

DCS Mslice User Manual

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Powder Sample

1. Select the data files, and press **Load Data** button.

Drive: G:\

Folder: G:\200307

Files:

- 20030807_010.dcs.gz
- 20030807_011.dcs.gz
- 20030807_012.dcs.gz
- 20030807_013.dcs.gz
- 20030807_014.dcs.gz
- 20030807_015.dcs.gz
- 20030807_016.dcs.gz
- 20030807_017.dcs.gz
- 20030807_018.dcs.gz

Sample: Powder

E Rebin Size: 1

Intensity Label: Intensity (arb. units)

Title Label:

Legend Label:

Buttons: Load Data, Add Data, Clear DCS Data

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

Viewing Axes:

		Label
u1	Q	Q
u2	Energy	E

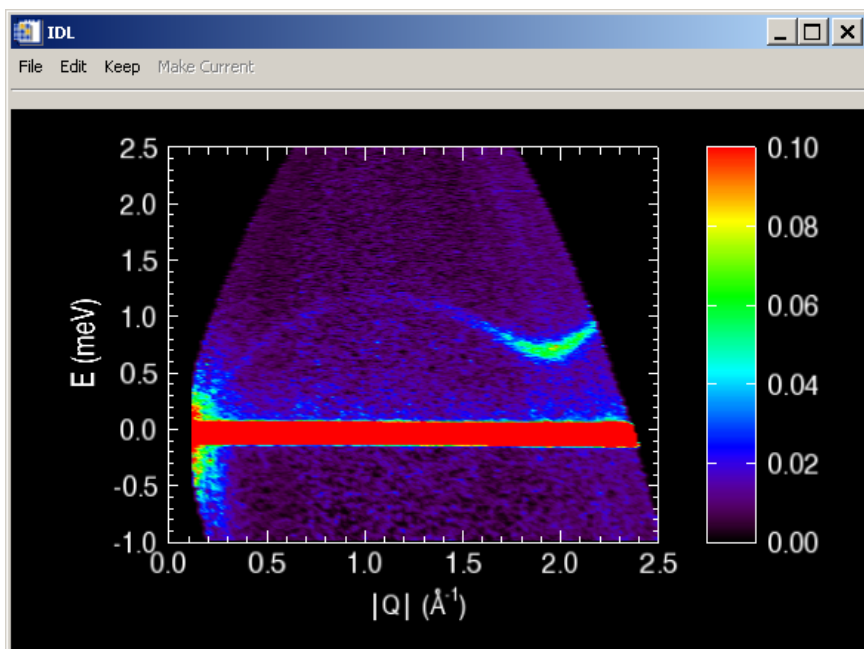
Buttons: Calculate Projections

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.

Display:

horizontal range Q	0	to:	2.5	step	0.015
vertical range E	-1	to:	2.5	step	
intensity range	0	to:	0.2	color map	RAINBOW
smoothing level	1	shading	Gourau	Buttons:	Plot Slice, Surf Slice

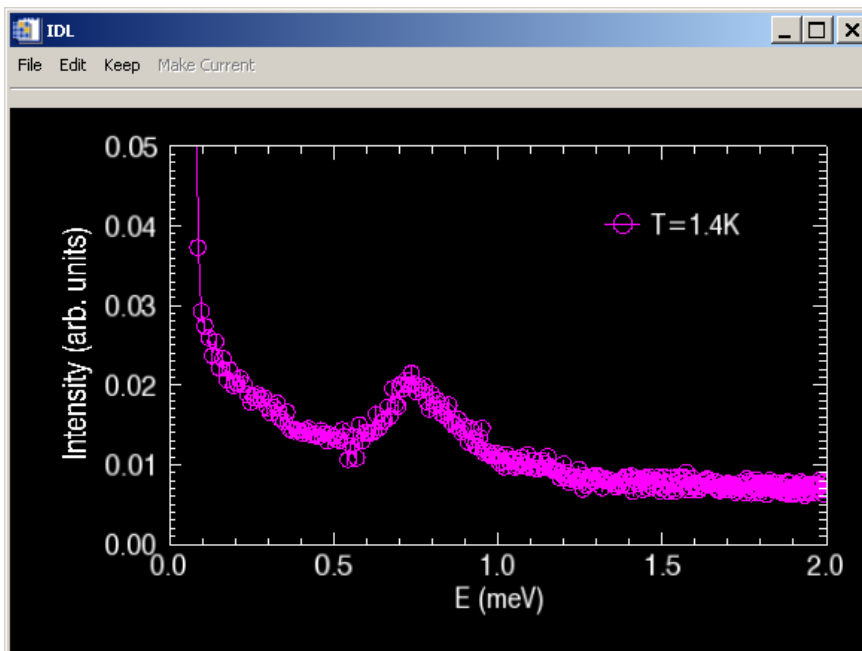
The plot will look like the following, which is a superfluid LHe4 roton spectrum.



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

Cut:
along **E** from: 0 to: 2 step
thickness range |Q| 0 to: 2.5 symbol **magent**
y **Intensity** range 0 to: 0.05 circle solid
Plot Cut Oplot Cut
save as none Browse Fit

The plot will look like the following.

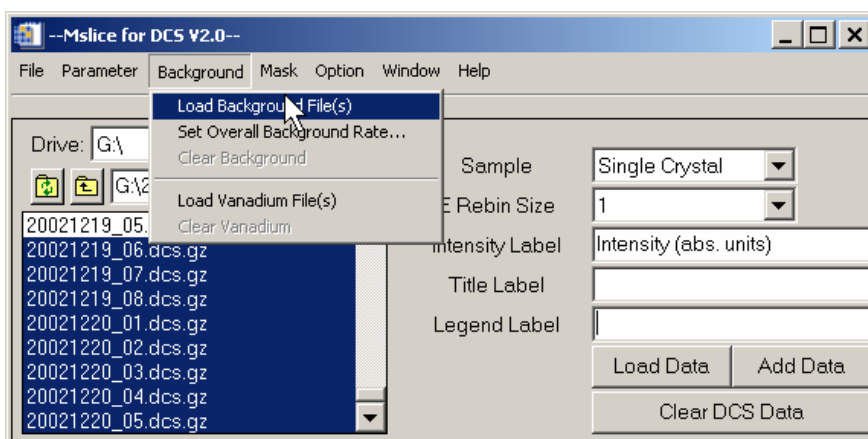


Single Crystal Sample

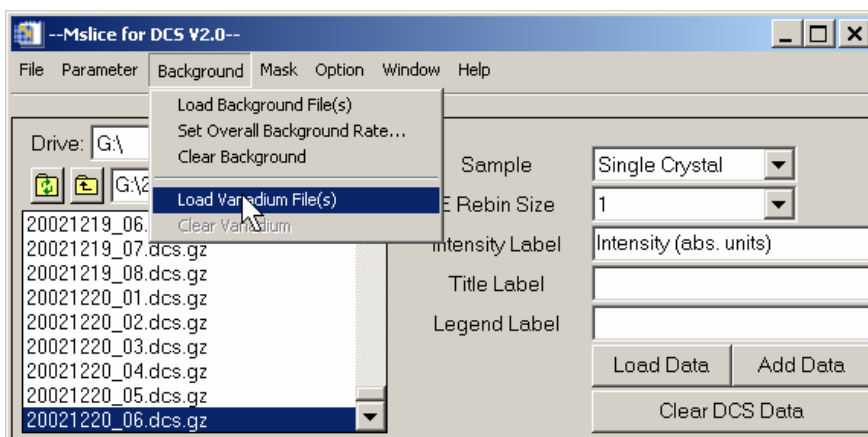
1. Select the data files, and press **Load Data** button.

Drive: G:\
G:\200211
20021218_06.dcs.gz
20021218_07.dcs.gz
20021218_08.dcs.gz
20021219_01.dcs.gz
20021219_02.dcs.gz
20021219_03.dcs.gz
20021219_04.dcs.gz
20021219_05.dcs.gz
20021219_06.dcs.gz
Sample: Single Crystal
E Rebin Size: 1
Intensity Label: Intensity (abs. units)
Title Label:
Legend Label:
Load Data Add Data
Clear DCS Data

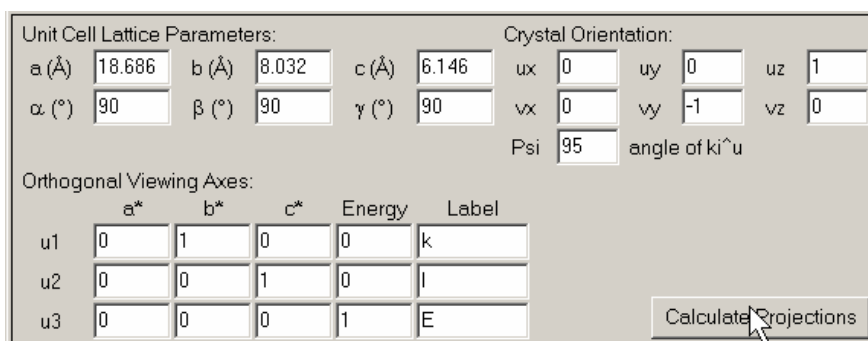
2. Select the background (empty can) files, then in **Background** menu, press **Load Background File(s)**.



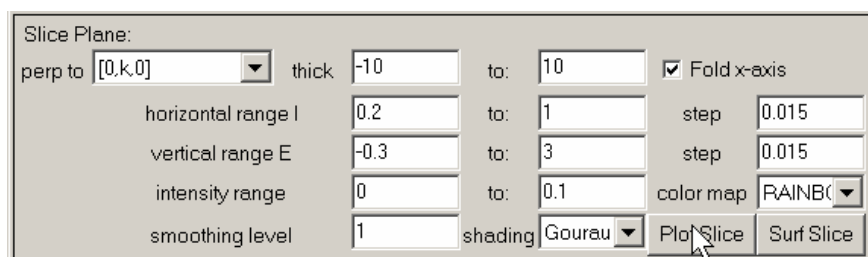
3. Choose the Vanadium file, and in **Background** menu, press **Load Vanadium File(s)**.



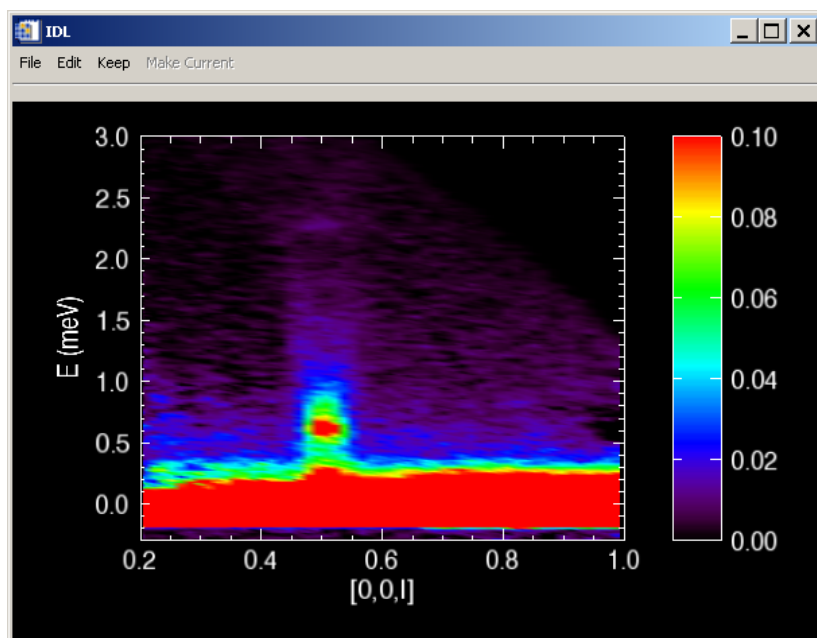
4. Enter the lattice parameters, crystal orientation, and the viewing axes, then press **Calculate Projection** button. Psi is the angle from k_i to u , with counterclockwise being the positive direction.



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.

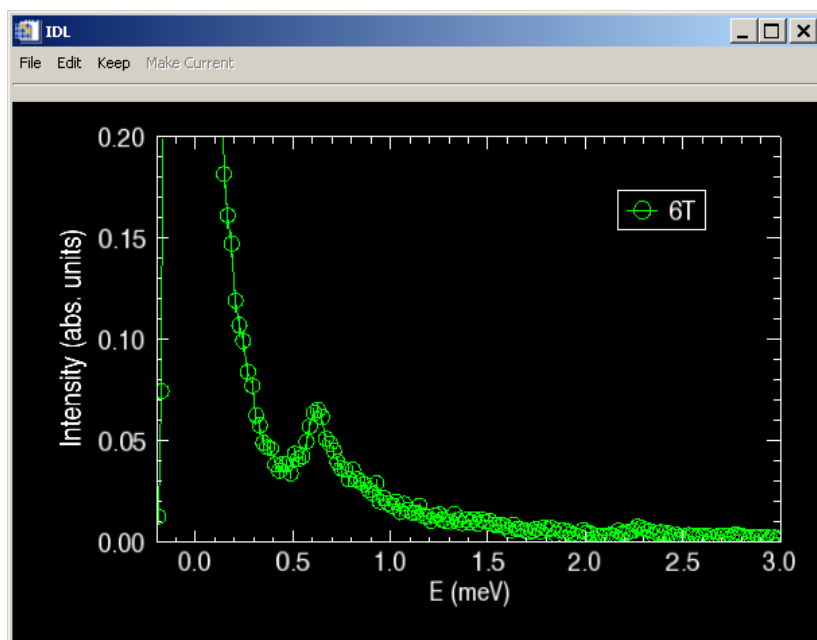


6. Choose the cutting axis and thickness over the other two axes, and press **Plot Cut** to plot the cut.

Cut:
 along from: to: step
 thickness range k to:
 thickness range l to:
 y range to:
 symbol

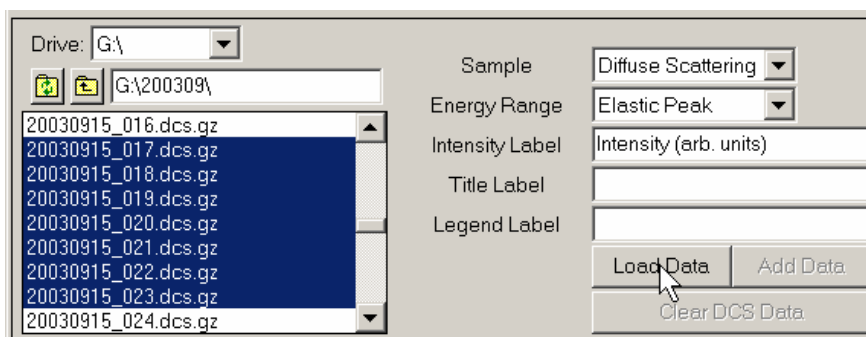
 save as

The plot will look like the following.

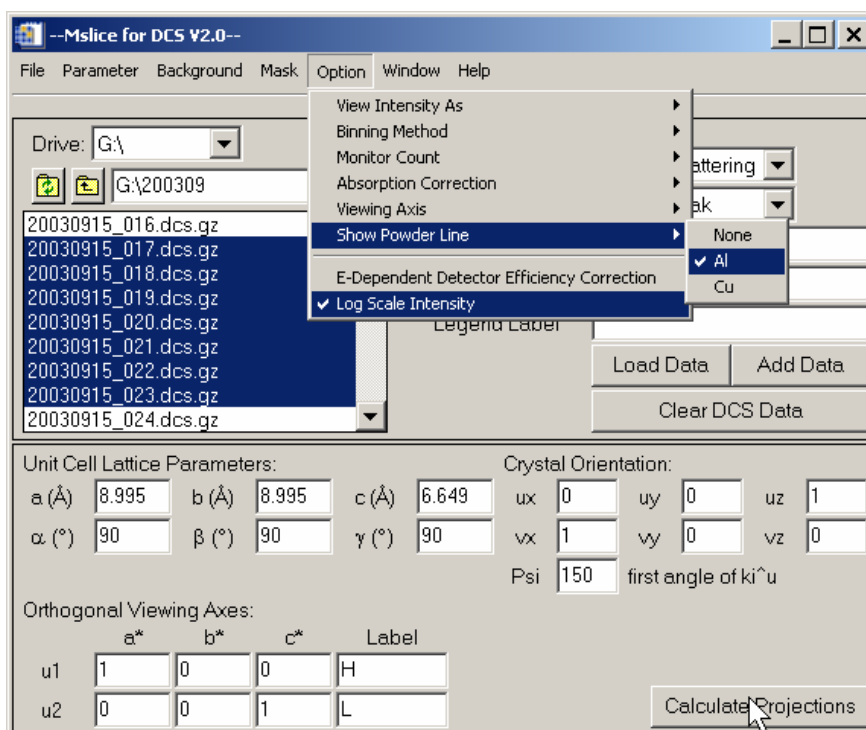


Single Crystal Diffuse Scattering

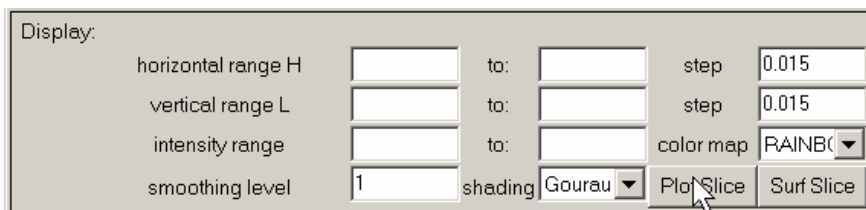
1. Select the data files, and press **Load Data** button.



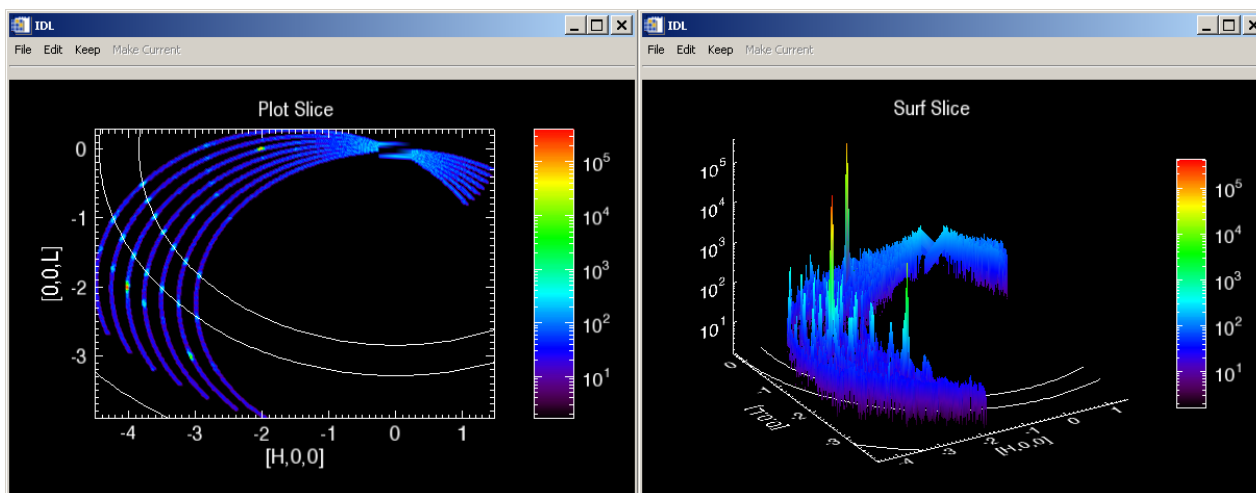
2. In the option menu, select the average binning method, show Al powder line, and log scale intensity. Enter the lattice parameters, crystal orientation, and the viewing axes, then press **Calculate Projection** button. Psi is the angle from k_i to u of the first file, with counterclockwise being the 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.



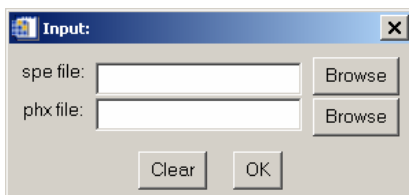
The plots will look like the following.



The white lines denote the positions of the Al powder line.

Load SPE File

To read a SPE file, use the **Load SPE File** button in the **File** menu. The following dialog window will appear. PHX file refers to the detector configuration file that is associated with the SPE file.



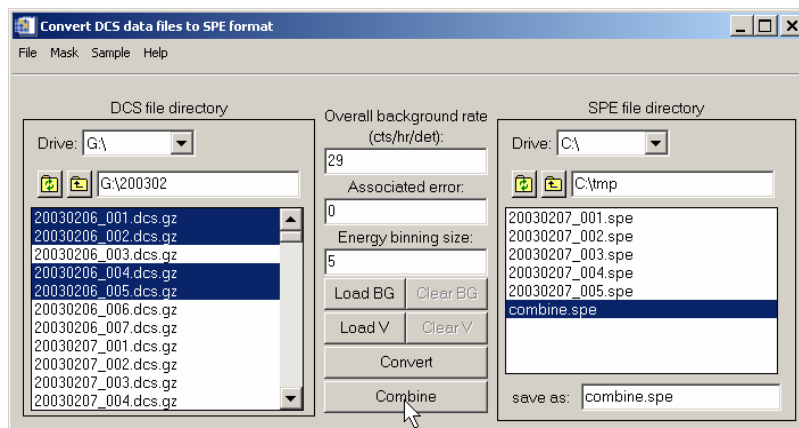
User will be asked to enter the incident neutron energy during the projection calculation.

Load DAVE File

To read a DAVE format file, use the **Load DAVE File** button in the **File** menu. The DAVE file should contain all necessary information, preferably a DAVE file reduced from the DCS files.

Convert DCS Files to SPE Format

Convert DCS Files To SPE Format button in the **File** menu starts a stand-alone application to convert DCS files into SPE format which can be processed by MATLAB [Mslice](#) program.



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. 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. 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 **Sample** menu. With the choice of powder sample, detectors with the same two theta angle will be combined.

Detector configuration file (*.phx) can be created during file conversion by choosing the **Yes** option in **Sample->Create Detector File**.

To exit the program, either go to **File->Exit** or simply close the window.

Recent Files

File->Recent Files menu stores the latest file loading history. Only files loaded by pressing **Load Data** button will be stored. The first file comment is used as the entry name. Up to five entries will be shown.

Exit

To exit the program, press the **File->Exit** button or simply close the window.

Load Parameters

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 DCS data and projection are not loaded.

Save 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.

Change Self-Shielding Factor

The self-shielding factor is used in [background subtraction](#) according to the following equation:

$$I = I_1 - \text{ssfactor} * I_2 ,$$
$$\text{Err} = \sqrt{\text{Err}_1^2 + (\text{ssfactor} * \text{Err}_2)^2} .$$

Change Overall Intensity Factor

The overall intensity factor is multiplied to the intensity during [projection calculation](#). This factor is reset to 1 every time a data file is loaded.

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.

Set Data Directory

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

Set Working Directory

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 Background File(s)

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

$$I = I_1 - \text{ssfactor} * I_2 ,$$
$$\text{Err} = \sqrt{\text{Err}_1^2 + (\text{ssfactor} * \text{Err}_2)^2} ,$$

where ssfactor is the average self-shielding factor.

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 handling in this process. Use **Background**->**Clear Background** to clear it from the memory.

Clear Background

Background->Clear Background button is used to clear the background file 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. 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.

Mask Upper and Lower Banks

To view the data from only the central bank detectors, press the **Mask Upper and Lower Banks** in the **Mask** menu. 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 Central and Lower Banks

To view the data from only the upper bank detectors, press the **Mask Central and Lower Banks** in the **Mask** menu. 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 Upper and Central Banks

To view the data from only the lower bank detectors, press the **Mask Upper and Central Banks** in the **Mask** menu. 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** 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.

Intensity Type

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

S(Q,omega) ----- a factor of $(ki/kf)^4$ is applied to the normalized intensity,

Symmetrized S(Q,omega) ----- a factor of $\exp(-E/2k_B T) * (ki/kf)^4$ is applied to the normalized intensity,

$d^2(\sigma)/d(\Omega)d(E_f)$ ----- a factor of $(k_i/k_f)^3$ is applied to the normalized intensity.

Binning Method

Two binning methods, **average** and **sum**, can be chosen from the **Option->Binning Method** menu button. The binning method is applied in rebinning time channel according to **E Rebin Size** for *powder* and *single crystal* or energy range in loading *diffuse scattering* data, and rebinning data in displaying slices and cuts.

Monitor Count

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.

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 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, either Al or Cu powder line 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 or Cu option in **Option->Show Powder Line** menu. The projection needs to be calculated to have the option in effect.

E-Dependent Detector Efficiency Correction

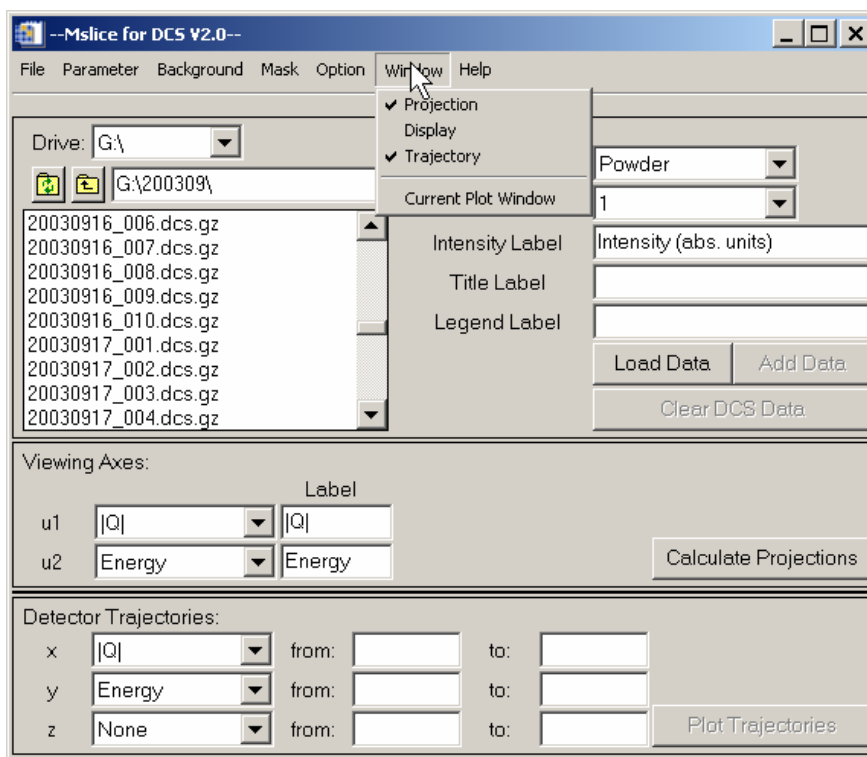
The energy dependent detector efficiency correction to the intensity can be applied to the data in projection calculation. To set this option on and off, press the **Option->E-Dependent Detector Efficiency Correction** button. When the program started, this option is on.

Log Scale Intensity

If **Option->Log Scale Intensity** menu button is set, subsequent plots will use log scale for the intensity. However, the log scale can be set back to linear in the plots.

Hiding Part of the Window

The projection, display, and detector trajectory frame of the window can be hidden by using the options in **Window** menu. This can be quite useful if the size of the window is larger than the screen. The following snapshot is an example.



View Current Plot Window

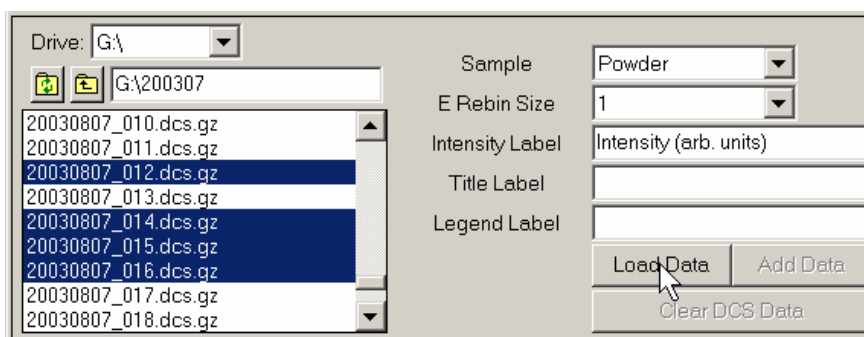
By pressing **Window**->**Current Plot Window** menu button, the current active (not kept) plot window will gain focus.

Load DCS File

To load DCS file(s) ending with .dcs or .dcs.gz, 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. 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.

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*. Press **Clear DCS Data** button to remove the data from memory.



Add Data

The **Add Data** button will be activated when DCS 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 wavelength, master speed, speed ratio, resolution mode, or tsdmin.

For *powder* and *single crystal* data, the data are added to existing data; for *diffuse scattering* sample type, 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:

$$\begin{aligned} I_3 &= (I_1 * W_1 + I_2 * W_2) / (W_1 + W_2) , \\ Err_3 &= \sqrt{[(Err_1 * W_1)^2 + (Err_2 * W_2)^2] / (W_1 + W_2)} , \\ W_3 &= W_1 + W_2 . \end{aligned}$$

Clear DCS Data

Press **Clear DCS Data** to clear from memory the loaded DCS data and calculated projection data if existed.

Sample Type

There are three sample types: *single crystal*, *powder*, and *diffuse scattering*.

For **single crystal** sample, [lattice parameters](#), [crystal orientation](#), and three [viewing axes](#) need to be given to enable proper [projection calculation](#). The data is plotted as 2D intensity color map on the plane defined by two of the viewing axes. The third axis is used to restrict the slice range. The data can also be cut along one of the three viewing axes with restrictions on the other two axes, and plotted as 1d plot.

For **powder** sample, 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 **diffuse scattering** sample type, [lattice parameters](#), [crystal orientation](#), and two [viewing axes](#) need to be given to enable proper [projection calculation](#). 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 viewing axes with restrictions on the other axis, and plotted as 1D plot.

When the sample type is changed, the projection data is cleared and need to be recalculated before any

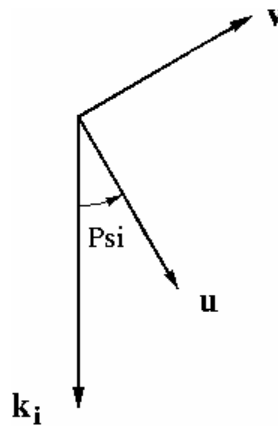
plots can be made. The raw data is still stored in the memory if the change is between *powder* and *single crystal* type.

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 **k_i**, and is positive if **k_i** x **u** is pointing to the vertically upward direction. It should be the same as DCS A2 angle if A2=0 when **k_i**//**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

The viewing axes for *single crystal* are either wave vector directions or energy. They must be orthogonal if the orthogonal option is chosen for the [viewing axis type](#). The energy axis is orthogonal to any wave vector direction. An example is

$$\begin{aligned} \mathbf{u1} &= [1 \ 0 \ 0 \ 0] ; \mathbf{a}^* \\ \mathbf{u2} &= [0 \ 1 \ 0 \ 0] ; \mathbf{b}^* \\ \mathbf{u3} &= [0 \ 0 \ 0 \ 1] ; E \end{aligned}$$

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.

Diffuse Scattering

The viewing axes for *diffuse scattering* are wave vector directions. They must be orthogonal if the orthogonal option is chosen for the [viewing axis type](#). An example is

$$u1 = [1 \ 0 \ 0] \quad ;a^*$$

$$u2 = [0 \ 1 \ 0] \quad ;b^*$$

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.

Energy Rebin

To reduce the amount of data being processed and plotted, the raw data can be rebinned in the [projection calculation](#) for *single crystal* and *powder* sample types. 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](#).

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. The intensity will be calculated as one of three 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. The projected data and the raw data are stored differently, i.e., the raw data are not changed by this calculation. If no DCS data has been loaded, the program will prompt for incident neutron energy E_i to calculate detector trajectories.

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

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

For *single crystal* and *diffuse scattering*, 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 DCS 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. It is set to the last word of the comment of a DCS data file after the file is loaded. The plot legend can be easily modified in the plot window.

Intensity Color Contour Plot and Slice

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

For single crystal data, the axis perpendicular to the slice plane is chosen from the **perp to** droplist which contains the three viewing axes. The choice of the perpendicular axis automatically defines the slice plane axes as the remaining two viewing axes, and the horizontal and vertical label will change accordingly.

To fold the symmetrical data, choose the **Fold x-axis** option. The data can be folded into either positive or negative range depending on the sign of the horizontal range.

Data can be rebinned by specifying the horizontal and/or vertical **step**. If not specified, the default binning size is 200 except for energy data. The binning algorithm is as follows: a grid of bins of size $xstep$ \times $ystep$ 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 energies from being changed by the binning process.

Cut

Cuts can be made along one of the viewing axes with integration over the other two directions for *single crystal* or the other one direction for *powder*. 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. If **save as** type is other than *none*, the cut data will be saved as a .xye(x, y, yerr) file whose name can be either entered in a the filename textbox or chosen by pressing **Browse** button.

The cut data can also be sent to the Peak Analysis (PAN) program for fitting. To do this, simply press the **Fit** button. The cut data will be saved in this operation if the saving file name is specified.

Tip: 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 energies from being changed by the binning process.

Plot Trajectories

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

