Helical Data Collection

Helical data collection will collect data across a larger volume of your sample, which can be very advantageous for radiation sensitive samples. It can also be used to collect data from different parts of the same crystal or from multiple crystals within the same loop.

The basic premise of the helical data collection with sergui is to define a vector across you sample. Data will then be collected across this vector in either a segmented or continuous manner.

Segmented Data Collection

In segmented data collection, the sample will make discrete jumps along the defined vector (or user selected positions) and a number of frames will be collected at each discrete location. This method can be used to collect data from different crystals.

Continuous Data Collection

In continuous data collection, the sample will move along the defined vector every frame. Which means that new sample will be introduced each frame. This method can't be used to collect data from different crystals.

The helical data collection gui is opened from the Automation menu pull down menu.
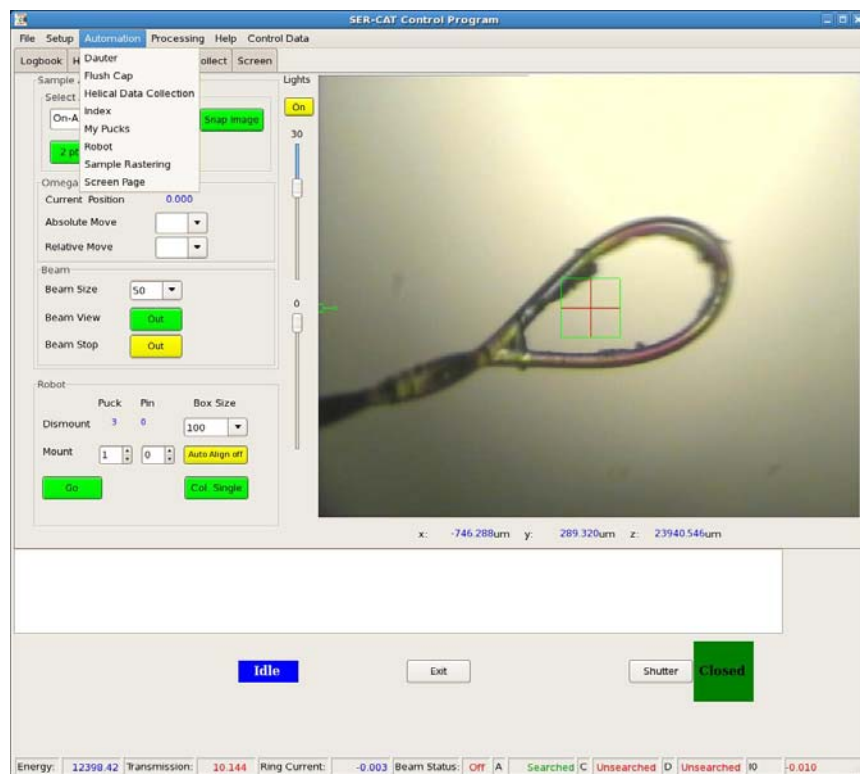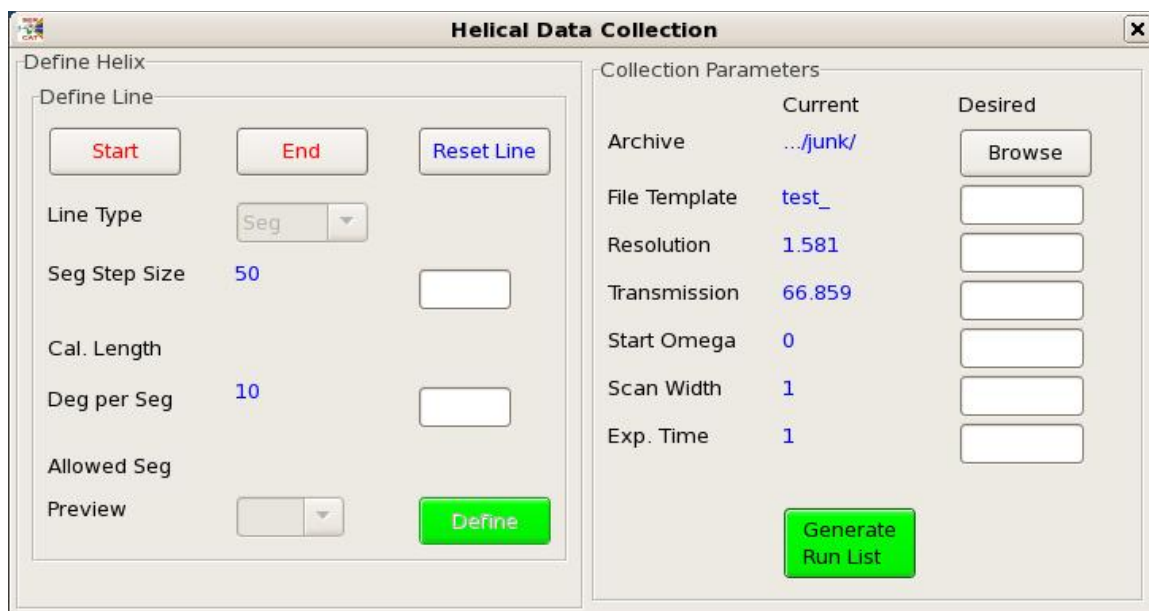
The Helical Data Collection gui is divided into 2 sections: Define Line and Collection Parameters.

Define Line

The start of any helical data collection is to define the initial vector across the sample

Step 1: Align the left most extent of your sample. This point will be used so make sure that it diffracts well. After you are satisfied with the alignment press the Start button.

Step 2: Align the right most extent of your sample and press the End button.

After you have finished setting the end points of the vector, the rest of this section will update. The length of the vector will be calculated and the default Line Type of Segmented (Seg) will be chosen.

Step 3: Select the Type of Line you want: Segmented or Continuous. You can freely go back and forth between these 2 options, but if you have made any modifications to the segment positions they will be lost.
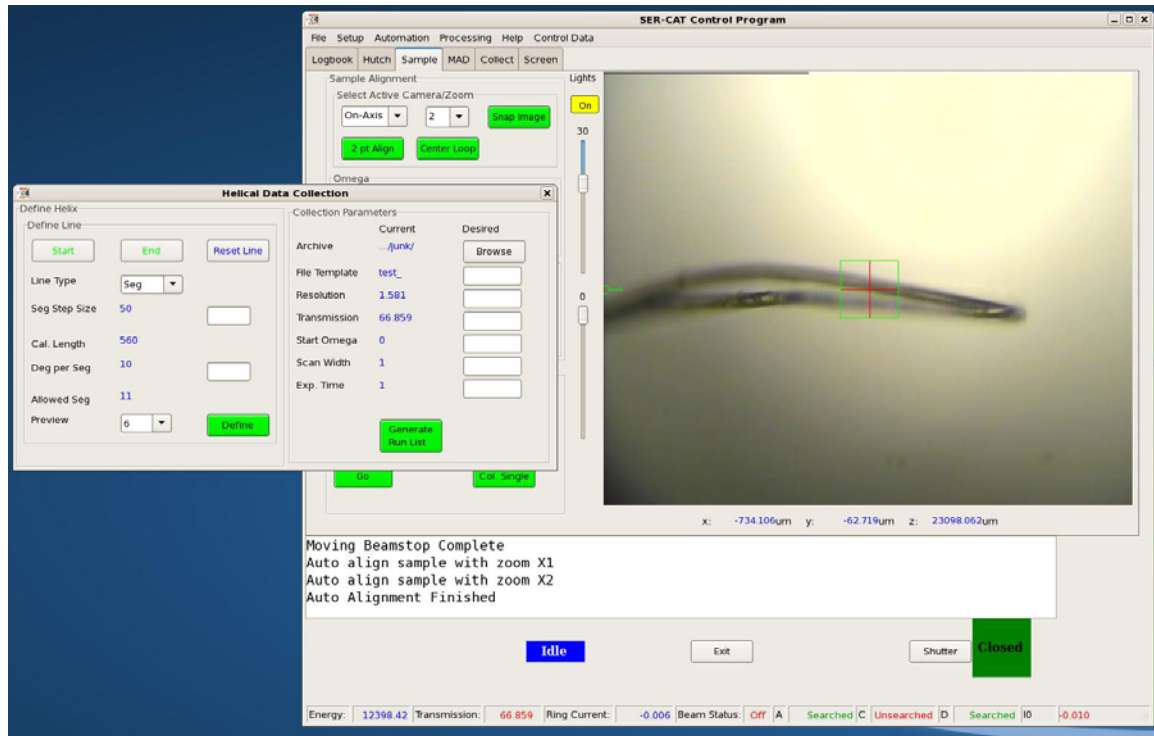
Segmented Data Collection
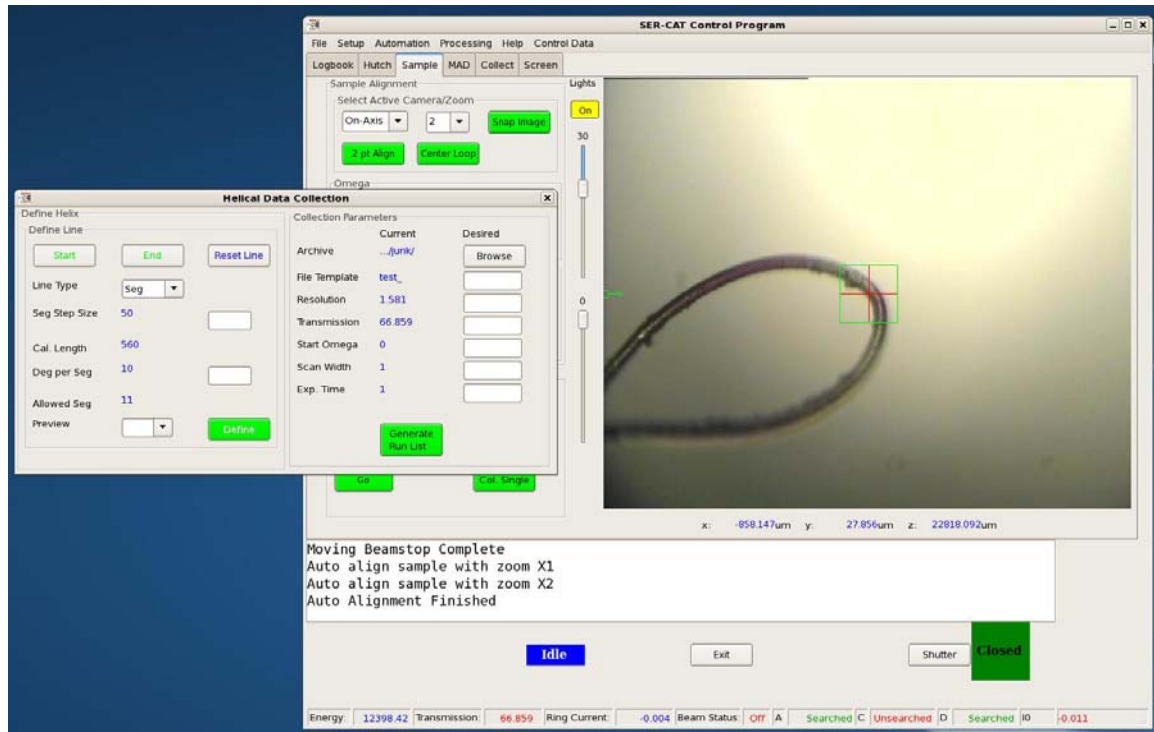
For the Segmented Data Collection mode, the length of the vector will be calculated and the default segment step size of 50 microns and 10 degrees per segment will be applied. The segment step size is used to determine the spacing between the centers of each segment. In the example above, the length of 560 microns results in 11 unique segments.

Note: The user is free to define what spacing (and therefore the number of segments) they prefer. So, if they want they can overlap segments or provide for a larger separation.

The Preview pull down allows the user to see the alignment position for each segment. For example, if 6 sixth (6) segment is chosen in this example the system will look as below. The user is free to collect images at these positions and realign the sample if required. To redefine the segment location just realign the sample and press the Define Button. The option to redefine segment locations can be used to move the segment to any location the user desires. The locations for segmented data collection ***DO NOT HAVE TO BE ON OR NEAR THE ORIGINAL LINE***. These locations can be anywhere! This can be used to select different locations or even crystals.

Note: For different crystals you can define 180 degrees per segment and modify the start position in the collect runs list to be 0 for each segment.

Continuous Data Collection

If the continuous data collection mode is chosen, Define Rotation section will be modified. The vector length will still be calculated but a default of 100 images will be applied. The movement along the vector for each frame will be determined by dividing the length by the number of images. In the example shown below, the length was calculated at 560 microns, so each frame will be incremented 5.6 microns along the vector. The user is free to choose the number of frames, and consequently the step per frame, by entering a different number of frames. The Preview button is less useful in this mode of data collection as it is tedious to go though the positions of all 100 locations to redefine the sample x,y,z position.

Note: Continuous data collection can't be used to collect data on radically different location, such as different crystals within the same loop. The data collection must stay on the defined vector.

Collection Parameters

This section is used to define the experiment. New values need to be entered into the appropriate field and then the Enter button must be pressed on the key board. Only the Blue entries will be use used. Press the Generate Run List Button to update the Collect Runs run list.

For segmented data collection, there will be a different ID and data set for each segment. The initial generation of the run list will assume that the data be collected sequentially, but this can be modified by the user. For example, the user could collect 100 degrees of data at each location by modifying each run list for a total of 100 frames and a start of omega 0 – this will collect 100 degrees of data at each segment location starting at omega = 0.

For continuous data collection there will be a single data set generated. The total number of frames can't be modified in this runlist or the system will eventually crash during data collection. The other parameters can be modified.

Segmented data collection run list

Continuous data collection run list

Pressing the Collect Button will start eh helical data collection. A gui will pop up asking if the user wants to do segmented data collection. Pressing yes will continue the segmented data collection. Pressing no will collect data but the sample will not move during the data collection and will stay wherever it happens to be.