Data Collection Procedure
Beamline 19ID

Setup Computer and Control Windows

1. Login to LINUX workstation in the 19ID operations area as “userYid” with Y as assigned.
2. Launch the 19-ID user toolbar:
   • Open an xterm session from any workspace on the LINUX desktop.
   • Type “SBCTOOLS”.
   • Iconify the xterm and medm windows.
   • Configure the user toolbar to “Put on All Workspaces”.
3. Launch windows used in beamline control:
   • Go to Beamline LINUX workspace.
   • From user toolbar, select 19-ID–Beamline→Quick Start… to open windows to control Energy…, Tune…, Timing Shutter/Attenuators… and I0 Monitor… automatically.
   • Arrange windows in the workspace.
   • Configure the Beam Intensity window for the I0 monitor to “Put on All Workspaces”.
   • This icon can be used to launch these and other windows individually (see List of User Toolbar Windows at the end of this document).
4. Launch windows used in diffraction image acquisition:
   • Go to sbcollect LINUX workspace.
   • From user toolbar, select 19-ID–sbcollect→Quick Start… to open windows to control sbcollect…, I0 Monitor…, and Beam Stop Position… automatically.
   • Arrange windows in the workspace.
   • This icon can be used to launch these and other windows individually (see List of User Toolbar Windows at the end of this document).
   • Select sbcollect window, choose “Collection” tab and enter initial parameters:

   [NOTE: Do not move between input fields using Tab key].
   • Verify “Exposure Mode” is “ScanOpen”.
   • Verify “Detector Mode” is “Full”, “Hbin” or “Sbin”; choose desired mode using menu button.

   [NOTE: “Full” mode images from the ADSC Quantum 315r detector are ~72 MB in size with 0.051-mm square pixels, while “Hbin” and “Sbin” mode images are ~19 MB in size with 0.102-mm pixels. “Hbin” mode should be used for weakly diffracting samples and “Sbin”, for more strongly diffracting samples.]
   • Note Energy in keV.
   • Verify detector Distance in mm, or input desired value.
   • Specify image template (e.g., test) and the directory into which images will be collected (/net/data/idwX/userYid/… with X = a or b and Y as assigned).

   [NOTE: Template directories should ONLY be changed or created using the browser window (“Click for Browse, Select or Create Template Directory”). Also, sbcollect will prompt you to choose to overwrite files if they already exist.]
   • Acquired images are displayed in “Display” tab window:
     • All pixels in the image are displayed.
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- Left-mouse-button clicking on the image yields positional information, including resolution, and intensity information, including $I/\sigma(I)$.
- Middle-mouse-button clicking and dragging on the image zooms in to a region of interest; middle-mouse-button clicking without dragging restores the unzoomed image.
- Checking “Auto update” displays images as they are acquired.
- Checking “Auto contrast” adjusts the contrast (i.e., “optimizes” black and white pixel values) as each image is displayed; contrast may be adjusted manually using the slide bar at the bottom of the image.
- A previously acquired image may be displayed using “Load file…”; the “Prev” and “Next” buttons allow images within a series to be displayed in sequence.

- Acquired images are also displayed in “Collection” tab window:
  - Every other pixel in the image is displayed.
  - Left-mouse-button clicking on the image yields positional information, including resolution.
  - Middle-mouse-button clicking and dragging on the image zooms in to a region of interest; middle-mouse-button clicking alone restores the unzoomed image.
  - Checking “Auto update” displays images as they are acquired.

5. Launch windows used in fluorescent scanning:
   - Go to Fluorescense LINUX workspace.
   - Open an xterm session on the LINUX desktop.
   - Change directory (“cd”) to the current data collection directory.
   - Run the command HKL3000 at the xterm prompt.
   - Left-mouse-click the “Data Collection” button under the “Data” tab.
   - Left-mouse-click the “Manual Control” button to launch the manual control window.
   - Left-mouse-click the “Energy Scan” tab in the manual control window.

6. For further information on logging in and configuring the data collection workspace, refer to documentation on the SBC web site.

Interlock D-Hutch and Verify Beam Stop Position

1. Go to sbcollect LINUX workspace, and select Fast X-Ray Shutter and Attenuators window:
   - Ensure that Fast X-Ray Shutter is “Close”.
2. Enter D-Hutch:
   - Remove the faceplate from Q315r detector.
   - Ensure beam stop is in place.
3. Interlock hutch and open “Station D Shutters” on PSS Control Panel.
4. Verify beam stop position:
   - From user toolbar, select 19-ID–sbcollect→Configure Attenuators→Verify Beam Stop Position….
   - In sbcollect “Collection” tab window:
     - Verify “Exposure Mode” is “ScanOpen”.
     - Set “Exposure Time” to 1 second; “Sequence Start” to 1, “Number of Images” to 1.
     - Enter a detector Distance of 200 mm.
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- Change the template name to see_beam_stop in the current directory.
- Click “Expose” to take an image.
- View see_beam_stop.0001.img in sbccollect “Display” tab window to verify that no direct beam spot appears on the image; if direct beam is visible, consult SBC staff.
- From user toolbar, select 19-ID–sbccollect→Configure Attenuators→ Restore Previous
  Configuration.…
- Repeat exposure and verification after removing all Al attenuators; if direct beam is visible, consult SBC staff.

Verify and/or Change Monochromator 2 Energy and Undulator Energy Settings

[NOTE: Monochromator 2 energies below 8 and above 13.5 keV should ONLY be accessed with SBC staff assistance.]

1. Go to Beamline LINUX workspace.
2. Select 19-ID Energy Setting window, and in the window:
   - The x-ray Energy/Wavelength can be verified or changed by moving Monochromator 2.
   - Ensure that “harmonic” is 1.
   - The “desired” Undulator Energy should be equal to the Monochromator 2 Energy plus 0.100 keV for Monochromator 2 energies between 8 and 13.5 keV.
   - To change the Undulator Energy:
     - Enter Monochromator 2 Energy plus 0.150 keV in the “desired” field.
     - Click “Start Undulator”; wait for “actual” to equal “desired” energy.

Tune Monochromator 2 to Maximize Photon Flux on Sample

[NOTE: The tuning procedure should be carried out after changing energy and after each APS Storage Ring fill.]

1. Go to Beamline LINUX workspace.
2. Select 19-BM Beam Intensity Optimization window.
3. Left-mouse-click the “Optimize Beam Intensity” button:
   - The “Status: tune” field indicates “Fast Tuning”.
   - The “tune:init” field indicates “busy”.
   - The “tune:busy” field indicates “busy”.
4. After about 20 seconds, beam optimization is complete:
   - The “Status: tune” field indicates “Completed”.
   - The “tune:init” field indicates “idle”.
   - The “tune:busy” field indicates “idle”.

Take Direct Beam Image

1. Go to sbccollect LINUX workspace, and in the sbccollect “Collection” tab window:
   - Note the detector Distance, and ensure that the “2Theta” angle is zero.
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- Insert the 3.0-mm, 0.75-mm, and 0.5-mm Al attenuators.

2. In the 19-ID Beam Stop Support window:
   - Click “store” under X and click “store” under Y.
   - Select “Man” mode for “Load Beam Stop” and “Start Beam Stop” buttons.
   - Set Y increment to 2.0.
   - Under Y, click “+” or “-” (whichever direction would move the beam stop closer to zero).
   - Click “Load Beam Stop”, then “Start Beam Stop”.

3. In the sbccollect “Collection” tab window:
   - Verify “Exposure Mode” is “ScanOpen”.
   - Set “Exposure Time” to 1 second; “Sequence Start” to 1, “Num of Images” to 1.
   - Change the template name to direct_\_distance in the current directory.
   - Click “Expose” to take an image.

4. View direct_\_distance.0001.img in sbccollect “Display” tab window:
   - Zoom in on direct beam position using middle mouse button.
   - If the direct beam spot has less than 10000 peak counts, retake the image for a longer time (e.g., 2 sec); if 65000 peak counts or greater, retake image for a shorter time, increase attenuation or both.
   - Click on spot, and record x and y coordinates in pixels.

5. Use HKL3000 on a LINUX workstation to determine the direct beam position using direct_\_distance.0001on /net/data/idwX/userYid/… with X = a or b and Y as assigned.

6. In the 19-ID Beam Stop Support window:
   - Under Y click “recall”.
   - Click “Load Beam Stop”, then “Start Beam Stop”.

7. Remove 3.0-mm Al attenuator in the sbccollect window, and verify that the beam stop is again in position (repeat Steps 3 and 4 above):
   - If direct beam is visible, consult SBC staff.

8. Repeat Steps 3 and 4 after removing all Al attenuators:
   - If direct beam is visible, consult SBC staff.

Align Nylon Loop and Mount Sample

1. Login to D-hutch LINUX workstation as “userYid”.

2. Launch the 19-ID user toolbar:
   - Open an xterm session from any workspace on the LINUX desktop.
   - Type “SBCTOOLS” in the xterm window to run the user toolbar.
   - Iconify the xterm and medm windows.
   - Configure the user toolbar to “Put on All Workspaces”.

3. Launch windows used in sample mounting and loop alignment:
   - Go to Miscellaneous LINUX workspace.
   - From user toolbar, select 19-ID–sbccollect→sbccollect… and choose “Alignment” tab window to view camera images of the sample for “point-and-click” alignment and to control sample lighting and reflector.

4. Align nylon loop of length typical to those containing samples using sbccollect:
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5. Mount and align sample on goniometer using sbccollect as in previous step (Step 4.).

Collect Test Images

1. Go to sbccollect workspace on the 19ID operations area LINUX workstation, and in sbccollect “Collection” tab window:
   • Insert attenuator(s), if desired:
     ▪ Start with 19-ID–sbccollect→Configure Attenuators→‘Standard’ Data Collection….
     ▪ Alternatively, enter the desired attenuation factor in the field under the “Shutters…” button.
   • Ensure that “Omega”, “Kappa”, “Phi”, “Distance” and “2Theta” parameters are at their desired values. If any are not:
     ▪ Change the value in the appropriate input field.

<table>
<thead>
<tr>
<th>Motion</th>
<th>Lower Limit</th>
<th>Upper Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance</td>
<td>145 mm</td>
<td>1200 mm</td>
</tr>
<tr>
<td>2Theta</td>
<td>0°</td>
<td>35°</td>
</tr>
<tr>
<td>Omega</td>
<td>-120°</td>
<td>120°</td>
</tr>
<tr>
<td>Kappa</td>
<td>-65°</td>
<td>5°</td>
</tr>
<tr>
<td>Phi</td>
<td>-185°</td>
<td>185°</td>
</tr>
</tbody>
</table>

   • Change template name for test crystal images (e.g., XTL01Aa_test) and new directory (/net/data/idwX/userYid/… with X = a or b and Y as assigned), if desired, using the “Template” browser and input field.
   • Verify “Exposure Mode” is “ScanOpen”.
   • Enter desired “Exposure Time” (3-sec minimum) and “Exposure Width” (e.g., 1.0°).
   • Set “Sequence Start” to 1, and “Number of Images” to 1.
   • Click “Expose” to take an image.

2. View XTL01Aa_test.0001.img in sbccollect “Display” tab window.

3. Verify crystal quality (may need exposures at 45 and 90° from initial Omega position):
   • If you wish to save the current and additional exposures, remember to change “Sequence Start” to 2, 3, etc. so that previous images are not overwritten.
   • Images are written to /net/data/idwX/userYid/… with X = a or b and Y as assigned.
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• Use HKL3000 on a LINUX workstation to index, refine orientation and crystal parameters, determine a data collection strategy, and simulate data collection to check for overlapping reflections using image(s) on /net/data/idwX/userYid/….

4. Establish exposure time based on test image(s).

Setup for Data Collection

1. Go to sbccollect LINUX workspace, and in sbccollect “Collection” tab window:
   • Verify beam attenuation for data collection.
   • “Open” timing Shutter.
2. In the PIN Diode I0 Monitor (elt12:pin) window, ensure “VOLTAGE” reads between 1 and 7 V:
   • If it doesn’t, increase or decrease “GAIN”, as appropriate.
3. In the sbccollect window:
   • “Close” timing Shutter.
4. Ensure that there is enough available disk space for the data scan:
   • Images will be written to /net/data/idwX/userYid/…; if not enough space is available, consult SBC staff and remove unnecessary images and other files from /net/data/idwX/userYid.

Start Data Collection

1. In sbccollect “Collection” tab window (sbccollect LINUX workspace):
   • Ensure that “Omega”, “Kappa”, “Phi”, “Distance” and “2Theta” parameters are at their desired values. If any are not:
     ▪ Change the value in the appropriate input field.
   [NOTE: Be mindful of the “Omega” motion limits (see above) when considering the scan range for the experiment. If “Phi” and “Omega” are coincident (i.e., “Kappa” is zero), “Phi” may be used to move desired crystal orientations into the “Omega” range.]
     ▪ Change the template to identify data scan (template name and directory – /net/data/idwX/userYid/…) to be collected.
     ▪ Verify “Exposure Mode” is “ScanOpen”.
     ▪ Change “Exposure Time” (3-sec minimum) and/or “Exposure Width”, if desired.
     ▪ Set “Sequence Start” to 1 and “Number of Images” to image number at Omega limit for scan.
     ▪ Click “Expose” to begin data collection:
       ▪ Images are written to /net/data/idwX/userYid/….
       ▪ View the first few images in sbccollect “Collection” tab or “Display” tab window to monitor them changing with rotation angle.
2. Process images on /net/data/idwX/userYid/… using either:
   • HKL3000 on an assigned LINUX workstation.
   • dtprocess/D*TREK in the dtprocess LINUX workspace.
     ▪ 19-ID–dtprocessÆLocal xterm… E launch local xterm window.
     ▪ Run the command dtprocess.SBC at the xterm prompt and answer the questions issued by the script.
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Archiving Files for Future Use

[NOTE: Files may be copied to user-supplied Firewire (IEEE1394a) or USB drives that are externally attached to either a user-provided portable computer, to an SBC workstation (running Linux) or to an SBC PC (Microsoft Windows XP). The SBC Linux workstations work well with “ext3” file systems. The SBC Windows PC’s work well with “ntfs”, “fat32”, and even Macintosh OS X file systems.]

1. If external drive is connected to a Windows PC:
   • Launch WinSCP and connect to the assigned Data Transfer Server as “userYid”.
   • Copy files from the “remote” directory (/net/data/idwX/userYid/…) to a “local” directory on the external drive.
     ▪ **DO NOT USE “drag and drop” to copy files.**

2. If external drive is connected to a LINUX workstation or Macintosh computer:
   • Open an xterm session on the workstation or computer.
   • Use “ssh” to connect to the assigned Data Transfer Server as “userYid”.
   • Use secure copy commands such as “scp” or “rsync” to copy files from the directory /net/data/idwX/userYid/… to the external drive.

3. If external drive is “ext3” formatted and is connected to a LINUX workstation:
   • Open an xterm session on the workstation or computer.
   • Run the command HomeArchiver at the xterm prompt and answer the questions issued by the script.
     ▪ HomeArchiver executes “rsync” commands in 10 minute intervals after the completion of the previous command to continuously copy files from the directory /net/data/idwX/userYid/… to the external drive.
     ▪ Monitor space on the external drive to ensure that the drive can accommodate all of your data files.

4. To copy files to your home institution via the network:
   • Open an xterm session on a LINUX workstation.
   • Use “ssh” to connect to the assigned Data Transfer Server as “userYid”.
   • Use secure copy commands such as “scp” or “rsync” to copy files from the directory /net/data/idwX/userYid/… to a computer at your home institution.

5. Consult SBC staff for further details.
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### List of User Toolbar Windows

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<tr>
<td></td>
<td>EPS→Module 1…</td>
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<td>Vacuum→Multi-Gauge Summary…</td>
<td>19-ID beamline vacuum gauge status.</td>
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<td>Scanning→Control…</td>
<td>Fluorescence Scanning Control.</td>
</tr>
<tr>
<td></td>
<td>Scanning→Detectors…</td>
<td>Scanning Detectors.</td>
</tr>
<tr>
<td></td>
<td>Scanning→Acquire &amp; Plot using IDL …</td>
<td>display fluorescence scans.</td>
</tr>
<tr>
<td></td>
<td>Scanning→Elements→Generic… etc.</td>
<td>setup Fluorescence Scanning Control for particular elements.</td>
</tr>
<tr>
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<td>Fast X-Ray Shutter and Attenuators.</td>
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<td>Intensity Monitors…</td>
<td>Beam Intensity.</td>
</tr>
<tr>
<td></td>
<td>Chooch xterm…</td>
<td>local xterm to execute Chooch.SBC script.</td>
</tr>
<tr>
<td>Beamlne</td>
<td>Timing Shutter/Attenuators…</td>
<td>Fast X-Ray Shutter and Attenuators.</td>
</tr>
<tr>
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<td>I0 Monitor…</td>
<td>Beam Intensity.</td>
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<td>Tune…</td>
<td>19-ID Beam Intensity Tuning.</td>
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<td>Collimation…</td>
<td>19-ID Collimation Setting.</td>
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<td>adxv.bin…</td>
<td>adxv display window and interface to display previously collected images.</td>
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<td>19-ID Sample and Q315R Detector Positioning.</td>
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<td>Local xterm…</td>
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<td>sbccollect graphical user interface.</td>
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<td>collect Watch diagnostic window.</td>
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<td>configure attenuators to verify beam stop position, to restore setting prior to beam stop verification or for “standard” data collection.</td>
</tr>
<tr>
<td>dtprocess</td>
<td>Local xterm…</td>
<td>local xterm window.</td>
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