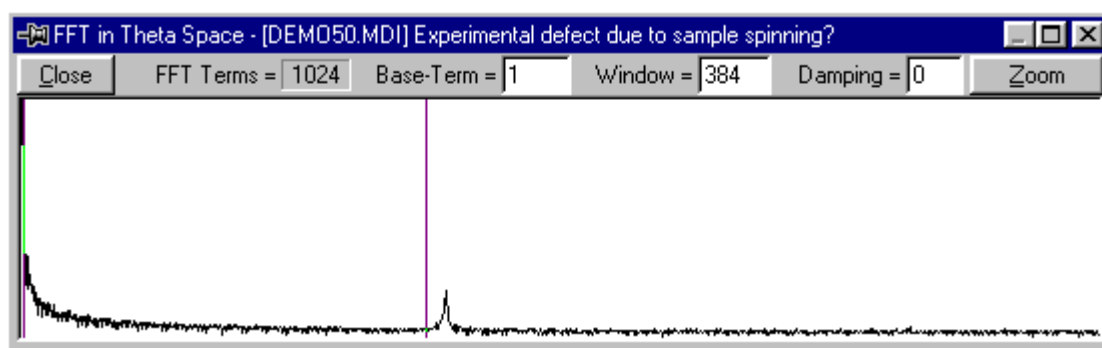
You can also display the 1st or 2nd derivative curve of the pattern using the 'Show Derivatives' options on the above dialog. Since Jade's peak search is based on the 2nd derivatives, you may be curious to see what the derivative curves look like for different filter types and lengths.

You can offset smoothed pattern up or down for a better view from [zoom & pan toolbar](#). You can display the difference pattern between the smoothed and the original using the difference button on the main toolbar. To accept the smoothed pattern for subsequent analysis, click the swap button  on the main toolbar. You can restore the original pattern by clicking the same button again.

You can also smooth the pattern in the frequency domain with the FFT (Fast Fourier Transform) filters described below, or using the 'Replace Data' option on [profile fitting](#) dialog after you profile-fit the peaks.

The **FFT Filters** enable manipulation of your data in Fourier frequency space for purposes such as data smoothing. You may find the FFT filter effective in eliminating noises that are periodic in theta or  $1/d$

space. An example of the transform is given below:



In this example, the signal peak in frequency space corresponds to a periodic noise in the pattern. Jade uses only the data in the zoom window in FFT analysis. The vertical lines on the graph mark the truncation of low and high frequency terms. The low frequency marker starts at the left edge of the graph if you can't see it. The Damping box allows for a Gaussian damping factor (zero or greater) to be applied to the amplitudes of frequency terms. The Zoom button toggles the graph between full range and truncated display. The untruncated and/or damped terms are then reverse-transformed to give the theta-space pattern that's overlaid in the zoom window for comparison and can be accepted for subsequent data analysis.

The **Remove Data Spikes** filter takes advantage of the fact that the electronic spikes are in general one step-size wide in peak detection. Such artifacts may be found in patterns obtained from older strip-chart instruments that were converted to digital acquisition. The problem existed with the original instrument but was masked by large RC constants that prevented the pen from recording the real data to the plotter. Some spikes may not be detected due to their multi-step nature. Nevertheless they can be removed manually using [data editing cursor](#).

The **Sample Displacement** correction applies the formula ' $\Delta 2\theta = D \times \cos(\theta)$ ' to the interpolation of data points in the current pattern, where the variable D is the angular shift in  $2\theta$  ( $2T(0)$ ) caused by sample displacement at the incident beam direction, and is related to the absolute displacement (S) and goniometer radius (R) in the form of  $D = 2 \times 57.2958 \times S/R$ . You can specify the goniometer radius (R) in millimeters on the Instrument tab of [user preferences](#) dialog. If you don't, Jade will accept and report sample displacement (D) at  $2T(0)$  in degrees. If you do, it will be presented as the S value in millimeters. If the d-l lines of the active PDF overlay match the peaks in the pattern, Jade automatically carries out a least-squares fit to compute the displacement and presents the results for comparison. Otherwise, you must enter the displacement on the input box to be prompted. The corrected pattern can be accepted the same way as the smoothed pattern. Notice that the displacement correction can be replaced by an offset of  $2\theta$  zero when the scan range is not wide.

The **Change Scan Stepsize** operation allows you to resample data points in a different step-size. Some resolution of data will be lost inevitably if you resample at a larger step-size. Certain algorithms in Jade (such as peak search and phase identification) are optimized for step-sizes in the range of 0.02 to 0.05

degree. This operation could render better analysis results for patterns that are collected with a step-size <0.02 or >0.05 degree. It's usually unnecessary to acquire data with a step-size less than 0.02 degree for most analyses on conventional diffractometers. Better data and analysis results will always be obtained if you can afford to count for longer times on each step. When you resample data in a larger step-size, Jade will add up or average adjacent data points to give better statistics. See [Jade's registry entries](#) topic for more information on this operation.

The **Fixed <-> Variable Slit** filters convert pattern intensities between fixed and theta-compensating slit scans in the relationship  $I(v) = I(f) * \sin(\theta)$ . The maximum counts of data are maintained in the conversion. Instead of converting the observed pattern, you can overlay PDF d-I lines in variable slit intensities. See the option on the Display tab of [user preferences](#) dialog.

The **Lp Correction** converts pattern intensities to what they should be if the Lorentz and polarization effects are removed from a powder diffraction pattern. The resultant peak intensities relate more closely to the structure factors of the reflections.

**Dead Time Correction** can be performed, if you have specified the detector dead time on the Instrument tab of [user preferences](#) dialog, to correct pattern intensity for the intense peaks which saturate the X-ray detector or counter. Refer to your detector manual for how to determine the dead time, which should be around 100 to 300 micro-seconds for a Geiger-Muller counter, and much shorter for a solid-state detector. Jade uses the following formula for the correction:

$$I(c) = I(o) / (1 - CPS \times T / 1000000)$$

where  $I(c)$  is the corrected intensity of a data point,  $I(o)$  is the observed intensity, CPS is the counts per second, and T is the detector dead time in micro-seconds. Jade will not perform the correction if the product of  $CPS \times T / 1000000$  is >0.9. Jade can perform the correction automatically on a newly-read pattern if you check the 'Dead Time Correction' box on the Instrument tab of [user preferences](#) dialog.

**Absorption & Transmission Corrections** are provided for processing Debye-Scherrer film data. The International Tables values for absorption corrections are built in, and linear interpolation of tabulated values are used within the allowed ranges of absorption coefficients. You are required to enter the absorption coefficient on the prompted input box.

The **Revert & Invert Scan Pattern** are provided in case you use Jade to view spectrum data.

The **Focus Scan Pattern** filter, which lights up only if there are located peaks in the zoom window, brings up the following dialog



to allow for sharpening and diffusing of the observed pattern. You may consider it as a quick pattern simulation tool which idealizes the observed data. The left slider on the dialog lets you alter the FWHM values of peaks while the right slide adds random noises to the simulated pattern. The  $K\alpha_2$  and BG buttons add  $K\alpha_2$  peaks and current background curve as you wish. You may find this kind of data

treatment useful in dealing with broad and noisy data in phase identification.

Note: 2nd-level filters under the 'Others (FFT, Film...)' item are accessible only with the [Jade Plus](#) package.