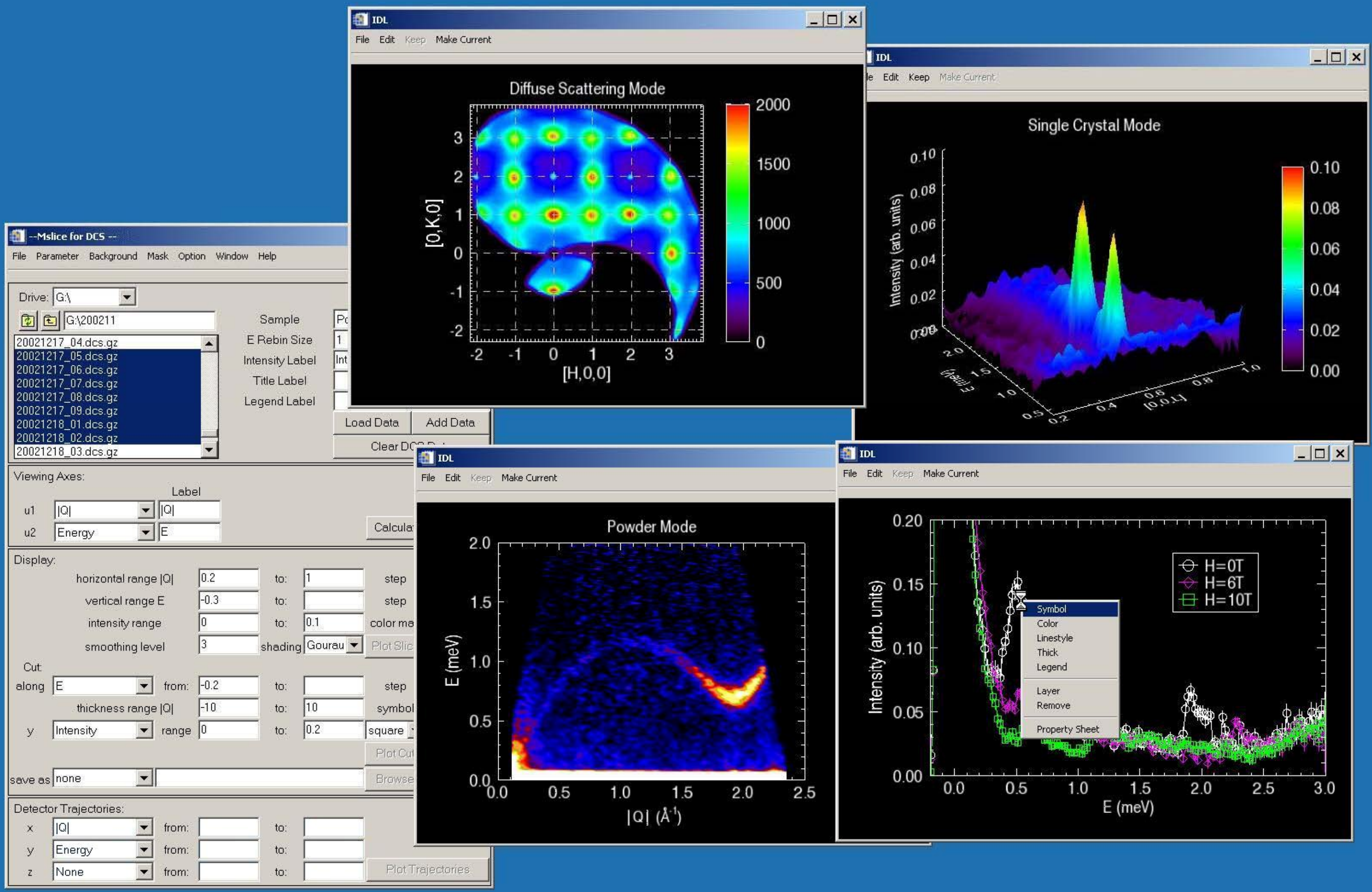
DCS-MSLICE



NIST Center for Neutron Research

DAVE

Data Analysis and Visualization Environment

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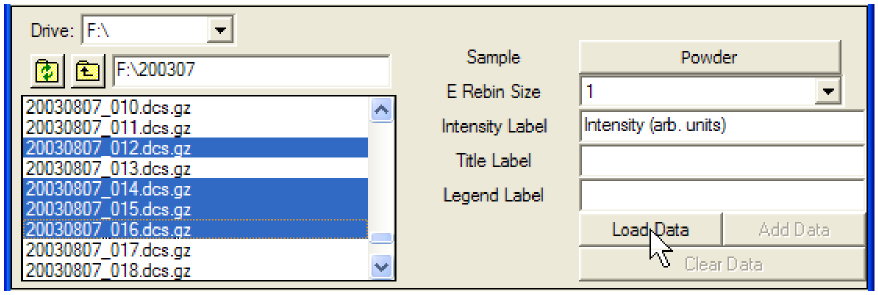
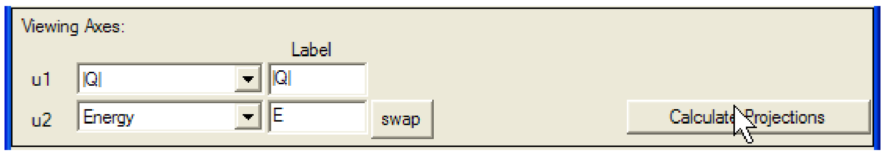
Powder Sample

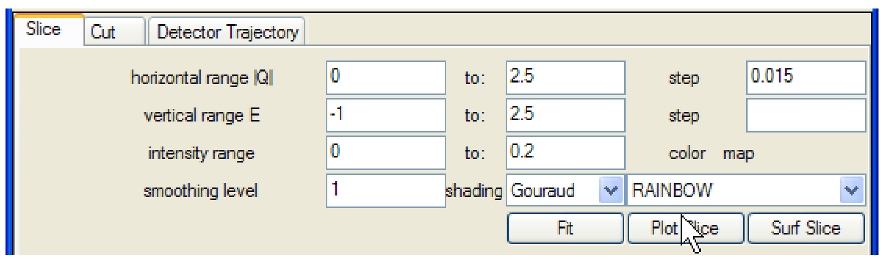
1. Change the sample type to Powder. Select the data files, and press **Load Data** button.



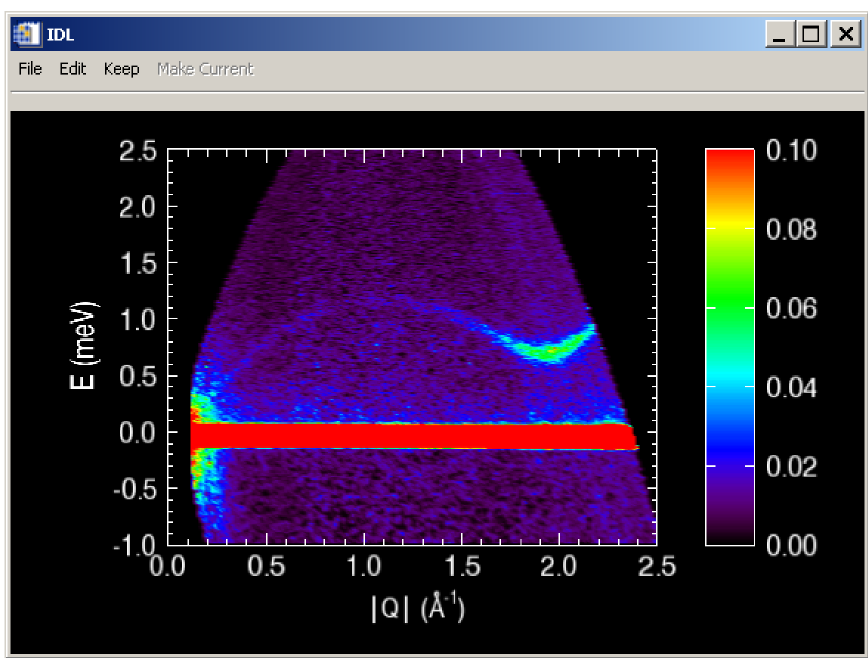
2. Choose the viewing axes, and press **Calculate Projection** button.



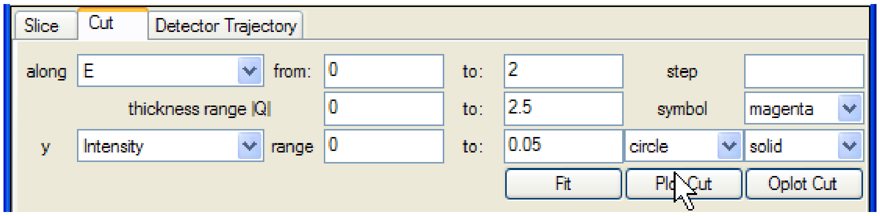
3. Press **Plot Slice** button to view the color contour plot of the intensity over the chosen viewing axes, or **Surf Slice** to view the 3D surface plot.



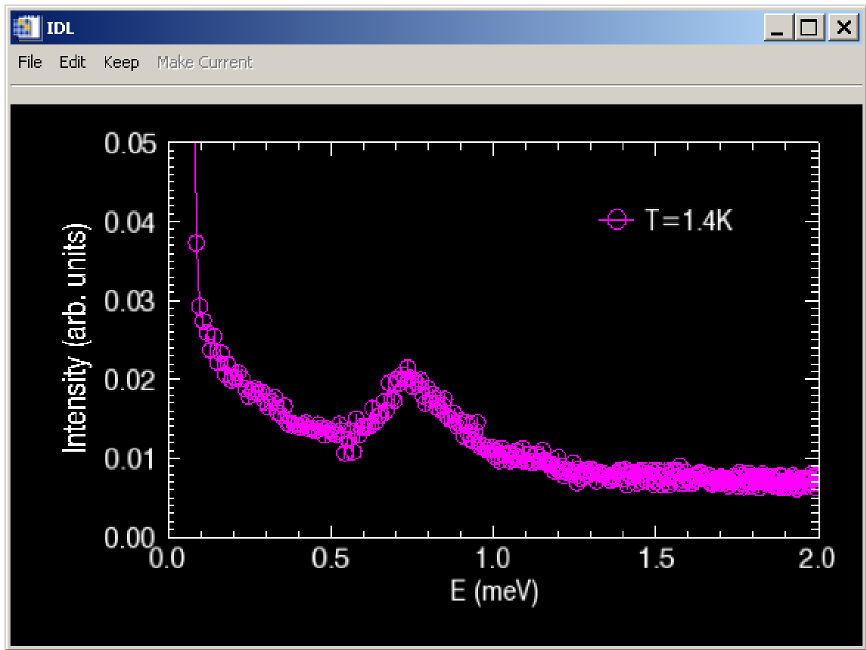
The plot will look like the following, which is a superfluid liquid He4 roton spectrum.



4. Choose the cutting axis, and press **Plot Cut** to plot the cut.

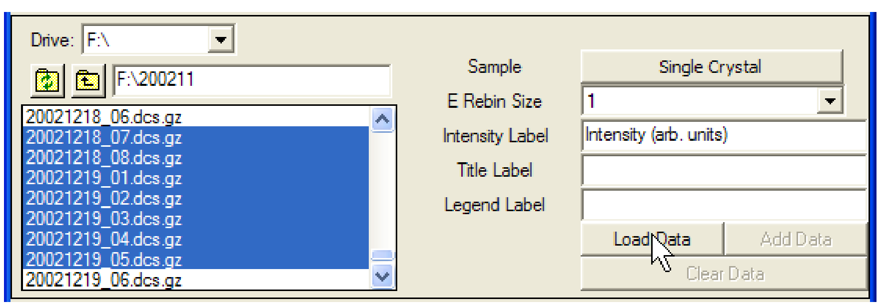


The plot will look like the following.

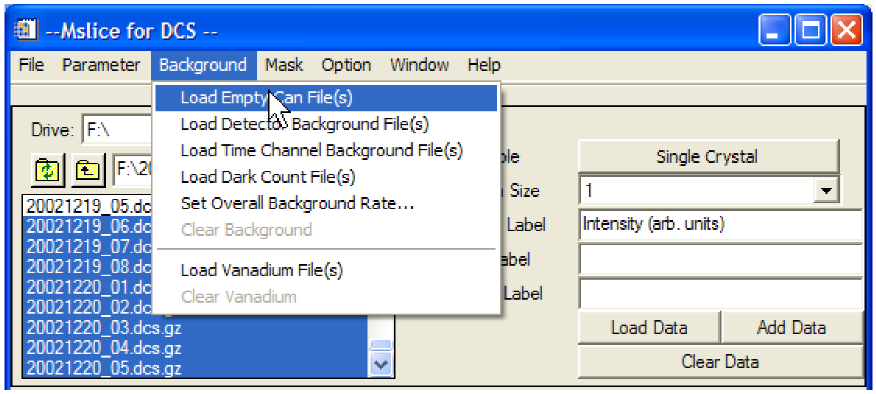


Single Crystal Sample

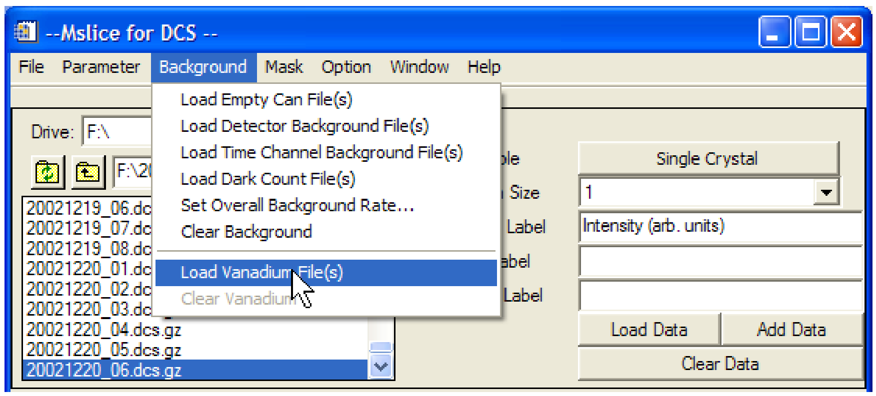
1. Change the sample type to Single Crystal. Select the data files, and press **Load Data** button.



2. Select the empty can files, then in **Background** menu, press **Load Empty Can File(s)**.

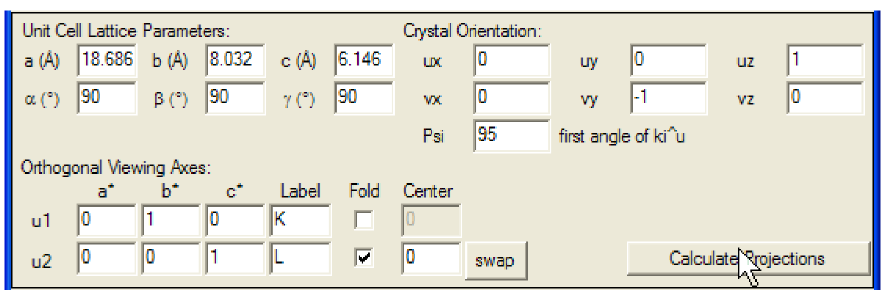


3. Choose the Vanadium file, and in **Background** menu, press **Load Vanadium File(s)**.

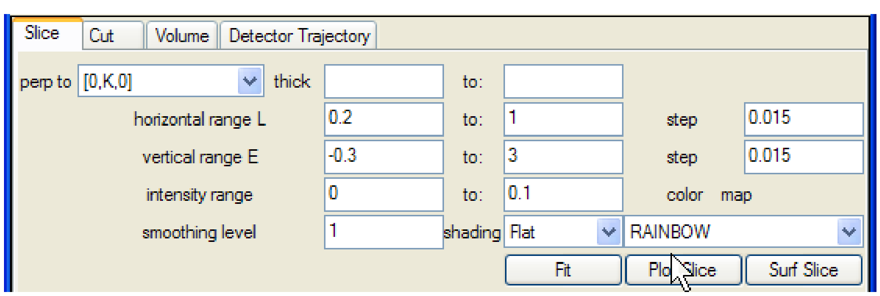


Press Yes for empty can subtraction and OK in the dialog window for absorption correction without filling in the size of the vanadium sample.

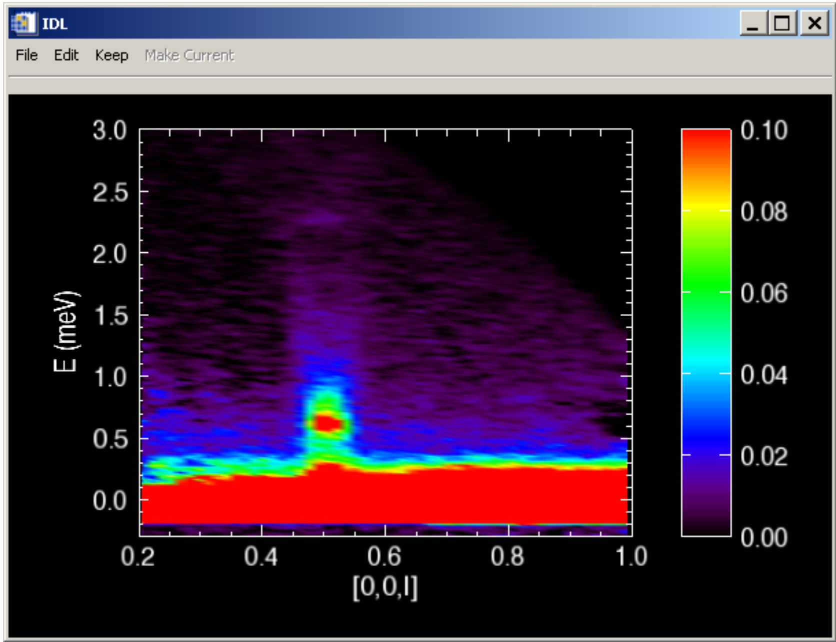
4. Enter the lattice parameters, crystal orientation, and the viewing axes, then press **Calculate Projection** button. Psi is the angle from ki to u, with counterclockwise being the positive direction.



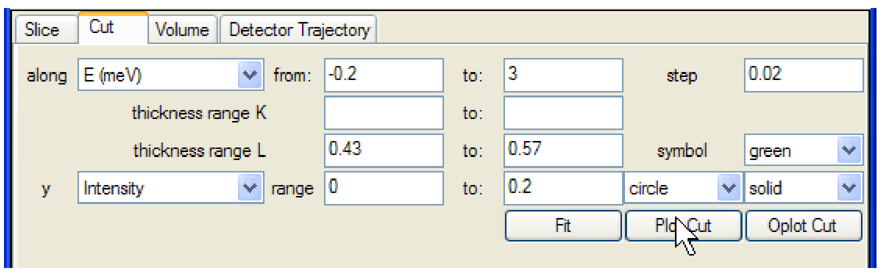
5. Choose the slice plane. Press **Plot Slice** button to view the color contour plot of the intensity over the slice plane, or **Surf Slice** to view the 3D surface plot.



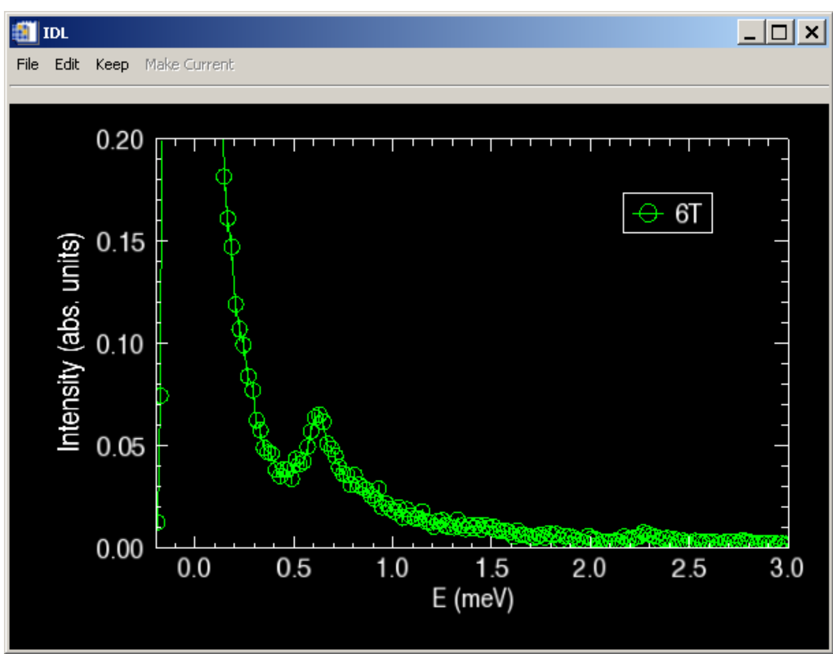
The plot will look like the following.



6. Choose the cutting axis and thickness over the other two axes, and press **Plot Cut** to plot the cut.

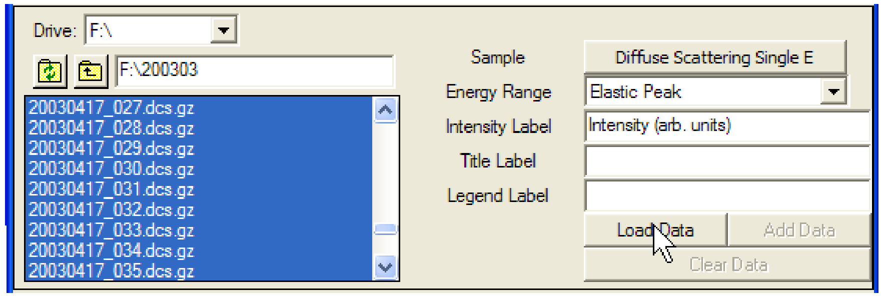


The plot will look like the following.

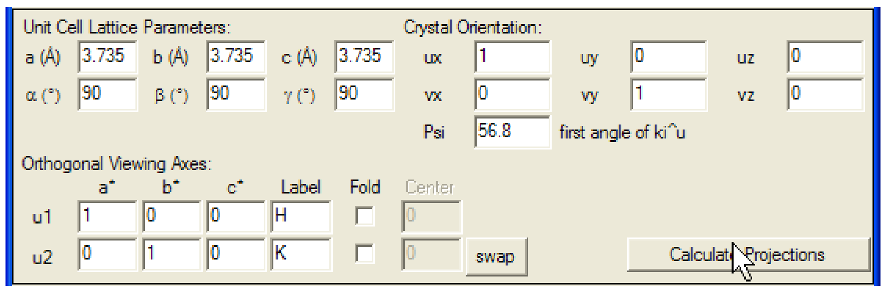


Single Crystal Diffuse Scattering

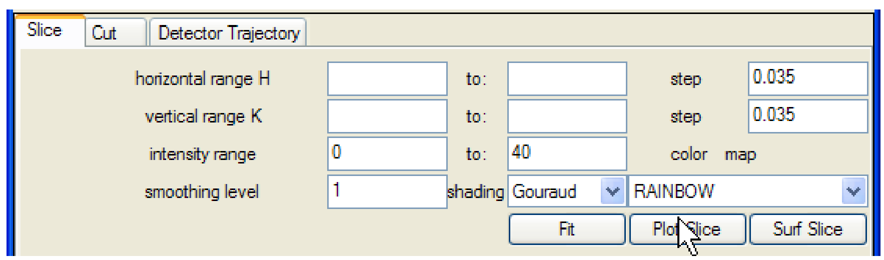
1. Change the sample type to Diffuse Scattering Single E and choose Elastic Peak as the energy range. Select the data files 20030415_095.dcs.gz to 20030417_035.dcs.gz, and press **Load Data** button.



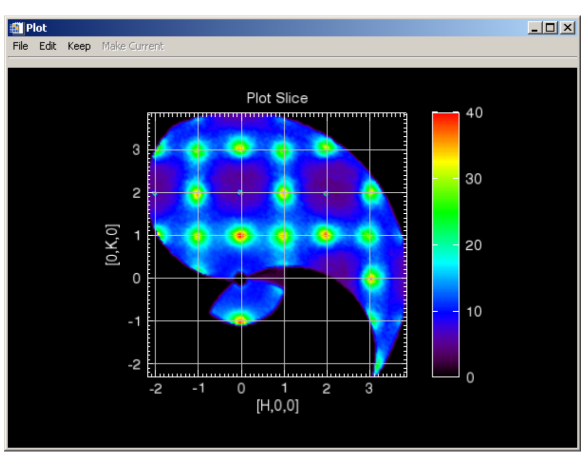
2. Enter the lattice parameters, crystal orientation, and the viewing axes, then press **Calculate Projection** button. Psi is the angle from **ki** to **u** of the first file, with counterclockwise being the positive direction.

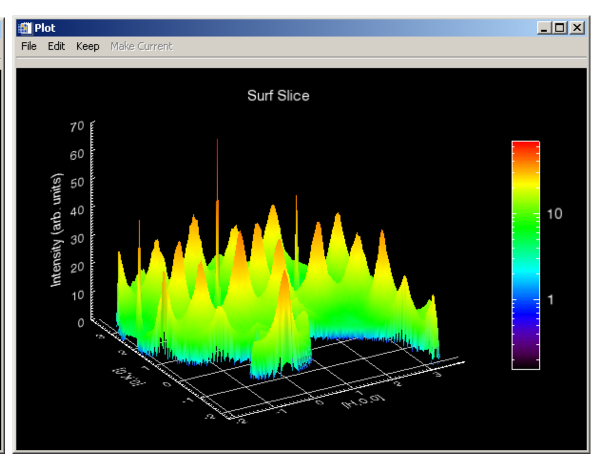


3. Press **Plot Slice** button to view the color contour plot of the intensity over the viewing axes, or **Surf Slice** to view the 3D surface plot.



The plots will look like the following.





File Type

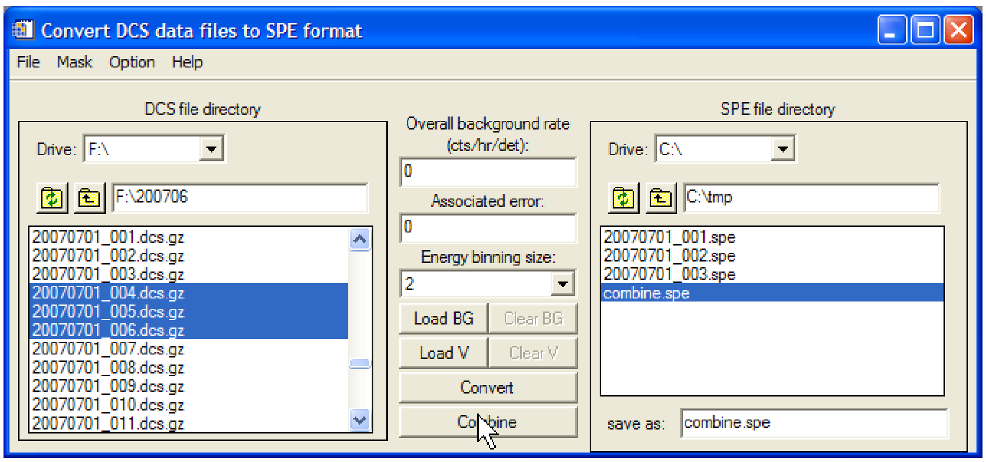
dcs_mslice is designed to handle multiple instrument and file formats. To switch among file types, go to **File**->**FileType** menu. If specific tools for the chosen file type are available, they are included in **File**->**FileTools** menu. Please refer to **Help**->**How to Add a New File Type** for the procedures of adding a new file type to the dcs_mslice program.

File Tools

File->**FileTools** menu contains specific tools for the current file type. This menu will be insensitive if no tools are available.

Convert DCS Files to SPE Files

For DCS file type, **Convert DCS Files to SPE Format** button in the **File**->**FileTools** menu starts a stand-alone application to convert DCS files into ASCII SPE format which can be processed by MATLAB Mslice or other programs.



Choose one or more DCS *.dcs or *.dcs.gz files in the DCS file directory, press **Convert** button to convert them into *.spe files. The converted files will have the same names as the DCS files except for the file extension and they are saved in the SPE file directory.

To combine two or more DCS files, choose them in the DCS file directory, then press **Combine** button. The name of the combined SPE file can be specified in the **save as:** textbox. If no name is given, the default is 'combine.spe'.

Overall background rate and **Associated error** are used to apply an overall background rate to all the detectors. The background will be subtracted in Convert and Combine operations.

Energy binning size is used to rebin the time channel to reduce the size of data.

Load BG button is used to load background files, which will be subtracted in Convert and Combine operations. There are two types of backgrounds: empty can and detector dependent energy gain side background. The types can be changed in **Option->BG File Type**. Once the background file is loaded, they will stay in the memory until **Clear BG** button is pressed. The **Clear BG** button will be sensitive only when a background file has been loaded.

Load V button is used to load vanadium files, which will be used to calculate the detector efficiencies. If the empty can background data are present, they can be subtracted from the vanadium data. The detector efficiencies are divided from data in **Convert** and **Combine** operation. Once the vanadium file is loaded, the detector efficiencies will stay in the memory until **Clear V** button is pressed. The **Clear V** button will be sensitive only when a vanadium file has been loaded.

Both background files and vanadium files are selected in the DCS file directory.

Detectors can be masked in various ways in the **Mask** menu. Once set, the mask will stay in the memory until **Mask->Clear the mask** is pressed.

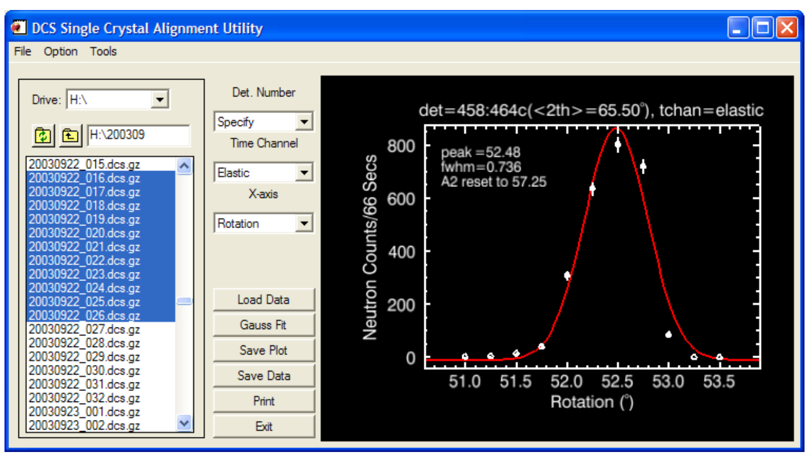
The data files can be saved as either single crystal or powder sample by choosing the corresponding sample type in the **Option->Sample Type** menu. With the choice of powder sample, detectors with the same two theta angle will be combined. The default is powder.

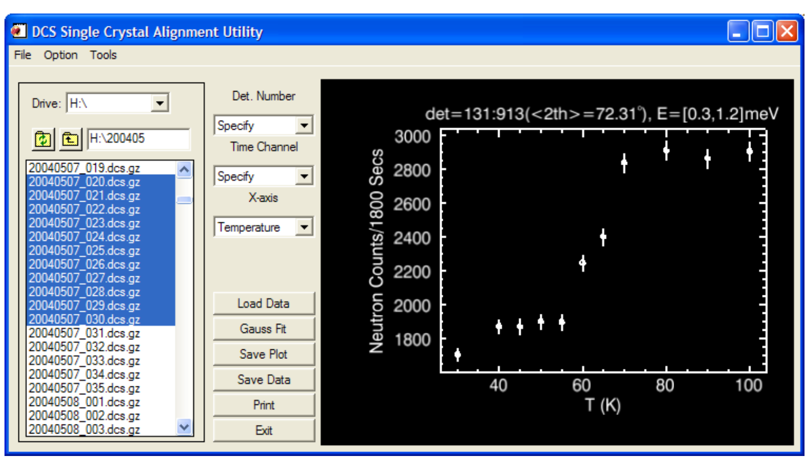
Detector configuration file (*.phx) can be created during file conversion by choosing the **Yes** option in **Option->Create Detector File**. The default is No.

The other options in the option menu are the same as those in the mslice option menu.

Plot DCS Crystal Alignment Files

This is one tool specific for DCS files. It allows you to easily plot the single crystal alignment files and fit the peak with a Gaussian function. The detector numbers corresponding to the Bragg peak need to be specified. The time channels can be all, elastic(time channels covering the whole elastic peak) or specified energy range. It also provides the capability of plotting temperature dependence of intensities in specified detectors and time channels.





Save Slice Data

File->**Save Slice Data As** menu allows you to save the current slice data in four formats: DAVE file, SPE file, (intensity, err, x, y) 4-column ascii file, or (x, y, intensity, err) matrix file. The following is an example of the matrix file for a 3x4 matrix data.

```
3 4                      ;nx  ny

0.2                      ;xdat
0.4
0.5

-1                       ;ydat
0
1
2

0.10   0.22   0.33       ;intensity
0.11   0.40   0.65
0.12  -2.80  -1.20
0.13   3.12   0.00

0.01   0.02   0.04       ;error bar
0.02   0.10   0.11
0.02   0.75   0.02
0.03   0.25  -1.00
```

The slice data are exactly the same as the data shown if **Plot Slice** button is pressed except that there is no smoothing of the data. -1 in the error bar signifies missing data in the grid. A filler of -1e20 is also used to represent the missing data intensity. Note that the error bar is not passed to the slice plot.

Save Cut Data

File->**Save Cut Data As** menu allows you to save the current cut data in two formats: (x, y, yerr) 3-column ascii file, or DAVE binary file.

The cut data are exactly the same as the data shown if **Plot Cut** button is pressed.

Save Projection

File->**Save Projection As** menu allows you to save the whole projection data in a multi-column ascii text format. The first line is the label of each column of data.

Save and Load Parameters

To save the current settings in the main window, click the **Parameter**-> **Save Parameters** button. A file selection window will pop up. The default extension of saved file is **.prm*. If no file name is entered or selected, no action is taken.

To load a previously saved parameter file, click the **Parameter**->**Load Parameters** button. A file selection window will pop up. All the parameters shown in the main window plus some options will be restored. However, previous data and projection are not loaded.

Change Self-Shielding Factor

The self-shielding factor is used in background subtraction according to the following equations:

$$I \;=\; I_1\text{-ssfactor}*I_2\ ,$$
$$Err \;=\; \sqrt{Err_1^{\,2} + (ssfactor * Err_2)^2}\ .$$

Change Smoothing Kernel

The smooth kernel for smoothing the 2D slice data can be changed in the **Parameter** menu. The default kernel is [[0.1,0.2,0.1],[0.2,0.8,0.2],[0.1,0.2,0.1]]. An error will be given if the entered matrix is not symmetric.

Change Binning Threshold

The binning threshold (f) is a factor that is used to remove bins that have too few number of data in them. Only bins that have at least f*NMAX number of data will be plotted. NMAX is the maximum number of data in a single bin. The default is f=0, which will include all data in the binning. This factor will be reset to 0 every time a new file is loaded.

Set Data and Working Directory

Set Data Directory in the **Parameter** menu will change the data directory to a new one.

Set Working Directory in the **Parameter** menu will change the working directory to a new one. The working directory is used as the default directory in saving files.

Load Empty Can File(s)

To load an empty can file, use the upper left file locator to select the empty can file(s). Then press the **Background**->**Load Empty Can File(s)** button. The empty can data will stay in the memory until the **Background**->**Clear Background** is pressed. The empty can data will be subtracted in projection calculation. The intensity (I) and error (Err) are calculated as follow:

$$I \;=\; I_1\text{-ssfactor}*I_2\ ,$$
$$Err = \sqrt{Err_1^{\,2} + (ssfactor * Err_2)^2}\ ,$$

where ssfactor is the average self-shielding factor.

Load Detector Background File(s)

This operation calculates the supposedly flat background from the specified background files. The result is an array with the size of the number of detectors. An energy range will be asked, which is used to locate the flat background. An example will be using a very low temperature measurement and an energy range in the energy gain side, where no scattering would be expected. The background data will stay in the memory until **Background**->**Clear Background** is pressed. The background will be subtracted in projection calculation.

Load Time Channel Background File(s)

This operation calculates the background of certain time channels averaged over a given 2theta range from the specified background files. The result is an array with the size of the number of time channels in the given energy range. The energy range and two theta range will be asked, which are used to locate the background. The background data will stay in the memory until **Background**-

>**Clear Background** is pressed. In projection calculation, the background in the relative time channels will subtracted from the data.

Load Dark Count File(s)

This operation loads a shutter closed dark count file. Use **Background**->**Clear Background** to clear it from the memory. This operation currently is only functional for DCS file type. If empty can data are present, the dark counts will be subtracted from them also. Dark count data and the overall background rate reside in the same memory.

Set Overall Background Rate

The **Set Overall Background Rate** button in the **Background** menu is used to input the overall background rate in counts/hour/detector. The value is then adjusted accordingly to be subtracted from DCS data in projection calculation. There is no error bar handling in this process. Use **Background**->**Clear Background** to clear it from the memory. This operation currently is only allowed for DCS file type. If empty can data are present, the overall background rate will be subtracted from them also.

Clear Background

Background->**Clear Background** button is used to clear the background data, empty can data, and/or overall background rate from memory. To take effect, projection needs to be recalculated.

Load Vanadium File(s)

To calculate the detector efficiency factor of the spectrometer, first highlight the vanadium file using the upper left file locator, then press the **Load Vanadium File(s)** button in the **Background** menu. If the empty can data are present when this operation is carried out, they can be subtracted from the vanadium data in the first two sample types. The absorption of the vanadium is taken into account if the dimensions of the annular vanadium sample are given. Press OK button without giving the dimensions will skip the absorption calculation. The detector efficiency factor is calculated as proportional to the integrated intensity of the elastic peak in each detector. This factor is divided from the raw data every time the projection is calculated. However, the raw data and the projection data are stored differently. Use **Background**->**Clear Vanadium** to clear the detector efficiency factor from memory.

Clear Vanadium

Background->**Clear Vanadium** button is used to clear the detector efficiency factor from memory. To take effect, projection needs to be recalculated.

DCS Mask

There are three detector banks in the DCS instrument, each of which can be masked. There is also a **Mask Negative Angle Detectors** option to mask the small amount of detectors on the west side. As for all masking operation, the mask takes effect when projection is calculated.

Once set, the mask stays in the memory. To clear the mask, press **Mask**->**Clear Mask** button.

Set Your Own Mask

To mask arbitrary detectors, press the **Set Mask** in the **Mask->Set Mask** menu. The detector number starts from 0. The mask takes effect when projection is calculated.

Once set, the mask stays in the memory. To clear the mask, press **Mask**->**Clear Mask** button.

Plot Mask

The **Plot Mask** in the **Mask->Set Mask** menu starts an interactive masking tool. You can read the help information in that tool to learn how to use it to mask detectors. This function is available only when data are loaded. The mask takes effect when projection is calculated.

Once set, the mask stays in the memory. To clear the mask, press **Mask**->**Clear Mask** button.

Mask Bragg Peaks

To automatically mask the detectors where the Bragg peaks occur, press the **Mask->Set Mask->Mask Bragg Peaks** menu button. An interactive plot mask window will appear to allow modifications. This function is available only when data are loaded. The mask takes effect when projection is calculated.

Once set, the mask stays in the memory. To clear the mask, press **Mask**->**Clear Mask** button.

Save and Read Mask File

The detector masks can be saved in a text file by pressing the **Save Mask File** in the **Mask** menu.

The index numbers of detectors to be masked can also be read from a text file. The numbers should be separated by space or comma, and can be in multiple lines. The detector number starts from either 0 or 1. The mask takes effect when projection is calculated.

Once set, the mask stays in the memory. To clear the mask, press **Mask**->**Clear Mask** button.

Instrument Geometry

There are two instrument geometries, **Direct** for fixed Ei instruments and **Inverse** for fixed Ef instruments. For a given instrument, this option may not be available.

Intensity Type

Use **Option**->**View Intensity As** button to choose the intensity type as one of the following:

S(Q,omega) --- a factor of $(ki/kf)^4$ is applied to the normalized intensity,
Symmetrized S(Q,omega) --- a factor of $exp(-E/2k_BT)*(ki/kf)^4$ is applied to the normalized intensity,
d2(sigma)/d(Omega)d(Ef) --- a factor of $(ki/kf)^3$ is applied to the normalized intensity,
Chi(Q,omega) --- a factor of $[1-exp(-E/k_BT)](ki/kf)^4$ is applied to the intensity,
GDOS --- a factor of $[1-exp(-E/k_BT)](ki/kf)^4$ *E/Q^2 is applied to the intensity,
VDOS --- a factor of $[1-exp(-E/k_BT)](ki/kf)^3$ *E*sin(2th)/(Q_{max}^4-Q_{min}^4) is applied to the intensity,
Unadjusted by ki/kf factor --- no *ki/kf* factor is applied to the normalized intensity.

The option **E-Integrated Intensity** in the **Option->View Intensity As** menu will cause the following calculation to be carried out in plotting cuts and slices:

$$\mathrm{I} = \frac{\sum \mathrm{I}\Delta\omega}{\sum \Delta\omega}\Delta\mathrm{E},$$

where $\Delta\omega$ is the energy width for the corresponding time channels, and $\Delta\mathrm{E}$ is the proper energy range, for example the energy thickness in a Q-cut, or the energy binning steps. A warning message will be given if this option is on when starting dcs_mslice program.

Binning Method

Two binning methods, **average** and **sum**, can be chosen from the **Option**->**Binning Method** menu button. The average or sum of the intensities in each bin is calculated respectively in the two methods. The binning method is applied in rebinning time channel according to **E Rebin Size** for *powder* and *single crystal* mode, and rebinning data in displaying slices and cuts.

Option->**Binning Method**->**Constant Intervals** menu provides the option of creating binned data at constant interval. If the option is **No**, then averaged values will be the output.

Monitor Count

This only affects DCS file type. There are two options to calculate the monitor count: sum of beam monitor counts or the integrated intensity of the beam monitor counts after fitted by a Gaussian. The option is set in **Option**->**Monitor Count**. The monitor count is used to normalize data in loading DCS files. The monitor type can be selected by **Option**->**Monitor Count->DCS Monitor Choice**. BM1 is the monitor at the guide exit, and FC0 is the upstream monitor before the choppers. BM1 is the default monitor, and only when it is selected will sum and integrated intensity option matter.

Absorption Correction

Absorption corrections for cylindrical, annular, and spherical sample geometries are implemented in the program. Go to **Option**->**Absorption Correction** menu to set the option. The absorption correction factor for every angle and energy is calculated using 360 (or 6480 for sphere) uniform sampling points on the sample cross section. Instead of calculating the correction for 913 detectors and 1000 time channels, which is time consuming, interpolation from 100 angles and 100 energies can be used. The correction is for equatorial scattering only. The effect of DCS radial collimator is not taken into account in the calculation.

Viewing Axis Type

For single crystal and diffuse scattering type, there are two options of viewing axis: orthogonal and arbitrary. They can be set in **Option->Viewing Axis**. If orthogonal option is chosen, the viewing axes given must be orthogonal to each other.

Show Powder Line

In diffuse scattering mode, Al, Cu, stainless steel, or specified powder lines can be overplotted to the intensity contour plots or detector trajectories (when the viewing axes are x and y axis). To do this, select the Al, Cu, or Stainless Steel option in **Option**->**Show Powder Line** menu. Arbitrary Q values can also be specified. The projection needs to be recalculated to have the option in effect.

Elastic Peak Position Adjustment

The elastic peak position adjustment operation in **Option**->**Elastic Peak Position Adjustment** rotates the data so that the maximum intensity(**Automatic**) or the time channel of specified energy(**Specify**) will be shifted to E=0. The energy values will not be changed. If **Check the First File Only** option is on, only the first file will be examined for how many time channels need to be shifted. After changing this option, you need to reload the data files.

Plot Window Background Color

The background color of the plot windows can be either black or white, selected in **Option**->**Plot Window Background Color**.

User Macro/Function/Procedure

To interact with the projected data, use the **Option**->**User Macro/Function/Procedure** menu. Either multiple strings of command macros or a string of call to user defined IDL function or procedure can be specified.

The user macro should be executable IDL statements. Multiple statements can be in a single line separated by "&". The user function and user procedure can be defined in any way. Only the call to the function or procedure needs to be entered in the menu dialog window. A list of the internal variables is shown in the dialog window. The array dimensions of the variables should not be altered. The user functions are executed during projection calculation.

Here are some of the available variables:

- *qty* --- intensity.
- *err* --- error bar.
- *Q* --- wave vector transfer in $Å^{-1}$. A vector in single crystal mode. Qx is along ki; Qx and Qy are in the scattering plane; Qz is pointing upward.
- *Qv* --- wave vector projected onto the viewing axes, in corresponding reciprocal lattice unit.
- *en* --- energy transfer.
- *det_tt* --- detector 2θ angle.

Tip 1: Specifying the user function after the projection has been calculated will enable the array dimensions of the available variables being shown. The projection needs to be recalculated after the user function specification.

Tip 2: To do a model calculation, generate qty and err so that they have the same array dimensions as Q in powder mode, or an array dimension of [D2, D3, …] in single crystal mode, where Qv has a dimension of [D1, D2, D3, …].

Allow Extra Viewing Axis

In single crystal and diffuse scattering modes, by default only two viewing axes plus the energy (except for diffuse scattering single energy) are available for projection. To have a third viewing axis, set **Option**->**Allow Extra Viewing Axis** on. The orthogonality of the viewing axes follows the **Option->Viewing Axis** setting. The projection needs to be recalculated.

Viewing Axis Folding

The viewing axis in single crystal and diffuse scattering modes can be folded around the specified folding center. The default folding direction is to the side with larger range. To always fold to the plus side, set **Option**->**Fold to the Plus Side** on. The projection needs to be recalculated.

Dark Angle Correction

In diffuse scattering measurement, if the incident neutron intensity is affected by the dark angle of the cryostat or magnet, a simple dark angle correction can be applied by assuming a constant scattering cross section (such as elastic incoherent scattering or vanadium) in specified energy transfer and two theta range. This option is in **Option**->**Dark Angle Correction**. You can choose the same data files for this purpose. The projection needs to be calculated to have the option in effect. After projection calculation, the overall intensity factor for each corresponding file is given the value of Imax/I, where I is the total neutron counts in the specified E and two theta range.

E-Dependent Detector Efficiency Correction

The energy dependent detector efficiency correction to the intensity can be applied to the data in projection calculation. To set this option on and off, press the **Option**->**E-Dependent Detector Efficiency Correction** button. When the program started, this option is on.

Hide Error Bar

Choose **Option**->**Hide Error Bar** to prevent the error bars been shown in plotting cuts. However, the error bar will still be present in fitting the cuts.

View Spurion Caused by Detector

Option->**View Spurion Caused by Detector** option will cause the program to calculate spurious scatterings by the detector wall of all elastic signals. If spurion exists, the program will use the current settings to plot a slice.

Check Bitflip Error

Right-click to the left of **Load Data** button to show the popup menu and this option. Use this option to enable or disable the bitflip error checking during DCS data file loading.

Preserve Negative 2theta Angle Value

Right-click to the left of **Load Data** button to show the popup menu and this option. In powder mode, after the projection is calculated, only the absolute values of the 2theta angles are saved, unless the **Preserve Negative 2theta Angle Value** option is turned on. The projection needs to be recalculated to have the new option in effect.

DCS 2theta Correction

Right-click to the left of **Load Data** button to show the popup menu and this option. Use this option to enable or disable the 2theta correction due to the length of the detectors for DCS instrument.

Allow Two Sets of Empty Can Files

Right-click to the left of **Load Data** button to show the popup menu and this option. Use this option to allow or disallow two sets of empty can files. If two sets are allowed, the empty can subtraction is as follows:

$$I = I_{sample} - ssfactor*(factor_1*I_{emptycan1} + factor_2*I_{emptycan2}),$$

where ssfactor is the self-shielding factor, and $factor_1$ and $factor_2$ are extra factors that can be changed in **Parameter**->**Change 2-Set Empty Can Factors**. The handling of the additional set of empty can files is the same as that of the first set.

Close All Plot Windows

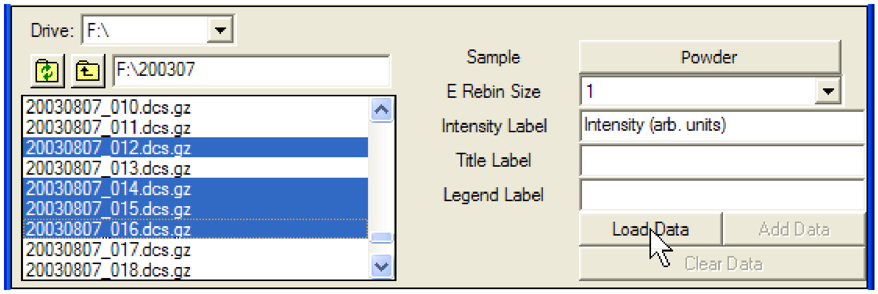
To close all plot windows, simply press **Window**->**Close All Plot Windows** button.

Load Data

To load data files, use the top left file locator to select one or more files. Press **Load Data** button to load the data. An error will be given if no file is highlighted. For DCS data, the data will be normalized by the monitor counts of beam monitor 1 if shutter is open.

For *powder* and *single crystal* sample type, the files will be combined. For *diffuse scattering* sample type, files are not combined, and energy range needs to be specified beforehand. For file types other than DCS, weights are required for proper data summation.

The loaded data will not be modified by the program until new data file is loaded or added, or the sample type is changed to or from *diffuse scattering* types. Press **Clear Data** button to remove the data from memory.



Tip 1: For DCS and INX file types, move the cursor over the highlighted files and right click to view the file information such as comment, wavelength, temperature, etc.

Tip 2: Move the cursor to the left of the **Load Data** button and right click to view the current settings of parameters.

Add Data

The **Add Data** button will be activated when data has been loaded.

Select the data files to be added by the upper left file locator. Then press the **Add Data** button. An error will be given if the file selected and the existing data are of different type. The criteria for DCS files are wavelength, master speed, speed ratio, resolution mode, and tsdmin.

For *powder* and *single crystal* data, the data are added to existing data; for *diffuse scattering* sample types, the data are appended to the existing data. The algorithm for computing added intensity(I) and error(Err) with weights(W) taken into account is as follows:

$$I_3 = (I_1 * W_1 + I_2 * W_2)/(W_1 + W_2),$$
$$Err_3 = \sqrt{(Err_1 * W_1)^2 + (Err_2 * W_2)^2} \Big/ (W_1 + W_2),$$
$$W_3 = W_1 + W_2.$$

Clear Data

Press **Clear Data** to clear from memory the loaded data and calculated projection data if existed. This operation is useful in planning experiments.

Sample Type

There are four sample types (more accurately modes of operation): *powder*, *single crystal*, *diffuse scattering singe E*, and *diffuse scattering multiple E*.

For **powder** mode, two viewing axes need to be specified. In the projection calculation, detectors with the same two-theta angle are combined. The data is plotted as 2D intensity color map on the plane defined by the viewing axes. The data can also be cut along one of the two viewing axes with restrictions on the other axis, and plotted as 1d plot.

For **single crystal** and **diffuse scattering** modes, lattice parameters, crystal orientation, and viewing axes need to be given to enable proper projection calculation. By default two viewing axes are available. To enable a third viewing axis, check **Option**->**Allow Extra Viewing Axis**. Except for **diffuse scattering single E** mode, the energy is also present as one axis. The data is plotted as 2D intensity color map on the plane defined by two of the axes (including the viewing axes and the energy if available). The other axes are used to restrict the slice range. The data can also be cut along one of the viewing axes with restrictions on the other axes, and plotted as a 1d plot.

The difference between diffuse scattering single E mode and multiple E mode is the treatment of the energy dimension. In single E mode, data within the specified energy range are combined to a single energy to save computer memory, while in multiple E mode, the data are not combined, which could sometimes lead to memory problem. If error occurs due to lack of computer memory, the solution is to reduce the specified energy range, increase the E-rebin size, or switch to single E mode.

When the sample type is changed, the projection data is cleared and need to be recalculated before any plots can be made. The raw data is still stored in the memory if the change is between *powder* and *single crystal* type.

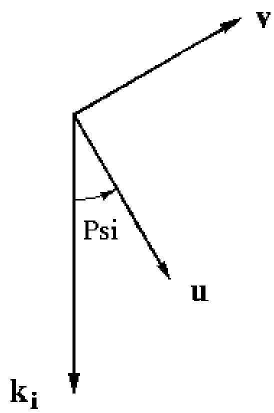
Lattice Parameters

For *single crystal* and *diffuse scattering* sample types, the direct lattice parameters of the unit cell are specified by **a**, **b**, **c**, α, β, and γ. α is the angle between **b** and **c**, β is the angle between **c** and **a**, and γ is the angle between **a** and **b**. An error will be given during projection calculation if any one of the six lattice parameters is missing.

Crystal Orientation

For *single crystal* and *diffuse scattering* sample types, the crystal orientation with respect to the spectrometer is defined by two reciprocal crystal axes (**u** & **v**) in the principal scattering plane of the spectrometer and one angle (Psi), which uniquely identifies the rotation of the crystal in this plane.

(**ux**, **uy**, **uz**) and (**vx**, **vy**, **vz**) specifies the two *reciprocal* crystal axes. u x v should point to the vertically *upward* direction.



Psi is the angle between u and ki, and is positive if ki x u is pointing to the vertically upward direction. For DCS file type, it should be the same as DCS A2 angle if A2=0 when ki//u. For *diffuse scattering*, Psi is the angle for the first file.

An error will be given in projection calculation if any value of u, v, or Psi is not set.

Viewing Axes

Powder

The viewing axes for *powder* are two axes out of (Energy, |Q|, 2Theta, and Det Group Number). They can be specified from the droplists. The labels of the viewing axes are used as corresponding axes titles in the 2d plots. The Most commonly used set of viewing axes for powder sample is u1=|Q| and u2=Energy.

Single Crystal and Diffuse Scattering

The viewing axes for *single crystal* and *diffuse scattering* are wave vector directions. They must be orthogonal if the orthogonal option is chosen for the viewing axis type. An example is :

u1 = [1 0 0] ;a*
u2 = [0 1 0] ;b*

An error will be given in projection calculation if any value of the viewing axes is not given or the axes are not orthogonal when required.

The viewing axes can be folded around a folding center. The default folding direction is to the side with larger range. To always fold to the plus side, set **Option**->**Fold to the Plus Side** on. The projection needs to be recalculated if any of the folding selections is changed.

Energy Rebin

To reduce the amount of data being processed and plotted, the raw data can be rebinned in the projection calculation for *powder*, *single crystal,* and *diffuse scattering multiple E* modes. Time channels are binned according to the size specified in the **E Rebin Size** textbox. No action is taken if the E rebin size is less than one or absent. The rebinning can be either average or sum according to the specified binning method. In *powder* and *single crystal* modes, the raw data is not affected by the rebinning, therefore changing the rebin size requires only the projection to be recalculated. In *diffuse scattering multiple E* mode, the raw data are rebinned, therefore changing the rebin size requires reloading the data.

Calculate Projection

Press **Calculate Projections** button to project the raw data into viewing axes. Detector masks and detector efficiency factors are applied if they are present. The background will also be subtracted if they have been previously loaded. Intensity data are also rebinned if E rebin size is greater than 1 for *powder* and *single crystal* modes. The intensity will be calculated as one of several options chosen in **Option**->**View Intensity As** menu. Energy dependent detector efficiency will be calculated if the option is set. Absorption correction factors will be calculated and multiplied to the intensity if so chosen. User function will also be executed if specified. The projected data and the raw data are stored differently, i.e., the raw data are not changed by this calculation. If no data has been loaded, the program will prompt for incident neutron energy Ei to calculate detector trajectories.

For *powder* mode, detectors with the same 2theta angle will be combined.

For *diffuse scattering* modes, data with the same sample rotation angles will be combined.

For *single crystal* and *diffuse scattering* modes, an error message will be given if any value of the lattice parameter, crystal orientation, and viewing axes is not given, or if the viewing axes are not orthogonal when required.

Intensity Label

The intensity label is used as the axis title for intensity in plots. If not given, the default is *Intensity*. IDL formatting codes are supported.

Title Label

The title label is used as title in plots. IDL formatting codes are supported. It is set to the comment of a data file after the file is loaded. The plot title can be easily modified in the plot window.

Legend Label

The legend label is used as the legend in plotting 1D cuts. For DCS files, it is set to the last word of the comment of the data file after it is loaded. The plot legend can be easily modified in the plot window.

2D Slice Plot

The intensity data projected into two viewing axes can be plotted as color contour plot by pressing the **Plot Slice** button.

In *Single Crystal* and *Diffuse Scattering* modes, the axis perpendicular to the slice plane is chosen from the **perp to** droplist, which includes the viewing axes and the energy(except *Diffuse Scattering Single E* mode). The choice of the perpendicular axis automatically defines the next two axes as the slice plane axes, and the horizontal and vertical label will change accordingly. The axes left will be used to further define the thickness of the slice.

Data can be rebinned by specifying the horizontal and/or vertical **step**. If not specified, the default binning size is 1000 except for energy data. The binning algorithm is as follows: a grid of bins of size xstep x ystep is constructed with the lower left corner at (xmin-xstep/2, ymin-ystep/2) and not exceeding xmax+xstep/2 along x and ymax+ystep/2 along y. The x and y values for each bin are calculated by taking the average of the x and y values of all the data in that bin, and the intensity is the average or sum of all the data in that bin according to the specified binning method. The limits are inclusive to the left and exclusive to the right.

The grid can be smoothed by choosing a nonzero **Smoothing level**. The default smoothing kernel is

0.1 0.2 0.1
0.2 0.8 0.2
0.1 0.2 0.1 .

The kernel can be changed in the **Parameter** menu.

The color map of the contour plot can be chosen from the **color map** droplist. The names are the same as the predefined IDL color table names.

Two types of shading are available: *Flat* and *Gouraud*.
Flat: The color has a constant intensity for each face of the surface, based on the normal vector.
Gouraud: The colors are interpolated between vertices, and then along scan lines from each of the edge intensities.

The 2D data can also be plotted as color surface plots by pressing the **Surf Slice** button.

Tip 1: Specify the horizontal and vertical range to reduce the amount of data and speed up the plotting.

Tip 2: If the energy step is not specified, the original energies corresponding to the time channels are used. This will prevent the energy values from being changed by the binning process.

Tip 3: For a large dataset, the binning will usually be much faster with the steps specified.

1D Cut

Cuts can be made along one of the viewing axes with integration over the other one or two viewing axes. Use **along** droplist to select the x axis, and **y** droplist to select the y axis. The plotted data are the average or summed values over the integrated volume according to the specified binning method.

X and y range, integration volume (thickness) can be specified by the **from:** and **to:** textboxes. Data can also be rebinned by specifying the cut **step**. The x-range is divided into bins of length *step* starting at xmin-step/2 and not exceeding xmax+step/2. The x and y value for each bin is calculated by taking the simple average of the x and y values of all data in that bin, where the limits are inclusive to the left and exclusive to the right.

Plot **symbols** can be specified by the color, symbol style, and line style droplists. White color will be switched to black when the figure is printed or saved as a file. Press **Plot Cut** to plot the cut in the current plot window, or press **Oplot Cut** to overplot the cut in the current plot window.

The cut data can also be sent to the Peak Analysis (PAN) program for fitting. To do this, simply press the **Fit** button.

Tip 1: If the cut is along energy and the step is not specified, the original energies corresponding to the time channels are used. This will prevent the energy values from being changed by the binning process.

Tip 2: For a large dataset, the binning will usually be much faster with the step specified.

3D Volume Plot

A volume plot can be made if the number of viewing axes (including the energy) is more than two. Proper steps need to be specified to achieve the ideal result. There are two interpolation methods: nearest neighbor and trilinear. The trilinear method gives a smoother look, but slower in rendering.

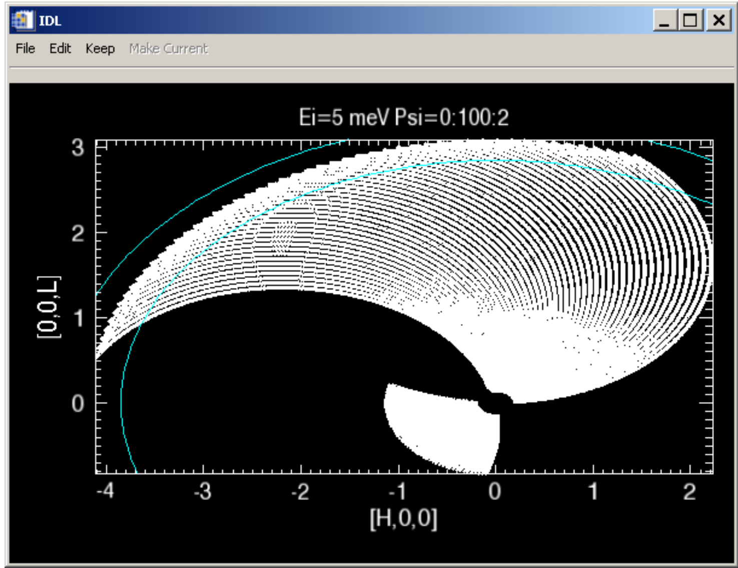
Fitting Data

Both the slice data and cut data can be sent to PAN program for fitting by pressing the **Fit** button.

Plot Trajectories

The **Plot Trajectories** button is insensitive until projection is calculated. The projection can be calculated without loading any data.

Detector trajectory is an x vs. y 1d plot. Both x and y are chosen from droplist. If None is chosen, the detector group number is used. Z can be used to restrict the range of data in extra dimension. If no ranges are set for x, y, and z, the default is to show all possible data. The following is an example in diffuse scattering mode. The color lines denote the aluminum powder line.



Oplot Trajectories

Oplot Trajectories button is used to overplot the trajectory in the current plot window. The button is insensitive until projection is calculated and in certain sample modes. The projection can be calculated without loading any data.