Preparing for remote data collection at NE-CAT

**Important Note:** The beamtime and remote login privileges are intended just for you and your group. You are not allowed to share these with any other person or group. If we notice any misuse of these privileges we reserve the right to cancel your current and future beamtime. Currently, remote data collection is available on both 24ID beamlines.

**Requirements:** NE-CAT remote data collection software is designed to connect to the beamlines via a web browser. Currently fully supported browser is the latest (no more than half year old) version of Firefox. You will need a computer with a high-speed internet connection and an optional webcam, speakers and microphone (for webex session). All graphical information is best reproduced on a computer monitor with screen resolution of 1680x1080 or higher. If you want to download diffraction images and inspect them locally, you would need a program like *adxv* installed.

**Dewar shipping:** Dewars should be shipped to arrive at NE-CAT at least one working day in advance of the beam time. Please note that dewars are not delivered to NE-CAT during the weekend and holidays. Provide the support staff with the tracking number. Mark your name on the dewar, if it is not obvious in the shipping label. Attach a return shipping FedEx label with the dewar. See [http://necat.chem.cornell.edu/userprogram/shippinginfo.htm](http://necat.chem.cornell.edu/userprogram/shippinginfo.htm). If you prefer to receive your data via a hard drive (rather than via the internet), you should send it along with the dewar.

**7 days before:** Users need to inform NE-CAT support staff of their intention to collect data remotely.

**3-4 days before:** If you are a first time user, a group login will be created for you on the remote server (https://remote.nec.aps.anl.gov:3001). Each group has a primary investigator (P.I.), an administrator, and regular users. The P.I. and the group administrator will be able to create/update/delete group users, taking responsibility for managing group members’ access privileges. Once a user is created, he/she can obtain a password by clicking on the password recovery link and entering their email address (which was entered by the administrator). Ship your dewars.

**1-2 days before:** You should provide your beamline support with a document detailing the pucks you have sent, and inform them which pucks (up to 14) you would like to have loaded when you start your data collection. You should also send a phone number where you and your group members can be reached. Your beamline support will email you details for a WebEx session to be used for communication during your data collection time, a script for syncing your remotely collected data to your home computers (the password is usually valid for 3-4 days only), as well as any additional details you may need.

**On the day:** Remote data collection experiments will start at 11am. However, support staff will let you know if an earlier start is possible. Your local support will load the first pucks you requested, enable remote control and then notify you that you are good to go.
When users log in to https://remote.nec.aps.anl.gov:3001 during their access time, they will have the option to control the session, observe the session, or to inspect the images from the session as they are collected. Note that only one web browser instance can have control at a time, while more than one web browser instances can observe and/or inspect images. You can interact with your local support via a WebEx video session, the telephone (24ID-C phone number is 630-252-1824) or using the chat session window inside the remote interface.

We will load pucks at 11am. Puck change can be requested only between 11am to 6pm. Note that puck change takes approximately 20-40 minutes. So, plan your beamtime accordingly, especially if there are multiple groups participating in a trip.

Afterward: Once your data collection is done, fill-out the end of the run form located at http://necat.chem.cornell.edu/userprogram/endofrunsummary.htm. Your dewar and hard drive will be shipped back to you using a FedEx label supplied by you. Your dewar will not be shipped back unless you provide a return-shipping label. You will be able to browse your images on the remote server for one week, and your local support will be able to help you with any problems you may have with your data.
Remote Data Collection on 24ID-C

short manual, version of October 2016

Note 1. All beamline software and hardware are under intense development: new features are constantly added or modified. Your support personnel will provide most up-to-date information. Please send your comments and suggestions about the manual to igor@anl.gov.

Note 2. Currently several beamline functions are not yet implemented in the remote session, including EXAFS scans (should be requested well in advance to be done by beamline personnel) and no mini-kappa support. Stay tuned for these features.

1. Starting the new session:

Once you receive an explicit permission from your support personnel, please login to https://remote.nec.aps.anl.gov:3001 with your registered email address and password. Initial password and forgotten password may be recovered by clicking on “Password Recovery” link in lower left menu and providing a registered email; after login you can change the password.

After a successful login you should accept NE-CAT user policy:

![Confirmation]

and you should see in your browser a screen similar to one in Figure 1.

![Figure 1. Selection of the remote session]

Your current session will have “OBSERVE”, “CONTROL” and “Images” buttons, assigned to your
group/institution (like a first line for NECAT on a figure above). The other sessions for your group (if any) will be grayed out. If you don’t see your group/institution, please call your support personnel. Only one member (IP address) of your group can “control” the beamline (data collection), while more than one can “observe” or browse “images”.

Press “GetSync” button to get the script for real-time data transfer (password is valid for 5 days only).

For real-time data processing results you should check RAPD processing in a separate browser instance: login to https://rapd.chem.cornell.edu/rapd (login/password for RAPD are currently different from remote session).

To collect data press “Control” button. This will bring you to a screen similar to one in Figure 2. This will be your main working environment for the remote session.

![Figure 2. Initial view of the main working environment for the remote session.](image)

The default view is “Collection”; “Images” tab may be used to visualize all diffraction images; “Scan” is used to setup different scans of the loop/crystal; “Tools” tab is used to start CHAT session with your support person and restart “Console”, all others functions under “Tools” tab are under development.

On the right side of the screen there are two small live video feeds of the sample/goniometer area: they can be stowed away or brought back to view window by clicking on the arrow. Top video feed is pre-assigned to three different views inside the experimental hutch: close-up view of the mounted crystal (“Sample”), view of the robot dewar (“Robot”) and the wide-angle view of the hutch (“Wide”). Have patience while camera switches the view. It may takes up to 20 sec. for the camera to switch.

On the bottom of the screen there are several informational boxes; moving the cursor over each box
will show some additional information. If the box is yellow, it means the corresponding value needs attention. Certain boxes can be double-clicked to change experimental parameters: double-clicking on “X beam pos.” or “Y beam pos.” will trigger a trimming of the beam position in the corresponding direction; double-clicking on “AutoalignTimer” will align the beam to the sample position; double-clicking on “Aperture” will allow change of aperture size; double-clicking on the box with mounted crystal ID (like B6 in Fig.2) will setup a crystal mounting dialog; double clicking on “Energy” will bring a pop-up dialog for energy change.

Click on “Main” button inside the “Light” box to illuminate the crystals; “Aux” will add a weak external illumination, which may not be apparent.

The central portion of the screen will show the mounted crystal and will be used for crystal centering. If you don’t see the sample after a mount, click on the “sample” on the top-left video feed and visually check if a sample is indeed mounted. If the sample is visible on the goniometer, set the zoom to 1 and rotate the crystal to bring it into the visual field of centering video feed and move it manually to the right by pressing on the > arrows.

To start a chat session with your support personnel, go to “Tools” tab and click on “Chat” bar. Click on “window” button and a new, floating chat window will appear: see figure below.

Move the small “Chat Window” to the bottom of the main window (above the lower menu) and re-size it; go back to “Collection” tab. Check Figure 3 for the best location of the chat window in the main window.

It is strongly advised that all members of the group have this small “chat” window open during remote data collection session.
II. Mounting and centering crystals

1. Click “Other” in “Change Sample” box – new pop-up “Robot Control” window will appear

Currently, crystal C10 is mounted; clicking on “previous” or “next” buttons will mount corresponding crystals, or you may make a selection using the two selection boxed below (C and 11 on the figure)

“Options” box includes “Unmount” button and the button to set “Load Position” - if your pins are constantly longer/shorter than 18mm, it is possible to save the current pin length; use with extreme caution!

If there is ice on the crystal, dismount it and mount again.

“Current pucks” may include information about the real names of your pucks (input is done by your support personnel)

2. Make selection (puck ID and crystal # - currently on the figure it is C11) and press “confirm”.

3. Wait; in ~75 seconds the crystal will be mounted, illuminated and visible in the central portion of the screen. “Robot mount in progress” will disappear and the bell will sound.

4. Center the crystal (step 5-10 below)

5. Change zoom to 1

6. Click in “3Click” button in “Centering” box – a number “1” will appear left from “3-Click” button.

7. Perform “3-Click” centering by clicking on your crystal – click once on the sample; wait, crystal rotates by 90 degree; click second time, etc. (total THREE clicks should be done). If you change your mind, “Abort” button may be used get out of “3-click” alignment cycle. It is recommended to finish 3-clicks centering without aborting the operation (“abort” function currently is not very stable).
8. Increase zoom (i.e. to 5) and repeat “3-Click” alignment.

9. Check crystal alignment by manually rotating it using “Omega” box buttons.

10. Repeat “3-click” centering again, if necessary.

11. If the goniometer is equipped with mini-kappa MK3, mini-kappa functions will be visible, otherwise only OMEGA rotation box will be present (as on Fig. 3). Use of mini-kappa should be requested couple days in advance and it is done only under supervision of the beamline scientist.

12. Proceed to data collections (section III below)

Figure 3. Main screen with illuminated mounted crystal (D2) and beam contour (50x70 micron).
For continuous (helical) data collection mode you should create a vector along the crystal:

a. Align the beginning of the vector, as described in steps 5-10 above. Press “Save” button to save the current centering position, number “1” will appear left of the “save” button.

b. Repeat the centering procedure for a second point along the crystal (endpoint of the vector) and save the second centering position, number “2” will appear left of the “save” button.

Once the vector is created, it will be drawn over your crystal/loop and will follow it during all omega rotations and during snaps/runs configuration setup.

**Note 1:** Re-drawing of the vector during all omega rotations is rather slow.

To clear previously saved vector, if necessary, press “Clear” button.

**Note 2:** The vector should be created for ALL operations in “Scan” tab – raster snaps or alignment by diffraction
III. Data Collection

a. Snapshots

Click on “Snap” button in “Data Collection” box; a new dialog will pop-up (see figure at right):

1. Type in the file prefix in the box “Prefix”. You will see the full final filename below. Change or reset filename index.
2. Select “Paired Snap Acquisition” ON and 90° Offset (highly recommended for RAPD to properly index and estimate the data collection strategy).
3. Type in parameters for the snapshot: initial (starting) angle, oscillation range, exposure time, detector distance and transmission (flux in %).
4. In the “resolution” box you will see corresponding values for current detector distance (you may also input desired resolution and the detector distance will be re-calculated).

*Please note: detector distance should be in the range of 1000 to 150 mm and exposure time should be in a range between 0.2 and 0.5 seconds. It is strongly advised to use”fine-slicing” strategy for data collection using PILATUS-6M detector. It is recommended to use detector distances less than 600mm because of increased air absorption (especially at low energies)*

6. Click “Execute” when ready to collect snapshots.

Now you can see incoming images by clicking on “Images” tab – Figure 4 below. Here you can select and see images and corresponding RAPD processing results, including best strategy for data collection and results of XDS integration.
Figure 4. “Images” tab

In this window it is possible to zoom in/out (1X, 2X and 3X buttons), draw resolution rings and view either single image or one degree slice during “fine-slicing” data collection.

It is possible to see any previously collected image by selecting filename from the history list on the left side of the window.

For high resolution pictures and more advanced viewing functions press “Viewer” button on the main session screen - another pop-up window will appear with high-resolution image.
B. Data Collection - Run Setup

Click on “Run” button in “Data Collection” box; the next dialog window will depend on whether the vector was defined for the crystal (helical scan) or not defined (single spot data collection).

B1. Conventional data collection

If the vector was NOT defined, you will see a simple dialog (above figure). Fill, check and double-check all fields before starting data collection by pressing “Execute”. Buttons in “Edit Runs” box allow you to add/remove extra runs, if necessary.

B2. Continuous vector scan (helical) data collection

If the vector was defined, continuous vector data collection is ON by default, and you will see a different dialog and the vector will be drawn over the crystal:
Once you change any numbers in the “Run Constructor” dialog, the software will draw the beam path on the crystal in green. Numbers under “Insets” (can be either positive and negative) determine the position and the length of the actual data collection vector relative to the initial vector. If “Vector Options” is off, no helical scan will be performed, and all data will be collected from the current centering spot on the crystal.

Currently, helical scan run doesn't use run_ID. Make sure you use a new and unique file_prefix. A problem of file overwriting may corrupt current remote session.

Always use “yes” for shutter-less operation of Pilatus detector.

During data collection all buttons that change the hardware configuration will be disabled. However, you can browse the images. Once data collection is done the bell will sound, and all buttons will be enabled for control. The illumination of the crystal is not ON automatically after snapshots or runs. You may need to press “Main” button in “lights” box (sometimes this button should be pressed two times). You can not see the crystal during data collection, however, auxiliary light can help to some extent, (accessible by pressing “Aux” button).

Please note: exposure time should be in a range between 0.2 and 0.5 seconds. It is strongly advised to use “fine-slicing” strategy for data collection using PILATUS-6M detector.
IV. **Crystal Analysis tools (under development)**

A. **Line scan**

Before any actions the vector along the crystal or the loop should be created in “Collection” tab!

![Image of Crystal Analysis Tab](image)

Figure 6. View of Crystal Analysis Tab (Line tool is selected)

1. Select “Line” in “Select Tools” box

2. In “Scan Setup” box change number of points to collect along the vector, aperture size, exposure time, detector distance and the transmission (flux in %). If necessary, press the “gear” button to access advanced parameters like resolution range for analysis (default 30-3A). Pressing “i” button will produce the detailed instructions in a separate window.

3. Adjust loop/crystal view by changing Omega and Zoom values

4. Once you are satisfied with the scanning protocol – press “Run”

5. The “Scan Progress” dialog will appear, do not abort the scan; during the scan all buttons will be grayed. Wait until you see the results – Figure 7 below.

Note – *The abort button should be used only rarely, as the system recovery time after any “abort” is up to 2 minutes.*
Figure 7. Results of the “line scan” and selection of the”best” spot

6. Browse through all images and statistics by selecting appropriate image number (lower left quadrant) or by choosing the highest number of spots (lower right quadrant)

7. Make selection and press “Selection” in “Move To” box ( “Click” box is not yet implemented). This step is mandatory to exit “scan mode”, even if there is no good diffraction.
B. Grid scan, *aka* “alignment by diffraction”

1. Select “Grid” in “Select Tools” box.

2. In “Grid Mode” box you select either 'Loop' (all loop will be scanned), 'Fill' (only the box created by dragging the mouse will be scanned) or 'Hybrid' – common selection between 'loop' and 'fill' selections (logical AND)

3. In “Scan Setup” box change aperture size, oscillation range, exposure time, detector distance, transmission (flux). If necessary, press the “gear” button to access advanced parameters like resolution range for analysis (default 30-3A). Pressing “i” button will produce the detailed instructions in a separate window.

4. Adjust loop/crystal view by changing Omega and Zoom values

5. Once you are satisfied with the scanning protocol – press “Run”

6. The “Scan Progress” dialog will appear, do not abort the scan; during the scan all buttons will be grayed. Be very patient! - wait until you see the results – Figure 8 below.

![Figure 8. Results of loop scan in “fill” mode](image)

6. Browse through all images and statistics by selecting appropriate image number (lower left quadrant) or by choosing the highest number of spots (lower right quadrant)

7. Make selection and press “Selection” in “Move To” box ( “Click” box is not yet implemented) – the goniometer will be centered at the selected point.

This step is mandatory to exit “scan mode”, even if there is no good diffraction.
C. Occluded view alignment (vertical scan)

1. To find a thin plate-like crystal or a needle-like crystal you may require to do a “vertical” scan. For better results it is recommended to rotate the loop, so its plane is perpendicular to the camera view.

2. Adjust loop/crystal view by changing Omega and Zoom values

3. Select “Vertical” in “Select Tools” box. There are two modes of operations: AUTO and DRAW. In AUTO mode the system will automatically create a vector for you; in DRAW mode you need manually draw the vector across the loop, using the mouse. Make sure the vector is covering the whole loop.

4. In “Scan Setup” box change aperture size, exposure time, detector distance and the transmission

5. Press “Run”; the “Scan Progress” dialog will appear, do not abort the scan; during the scan all buttons will be grayed. Be very patient! - wait until you see the results – figure below.

6. Browse through all images and statistics by selecting appropriate image number.

7. Make selection and press “Selection” in “Move To” box – the goniometer will be centered at the selected point. This step is mandatory to exit “scan mode”, even if there is no good diffraction.
V. Energy Change

To change the energy, double click on “Energy” box in low menu; a new pop-up dialog will appear:

![Energy Change Dialog](image)

Input new energy value and click confirm; wait until it finish. Please note, that any energy change going over 8300eV requires a change in the mirror strip (~12 minutes to finish).

VI. Data Backup

Press “GetSync” button on the main session screen (Figure 1) to get the script for real-time data transfer (password is valid for 5 days only). A new click on “GetSync” will generate a new password inside the script. To run it, open a terminal, go to directory where you want the data to be downloaded (and has enough disk space) and run it as "python sync_script.py -ar". Kill the script once all data is downloaded. You may choose to provide an external hard drive for additional data backup, which will be shipped back with the dewar.

VII. Troubleshooting

The most important advice for a stable remote session is to be patient, and not to use any double-clicking, unless specifically required (i.e. to change the aperture size or to do auto-alignment): Click once and wait for something to happen or the operation to finish.

The remote session is able to automatically reconnect to the beamline control software – it may take couple minutes. If your session is not responsive, – close the current browser, wait one minute and login again.

Still no connection/response? : go to "Tools" tab, select "User Interface Controls" and there is a button called “Restart RAC” you should click on it, wait 30 seconds, next press "Restart Console”; wait one minute for all sockets to re-connect, close the browser and re-login again.

![User Interface Controls](image)

Please use with extreme caution!
If none of these helped, call the beamline (630) 252-1824, or any other number supplied by your support personnel.
Press “Reset Video” button to fix a corrupted video stream.

If you experience a very slow network connection, the remote GUI now includes an option to use “low bandwidth” - the video quality will have low refresh rate and images will have low resolution. To enable - go to "Tools" tab, select "User Interface Controls"