

CrystalPlan 1.0 User Guide

by Janik Zikovsky (zikovskyjl@ornl.gov)

Document started April 14, 2010;



Introduction

CrystalPlan is an experiment planning tool for crystallography;
CrystalPlan...

- Lets you put in a list of sample orientation angles, and...
- ...calculates the coverage of detectors in reciprocal space.
- When you give it your sample's lattice parameters and UB matrix, it...
- ...predicts the positions of single-crystal peaks.
- You can then optimize your experiment by trying different orientations and seeing if your coverage statistics will still be adequate.

Step-by-Step Tutorial

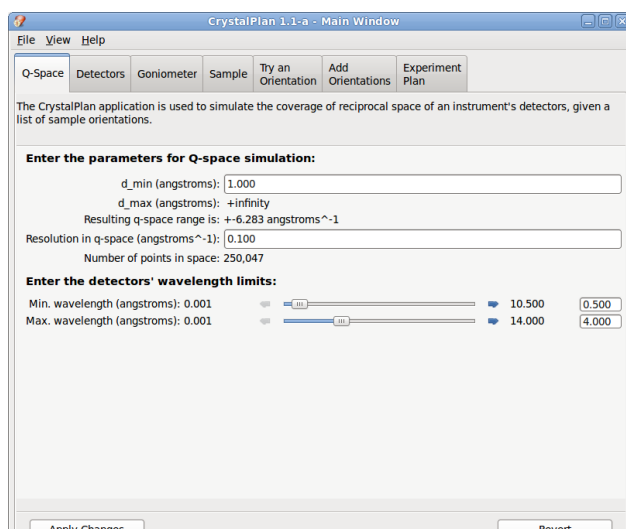
This tutorial will show you how to use most of the features of CrystalPlan by going through a typical run, step-by-step.

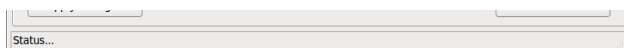
1. Starting CrystalPlan

From the terminal command line, type:

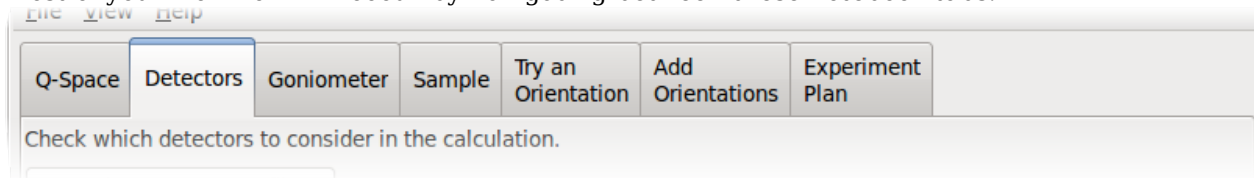
```
crystalplan.py
```

The GUI launches in two new windows. Select the main window:





Most of your workflow will occur by navigating between these notebook tabs:



2. Defining the Reciprocal Space of Interest and Wavelengths

Here you will set the general parameters of your experiment.

- Click the "Q-Space" tab, if it not already selected. If necessary, change the parameters so that it matches those shown below:

Enter the parameters for Q-space simulation:

d_min (angstroms): 1.000

d_max (angstroms): +infinity

Resulting q-space range is: +-6.283 angstroms⁻¹

Resolution in q-space (angstroms⁻¹): 0.100

Number of points in space: 250,047

Enter the detectors' wavelength limits:

Min. wavelength (angstroms): 0.001

Max. wavelength (angstroms): 0.001

10.500 0.500

14.000 4.000

- **d_min**

The smallest d-spacing allowed. Your simulated q-space will be limited to a maximum $q_{max} = 2\pi/d_{min}$

- **q-resolution**

The size of a voxel (smallest volume element) simulated, in Å⁻¹. The # of points will be calculated and shown below; you will get a warning if you try to make very high-resolution calculations, because memory consumption, etc. will be very high.

- **wavelength limits**

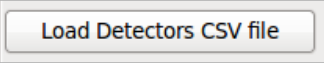
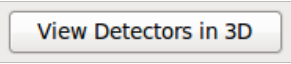
Specify your experiment's wavelength limits, in Angstroms; this could be due to limits on your neutron source or your detectors.

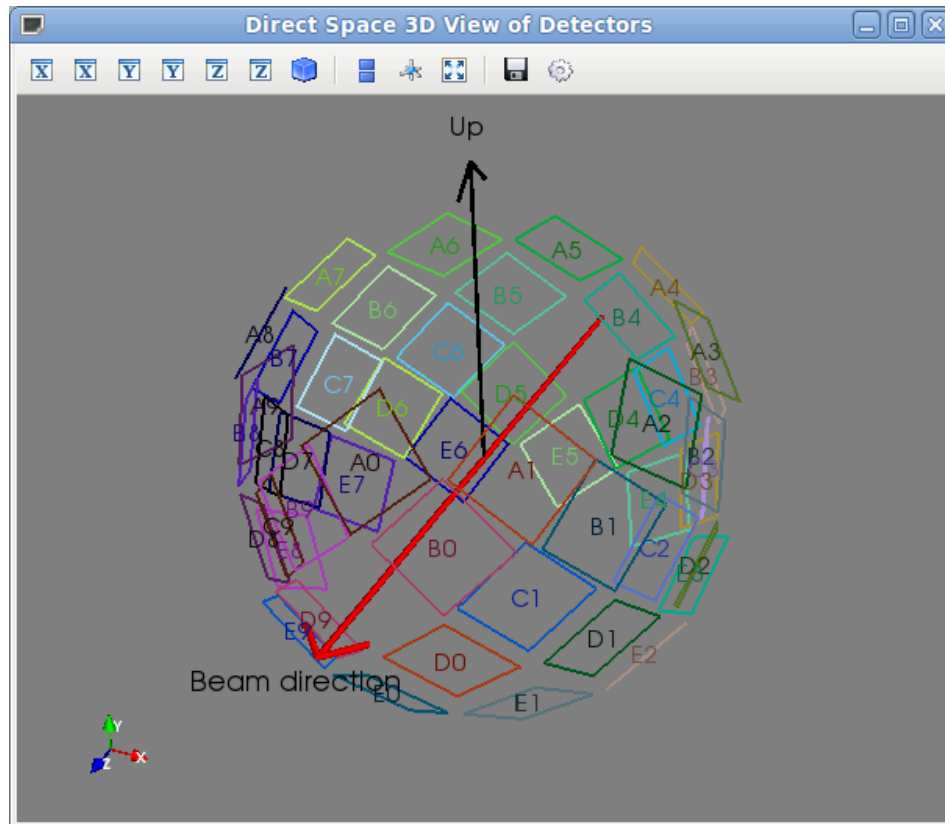
- When done, click the **Apply Changes** button. Changing these settings requires re-doing a lot of calculations, which may take some time if you have a lot of orientations saved.

3. Detectors

Here, you ensure that CrystalPlan has the correct detector geometry loaded.

- Click the "Detectors" tab.

- Load a detector geometry by clicking the  button. In the File Loading dialog that opens, select the "TOPAZ_detectors_all.csv" file.
- After a few seconds, the detector geometry is loaded. To confirm that the detectors are in the correct positions, you can visualize them in direct space by clicking , which displays them in a window like this one:

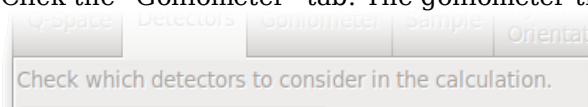


- There are additional controls on this tab that are not commonly used:
 - The list of detectors has checkboxes. You can uncheck a detector to indicate that it will not be used in the experiment (perhaps it is obscured or malfunctioning).
 - The Coverage Stats button calculates the coverage of each detector. The Select Best Detectors selects the best detectors based on these coverage statistics.

4. Goniometer

Now, you want to make sure that CrystalPlan is aware of which goniometer is currently in use in your instrument.

- Click the "Goniometer" tab. The goniometer that is currently selected is shown at the top:



- Select the TOPAZ in-house goniometer:

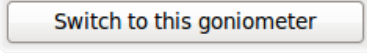


- Some general information about the goniometer is shown:

Description:

3-legged goniometer for TOPAZ, which allows for sample cooling. Has full phi rotation freedom, but is limited in chi and omega due to the travel range of the legs.

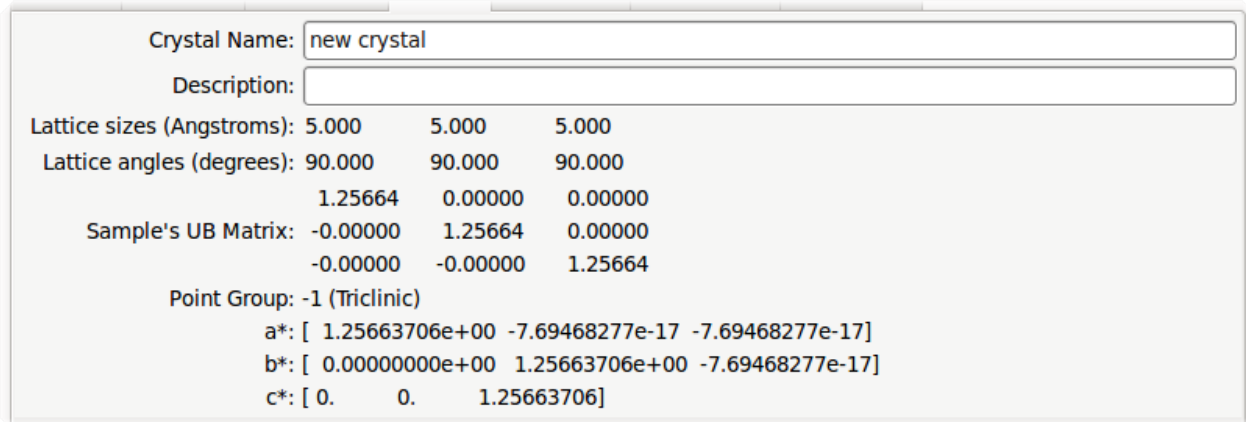
Phi, angle, ranges from -180.0 to 180.0 deg
 Chi, angle, ranges from -180.0 to 180.0 deg
 Omega, angle, ranges from -180.0 to 180.0 deg

- But your selection is not complete until you click 
- The program will now be aware of the sample orientation angle limitations that your instrument has, and will give you warnings if you try to use an inaccessible sample orientation.

5. Sample Settings

Now, you will want to enter or load in information about your sample: crystal lattice parameters, UB matrix, etc.

- Click the "Sample" tab. You are presented with an overview of the crystal parameters



Crystal Name:

Description:

Lattice sizes (Angstroms): 5.000 5.000 5.000

Lattice angles (degrees): 90.000 90.000 90.000

Sample's UB Matrix:

	1.25664	0.00000	0.00000
-0.00000	1.25664	0.00000	
-0.00000	-0.00000	1.25664	

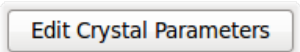
Point Group: -1 (Triclinic)

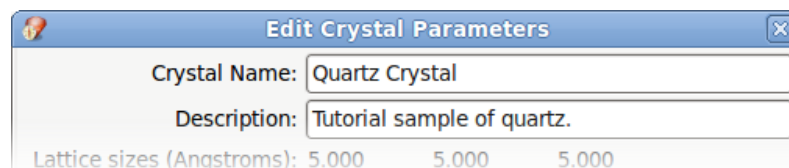
a*: [1.25663706e+00 -7.69468277e-17 -7.69468277e-17]

b*: [0.00000000e+00 1.25663706e+00 -7.69468277e-17]

c*: [0. 0. 1.25663706]

5.1. Edit Crystal Parameters dialog

- Click .
 - This brings up the "Edit Crystal Parameters" dialog box. You may edit the name and description:




Edit Crystal Parameters

Crystal Name:

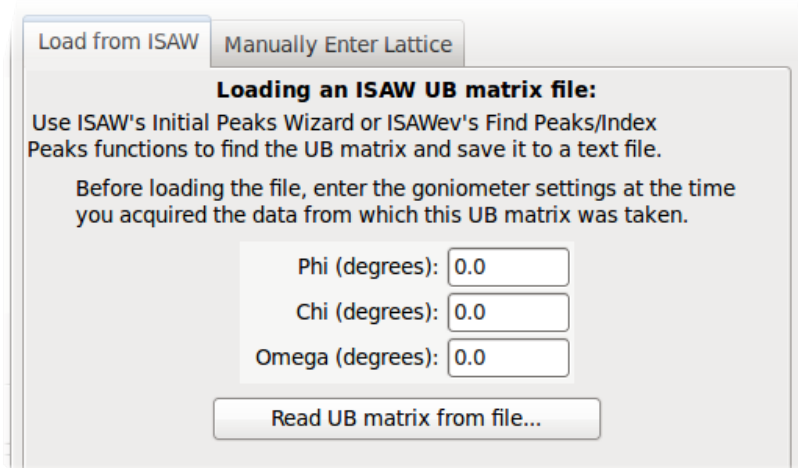
Description:

Lattice sizes (Angstroms): 5.000 5.000 5.000

- The top of the dialog shows you the current crystal parameters.
- The ["Manually Enter Lattice" tab](#) allows you to try out the program by typing in your lattice

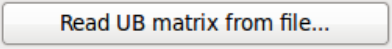
parameters and the sample mounting. Clicking the  button would create a UB matrix that you can use to test features of the program; however we will not be doing that in this tutorial.

- Instead, go to the "Load from ISAW" tab:



- If this were a real experiment, at this point you would have had acquired an adequate set of data at a starting sample orientation, and saved the run.
- You would then load that data into ISAW in order to find the sample orientation.
- ISAW can generate a UB matrix file that contains:
 - The crystal's *measured* UB matrix - this contains information about how the crystal is mounted relative to
 - The crystal's lattice lengths and angles.
- To learn how to calculate a UB matrix, please refer to ISAW's documentation. Using ISAW, you will be using the Initial Peaks wizard to locate and index the peaks. This method can be used to find both the lattice parameters and UB matrix, or you can specify the lattice parameters if known.
- You can also generate the same file using ISAWev (the ISAW event viewer), working directly from event data in reciprocal space. The procedure is the same (find and index the peaks) though the interface is a little different. Both methods generate exactly the same file format.
- However, the UB matrix output by ISAW **includes the orientation due to the goniometer** and not just the crystal mounting orientation.
 - The UB matrix needs to be corrected to account for this extra rotation.
 - This requires you to enter the goniometer angles corresponding to the sample orientation in the UB matrix file to load - the goniometer settings at the time that data was acquired.

- Enter these angles, in degrees, here:

- A sample UB matrix file can be found in the "model/data/quartzub.txt" file. Click the  button and select this file in the dialog.
- The top of the dialog shows you the loaded lattice parameters and UB matrix.

Crystal Name: Quartz Crystal

Description: Tutorial sample of quartz.

Lattice sizes (Angstroms): 4.908 4.917 5.366

Lattice angles (degrees): 89.853 89.808 60.341

Point Group: -1 (Triclinic)

Sample's UB Matrix: -0.22946 0.59245 -1.07069
 0.66577 0.75697 0.31423
 1.29413 -1.11274 -0.35468

UB matrix obtained from: ISAW UB matrix file at
 ../model/data/quartzub.txt
 modified by phi, chi, omega of 30.0, 15.0, 60.0

- From here, you can set the crystal's point group symmetry; however, we will leave it as "-1 (Triclinic)", as shown.
- Click **Ok** to apply the changes; clicking **Cancel** would revert all the changed made in the dialog.
- Some recalculations will occur when changing the crystal lattice parameters or orientation.

5.2. Choosing H,K,L ranges

- Still in the Sample tab, the following GUI allows you to pick which HKL to display:

H range: -5.0 5.0

K range: -7.0 7.0

L range: -5.0 5.0

Automatically fit to experiment's min d-spacing? ☒

Limit to a sphere of radius corresponding to d_min? ☒

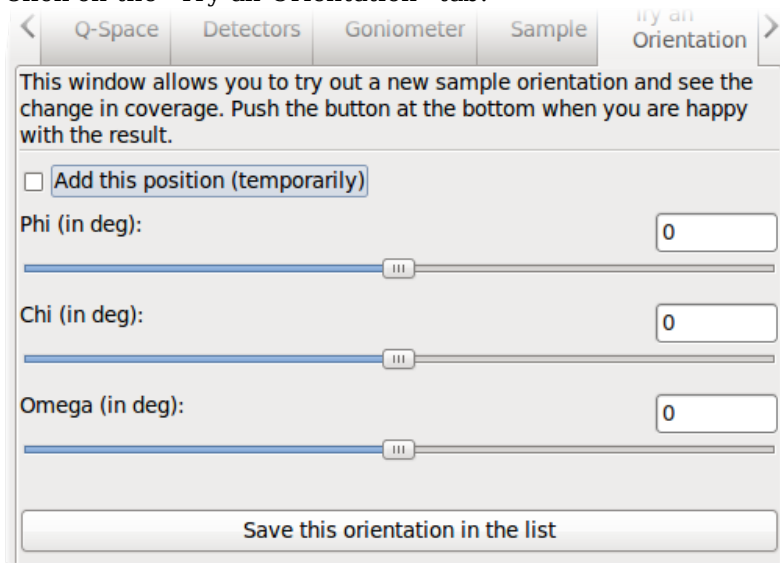
- These H,K,L ranges limit which peak indices that CrystalPlan will calculate and display.
- You can type in your ranges manually, however, I recommend that you keep both checkboxes checked:
 - They use the d_{min} parameter you set earlier in the "Q-Space" tab.
 - The first checkbox tells CrystalPlan to calculate the H,K,L ranges that fill a box of side in q-space corresponding to d_{min} .
 - But, the resulting peaks will form a cube only if all the lattice angles are 90 degrees.
 - By checking the second box, any peaks with a d-spacing smaller that d_{min} will be rejected, leaving a sphere of reflections in q-space.
- Click the **Apply New Range** button to apply any changes you have made. All reflections are re-calculated.
- Be aware that for large cells, the number of reflections within a given d_{min} may be very large, slowing down calculations and requiring a lot of memory.

6. Trying Sample Orientations

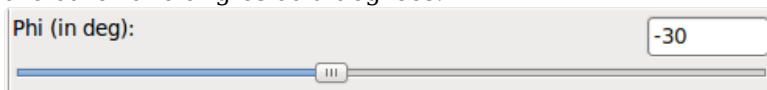
At this point, we have given the program all the information it needs to start predicting what we can

measure. We will now tell it what sample orientations we will try.

- Click on the "Try an Orientation" tab.



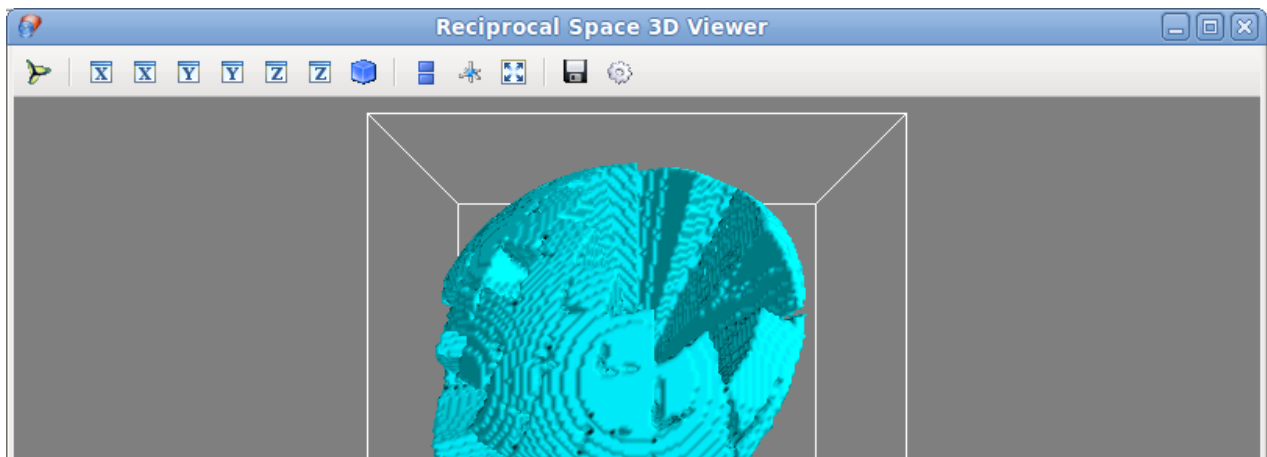
- Check the ☒ **Add this position (temporarily)** box.
- Now, you simulate a sample orientation.
 - As you change the values, the coverage calculation is re-done and updated in the 3D viewer (which we will look at next).
 - Use the slider or type in (and press Enter) to set a Phi angle of 30 degrees, while keeping the other two angles at 0 degrees.

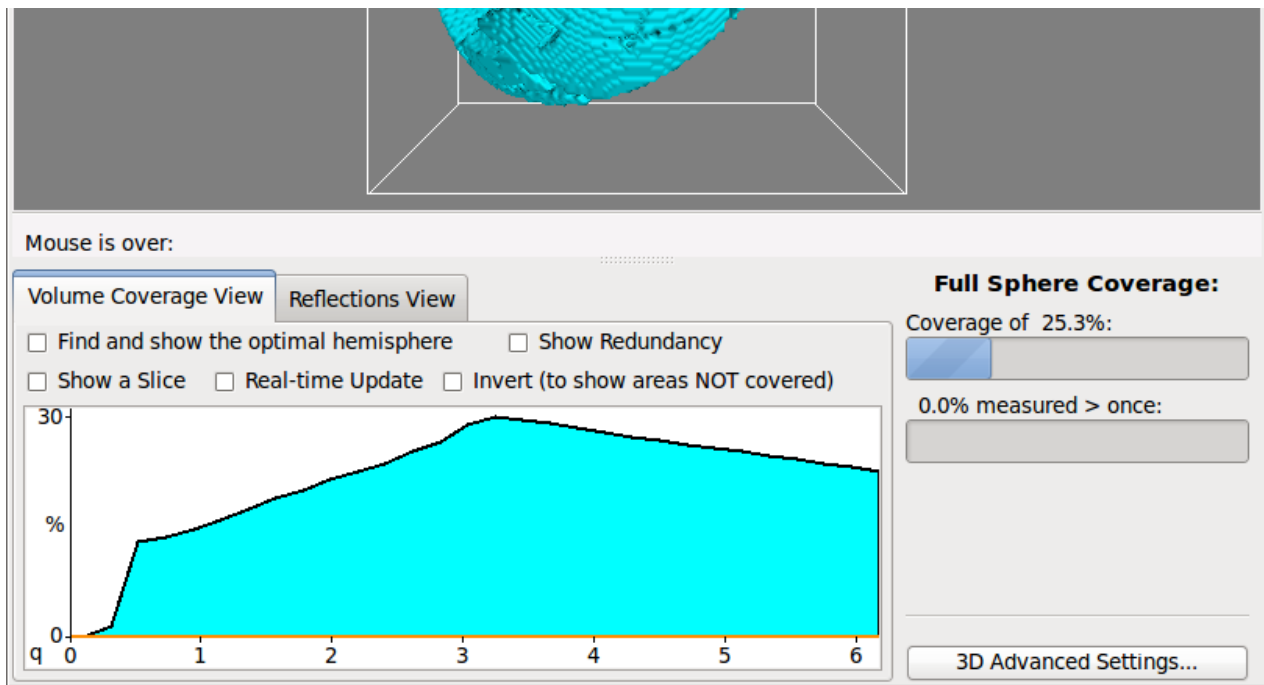


7. The Reciprocal Space 3D Viewer

Congratulations on making it this far! We will now look at the result of our simulated detector coverage.

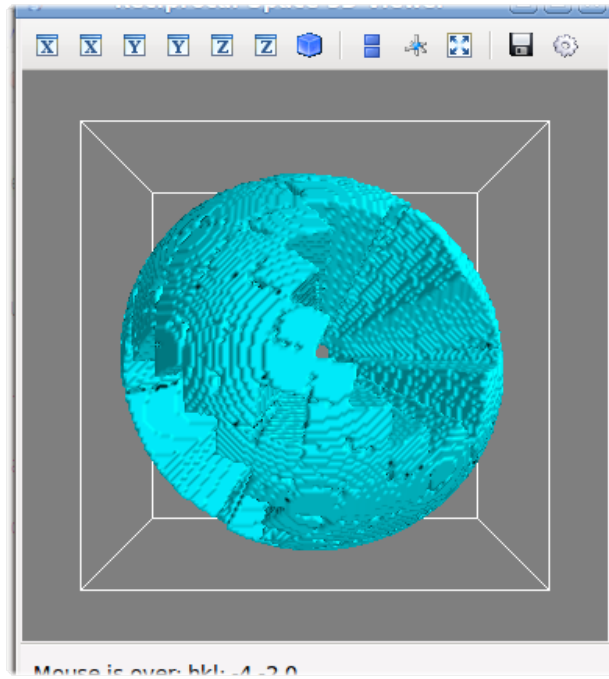
- Switch window to the Reciprocal Space 3D Viewer (this window opens with CrystalPlan, so it should already be open - otherwise, you can open it from the "View" menu).



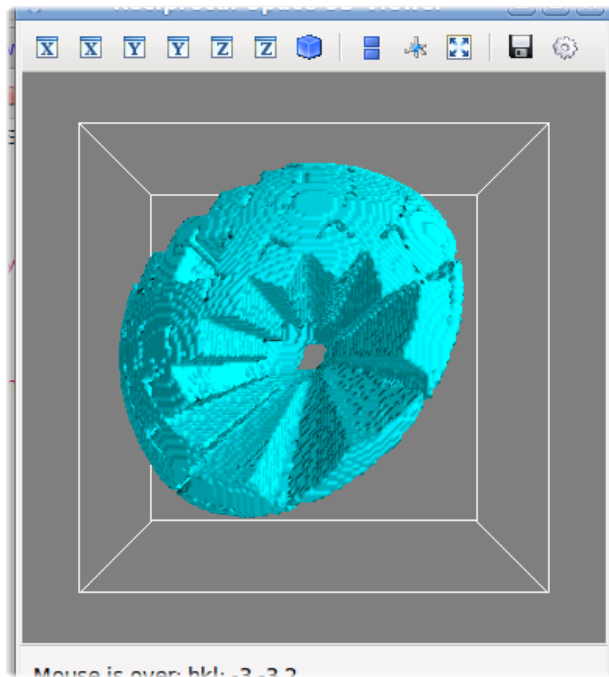


- The main part of the window is a 3D view of reciprocal space.
 - The white cube outline represents the extent of q-space that is simulated.
 - The center of the cube is $q = [0,0,0]$, which corresponds of course to $h,k,l = [0,0,0]$
 - The cube is sized so as to *just* hold a sphere of radius $q = \frac{2\pi}{d_{min}}$
- Right now, we are in "volume coverage" mode, which means that the shapes shown in cyan correspond to the *volume* in reciprocal space that has been measured by a detector.
 - When a "voxel" (volume pixel) has been measured once, it is marked as a value of "1".
 - The surface you see is the isosurface (the edge between 0 measurements and 1 measurement).
 - The "sharpness" of this 3D view is determined by the q-resolution you specified in the "Q-Space" tab at the beginning. You can change this resolution at any time, and the coverage will be recalculated at this new resolution.
- You can interact with the 3D view in a number of ways:
 - Click the left mouse button and drag to rotate the view around the center.
 - Hold SHIFT (or use the middle mouse button) to pan the scene around.
 - Hold CTRL to rotate the scene only around the camera's axis (roll).
 - Hold SHIFT+CTRL (or use the right mouse button) to zoom in and out by moving the mouse.
 - Use the mouse wheel to zoom in and out.
 - Press = and - to zoom in and out.
 - Press R to reset the zoom level and center the camera.
 - Press 3 to enable two-colour 3D rendering (with cyan/blue glasses you could see it in "real" 3D *a la* a 1950's B-movie :-)
- The buttons at the top of the view, from left to right, are:
 - 6 buttons to reset the views quickly, facing the given directions.
 - Default isometric view.
 - Turn on orthographic projection (no perspective effects - this is very handy when looking a ordered peaks).
 - Display the 3D axes.

- Go fullscreen (press Esc to go back)
- Save a screenshot.
- We will return to this window to explain the elements in more detail.
- For now, you can change the Phi angle in the "Try An Orientation" tab and visualize how that affects the reciprocal space coverage in this window. This animation shows the effect of changing the phi of the sample from -180 to +180 degrees:

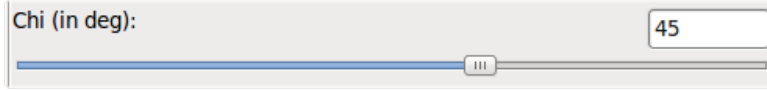


- And this animation shows a chi (tilt) rotation from -180 to +180 degrees, with phi kept constant:



9. Goniometer Limits

- Back in the Main Window's "Try Position" tab, try to set a Chi angle of +45 degrees:



Chi (in deg): 45

- ... and you will see the following warning message:

Warning! The angles cannot be achieved by the goniometer!
Reason: Limit to leg positions

informing you that you have tried a sample orientation that is not achievable by the selected goniometer.

- Not all goniometers have such limitations; for instance, if you select the "Simple Goniometer", there are no limits to the angles you can reach.
- However, the currently selected "TOPAZ In-House Goniometer" is limited in Chi tilt because of its design (a 3-legged "tripod" design). It can only tilt by a few degrees above or below zero.
- CrystalPlan calculated which angles are possible and warns you if they are not. A string describing the *reason* why this angle is not possible is displayed, if available.
- You can still simulate this sample orientation, but be aware that you will not be able to achieve it experimentally.

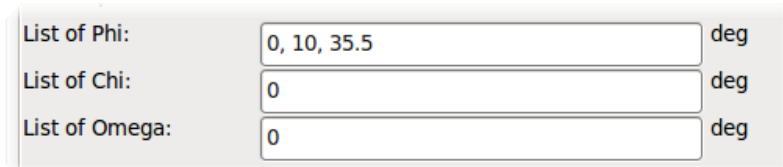
10. Adding Several Sample Orientations

Now, we will start building up an experiment plan by adding sample orientations.

- First, uncheck the ☒ Add this position (temporarily) box; this will remove the "trial" position from the coverage calculation.
- Switch to the "Add Orientations" tab.

10.1. Entering Lists of Angles

- Near the top of the window, you will see 3 text boxes where you can enter lists of angles to simulate:



List of Phi: 0, 10, 35.5 deg
List of Chi: 0 deg
List of Omega: 0 deg

- You can enter lists in 3 ways, based on Python script:
 - A simple list separated by commas: "**10, 22.5, -180**". You do not need to include square brackets.
 - An evenly divided linear range: "**linspace(start, stop, steps)**" will give you *steps* points, evenly divided from *start* to *stop* (inclusive).
 - A range of values in fixed steps: "**arange(start, stop, step_size)**" will step starting at *start*, go up in steps of *step_size*, until you reach *stop* - but does not include *stop*.
- Angles are stepped through for each list: for example, if you put lists containing 5 phi angles, 4 chi angles, and 2 omega angles, your resulting list of sample orientations will have 40 phi, chi,

omega combinations.

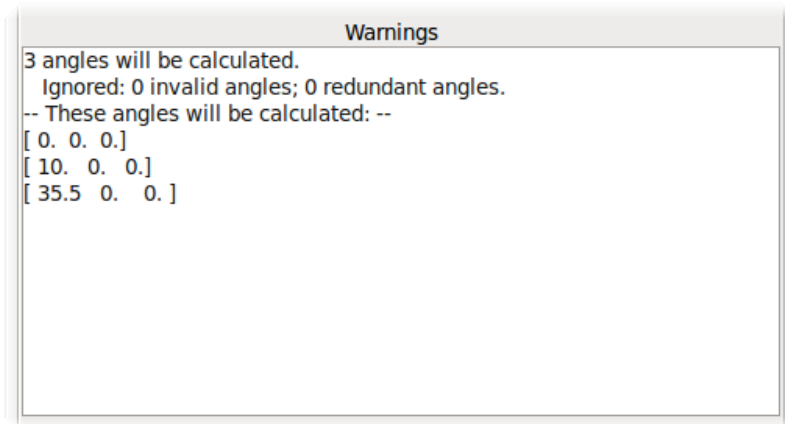
- You don't *have* to put in lists - you can also put in a single value for each angle, giving a single sample orientation.

10.2. Checking Validity of Orientations

- Enter the following values in the angle lists:

List of Phi:	<input type="text" value="0"/>	deg
List of Chi:	<input type="text" value="arange(-20, 20, 5)"/>	deg
List of Omega:	<input type="text" value="0"/>	deg

- You should see the following text below the angles:



- This box tells you that some of the angles you supplied were not achievable with the goniometer, and why. These angles will not be calculated.
- The remaining sample orientations will be calculated.

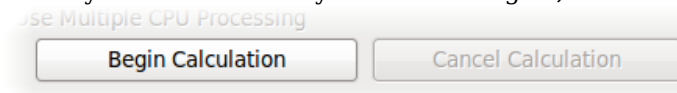
10.3. Adding Sample Orientations To Plan

- Enter the following values in the angle lists:

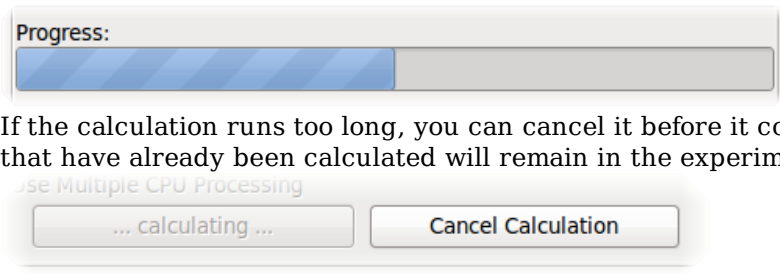
List of Phi:	<input type="text" value="0, 30, 60, 90"/>	deg
List of Chi:	<input type="text" value="0"/>	deg
List of Omega:	<input type="text" value="0"/>	deg

All of these sample orientations are possible.

- When you have entered your lists of angles, click the "Start" button to begin the calculation.

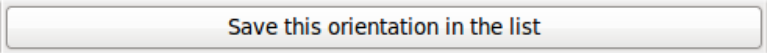


- The program now calculates the coverage at each sample orientation, and saves it in the experiment plan (which we will see in the next section).
- The calculation progress will be shown in this progress bar:



- If the calculation runs too long, you can cancel it before it completes. Sample orientations that have already been calculated will remain in the experiment plan.

- Another way to add sample orientations is to click the



button,

in the "Try an Orientation" tab. This adds to the experiment plan whatever sample orientation angles you tried by setting those sliders.

11. The Experiment Plan

- Switch to the "Experiment Plan" tab. Here, you see a grid with a list of all the sample orientations that have been calculated up to now:

	Use?	Phi (deg)	Chi (deg)	Omega (deg)	Stopping Criterion	Criterion Value	Comment
1	X	0.00	0.00	0.00	runtime (seconds)	60	
2	X	30.00	0.00	0.00	runtime (seconds)	60	
3	X	60.00	0.00	0.00	runtime (seconds)	60	
4	X	90.00	0.00	0.00	runtime (seconds)	60	

- Each row lists the sample orientation angles you will use (typically 3 angles, phi, chi, omega).
- The first column has a checkbox (X) if you are going to use this sample orientation in the experiment. Double-click to uncheck or recheck the box.
 - When you do so, the coverage corresponding to this sample orientation is removed from the total.
- The **Stopping Criterion** and **Criterion Value** columns allows you to specify *how long* to do the measurement for that particular sample orientation. You get a drop-down list of a few options (the exact list and function is determined by the DAS group):
 - **runtime**
The time to acquire data, in seconds.
 - **proton charge (or pcharge)**
The accelerator proton charge total, in picoCoulombs. This criterion has the advantage of

giving consistent counts, even if the accelerator goes down for some time during your run.

- **counts**

The total neutron count (over all detectors).

- **monitor counts**

The neutron count at the monitor.

- **roi counts**

The neutron count only in the region-of-interest (roi) on a detector. The roi will be defined on the DAS computers.

- As you change the runtime criteria, the following text box gives you an estimate of the total experiment time:

Estimated run time: 04m 00s

Some of the criteria, such as the counts, do not allow a time to be estimated, since the counts/second cannot be known ahead of time.

- You can manipulate the entries in the following ways:
 - You can highlight one or more rows (try Ctrl-clicking on the row numbers, or select a block with the mouse).
 - These buttons allow you to select orientations to use in the experiment:

☒ Use All Highlighted Rows: Use Don't Use

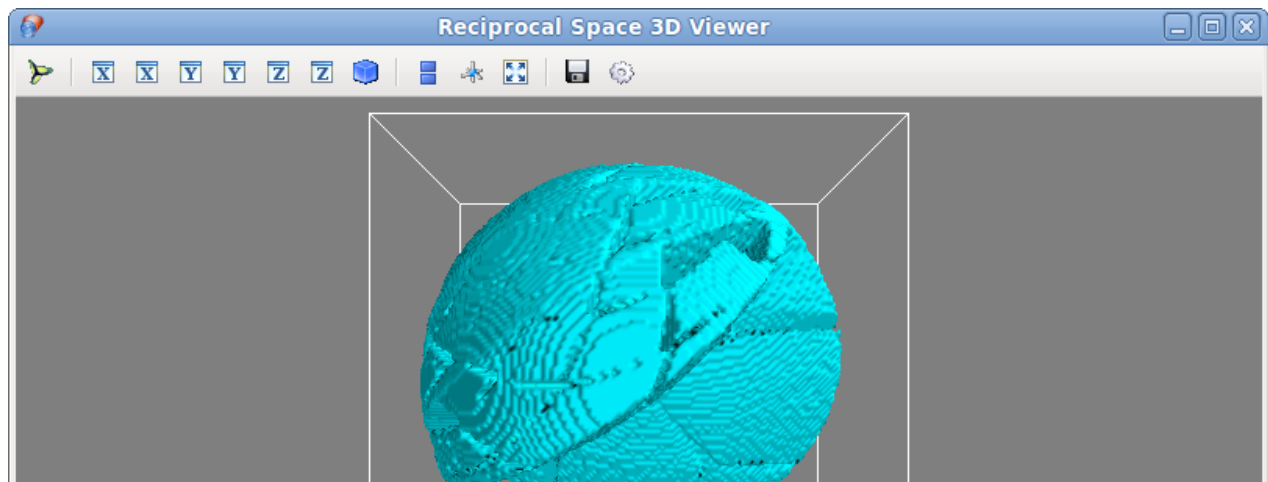
- These buttons allow you to delete orientations from the experiment:

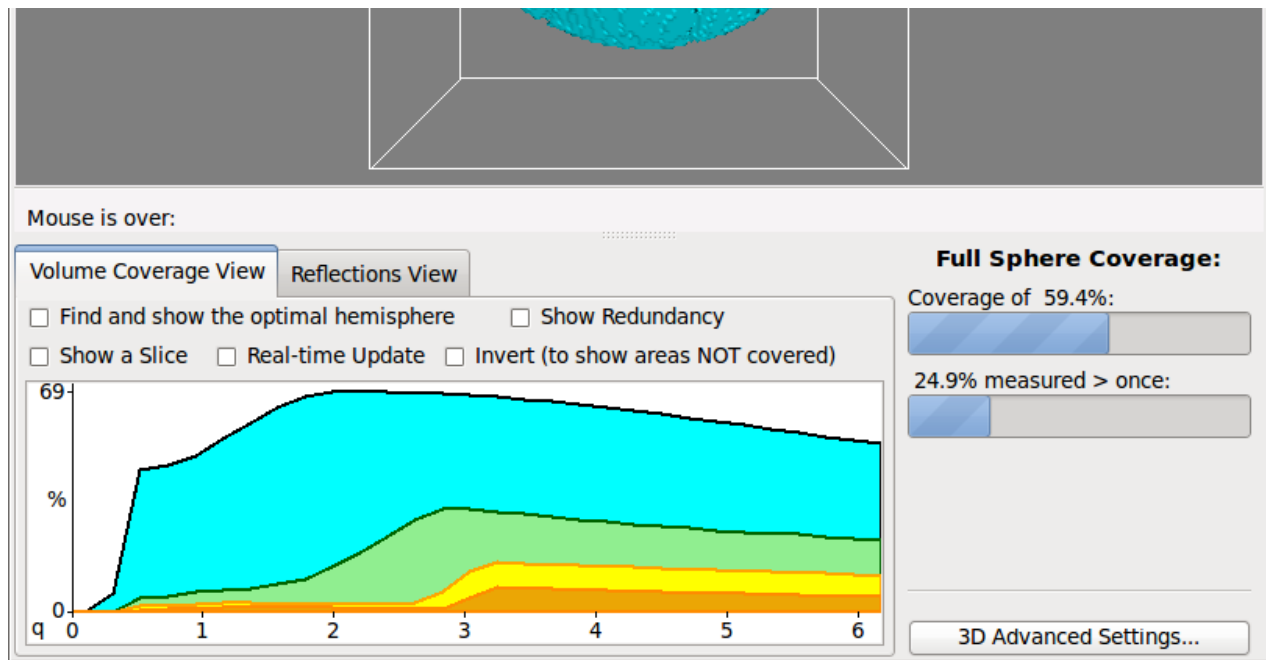
Delete All Delete Highlighted Delete Unused

- When you are happy with your experiment plan, click the Save to .CSV file button to make a CSV (comma-separated values) file containing the list of sample orientation and runtime criteria. This file can then be loaded on the DAS computers (using PyDas, for example) to run the experiment.

12. More Reciprocal Space 3D Viewer Options

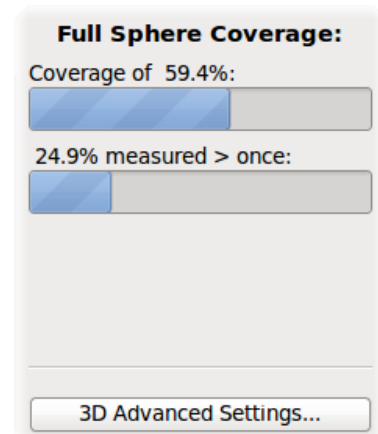
Now that we have more sample orientations in our plan, we return to the 3D viewer and explore some of its options. Here is what the 3D view looks like with the 4 orientations we have calculated:





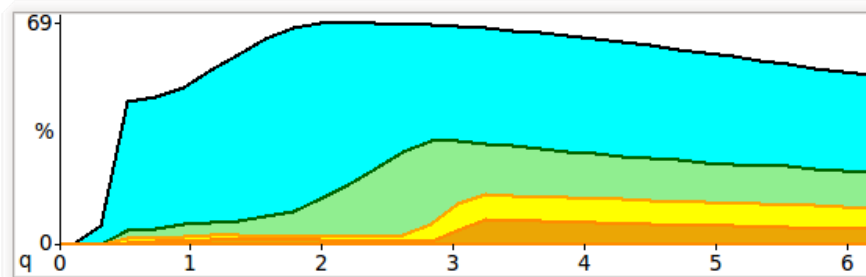
12.1. Coverage Statistics

- On the bottom right, you can see the coverage statistics panel:
 - The first bar indicates what percentage of reciprocal space volume was measured (at least once).
 - The second bar shows the redundant measurements - the proportion of q -space that was measured at least twice.



12.2. Slice Plot

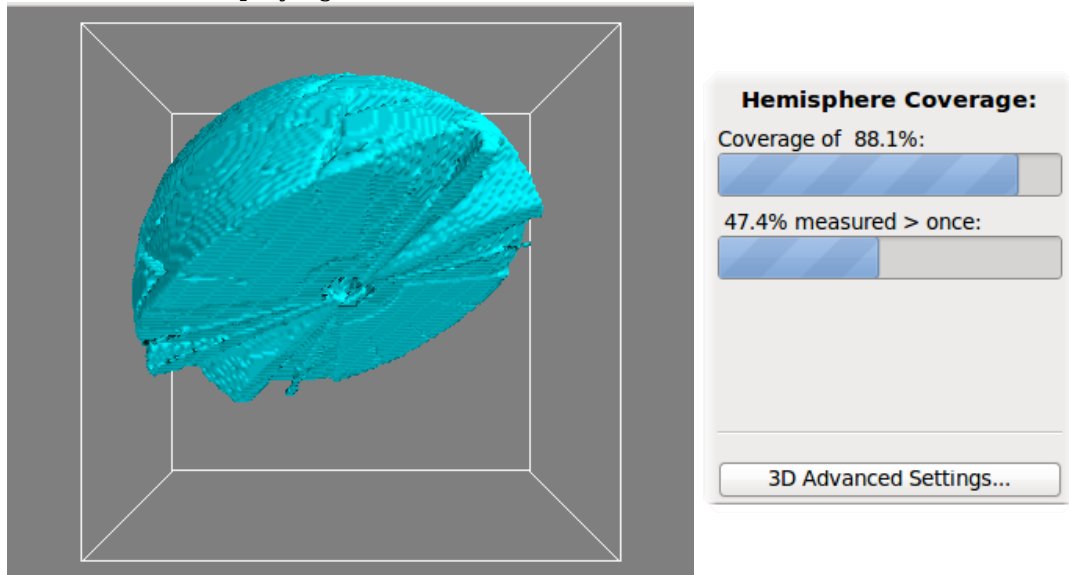
- On the bottom left is the slice statistics plot:



- This plot calculates the % coverage of a thin shell centered on a q starting at 0 and ending at $q_{max} = 2\pi/d_{min}$.
- The light blue plot is the percentage measured at least ones; in green is the percentage measured twice, yellow for measured 3 times, and orange for 4 times or more.
- This plot can use d-spacing for its horizontal axis. This is set in the Preferences, under the Main Window's "File" menu. Minimize and restore the window after changing the setting in order to refresh the display.

12.3. Hemisphere View

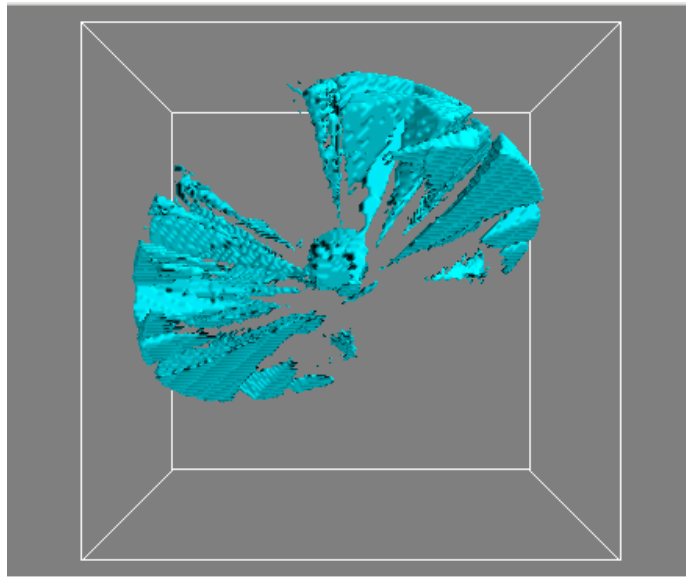
- Since all crystals have at least inversion symmetry (-1 point group) in scattering, that means that measuring a hemisphere of reciprocal space is enough to fully characterize your sample.
 - Check the ☐ Find and show the optimal hemisphere box to find and display only the "optimal" hemisphere. The program will find the side of reciprocal space with the most coverage, and ignore the rest, not displaying it at all:



- The coverage stats also reflect this choice - the coverage is compared to the volume of the optimal hemisphere, not the whole sphere; therefore your % covered will typically be higher, as seen above.

12.4. Inverted View

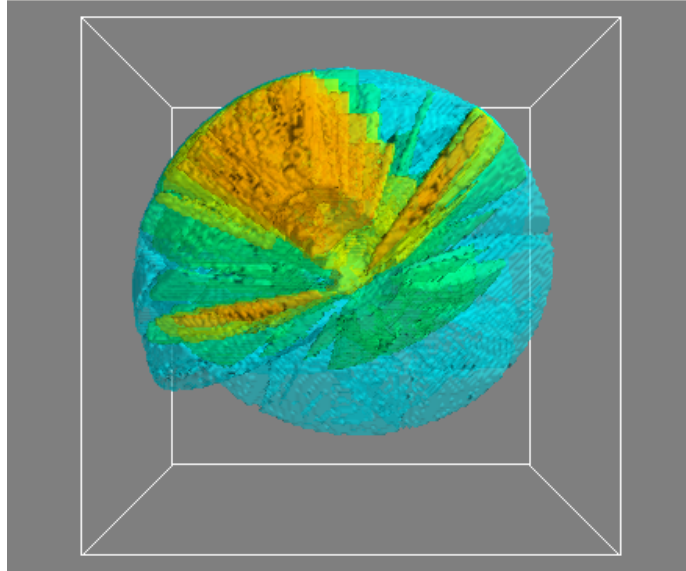
- You can also check the ☐ Invert (to show areas NOT covered) box to *invert* the coverage map, and show the volumes *not* measured. The next image shows the inverted coverage with the hemisphere box still checked - showing the volumes not covered but only in the hemisphere of interest.



- This can make it a lot easier to see spots you have missed, especially if they are hidden by covered volume.

12.5. Redundancy View

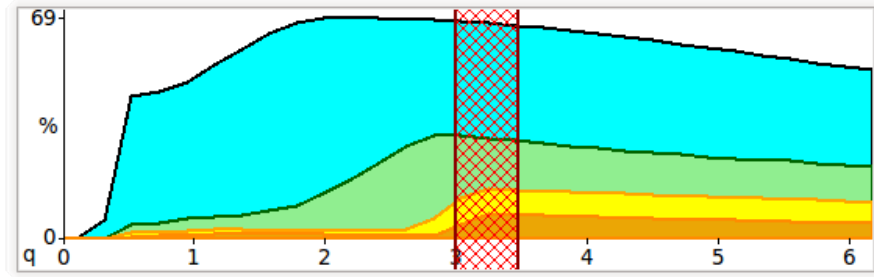
- If you check the ☒ Show Redundancy box, you will get a view of the redundancy of the measurement - how many times each voxel was measured. Semi-transparent isosurfaces are color-coded to show a single measurement, then 2, then 3, and finally 4 or more measurement.



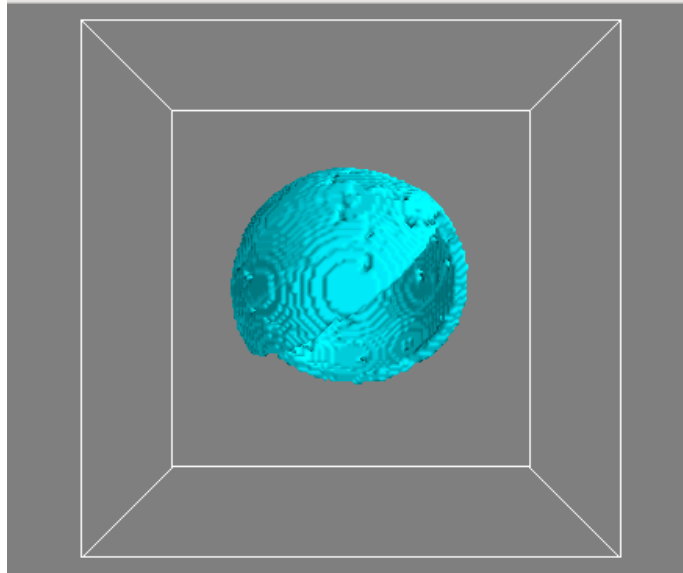
12.6. Slice View

- Check the ☐ Show a Slice box to view only a slice, (or shell) at a given q radius and given thickness.
- The Slice Plot now shows a hatched bar that you can move with the mouse to change the shell

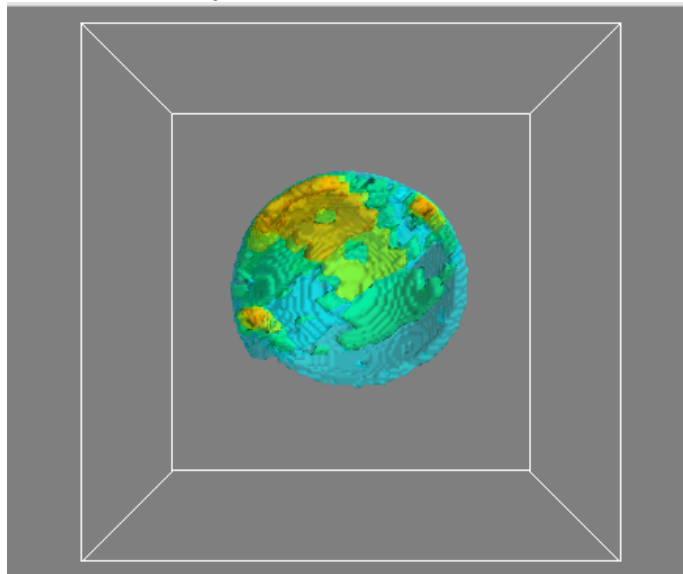
position and thickness.



- Click and drag the center of the area to change the q-radius
- Click and drag the edges of the area to change the thickness.
- The 3D view is updated to show only the selected slice of q-space:



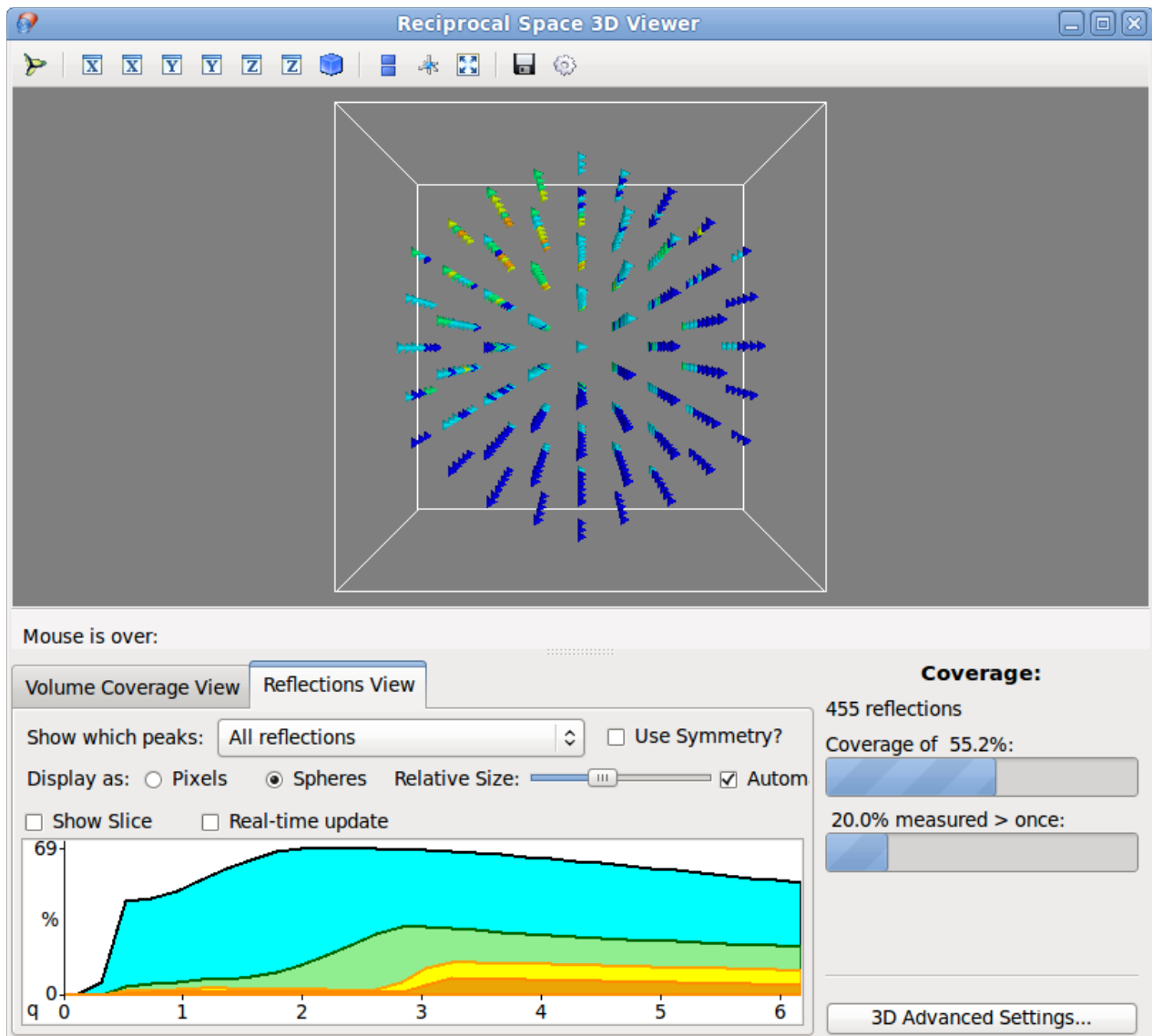
- ... and this also works with redundancy:



13. 3D Reflections View

Another way to measure your experimental coverage is by looking at single reflections, instead of viewing volume coverage in reciprocal space, as we have been doing before.

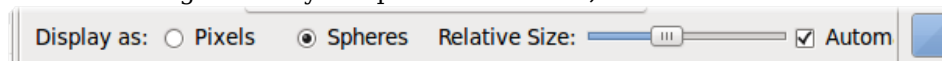
- To switch to reflection view, click on the "Reflections View" tab. Instead of volumes, you now see a number of color-coded points:



- The color-coding matches those in the volume view and the slice plot, with the addition of the dark blue peaks: those are peaks that were not measured.

13.1. How to Display Reflections

- You can change the way the peaks are drawn, in order to make the rendering clearer.

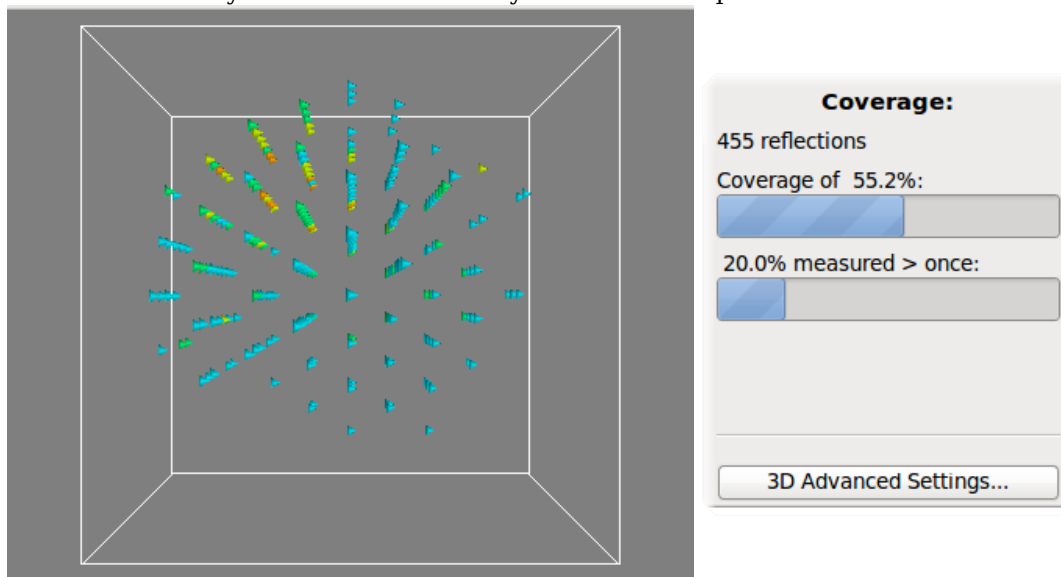


- Peaks can be displayed as small spheres (which look bigger when you zoom in) or pixels (which remain the same size).

- You can adjust the size of the spheres/pixels, or use the "Automatic" checkbox to let the program pick.

13.2. Which Reflections to Display

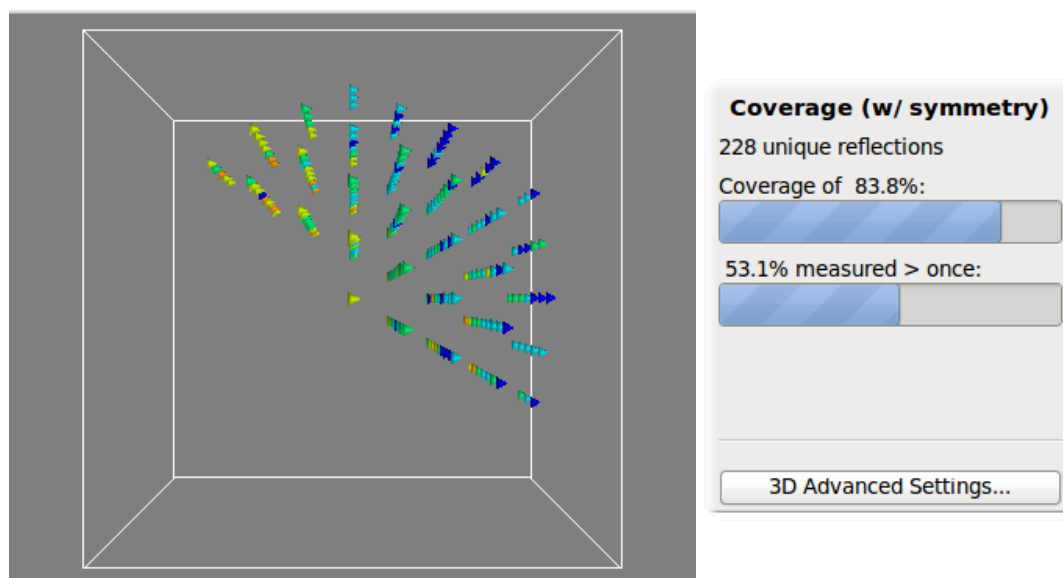
- In the drop-down box **Show which peaks:** **Measured reflections only**, you can pick whether to show all reflections, only those that have at least one measurement, or only the ones that were never measured.
- Here is what is shown if you select to show only the measured peaks



- The statistics panel tells you how many reflections are in the experiment, and what percentage were measured once, and twice or more.


13.3. Using Crystal Symmetry

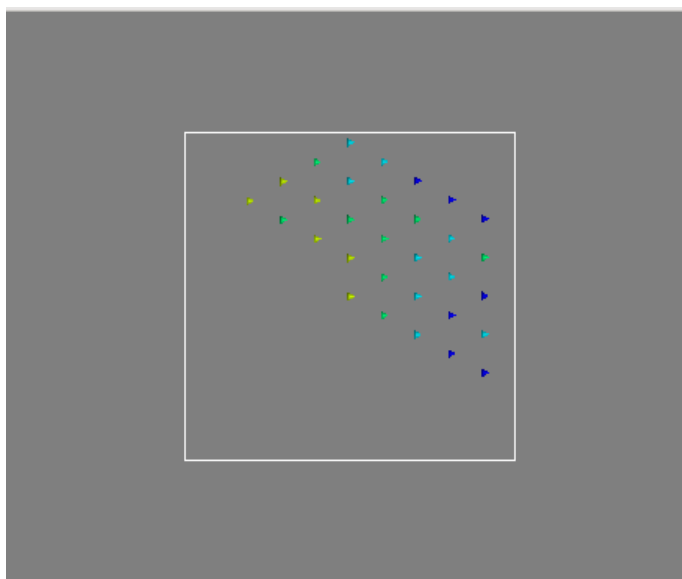
- By checking the ☐ **Use Symmetry?** box, you will take the crystal symmetry into account when considering peaks.
- HKL peaks that are equivalent, due to symmetry, are considered to be the same.
- Here is what is shown if you use symmetry:



- Note how only half of the reflections are visible. This is because the crystal is set to inversion (-1) point group symmetry, meaning that every $[h, k, l]$ has one equivalent reflection at $[-h, -k, -l]$.
- The program only displays the "primary" $[h, k, l]$, and the number of measurements of $[h, k, l]$ and $[-h, -k, -l]$ are added together to do the color-coding.
- Note how the statistics tab now shows a much higher percentage of reflections having been measured at least once, thanks to the symmetry of the crystal. The number of *unique* reflections is also shown.
- Higher symmetries will show even fewer points.

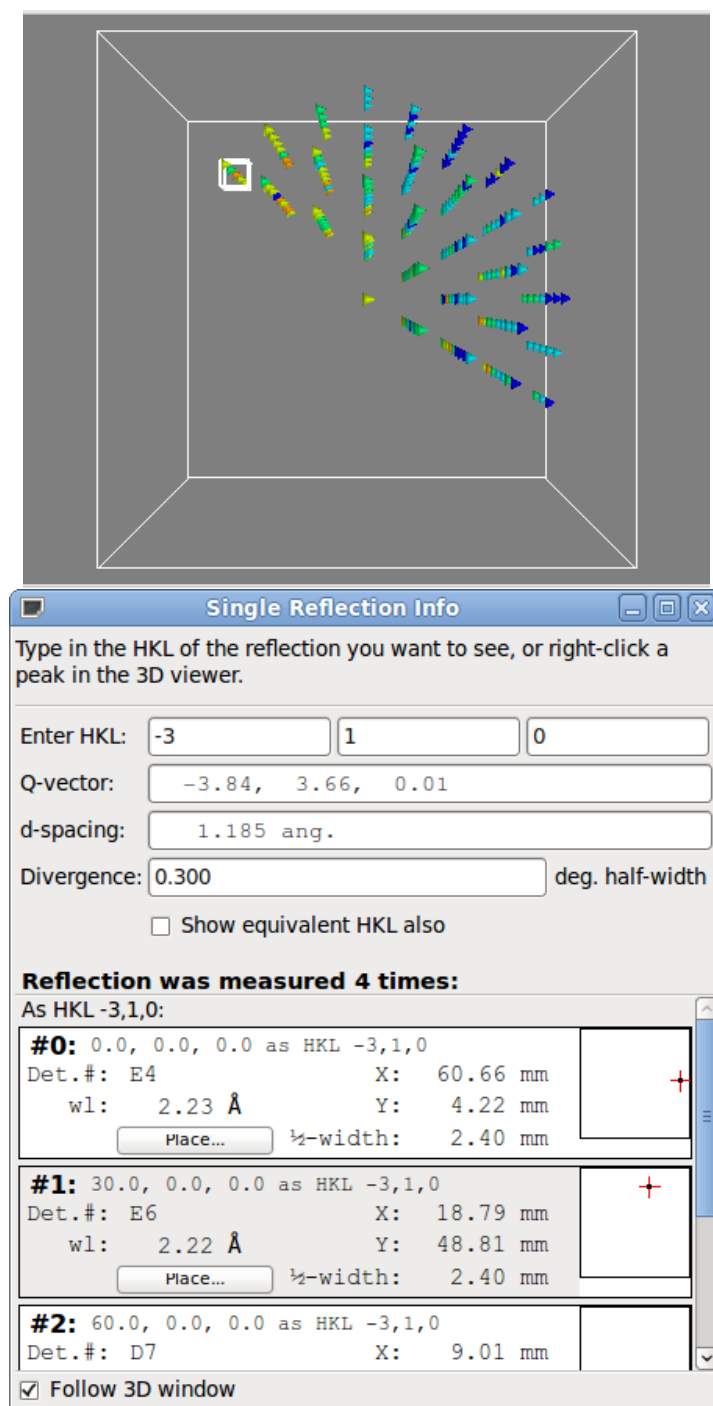
13.4. Parallel Projection

- Parallel projection (as opposed to perspective projection) can be a useful way to visualize reflections in reciprocal space.
- Click the  icon in order to toggle parallel projection on/off. With parallel projection, our crystal looks like this:



13.5. Selecting Reflections

- Right-click on a point in the reflection view to select it. It becomes highlighted with a small cube, and a separate window ("Single Reflection Info") pops up, as shown below:



- When the Single Reflection Info window is up, another way to select a reflection is to type in the H K L indices of the peak of interest. If the peak is out of range (was not calculated), the boxes turn red:

Enter HKL:

- Type in an H,K,L of 3, 2, and -4, and the selected reflection changes:

Enter HKL:

Q-vector:

d-spacing:

Divergence: deg. half-width

☐ Show equivalent HKL also

Reflection was measured 2 times:

As HKL 3,2,-4:

#0: 60.0, 0.0, 0.0 as HKL 3,2,-4 Det.#: B1 wl: 0.87 Å X: -18.58 mm Y: 43.60 mm 1/2-width: 2.24 mm <input type="button" value="Place..."/>	
#1: 90.0, 0.0, 0.0 as HKL 3,2,-4 Det.#: A3 wl: 1.61 Å X: 7.82 mm Y: 28.37 mm 1/2-width: 2.39 mm <input type="button" value="Place..."/>	

- Check the ☒ **Show equivalent HKL also** box and the equivalent hkl's will be displayed in the same list. In this case, -3, -2, 4 is the equivalent HKL:

Enter HKL:

Q-vector:

d-spacing:

Divergence: deg. half-width

☒ Show equivalent HKL also

Reflection was measured 3 times:

As HKL -3,-2,4:

#0: 0.0, 0.0, 0.0 as HKL -3,-2,4	
Det.#: D8 X: -49.59 mm	
wl: 1.03 Å Y: -11.66 mm	
<input type="button" value="Place..."/> 1/2-width: 2.24 mm	

As HKL 3,2,-4:

#0: 60.0, 0.0, 0.0 as HKL 3,2,-4	
Det.#: B1 X: -18.58 mm	
wl: 0.87 Å Y: 43.60 mm	
<input type="button" value="Place..."/> 1/2-width: 2.24 mm	

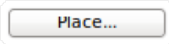
#1: 90.0, 0.0, 0.0 as HKL 3,2,-4	
Det.#: A3 X: 7.82 mm	
wl: 1.61 Å Y: 28.37 mm	
<input type="button" value="Place..."/> 1/2-width: 2.39 mm	

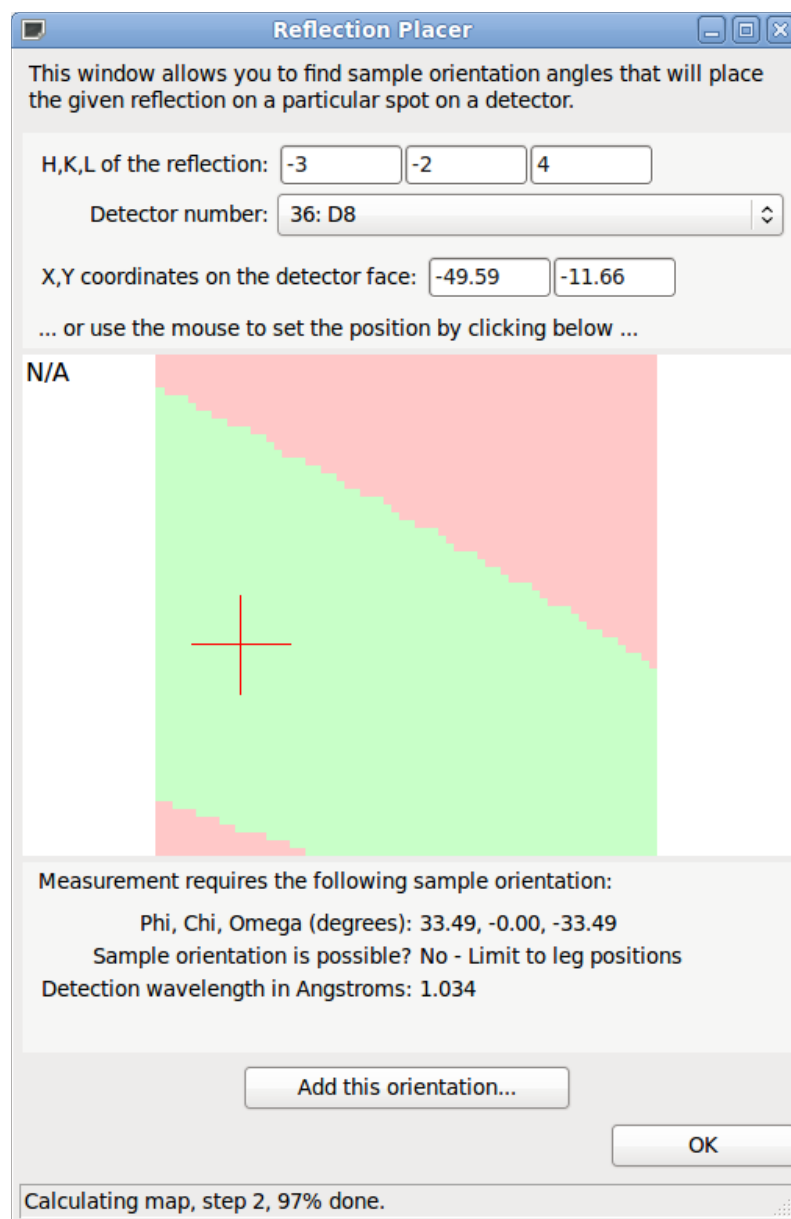
- The Q-vector and corresponding d-spacing of this hkl are shown.
- Each entry corresponds to a different sample orientation where the reflection was measured.

#0: 0.0, 0.0, 0.0 as HKL -3,-2,4	
Det.#: D8 X: -49.59 mm	
wl: 1.03 Å Y: -11.66 mm	
<input type="button" value="Place..."/> 1/2-width: 2.24 mm	

- Several pieces of information are shown:
 - The top line shows the sample orientation angles of that particular measurement, and the HKL at which the reflection was measured (relevant when the ☒ Show equivalent HKL also box is checked.
 - **wl**
The wavelength at which the peak is measured.
 - **Det.#**
The name of the detector on which this peak is measured.
 - **X and Y**
Positions on the detector face, with 0 as the center of the detector.
 - **1/2-width**
The half-width of the spot, assuming the scattered beam has a divergence entered here: deg. half-width . The black spot on the graphic also represents this divergence.

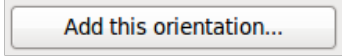
13.6. The Reflection Placer

- Click the  to bring up the reflection placer window:



- The HKL of the reflection you had selected, and the detector on which it was are pre-selected; but you can type in your own selections if you wish to place a particular HKL on a particular detector.
- The map in the center of the window represents the detector face.
- Click on the detector with the mouse, or type in values for the X/Y coordinates you want on the detector.
- The program calculates the sample orientation angles phi, chi and omega that will place the peak at that point.
- Note that the currently selected goniometer has limitations in chi tilt that make some areas not reachable - these are shown in red in the map. Green areas can be achieved; yellow areas are spots where the orientation is possible but the peak will be detected in a wavelength range that is outside the current range set in the Q-Space tab in the main window.
- With an unrestrained goniometer, there is a range of sample orientation angles that will place a peak at a particular point (think of it as performing a rotation of the peaks while keeping your

peak of interest centered). However, for this goniometer, the program attempts to find a chi angle as close to zero as possible (since the goniometer is limited to a few degrees near zero).

- Click the  button and the calculated sample orientation will be added to the current experiment plan.