

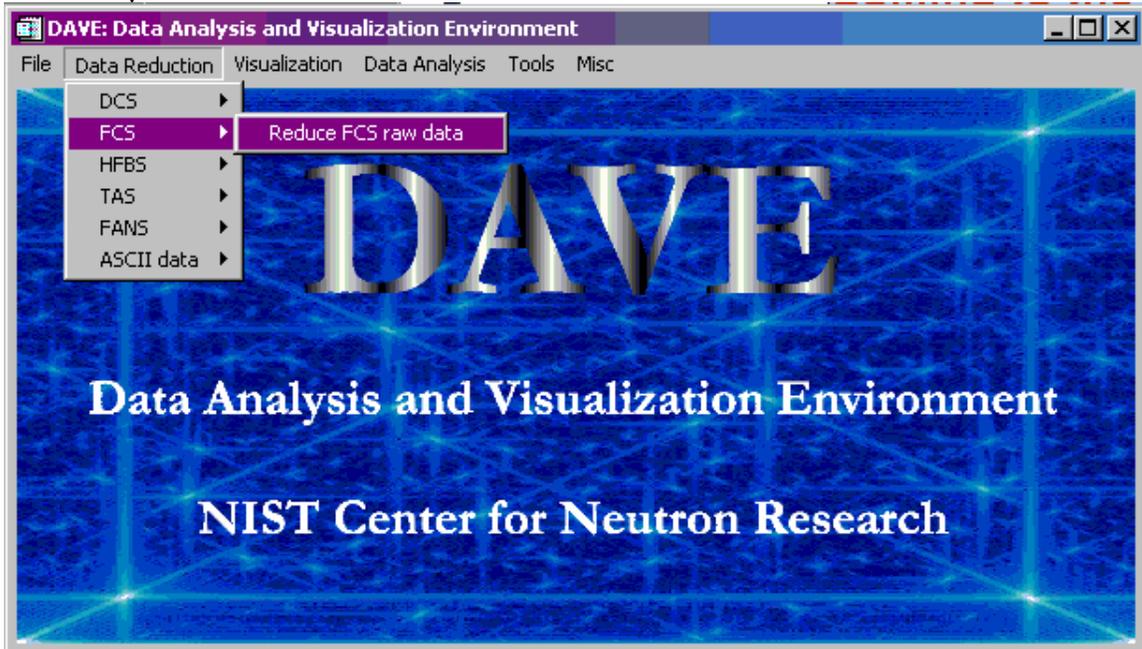
## FCS Data Reduction Using DAVE

Users of FCS can reduce and analyze their data sets using the software package called DAVE (Data Analysis and Visualization Environment). This package is freely available from the NIST Center for Neutron Research and can be downloaded from <http://www.ncnr.nist.gov/dave>.

In this document we will describe how to reduce your data using the tools within DAVE.

### Getting started

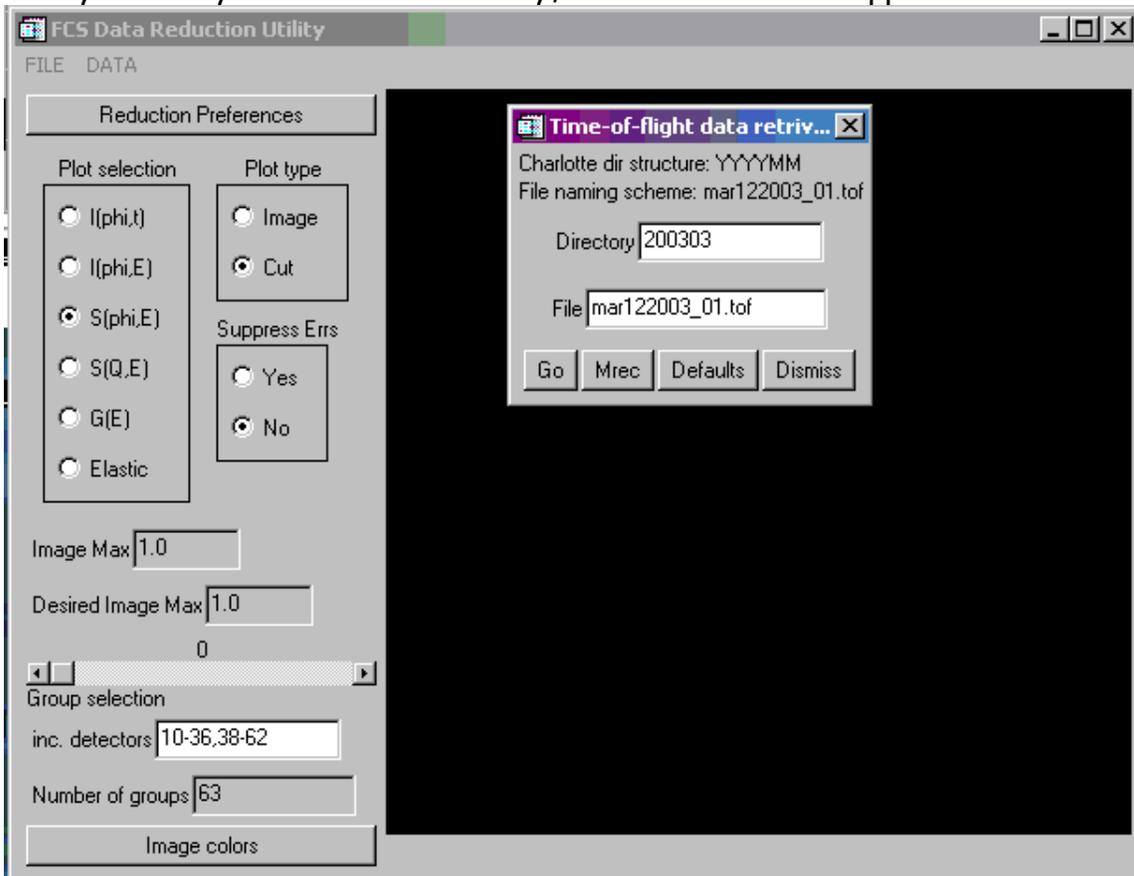
First, launch DAVE. You should set up the working environment so that your files are easily accessible. This can be done using the "File-Raw data directory" and "File-Working directory" menu items. As the names imply, you should choose the location for the raw .tof (and/or \_raw.dave) files as your raw data directory and the reduced data should be placed in the working directory.



Now that the environment is set up, you can proceed with the file manipulation and reduction of your data by launching Data Reduction->FCS->Reduce FCS Raw Data. For your information, data files on the VAX instrument computer are in a complicated, non-transportable binary format, with the extension .fcs. These files should only be used to extract ASCII

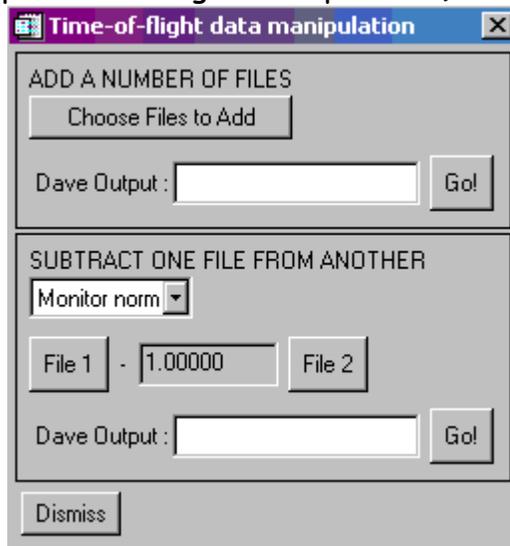
data using 'tof2ascii' on the VMS. In principle, this should already be done and the data stored on charlotte.ncnr.nist.gov along with any available instrument and temperature log files. These should be copied to your local computer via the network and/or somehow packaged to take with you.

If you are on a local NIST UNIX or Windows NT type machine, there is an option in the fcs reduction program to fetch .tof files, 'DATA->Get TOF Files'. If you need to check the file headers before fetching them, look at the monthly .mrec files (in the mrec directory on Charlotte). NOTE: I use a unix 'spawn' command to 'wget' to fetch the files (most UNIX systems already have this installed, if not, a simple www search for 'wget' will help you to install it.) For windows I execute a script the uses anonymous FTP. I guarantee that this will NOT work outside of the NIST campus, so make sure you have your data. Incidentally, the '\*' wildcard is supported.



### Adding/subtracting files

Selecting 'DATA->ADD/SUB TOF files' launches a new widget program that allows you to manipulate both .tof files and \_raw.dave files if you have created and saved the latter. You do not have to specify which type of file you have selected, however it does make sense to maintain each file type with the correct extension. The program performs automatic elastic line alignment (There might be cases where this is an extreme shift and not the few channels I anticipate. This might be a problem).

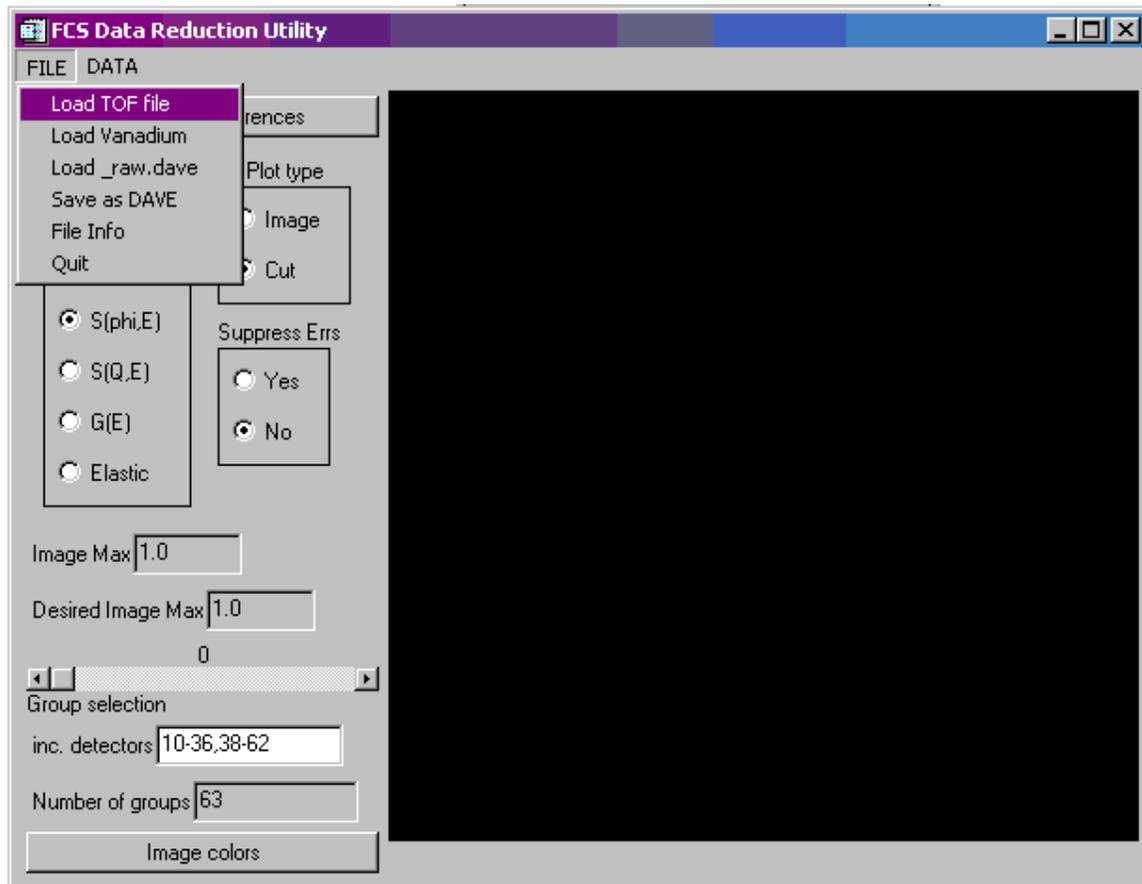


Any number of files can be added together. The monitors and counts are summed, and errors added in quadrature. The temperature is the mean of the files.

Only one file at a time can be subtracted from any other. The drop down list shows the allowed methods of normalizing the second file. If the value is taken from the ratio of monitors or length of run, then the value is displayed in the text box. If you wish to use an arbitrary scaling, then input the desired factor in the text box.

Pressing 'Go' will perform the addition/subtraction and also pass the resultant back to the main FCS program. If you supply text in the 'dave output' field this is taken to be a file name and the \_raw.dave file will also be saved.

## The Main Interface



Data can be loaded into the main program from the 'File' menu. Loading a TOF or `_raw.dave` file has essentially the same data reduction scheme, while a vanadium file is treated differently and behind the scenes (a gaussian is fitted to the raw elastic line and the resulting intensity is used to scale the detectors). At any point you can see what data file is loaded and previous file treatments by selecting 'File Info'.

The main outlined box on the left contains the possible data reduction routes available, with the plotting options immediately to the right.

- If the data has angle/Q and Energy/Time dependence then a 2D contour plot is available along with the traditional data cuts.
- Changing the 'Desired Image Max' and the 'Image Colors' button controls the 2D image.
- Suppressing error bars removes the from the plot graphic.

Detectors are specified between 0 and 62. They have been reversed (compared with what is physically the case on the spectrometer) in their ordering so that low angle detectors are low number detectors. Ranges must be specified with dashes between numbers and commas separate lists. There is currently no syntax error handling procedure here, so get it right!

The detectors can be grouped by inputting how many groups are desired. While this function uses all detectors in your list and tries to allocate the same number of detectors per group, this does mean that you might be spanning a large detector range in one or more groups. On the plus side, you cannot specify more groups than detectors and less than 1 group.

The 'Group selection' slider shows the current active group in the plot (if doing 'cuts').

### **Data Reduction Details**

#### **I(Phi,t)**

Plots the raw data counts in time channels with detector angle as the grouping parameter. All data recorded from half height detectors at low angles are scaled to those of full height.

#### **I(Phi,E)**

Plots the raw data counts against energy with detector angle as the grouping parameter. The energy transfer is determined from the average time channel with most counts or can be input from the 'reduction preferences' dialog.

#### **S(Phi,E)**

Plots the corrected scattering law against energy with detector angle as the grouping parameter.

Including an arbitrary scaling factor (all constants lumped together really) the data are treated as follows:

- Flat background is subtracted. The time channels should be chosen from the I(phi,t) plot and input from the 'reduction preferences' dialog.
- Corrected for the  $K_0/K_f$  term.

- Corrected for detector efficiency with respect to neutron energy.
- If vanadium normalization is requested (and valid), it is performed.
- If symmetrizing is requested it is performed. Both sides of the data are multiplied by  $e^{(E/2kT)}$

### S(Q,E)

Plots the corrected scattering law against energy with momentum Transfer as the grouping parameter. The Q interpolation needs to be specified in the 'reduction preferences' dialog.

### G(E)

Plots a generalized phonon density of states. This is approximately given by  $S(Q,E) * (1 - e^{(-E/kT)}) * E/Q^2$ . There should also be, at least, a Debye-Waller factor here.

### Elastic

Plots the intensity of a gaussian fitted to the elastic peak position as a function of detector angle. It is useful in determining Bragg scattering and strange detectors.

## Reduction Preferences

Time-of-flight reduction preferences

Elastic Channel   Apply

Background range: Low  High

Temperature (K)  Sigma

Constant E binning

Low  High  # E bins   Apply

Constant Q binning

Low  High  # Q bins   Apply

Symmetrize S(Q,E)  Vanadium Norm.

Save as DAVE (select as many as you like)

I(phi,t)  I(phi,E)  S(phi,E)  S(Q,E)  G(E)  Raw

Defaults Apply Dismiss

Elastic channel choice, background range and temperature are self-explanatory. Sigma is a general scaling parameter that you can use to allow for changes in scatter and scattering cross-section between samples.

Constant E binning, is useful if you wish to use the DAVE utility for peak fitting with a convoluted resolution function. Trial and error over your data range will show what numbers are best. Bear in mind that you need to adequately describe the elastic line, but do not want to extrapolate between data points at larger neutron energy gains.

Constant Q binning is necessary to plot  $S(Q,E)$

Symmetrization and vanadium normalization flag can be set here.

To save .dave files, just select the files you want here and then from the main menu choose File-> Save as Dave. The raw data file selector is useful if you wish to save the data in a dave format that is not adjusted in anyway. It allows you to add and subtract data from FCS down the road.