Data Collection Procedure
Beamline 19BM

Setup Computer and Control Windows

1. Login to LINUX workstation in the 19BM operations area as "userYbm" with Y as assigned.
2. Launch the 19-BM 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 <u>All</u> Workspaces".
3. Launch windows used in beamline control:
   - Go to **Beamline** LINUX workspace.
   - From user toolbar, select 19-BM–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 <u>All</u> 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 **sbccollect** LINUX workspace.
   - From user toolbar, select 19-BM–sbccollect→sbccollect… to open the sbccollect graphical user interface.
   - Arrange windows in the workspace.
   - This icon can be used to launch this 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 "Full", "Hbin" or "Sbin"; choose desired mode using menu button.

[**NOTE: "Full" mode images from the ADSC Quantum 210r detector are ~32 MB in size with 0.051-mm square pixels, while "Hbin" and "Sbin" mode images are ~8 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/bmwX/userYbm/… 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.
5. Launch windows used in fluorescense 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.

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 the faceplate from Q210r 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-BM–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.
  - View see_beam_stop.0001 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-BM–sbccollect→Configure Attenuators→Restore Previous Configuration....
  - Repeat exposure and verification after removing all Al attenuators; if direct beam is visible, consult SBC staff.

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Verify and/or Change Monochromator Energy Setting

[NOTE: Monochromator energy changes greater that 0.020 keV should ONLY be accessed with SBC staff assistance.]

1. Go to **Beamline** LINUX workspace.
2. Select 19-BM Energy Setting window, and in the window:
   - The x-ray Energy/Wavelength can be verified or changed by moving Monochromator.

Tune Monochromator 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.
   - Insert the 3.12-mm, 0.70-mm, and 0.56-mm Al attenuators.
2. In the sbccollect "Motion/Energy tab window:
   - Set Y increment to 2.0.
   - Under Y, click "-" to move beam stop down 2 mm from intercepting direct beam.
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 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/bmwX/userYbm/… with X = a or b and Y as assigned.
6. In the sbccollect "Motion/Energy tab window:
   - Under Y click "+" to move beam stop up 2 mm to restore it to intercepting direct beam.

7. Remove 3.12-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 Crystal

1. Login to D-hutch LINUX workstation as "userYbm".
2. Launch the 19-BM 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 <u>All</u> Workspaces".
3. Launch windows used in sample mounting and loop alignment:
    *   Go to **Miscellaneous** LINUX workspace.
    *   From user toolbar, select 19-BM–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:
    *   Left-mouse-click "Move to Mount" button in "Alignment" tab window, and after goniometer head has moved perpendicular to the cold stream, mount empty loop on goniometer head.
    *   Left-mouse-click "Auto Loop Align" in "Alignment" tab window, and after goniometer has moved and sample reflector is visible in the lower left and right images of "Alignment" tab window (approximately 30 seconds), loop should be aligned in upper left image of "Alignment" tab window.
    *   Left-mouse-click in lower left and right images of "Alignment" tab window and rotate omega between –90, 0 and 90 ° to complete alignment of empty loop.
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 19BM operations area LINUX workstation, and in the sbccollect "Collection" tab window:
    *   Insert attenuator(s), if desired:
        *   Start with 19-BM–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.

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Current Motion Ranges

Motion	Lower Limit	Upper Limit
Distance	125 mm	850 mm
2Theta	0°	30°
Omega	-120°	120°
Kappa	-5°	45°
Phi	-185°	185°

- Change template name for test crystal images (e.g., XTL01Aa_test) and new directory (/net/data/bmwX/userYbm/… 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., 1.0º).
- Set "Sequence Start" to 1, and "Number of Images" to 1.
- Click "Expose" to take an image.
2. View XTL01Aa_test.0001 in sbccollect "Display" tab window.
3. Verify crystal quality (may need exposures at 45 and 90º 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/bmwX/userYbm/… 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/bmwX/userYbm/….
4. Establish exposure time based on test image(s).

Setup for Data Collection

1. Go to **sbccollect** LINUX workspace, and in the 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/bmwX/userYbm/…; if not enough space is available, consult SBC staff and remove unnecessary images and other files from /net/data/bmwX/userYbm.

Start Data Collection

1. In the sbccollect "Collection" tab window (**sbccollect** LINUX workspace):
    - Ensure "Omega", "Kappa", "Phi", "Distance" and "2Theta" parameters are at their desired values. If any are not:
        - Change the value in the appropriate input field.

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[**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/bmwX/userYbm/…) 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/bmwX/userYbm/….
  - 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/bmwX/userYbm/… using either:
  - HKL3000 on an assigned LINUX workstation:
    - Run the command HKL3000 at the xterm prompt.
  - dtprocess/D*TREK on an assigned LINUX workstation:
    - Run the command dtprocess.SBC at the xterm prompt and answer the questions issued by the script.

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 "userYbm".
  - Copy files from the "remote" directory (/net/data/bmwX/userYbm/…) 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 "userYbm".
  - Use secure copy commands such as "scp" or "rsync" to copy files from the directory /net/data/bmwX/userYbm/… 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/bmwX/userYbm/… to the external drive.
    - Monitor space on the external drive to ensure that the drive can accommodate all of your data files.

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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 "userYbm".
    - Use secure copy commands such as "scp" or "rsync" to copy files from the directory /net/data/bmwX/userYbm/… to a computer at your home institution.
5. Consult SBC staff for further details.

Restarting SBCServer Process

[NOTE: If sbccollect appears unresponsive and/or the sbccollect "Collection" tab window shows "Offline", the SBCServer process needs to be restarted. Restarting SBCServer during data collection should not interrupt or terminate data collection.]

1. From user toolbar, select 19-BM–TOOLS➔Restart SBCServer… .
    - sbccollect "Collection" tab window should show "Offline" and input fields might go blank.
    - Within 20 seconds, sbccollect "Collection" tab window should show "Connected", input fields should show proper values and sbccollect should again appear responsive.
2. If sbccollect remains unresponsive, repeat procedure (19-BM–TOOLS➔Restart SBCServer…).
3. If sbccollect still remains unresponsive, repeat procedure (19-BM–TOOLS➔Restart SBCServer…) a third time.
4. If sbccollect still remains unresponsive, consult SBC staff.

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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-BM Equipment Protection System status and reset.
	Vacuum→Multi-Gauge Summary…	19-BM beamline vacuum gauge status.
Fluorescense	Scanning→Control…	Fluorescense Scanning Control.
	Scanning→Detectors…	Scanning Detectors.
	Scanning→Acquire & Plot using IDL …	display fluorescense scans.
	Scanning→Elements→Generic…, etc.	setup Fluorescense 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…	Fast X-Ray Shutter and Attenuators.
	I0 Monitor…	Beam Intensity.
	Energy…	19-BM Energy Setting.
	Tune…	19-BM Beam Intensity Tuning.
	High/Low Energy Operation…	19-BM Setup for High/Low Energy Operation.
dtdisplay	adxv…	adxv display window and interface to display images as they are collected.
	adxv.bin…	adxv display window and interface to display previously collected images.
	dtdisplaybm…	dtdisplay display window and interface.
Miscellaneous	Sample Positioning…	19-BM Sample and Q210r Detector Positioning.
	Local xterm…	local xterm window.
sbccollect	sbccollect…	sbccollect graphical user interface.
	I0 Monitor…	Beam Intensity.
	sbccollect Watch…	collect Watch diagnostic window.
	Configure Attenuators→Verify Beam Stop Position…, etc.dtcollect Watch…	configure attenuators to verify beam stop position, to restore setting prior to beam stop verification or for "standard" data collection.
TOOLS	Restart SBCServer…	restart SBCServer process on 19BM beamline server computer.