Preparing for remote data collection at NE-CAT

Requirements: NE-CAT remote data collection software is designed to connect to the beamlines via a web browser. Remote runs in recent versions (less than half a year old) of Safari, Chrome, and Firefox; although Firefox is the only full supported browser. To run Remote, you need a computer with a high-speed internet connection. Graphical information is rendered best on a computer screen with resolution of 1680x1080 or higher. If you intend to communicate with your support staff through a web conference your computer will also need speakers, a microphone, and optionally a webcam. If you want to inspect downloaded diffraction images locally, you will 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 your beam time. Please note that dewars are not delivered to NE-CAT during weekends 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. 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. ESAF form should be submitted by your group spokesperson. Only approved people on ESAF can login to ANL network to control the beamline.

3-4 days before: If you are a first time user, a login will be created for you on the remote server (https://remote.nec.aps.anl.gov:3001) and associated with your group. Once a user account is created, you can obtain a password by clicking on the password recovery link and entering your email address (which was entered by the administrator). The new user account info is also included in the automated e-mail.

Time to 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 you would like to have loaded when you start your data collection (up to 14 pucks can be loaded for a full day of 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 WebConf session to be used for training or communication during your data collection time, (if required or requested by you), as well as any additional details you may need.

On the day: Daytime remote data collection experiments will start at 11am; second shift (if any) will start based on the approved schedule. However, support staff will let you know if an earlier start is possible. Your local support will load the 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 (including the inspection of 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. You can
interact with your local support via a WebConf video session, the telephone (provided by you support personnel) or using the chat session window inside the remote interface.

We will load pucks before 11am. Additional puck changes 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](http://necat.chem.cornell.edu/userprogram/endofrunsummary.htm). Your dewar and hard drive will be shipped back to you using the 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 via the Review option, and your local support will be able to help you with any problems you may have with your data.

**Important Note**: Beam time privileges are intended for you and your group. All persons participating during your beam time should be listed on the ESAF and you are not allowed to share access to your remote session with another person or group who have not been listed on the ESAF prior to your experiment. Additionally, your remote login privileges are intended for you only. If another person wishes to control the beamline - they should log in with their own credentials. If we notice any misuse of these privileges we reserve the right to cancel your current and future beamtime.
Remote Data Collection on 24ID-C

short manual, version of April 2020

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 or emission scans for metal identification (should be requested well in advance to be done by beamline personnel only during the daytime). The use of mini-kappa should be discussed in advance with your support personnel.

1. Starting the new session:

The remote session starts when you login to https://remote.nec.aps.anl.gov:3001 with your registered email address and password. Initial, forgotten, or expired passwords 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:

![NE-CAT User Operation Policy](image)

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

![Selection of the remote session](image)

Figure 1. Selection of the remote session
Your current session will have “Sync”, “Observe” and “Control” buttons, assigned to your group/institution (like a first line for NECAT on a figure above). The Webconf button will also be present if your support person has set this option - you may request it if you desire real time video support. The other (old) sessions for your group (if any) will have only “Sync” and “Review” buttons. 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”. Only users with approved APS access and listed on the current ESAF can take control of remote.

Press “Sync” button to get the script for real-time data transfer (password is valid for 4-5 days only). Once the password expires, download the sync script again if you need to continue to transfer files.

For real-time data processing results you should check RAPD processing in a separate browser instance: login to https://rapd.nec.aps.anl.gov/. Credentials for RAPD are provided to each lab and are different from your individual remote credentials.

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”, where crystals are centered and data collection is initiated; “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 for troubleshooting, all others functions under “Tools” tab are under development.

On the right side of the screen there are two small live image streams of the sample/goniometer area: they can be stowed away or brought back to view window by clicking on the arrow, attached to the left
side of the image stream tab. The top image 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. The bottom image stream is a fixed camera mounted directly above the sample mounting area and looking down.

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 may need attention. Certain boxes can be double-clicked to change experimental parameters: 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 switch On/Off the illumination of the loop; “Aux” will add a weak external illumination, which may not be apparent. The Aux light may cause a glare on the loop that makes seeing the crystal hard. Turning Aux off will eliminate the glare.

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 the mount, check step #10 on page 7 for more details.

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 (see below on page 7) for the best location of the chat window in the main window. It is strongly advised that all members of the group who are controlling or observing the session have this small “chat” window open during remote data collection session, so that they can easily see any discussion taking place.
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 in sequential order, 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! We recommend that you use “Unmount” to dismount your last crystal (to prevent frost building up on the sample pin) after you have finished data collection session.

If there is ice on the crystal - dismount it and mount again. This procedure will usually clear off any ice that is loosely bound to the surface of the crystal.

“Current pucks” box 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 a bell will sound when the mount is complete.

4. Center the crystal (step 5-9 below) ; if the loop is not visible – see #10.

5. Click “3-Click” button in “3-click Centering &Saving” box – a number “1” will appear left from “3-Click” button and a green box will surround the central view screen.

6. 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). You should wait until the number left of the "3-click" button increments to the next value before proceeding with the next click. 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).
7. Increase zoom (5 or 6 is a typical value) and repeat “3-Click” alignment. Make sure the crystal is properly centered at zoom 1 before increasing zoom.

8. Check crystal alignment by manually rotating it using “Omega” box buttons – on the right side of the viewing window (Figure 3).

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

10. If the loop/crystal is not visible, confirm the sample was successfully mounted using the image streams on the tab on the right side of the screen. Once it's confirmed that the crystal was mounted on the goniometer, proceed with the following procedure – first, make sure zoom is 1; next rotate the loop in 45° steps either through, or more often into the field of view (the loop will be out of focus). When you see the crystal, initiate 3-click centering and if crystal rotates out of the field of view again, click edge of screen where you saw it disappear. This should result in a more centered crystal that will hopefully stay in the field of view for further centering.

If the loop is too far to the left, you won't see anything as you rotate omega (if lucky, might see the end of the loop at the far left) - use horizontal movements to the right combined with occasional omega rotations until you can see some portion of the loop. Then proceed with “3-click centering”. If only the pin is visible as you rotate omega, use horizontal movements to the left until you can see the loop.

11. Proceed to data collections (section III – page 9)

Figure 3. Main screen with illuminated mounted crystal (D2) and beam contour (50x70 micron).
**Vector creation**

For continuous (helical) data collection mode or line and grid scans you should create a vector along the crystal. To create a vector, you must center on and save the two endpoints of the vector.

a. Center at where you want the vector to begin, as described in steps 5-9 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.

![Vector creation along the crystal](Figure 4)

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.

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

*Note 1:* Re-drawing of the vector during all omega rotations is rather slow, so you may see a lag in the vector position before it is updated.

*Note 2:* The vector should be created for line scan or grid scan (alignment by diffraction). For a line scan, it should only span the region of interest, i.e. the length of the crystal. For a grid scan the vector should cover the whole loop, not only “region of interest”.

*Note 3.* Do NOT create/use vertical vector. The vector should be mostly parallel to the omega rotation axis (+/- 45 degrees).

*Note 4.* Multiple vectors (more than 2 saved points) are not supported and will cause system error. If three or more points were saved – press “Clear” button and start again creating the new vector.
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 can also use the optional project name field – if a project name is entered, an additional sub-directory will be created. You will see the full final filename below.

2. Change or reset filename index. The index resets to 1 after a crystal is mounted and it increments as snapshots are taken.

3. Select “Paired Snap Acquisition” ON and 90° Offset (highly recommended for RAPD to properly index and estimate the data collection strategy). This instructs the beamline to take two images, the first at the indicated initial omega and the second at +90 degrees from the initial omega.

4. Type (or change) parameters for the snapshot: initial (starting) omega angle, Delta omega (oscillation range) – should be ~1 degree, exposure time, detector distance and transmission (flux in %).

5. 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).

6. AutoNaming ON will automatically fill file prefix with PuckID (either the puck name if entered by support personnel or the puck position letter if no name was entered) and crystal ID.

7. AutoTab ON will let the system automatically switch tabs, i.e. the “Images” tab will be open after completion of the snaps.

Please note: detector distance should be in the range of 1000 to 150 mm, delta omega (oscillation range) should be 1° and exposure time should be in a range between 0.5 and 1 second. We recommend to use detector distances less than 600mm because of increased air absorption (especially at low energies).

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

Now you can see incoming images by clicking on “Images” tab – Figure 5 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 5. “Images” tab view**

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. The pop-up blocker should be disabled in your browser.
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 a vector was NOT defined, you will see a simple dialog (above figure).
Fill file prefix and project (optional) fields, input total number of images to be collected, detector distance (or resolution), flux, starting omega (based on the optimal strategy), oscillation range and exposure time. Check and double-check all fields before starting data collection by pressing “Execute”.

*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 EIGER-2 detector (delta omega 0.1°-0.5°).*

Buttons in “Edit Runs” box allow you to add/remove extra runs, or setup the inverse beam data collection, if necessary (see below).
B2. Continuous vector scan (helical) data collection

If a 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 (Figure 6):

![Image of Run Constructor dialog]

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 or 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.

During data collection all buttons that change the hardware configuration will be disabled. However, you can browse the images. Once data collection is done, a 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 will need to be pressed two times before the light will come on) two times). You can not see the crystal during data collection, however, the auxiliary light can help (accessible by pressing “Aux” button).
IV. Crystal Analysis tools (under constant development)

A. Line scan

*Note: Before any actions the vector along the “region of interest” or the crystal should be created in “Collection” tab!*

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 30-3.6 Å). 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 “Define Scan”

5. In a while (~10-15 sec) the vector will be covered with red circles/ovals and the “Scan Commit” window will appear. Press “Go” to start the scan, “Modify” to go back to the setup window or press “Abandon” if you changed your mind.

6. After pressing “Go”, in about ~10-30 sec. a pop-up window “Scan Progress” will appear. During the scan the empty circles/ovals will change color, based on the number of “good” diffraction spots, if any. In the bottom part two windows will open with “table” and graphical view of the number of “good” spots. Wait patiently until “Scan Progress” window will disappear.

*Note – The abort button should be used with caution, as the system recovery time is up to 2 minutes.*
Figure 8. Results of the “line scan” and selection of the “best” spot

7. Browse through all images and statistics by selecting appropriate image number (lower right quadrant) or by choosing the highest number of spots (lower center table) – figure 8.

8. Make selection and press “Move To 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.
B. Grid scan, *aka* “alignment by diffraction”

*Note: Before any action a vector along the whole loop should be created in “Collection” tab!*

The vector should cover the WHOLE loop, not just a region of interest!

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

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

*Figure 9. General view of the Grid Scan initial setup*
3. In “Grid Scan - Primary” box you may change aperture size (starting with bigger aperture is recommended), overlap % between nearby spots during the scan (10-30% is a good choice), detector distance, transmission (flux). If necessary, press the “gear” button to access advanced parameters like resolution range for analysis (default 30-5A). Pressing “i” button will produce the detailed instructions in a separate window.

4. Switch On/Off the light; adjust loop/crystal view by changing Omega and Zoom values. It is recommended to perform the grid scan when the loop is nearly perpendicular to the camera view (and x-ray beam).

5. Once you are satisfied with the scanning protocol – press “Define Primary Scan”

6. In a while (~10-15 sec) the loop will be covered with red circles/ovals and the “Scan Commit” window will appear. Press “Go” to start the scan, “Modify” to go back to the setup window (Figure 8) or press “Abandon” if you changed your mind.

After pressing “Go”, in about ~20-40 sec. the following screen will appear with pop-up “ScanProgress”:
During the scan the empty circles/ovals will change color, based on the number of “good” diffraction spots, if any. In the bottom part two windows will open with “table” and graphical view of the number of “good” spots. Wait patiently until “Scan Progress” window will disappear.

7. Browse through all images and statistics by selecting appropriate image number (lower right quadrant) or by choosing the highest number of spots (lower center table) – figure 10.

![Figure 10. The results of the primary grid scan](image)

8. Make selection and press “Move To 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.

At this point you have three options: 1) if you are satisfied with the search results – you proceed to collect snaps or runs; 2) rotate your crystal 90° and do a vertical scan, or 3) if you need to perform a fine/detailed search of the crystal you may do a “secondary” fine search. Please notice that a new button “Secondary” appeared in “Select Tools” box.
9. If a fine, more detailed grid scan is required, press “Secondary” button and check new parameters for scan, like aperture size (in most cases 30 micron is a good choice), overlap value, distance, transmission (flux in %) - (should be higher for smaller aperture). Once satisfied, press “Define Secondary Scan” button. The new loop view will be generated:

And you will need to draw (by dragging the mouse) the box in the area where you want to perform a secondary fine search:
10. Press “Done”. In a while (~10-20 sec) the box will be covered with red circles/ovals and the “Scan Commit” window will appear. Press “Go” to start the scan, “Modify” to go back to the setup window or press “Abandon” if you changed your mind – see image below:

11. Be patient until the beamline finish the scan and the result will appear:
12. Make selection and press “Move To 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.

13. It is possible to go back to the original “primary” scan and select another area for fine search. Make selection in the “Select Data” box on the top right corner – see figure below

Please note that only scans associated with the currently mounted crystal will have a “correct” coordinate values.
C. 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. Select “Vertical” in “Select Tools” box. Adjust loop/crystal view by changing Omega and Zoom values. Switch lights ON, if necessary. Vector is not needed for vertical scan, if present it'll be ignored.

3. In “Vertical Line Scan” box you can change aperture size (smaller size like 10 or 30 microns is recommended), overlap values (30-50% is a good choice), omega, detector distance and the transmission (flux in %%).

4. Draw the box (by dragging the mouse across the loop view) through the center of the loop; the box should always extend outside of loop:
5. Press “Define Scan” button; in a while (~10-20sec.) the “Scan Commit” dialog will appear :

![Scan Commit dialog](image)

Press “Go” to start the scan, “Modify” to go back to the setup window or press “Abandon” if you changed your mind.

6. After pressing “Go”, in about ~20-30 sec. the following screen with results will appear :

![Scan results](image)

Figure 11. The results of the vertical grid scan
7. Browse through all images and statistics by selecting appropriate image number (lower right quadrant) or by choosing the highest number of spots (lower center table).

8. Make selection and press “Move To 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:

![Changing Energy](image)

Input new energy value and click confirm; wait until it finish. Please note, that any energy change going across 8200eV requires a change in the mirror strip (~12 minutes extra to finish).

VI. Data Backup

Press “Sync” button on the main session screen (Figure 1) to download the script for real-time data transfer (password is valid for 5 days only). A new click on “Sync” 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 and wait one FULL minute for all sockets to re-connect.
Still no connection/response? : Go again to "Tools" tab, select "user interface controls" and next press "Restart Console"; wait TWO full minutes for all sockets to re-connect, close the browser and re-login again.

![User Interface Controls](image)

Please use with extreme caution!
Note: After “restarting console” it is necessary to do “beam alignment” before running any scans!

If none of these helped, call 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" and press “Low Bandwidth”
Lost beam – if you see a pop-up window about lost beam, first check APS beam status web-page:

You may see image similar to:

![APS Storage Ring Status](image)

If the “Storage Ring Current” is 0.0 and “Operation Mode” NO BEAM, APS lost the beam and there is no point to call your support personnel...
Keep refreshing this page, until you see some information about “Next Fill Info” - in the current example you should expect the beam only @17:00.

Only if “Storage Ring Current” is ~100mA and “Operation Mode” Delivered BEAM, should you call your support personnel, so they can open the main shutter for your operations.