

Data Collection Procedure

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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 fluorescence scanning:
 - Go to **Fluorescence** LINUX workspace.
 - From user toolbar, select (left mouse button) 19-ID–Fluorescence→Quick Start... to open windows for Scanning →Control..., Scanning→Acquire & Plot using IDL..., Timing Shutter/Attenuators..., Intensity Monitors..., and Chooch xterm... automatically.
 - Arrange windows in the workspace.
 - Configure the Fast X-ray Shutter and Attenuators window 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 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).
5. Launch windows used in diffraction image acquisition:
 - Go to **sbccollect** LINUX workspace.
 - From user toolbar, select 19-ID–sbccollect→Quick Start... to open windows to control sbccollect..., 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 sbccollect 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 either “Full”, “Hbin” or “Sbin”; choose desired mode using menu button.

[NOTE: **“Full” mode images from the ADSC Quantum 315 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.

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- 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, sbccollect 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.
 - 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.
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 **sbccollect** LINUX workspace, and select Fast X-Ray Shutter and Attenuators window:
 - Ensure that Fast X-Ray Shutter is “Close”d.
2. Enter D-Hutch:
 - Remove lead faceplate from ADSC Quantum 315 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–sbccollect→Configure Attenuators→ Verify Beam Stop Position....
 - In sbccollect “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.
 - Change the template name to see_beam_stop in the current directory.
 - Click “Expose” to take an image.

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- 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 0.100 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-ID Beam Intensity Tuning window, and in the window:
 - Select “Auto” mode for “Load Value” and “Start” buttons.
 - Ensure that “Backlash” is selected from the “motion” menu button.
 - Set “Gain” on both the Inboard (elt23) and Outboard (elt24) detectors of the PIN Diode Detector Array until “Voltage” is between 1 and 7 V (increase and decrease by clicking “>” and “<” buttons, respectively).
 - Normalize the Current readings for both detectors to the APS Storage Ring Current by selecting “aps1” from the “Normalized by” menu button.
4. Use Monochromator 2 Tune to maximize photon flux as measured by the Inboard (elt23) and Outboard (elt24) detectors of the PIN Diode Detector Array *without* opening Fast X-ray Shutter and exposing sample:
 - Set Monochromator 2 Tune increment to 10.
 - Click “store” to record starting value.
 - Click “+” or “-” and observe “Current” values on elt23 and elt24 detectors; continue until values are maximized.
 - If “Voltage” rises above 10 V on either or both detectors, reduce “Gain” by the same amount on both detectors until “Voltage” is between 1 and 7 V.

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- Near maximum “Current” values, change increment to 2 for finer adjustments; continue clicking “+” or “-” again until “Current” values are maximized.
5. Select window for PIN Diode I0 Monitor (elt12:pin); this detector is located downstream of Fast X-ray Shutter to measure photon flux on sample:
 - Click “Load” under OFFSET RATE to set gain offset in Beam Intensity monitor elt12:pin window.
 - Open Fast X-Ray Shutter in Fast X-ray Shutter and Attenuators window.
 - Set “GAIN” until “VOLTAGE” is between 1 and 7 V in Beam Intensity monitor window.
 - Close Fast X-Ray Shutter.
 - If attenuators are later placed in the beam, recheck elt12:pin “VOLTAGE” to make sure it is in proper operating range **before beginning data collection** (see Setup for Data Collection below).

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.
 - 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_date_distance* in the current directory.
 - Click “Expose” to take an image.
4. View *direct_date_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_date_distance.0001* on `/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.

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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 “ssh plum SBCTOOLS” in the xterm window to run the user toolbar remotely from the LINUX workstation plum in the 19ID operations area.
 - Iconify the xterm and medm windows.
 - Configure the user toolbar to “Put on All Workspaces”.
3. Launch windows used in loop alignment and sample mounting:
 - Go to **Miscellaneous** LINUX workspace.
 - From user toolbar, select 19-ID–Miscellaneous→Sample Positioning... to open window to control goniometer and detector positioning.
 - From user toolbar, select 19-ID–sbccollect→sbccollect... and choose “Alignment” tab window to view camera images of the sample and to control sample lighting and reflector.
 - Arrange windows in the workspace.
4. Align nylon loop of length typical to those containing samples.
5. Mount and align sample.

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.

Current Motion Ranges

Motion	Lower Limit	Upper Limit
Distance	145 mm	1200 mm
2Theta	0°	35°
Omega	-120°	120°
Kappa	-65°	5°
Phi	-185°	185°

- 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°).

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- Set “Sequence Start” to 1, and “Number of Images” to 1.
- Click “Expose” to take an image.

[NOTE: The Quantum 315 detector collects 2 shutter-closed (i.e., dark) images for the specified “Exposure Time” before the timing shutter opens to collect the x-ray 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.
 - 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:

[NOTE: The Quantum 315 detector collects 2 shutter-closed (i.e., dark) images for the specified “Exposure Time” before the timing shutter opens to collect the first of a series of images.]

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- 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-dtprocess → Local xterm... ☛ launch local xterm window.

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. 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.
4. Consult SBC staff for further details.

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List of User Toolbar Windows

Icon	Menu Item	Window/Function
EQUIPMENT	APS→Storage Ring History...	APS Storage Ring information and status.
	EPS→Module 1...	19-ID Equipment Protection System status and reset.
	Vacuum→Multi-Gauge Summary...	19-ID beamline vacuum gauge status.
Fluorescence	Scanning→Control...	Fluorescence Scanning Control.
	Scanning→Detectors...	Scanning Detectors.
	Scanning→Acquire & Plot using IDL ...	display fluorescence scans.
	Scanning→Elements→Generic..., etc.	setup Fluorescence Scanning Control for particular elements.
	Timing Shutter/Attenuators...	Fast X-Ray Shutter and Attenuators.
	Intensity Monitors...	Beam Intensity.
	Chooch xterm...	local xterm to execute Chooch.SBC script.
	Beamline	Timing Shutter/Attenuators...
I0 Monitor...		Beam Intensity.
Energy...		19-ID Energy Setting.
Tune...		19-ID Beam Intensity Tuning.
Collimation...		19-ID Collimation Setting.
High/Low Energy Operation...		19-ID Setup for High/Low Energy Operation.
dtdisplay		adxv...
	adxv.bin...	adxv display window and interface to display previously collected images.
	dtdisplayid...	dtdisplay display window and interface.
Miscellaneous	Sample Positioning...	19-ID Sample and Q315 Detector Positioning.
	Local xterm...	local xterm window.
sbccollect	sbccollect...	sbccollect graphical user interface.
	Beam Stop Position...	19-ID Beam Stop Position.
	I0 Monitor...	Beam Intensity.
	sbccollect Watch...	collect Watch diagnostic window.
	Configure Attenuators→Verify Beam Stop Position..., etc.	configure attenuators to verify beam stop position, to restore setting prior to beam stop verification or for “standard” data collection.
dtprocess	Local xterm...	local xterm window.