Using Python Data Shell (PDS) to process SPEC data and Pilatus images

1. To look at your Master file, filter your data, and create a Project file:
   1. Launch run\_filter.exe
   2. Click “Load Master File…” and choose your master (.mh5) file.
   3. Filter the scan list (using the buttons) if you wish.
   4. Select attributes you wish to apply, or load an attribute file.-
   5. Select the scans you wish to include in your project file and move them to the right using the arrow keys. You can remove scans from the project list by using the left arrow keys.
   6. Edit the Project Name if you wish.
   7. Click either “New Project File” or “Append Scans To…”
2. To integrate your data:
   1. Launch run\_integrator.exe
   2. Select File>Load Project File and choose your project (.ph5) file
   3. Use the tree at the left to navigate. Hit the “esc” key to return focus to the tree.
   4. To delete a scan from the Project, simply select it and press the “delete” key
   5. Each point is integrated with its current parameters when it is selected. You can integrate multiple data points using the “Integrate Scan” and “Integrate Custom” buttons
   6. For more information about individual parameters, hover over their names for tool tips.
   7. Use the “Apply to Scan” and “Apply to Custom” buttons to apply to multiple points
   8. Use the “Freeze” checkboxes to apply parameters to subsequently selected points. F2 toggles the “Freeze” check box for the ROI
   9. Use the “Bad Point” checkbox to exclude a point from your data set (use F4 to toggle)
   10. Use Image Max to choose a maximum value for scaling the image plots. The default (-1) autoscales on the ROI.
   11. To include a Pilatus bad pixel map, the file must be in the integrator’s current directory, and must have a single empty line at the end. Enter the file name only with no punctuation, then hit Apply above to Custom and choose points/scans.
   12. To copy parameters from one collection of points to another, select Edit>Copy parameters. Choose the points to copy FROM and click “OK”. Choose the points to copy TO and click “OK”. This copies parameters in the FROM list to those in the TO list with the nearest L-values. This is very useful when comparing chemical treatments.
   13. To save the parameters from the current point to an Attribute file (for later use with the Filter), select File>Save attributes
   14. To see the results of the area correction (spill-off and beam footprint), select View>Area Correction
   15. To save an ASCII file with columns for H, K, L, structure factors, and esd’s, select File>Save HKLFFerr. If you did energy scans (escan) with SPEC for RAXR/RIDS, you can save a file with an additional column for energy (File>Save HKLEFFerr)
3. File locking:

The HDF5 file format used by PDS is powerful and efficient, but it is possible to corrupt the files if someone attempts to write to a file that is open elsewhere. Thus, PDS has file locking capability built into it. If you are unable to open a file (Master or Project) because it is locked, go to the directory that contains the file and look for a .lock file. Open it with a text editor to see who owns the lock, and then ask that user to close the Master or Project file. If you feel confident that the lock file is orphaned and that the main file is not really open, you may delete the lock file, but do so with caution.