TAS SCAN MAPPER

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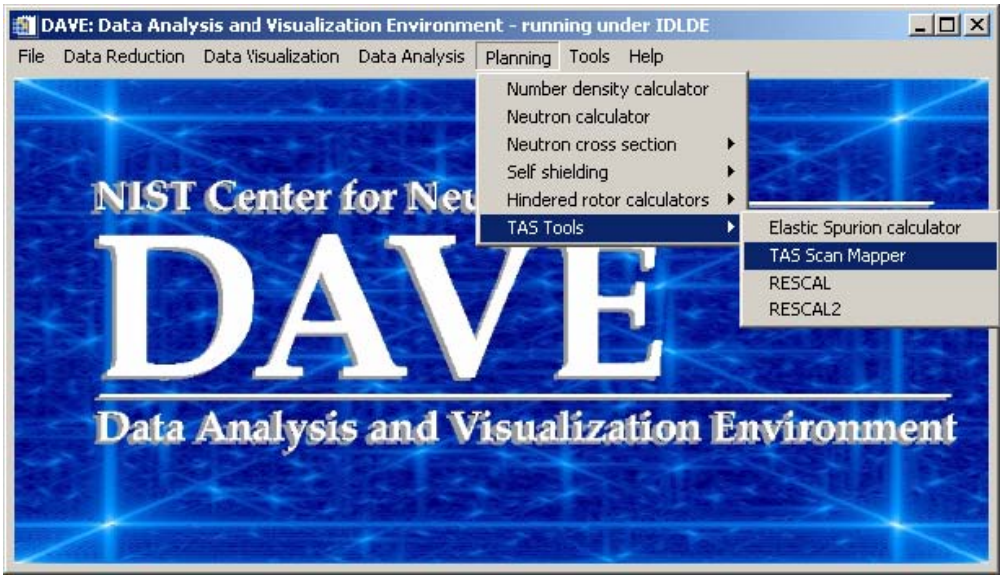
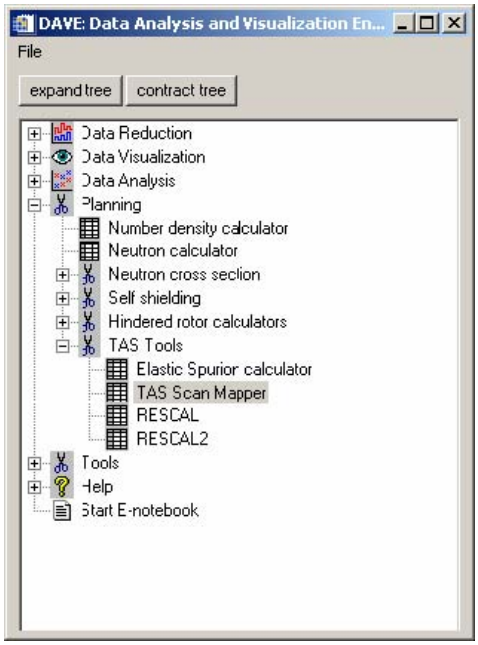
QUICKSTART GUIDE

1. Startup

TAS Scan Mapper displays the position in reciprocal space of the points in your scan and the location of possible spurious features in your triple axis scan. To begin open DAVE and select Planning->TAS Tools->TAS Scan Mapper



or

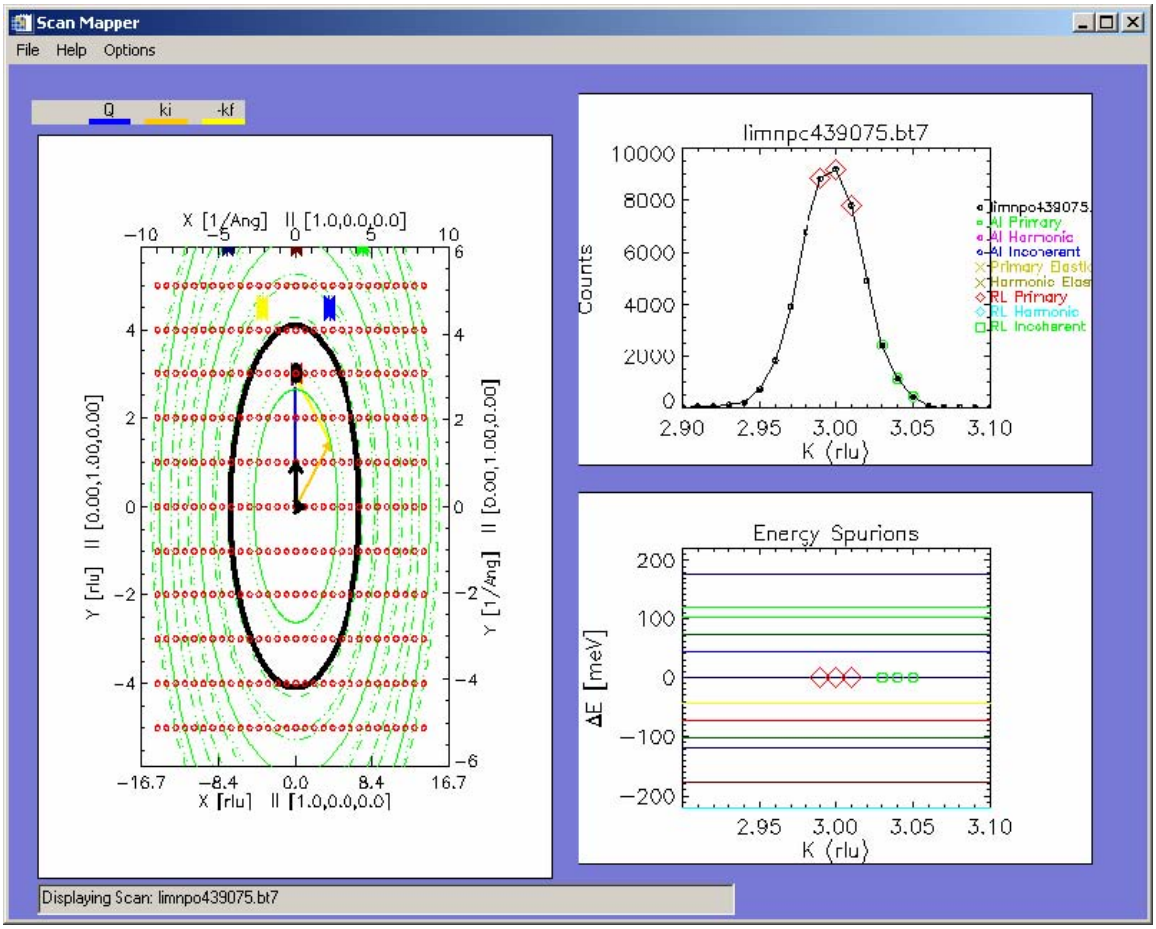


2. TAS Scan Mapper Interface

Two windows will appear, TAS Scan Mapper and TAS Scan Mapper Controls.

a. Main Window

The Scan Mapper window contains 3 plots. There is a plot of features in the scattering plane (Scattering Plane, left side), a plot of the current scan (Scan Plot, upper right), and a plot of the energy transfer measured (Energy Plot, lower right). The scattering plane and the energy plot both label the scan points and all of the harmonics. The color coding is consistent between the two plots. The different harmonics can be selected for display by using the color-coded checkbox controls under the "Display Choices" tab (see below.)

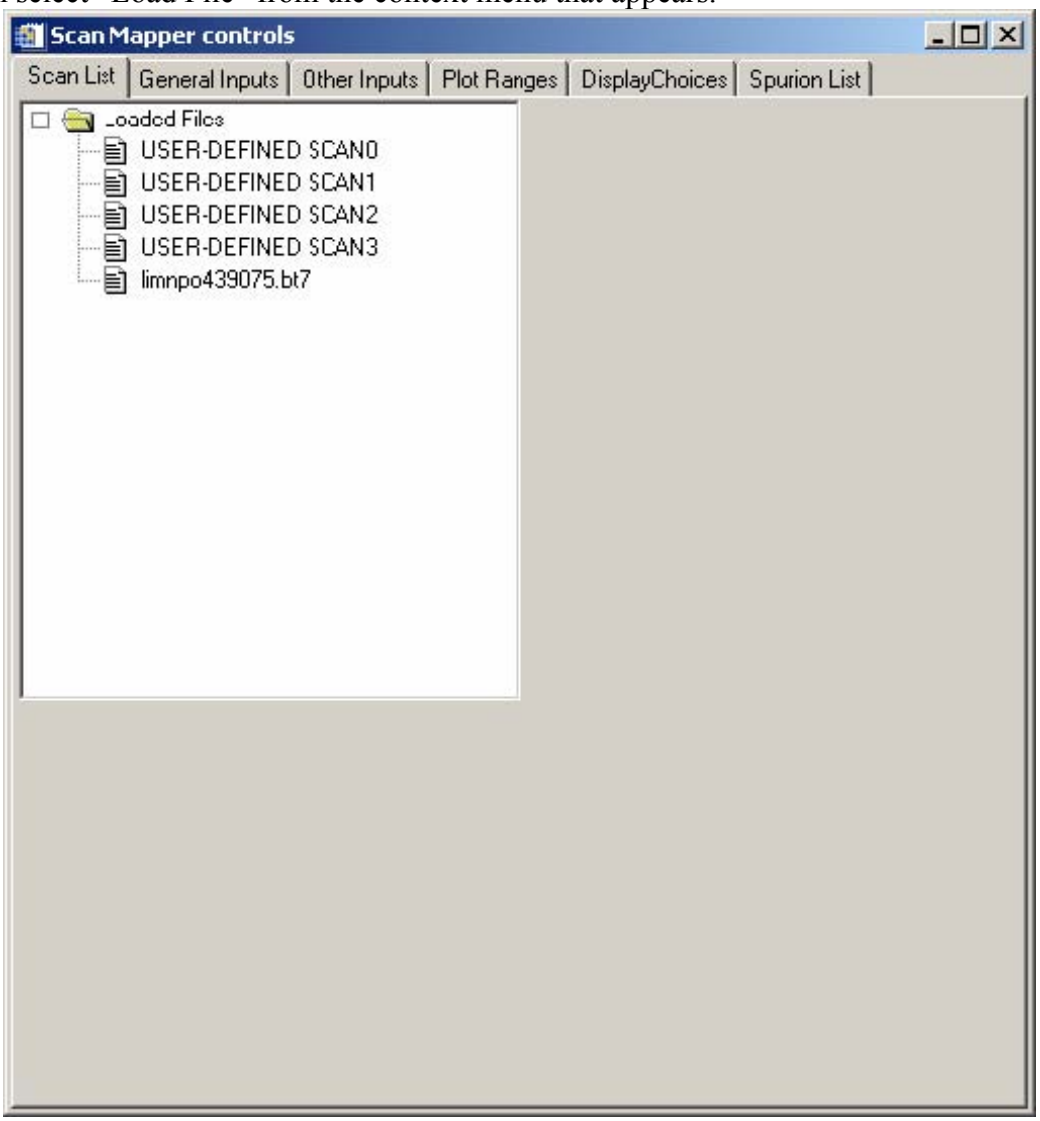


b. TAS Scan Mapper Controls

The controls for the application are on a floating control window. If you delete the controls, you can restore them under the "Options" menu at the top of the main window. The controls consist of six tabs: Scan List, General Inputs, Other Inputs, Plot Ranges, Display Choices, and Spurion List.

i. Scan List

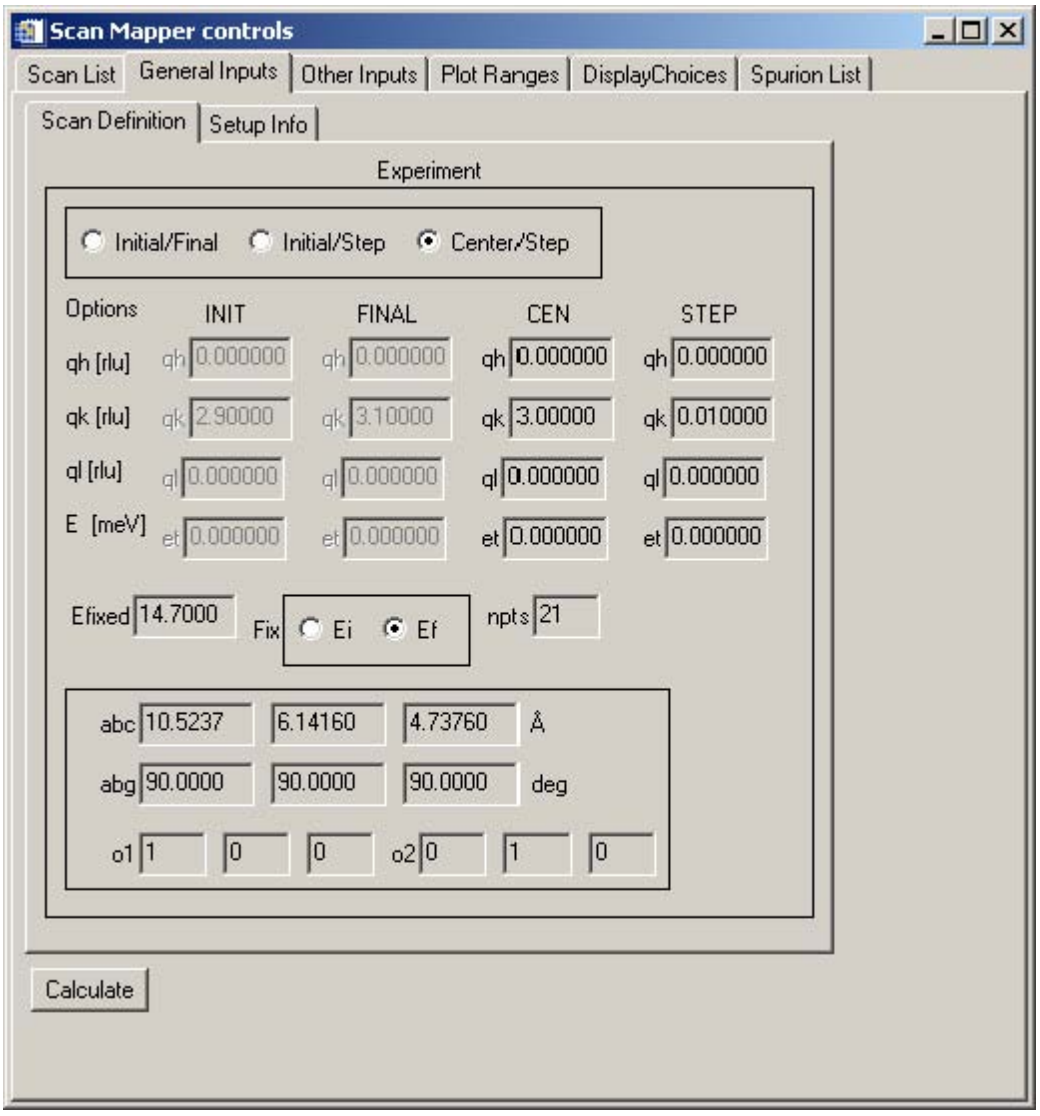
All of the scans entered by the user (via the "General Inputs", see below) or read in from file (via File->Open) will appear in the Scan list in the Scan Mapper controls. Any of the scans in the list can be re-displayed by clicking on its item in the scan tree. The session can be saved by going to File->Save. This will save your work in a .spu file. Saved sessions can be recovered by selecting File->Restore Session. Note that this will restore the previous file and remove your current scans, so be sure to save your scans before restoring old work. If you want to open a new file, you can right-click on an empty space inside the tree displaying loaded scans and then select "Load File" from the context menu that appears.

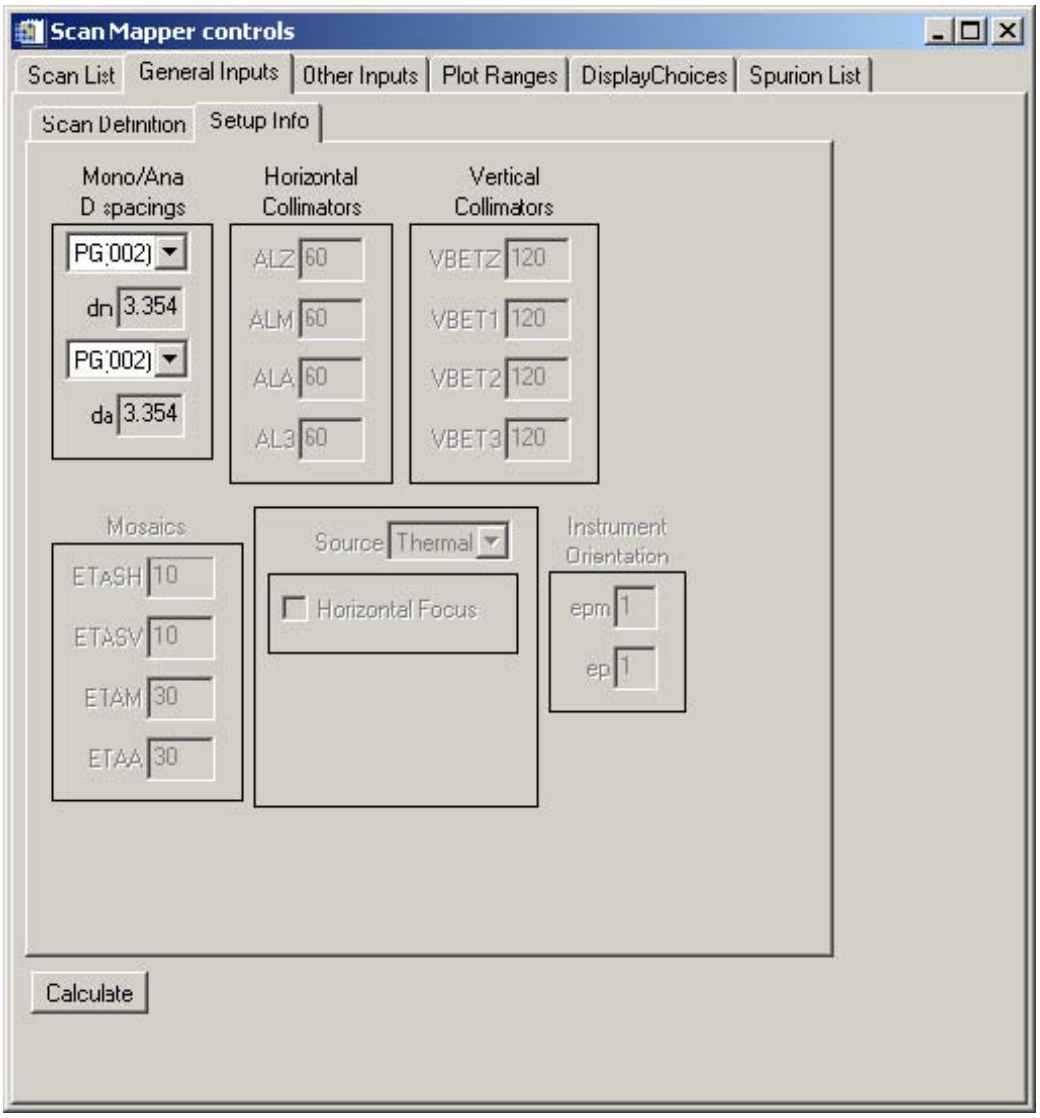


ii. General Inputs

The General Inputs tab contains two sub-tabs. The "Scan Definition" tab is currently implemented. The "Setup Info" tab is implemented but its inputs are not currently used. The

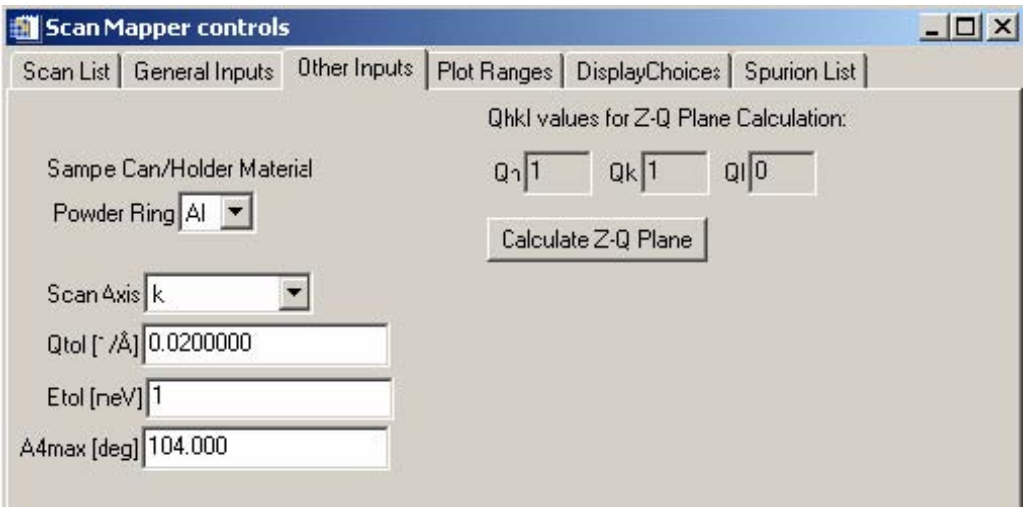
Setup Info tab inputs information for the resolution function, which will be implemented at a later time.





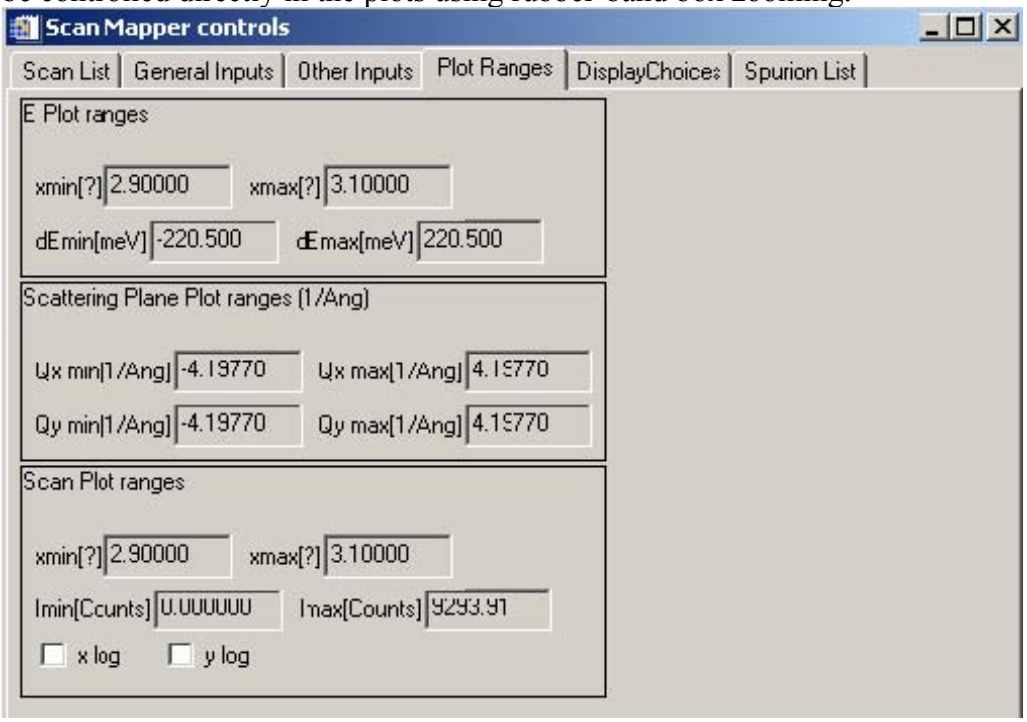
iii. Other Inputs

The "Other Inputs" tab contains some important input values. Notably, the sample holder/can material, the axis to use for the scan and energy plots, the tolerances in Q and energy for determining whether points in the scan are likely to give rise to spurious data, and the maximum 2-theta angle available for the spectrometer.



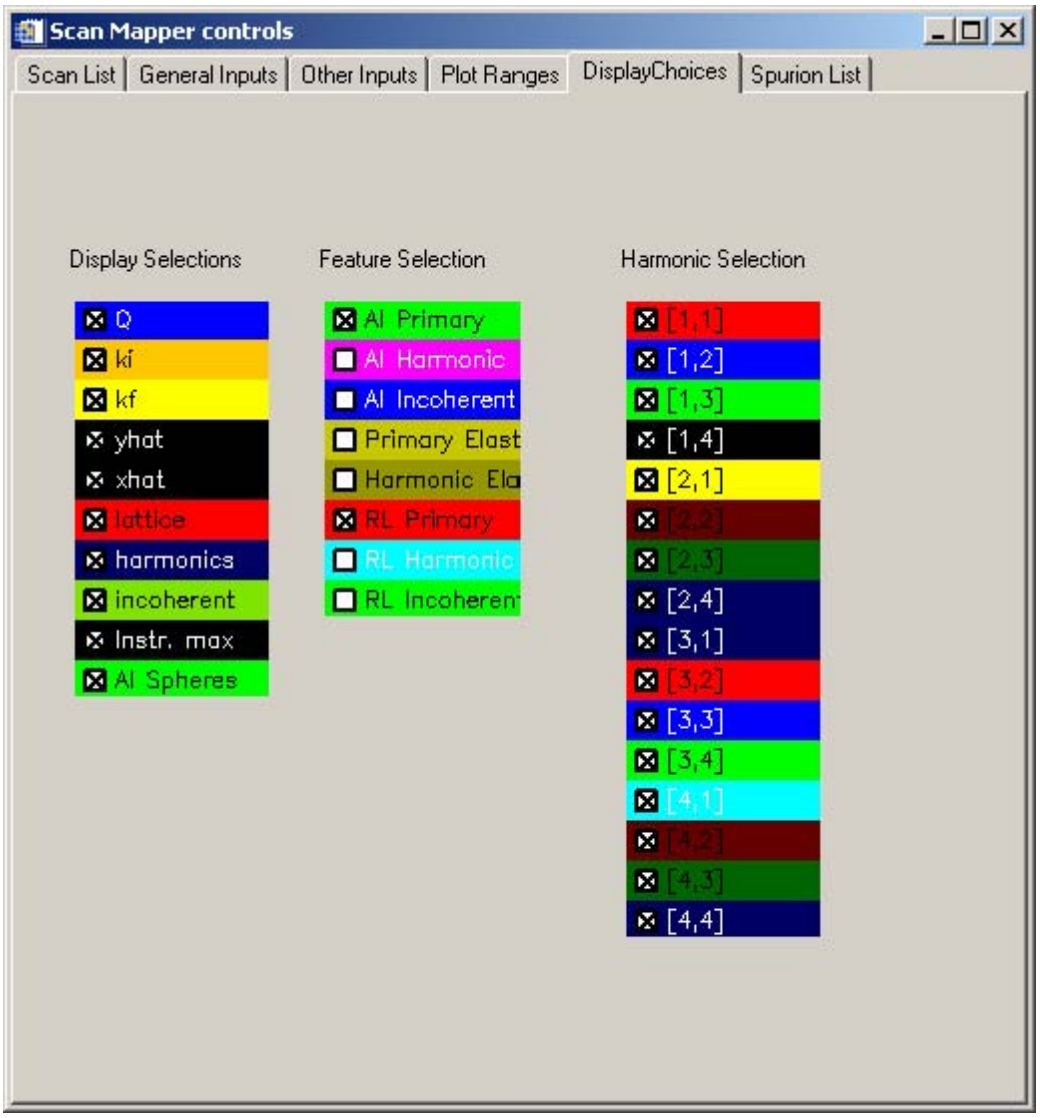
iv. Plot Ranges

The "Plot Ranges" tab gives the user control over the ranges in the three plots. The plot ranges also can be controlled directly in the plots using rubber-band box zooming.



v. Display Choices

The "Display Choices" tab provides checkboxes so that the user can decide which features to display in the plots. The first set chooses items displayed in the Scattering Plane plot, such as Q vector display, incoherent, scan trajectory, sample can/holder spheres, etc. The second set of checkboxes determines which types of spurions to display in the Scan and Energy plots. The final set of checkboxes determines which harmonics to include in the scattering plane and energy plots. These harmonics are specified as [n,m] pairs.



vi. Spurion List

The final tab in the controls panel lists the set of spurious features along with their sources. You can display all of the possible spurious features at once, but that listing may be too long for the window. Instead you can uncheck the box, "Select All Points", and then the slider can be used to choose the point number for display. This will update the spurion listing, the scan plot and the energy plot. In those plots only the possible spurions for the currently selected point will be highlighted.

For each potential spurion, the listing tells:

1) The harmonic or incoherent component of the beam that is the source of the spurion, e.g. {2*ki,3*kf} or QmonoIncoherent.

2) The actual feature in reciprocal space that this harmonic explores,

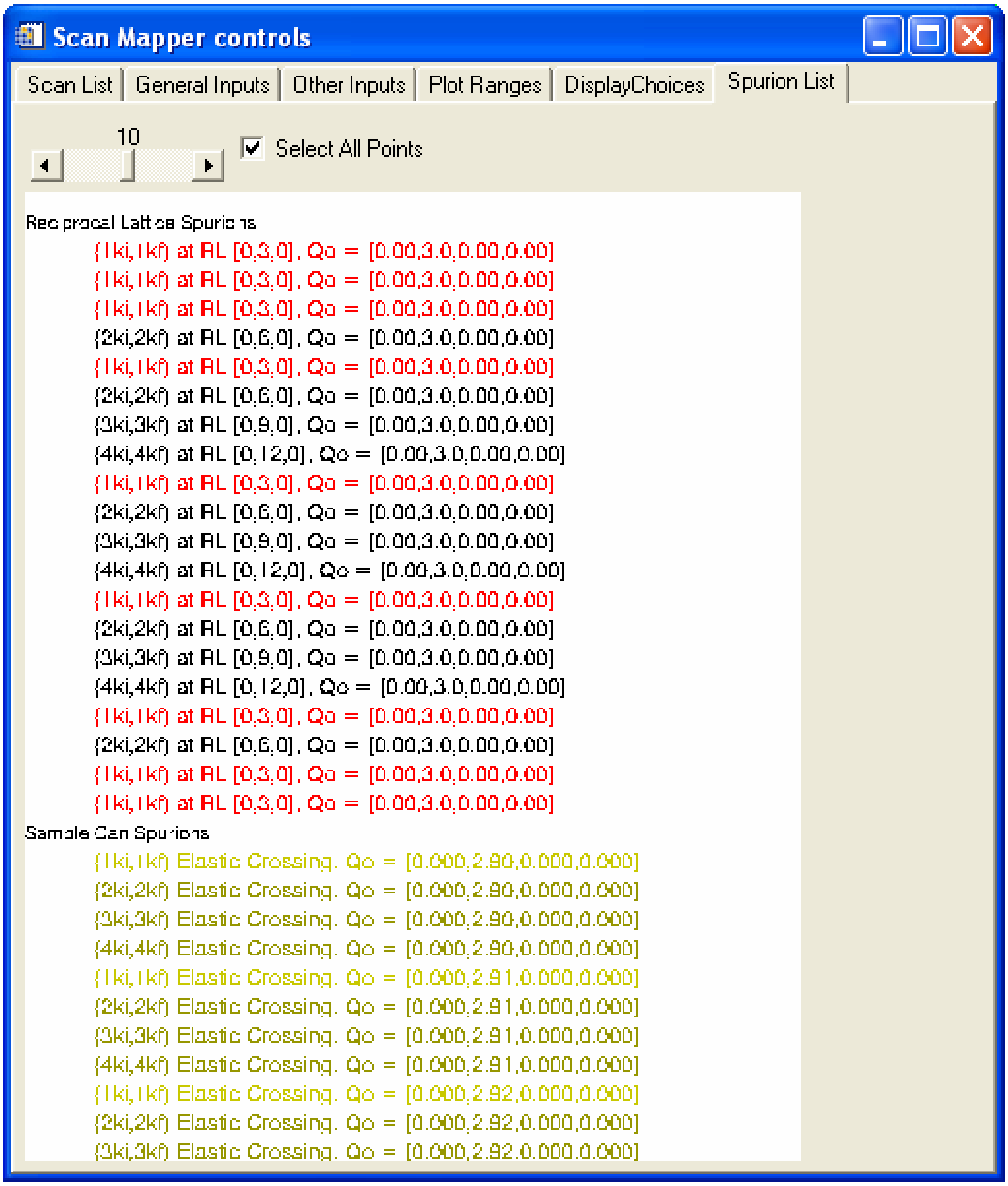
   a. RL[0,3,0] is the reciprocal lattice point [0,3,0]

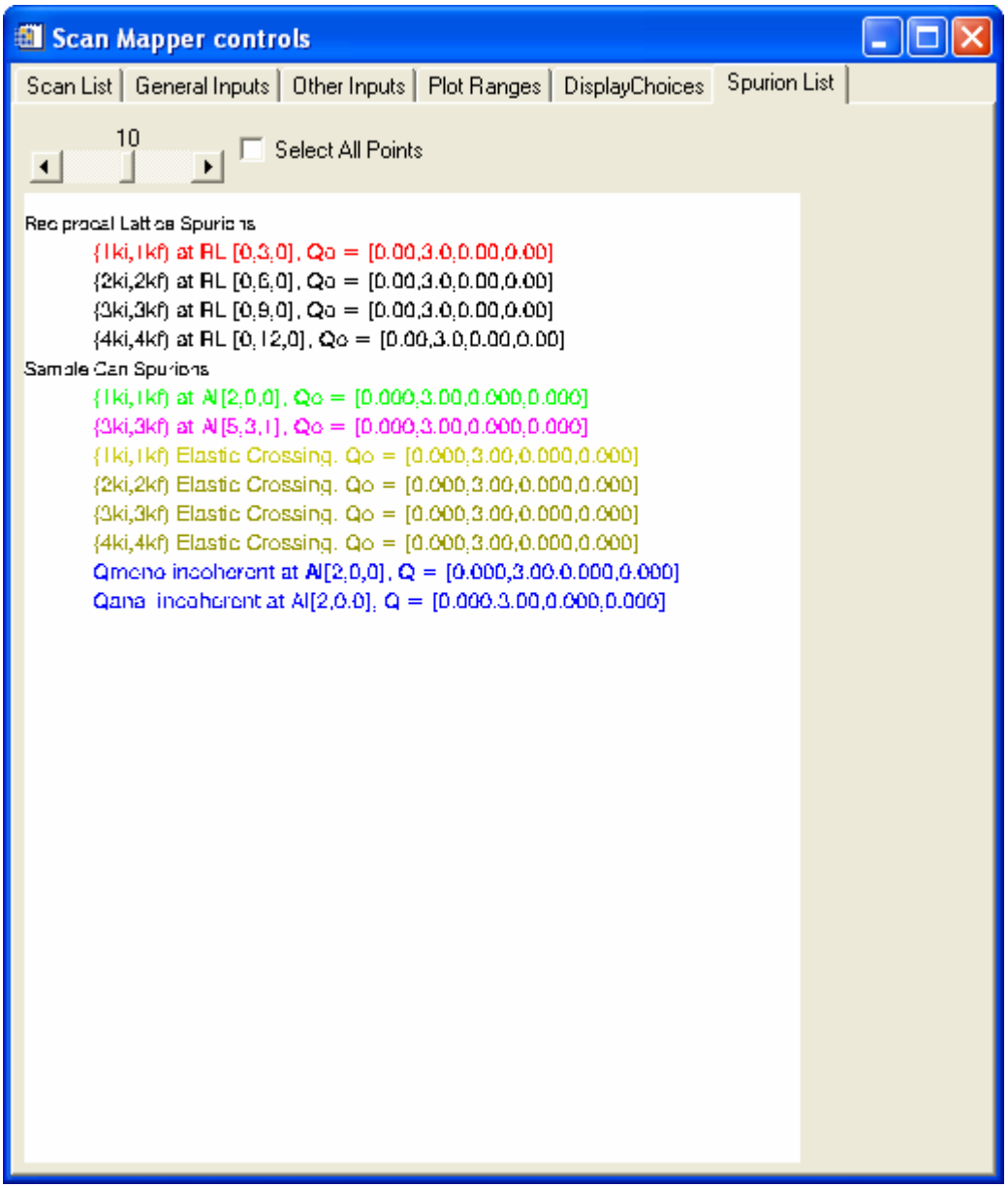
   b. Elastic Crossing means that the component of the scan crosses the elastic line at that

point.

c. Al[2,0,0] means indicates that the scan approaches the [2,0,0] powder ring for the sample holder material.

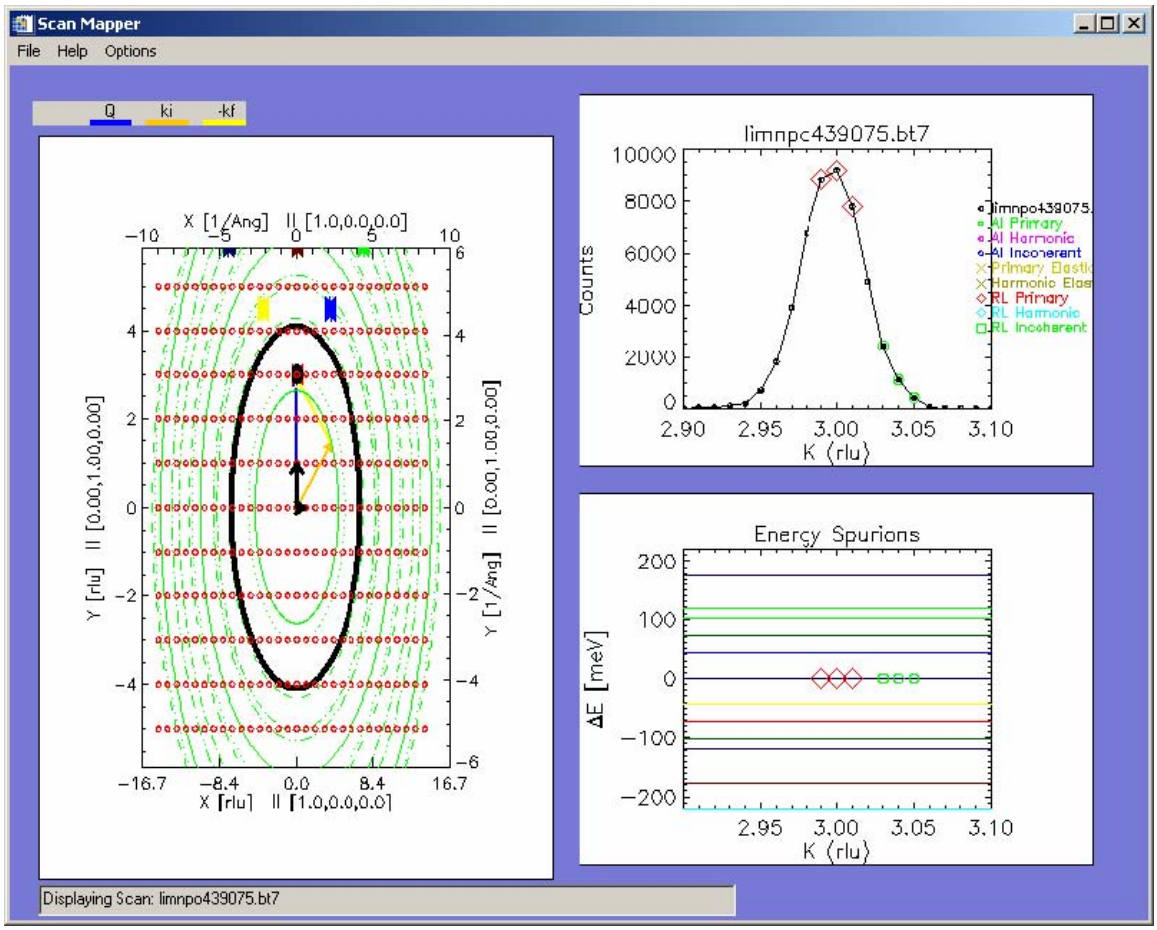
3) Finally, Qo = [**Q**] is the Q vector of the primary beam.



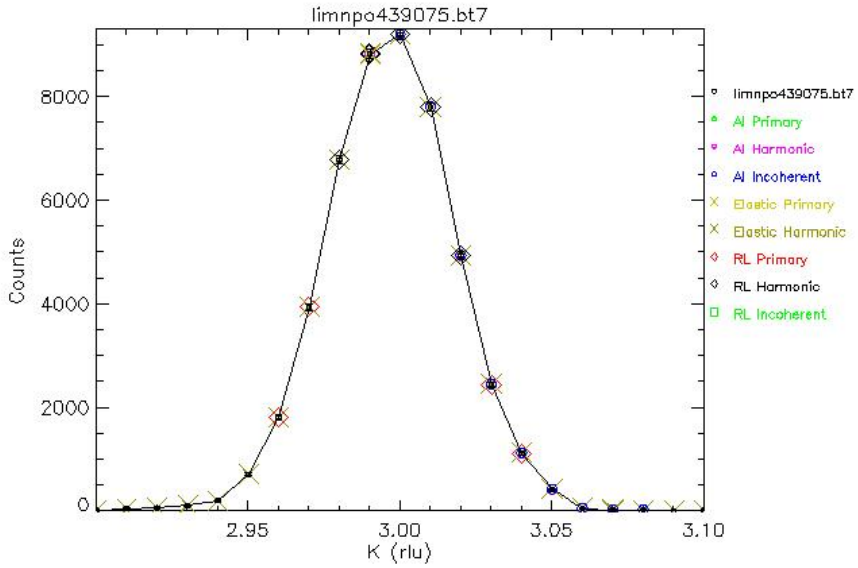


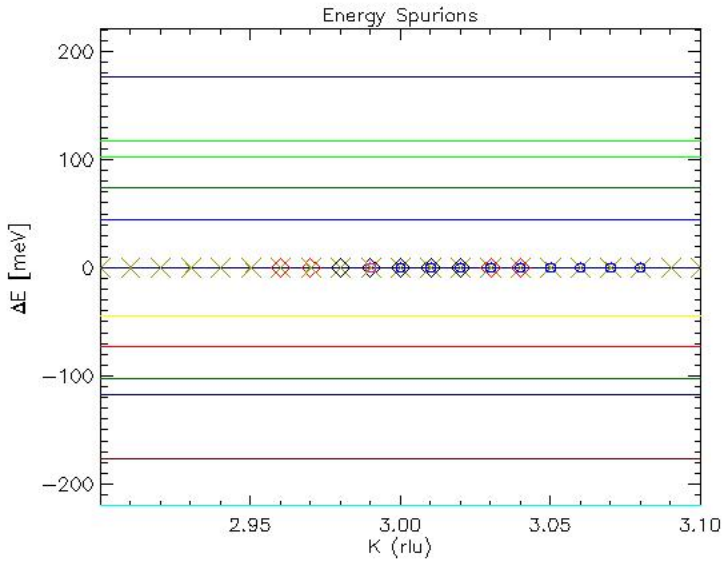
3. Scan Definition

A scan is defined when you either: 1) enter it manually via the "Scan Definition" tab in the controls, or 2) read in a data file. If you read in a data file, the data in the file will be displayed in the scan plot with possibly spurious features highlighted with the symbols indicating their respective sources. A text listing of the expected spurions for the scan will be in the "Spurion List" tab, and there will be symbols plotted on the both "Scan Plot" and the "Energy Plot" to indicate graphically the locations of the spurions.


Scan Mapper
File Help Options
Q ki -kf
X [1/Ang] || [1.0,0.0,0.0]
Y [rlu] || [0.00,1.00,0.00]
Y [1/Ang] || [0.00,1.00,0.00]
X [rlu] || [1.0,0.0,0.0]
limnpc439075.bt7
Counts
K (rlu)
Al Primary
Al Harmonic
Al Incoherent
Primary Elastic
Harmonic Elas
RL Primary
RL Harmonic
RL Incoherent
Energy Spurions
ΔE [meV]
Displaying Scan: limnpo439075.bt7

4. Spurion Calculations





Each item in the Scan Plot is labeled with what may at first appear to be a cryptic legend. The same legends apply to both the Scan Plot and the Energy Plot directly below it. The following attempts to explain the items in the legend and how they are calculated.

For each of the options below, $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$ and $E = E_i - E_f$. The term **"primary"** below indicates

that the feature was due to ($1*\mathbf{k}_i - 1*\mathbf{k}_f$) for the Scan Plot and $E_i - E_f$ for the Energy Plot. The term **"harmonic"** indicates that the feature originates from $n*\mathbf{k}_i - m*\mathbf{k}_f$ for the Scan Plot and $n^2E_i - m^2E_f$ for the Energy Plot, where at least one of n or m is greater than 1. The components of each **Q** vector and each item in the scattering plane are broken down into Q_x and Q_y, where x and y indicate the vectors that define the scattering plane.

The Al spheres and reciprocal lattice points are considered only in the scattering plane. It should be noted that a crystal with a large unit cell length perpendicular to the scattering plane may have features that approach the scattering plane. The possible effects of such features are not considered here, even though they may have effects in real scans.

Scan Plot/Energy Plot legends:

1. The first legend is the name of the data set. If this is from a file it will be actual data, if it is from a user-defined scan then it will be a set of points, all with value 1.

2. The second one is **"Al Primary", green circle**. These points indicate where a point in the primary beam (1*ki,1*kf) scan approaches a powder sphere from the sample holder (possible made of Al, Cu, or Mo). Calculating Qxy in the scattering plane, these points are selected where the distance $r = \sqrt{((Q_x - Q_{Al}\cos(\theta))^2 + (Q_y - Q_{Al}\sin(\theta))^2)}$ is less than the tolerance distance (specified in the "Qtol" field on the "Other Inputs" tab).

3. The third item is **"Al Harmonic", purple circle**. These are points where the harmonic beam scans (n*ki,m*kf) approach a sample holder powder ring. Once again, calculating Qxy in the scattering plane, these points are selected where the distance $r = \sqrt{((Q_x - Q_{Al}\cos(\theta))^2 + (Q_y - Q_{Al}\sin(\theta))^2)}$ is less than the tolerance distance (specified in the "Qtol" field on the "Other Inputs" tab).

4. The fourth item is **"Al Incoherent", blue circle**. These occur when the incoherent scan (when kf=ki off the mono or when ki=kf the analyzer) approach an Al (or other sample holder material) powder ring. $\mathbf{Q_{mono}} = \mathbf{k}_i - k_i\,(\mathbf{k}_f/|\,\mathbf{k}_f\,|)$ and $\mathbf{Q_{ana}} = \mathbf{k}_f\,(\mathbf{k}_i/|\,\mathbf{k}_i\,|) - \mathbf{k}_f$. Once again, calculating Qxy from in the $\mathbf{Q_{mono}}$ or $\mathbf{Q_{ana}}$ in the scattering plane, these points are selected where the distance $r = \sqrt{((Q_x - Q_{Al}\cos(\theta))^2 + (Q_y - Q_{Al}\sin(\theta))^2)}$ is less than the tolerance distance (specified in the "Qtol" field on the "Other Inputs" tab).

5. The fifth item is **"Elastic Primary", dark yellow X**. This occurs when the primary beam (1*ki,1*kf) passes through E=0, namely when $(E_i - E_f) < E_{tol}$ specified in the "Etol" of the "Other Inputs" tab.

6. The sixth item is **"Elastic Harmonic", olive X**. This occurs when one of the harmonic beams (n*ki,m*kf) passes through E=0, namely when $(n^2E_i - m^2E_f) < E_{tol}$ specified in the "Etol" of the "Other Inputs" tab.

7. The seventh item is **"RL Primary", red diamond**. This occurs when the primary beam scan passes through a reciprocal lattice point of the sample, as specified by a, b, c, α, β, γ. Calculating Qxy in the scattering plane, these points are selected where the distance $r = \sqrt{((Q_x - Q_x[RL])^2 + (Q_y - Q_y[RL])^2)}$ is less than the tolerance distance (specified in the "Qtol" field on

the “Other Inputs” tab).

8. The eighth item is **“RL Harmonic”, black diamond**. This occurs when the one of the harmonic beam scans (n*ki,m*kf) approaches a reciprocal lattice point of the sample, as specified by a, b, c, α, β, γ for the sample. Calculating Qxy in the scattering plane, these points are selected where the distance $r = \sqrt{((Q_x - Q_x[RL])^2 + (Q_y - Q_y[RL])^2)}$ is less than the tolerance distance (specified in the “Qtol” field on the “Other Inputs” tab).

9. The ninth item is **“RL Incoherent”, green square**. These occur when the incoherent components of the scan (when kf=ki off the mono or when ki=kf the analyzer) approache a reciprocal lattice point of the sample, as specified by a, b, c, α, β, γ for the sample. $\mathbf{Q_{mono}} = \mathbf{k_i} - k_i (\mathbf{k_f}/|\mathbf{k_f}|)$ and $\mathbf{Q_{ana}} = \mathbf{k_f} (\mathbf{k_i}/|\mathbf{k_i}|) - \mathbf{k_f}$. Once again, calculating Qxy from in the $\mathbf{Q_{mono}}$ or $\mathbf{Q_{ana}}$ in the scattering plane, these points are selected where the distance $r = \sqrt{((Q_x - Q_x[RL])^2 + (Q_y - Q_y[RL])^2)}$ is less than the tolerance distance (specified in the “Qtol” field on the “Other Inputs” tab).

Future Features

1. Calculated scan of resolution-limited feature. Resolution Ellipsoid calculations (for display and determination of spurious data)

2. Reciprocal Lattice calculator (Allow user input of unit cell information) Auxiliary 3d view of reciprocal space Output features as requested and defined by users