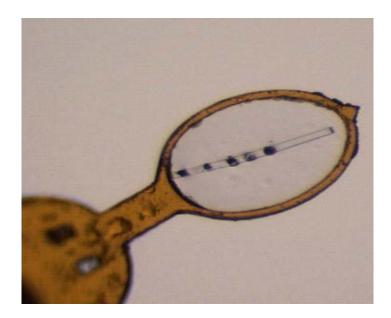
24ID-E operation manual

and troubleshooting



(under permanent construction and improvements)



This manual is NOT finished and will be NEVER finished (version of October 2012)

General Computer Layout

Our computer network can be roughly separated into five parts: (1) ADSC data collection computers, (2) MD2 operation computer, (3) two computers for the beamline control, (4) three computers for data processing and structure solution and (5) data storage and backup. You should use computers in category (1), (2) or (3) ONLY for data collection and the beamline controls (no Web browsing, games, music etc). In addition, there are two more shared computers in the back user area.

The control room for 24ID-E station is pictured in Figure 1.

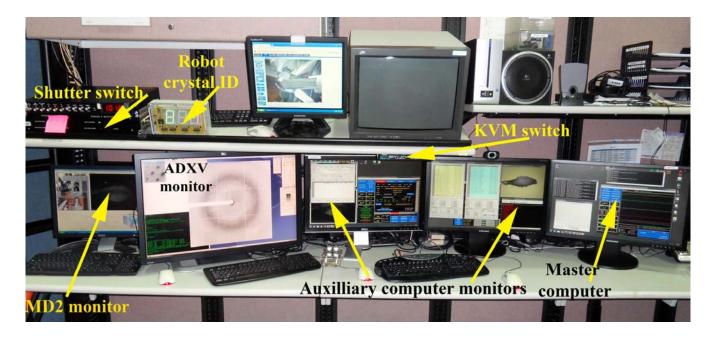


Figure 1. General view of the main working area on 24 ID-E.

<u>MD-2 Operation computer</u> is NOT used by users. Two programs should be always running: <u>MD2_RPC_comwrapper Server</u> (usually minimized to the task bar) and <u>MD2 Control GUI NE-CAT2</u>.

Check Troubleshooting section on how to restart the whole MD-2 and how to restart ALL user beamline control software.

<u>ADSC computer</u> is used only for current diffraction image visualization, using *ADXV* software. To start the ADSC software: find on the desktop a diamond-shaped icon called "AutoADSC" and double – click on it, a new window with green font will open. Next on "auxiliary" computer in the CONSOLE script under detector tab select "UTILITIES" and choose "Restart ADSC system" – a new GUI will start after in a while. All other functions of the ADSC GUI are for exclusive use of the beamline personnel.

Beamline Control Computers The beamline control software runs on two different Windows computers, namely "**master**" and "**auxiliary**". The video from these computers is output to 3 rightmost LCD monitors (see picture above). You can switch between these computers by pressing corresponding buttons on KVM switch (below the top shelf). All user operations are done on "auxiliary" computer only.

To start the main script, find on the desktop the icon EXEC_Intel (or it may be called EXECUTOR).



A new empty window will appear.

Click on **File** and choose "Prior .CXE Selection", drag the mouse to the right to select the script "C:\CONHEAP\PHII_MD2_FULL_REDIS_N EW.CXE". As the beamline is under constant development, the current name of the script may be different; the support beamline personnel will notify you. Click on "Execution Option" and choose "Execute Script"

EXECUTOR Current Script: C:\CO	NHEAP\PHII_MD2_FULL_REDIS_NEW.cxe PID: 2:				
File Execution Options Debugging (Options System Diagnostics Configurators Sy:				
Select .CXE File					
Prior .CXE Selections	C:\CONHEAP\PHI_MD2_FULL_REDIS_NEW.CXE				
Compile .CXE File	C:\CONHEAP\S24_FRONT_END.CXE				
Map Network Share	C:\CONHEAP\RUN_TRACKER.CXE C:\CONHEAP\SURVEY_TRACKER.CXE C:\CONHEAP\PHII_MD2_FULL_REDIS.CXE				
Print Screen					
Start Console Server	C:\CONHEAP\IMG_OCV_HOUGH_TWO.CXE				
Stan Cancola Saniar	CICONHEAPIPHT MD2 FULL REDISS CXF				

Now you should see the new window coming (Figure 2):

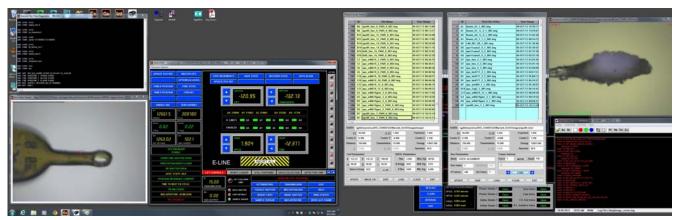


Figure 2. MD2 support table script PHII_MD2_FULL_REDIS.cxe"

This is your MAIN working area and you can do all following functions:

- Access the crystal centering interface (3-click alignment, focusing, lights, snapshots collection, basic robot operations) **XTAL CENTERING tab**
- Access data collections interface with different protocols DATA COLLECTION tab
- adjust the orientation of the MD2 table relative to the beam (MD2 AUTOALIGN)
- change the size of the beam aperture (MD2 APPERTURE); check he current aperture value
- maximize the flux and optimize the beam position (**TRIM_X** and **TRIM_Y POSITIONs**);
- Access the robot control script by pressing **ROBOT LOADER** (see next chapter)
- move in/out the sample sensor **RETRACT/INSERT SS**;
- retract/insert the cold-steam nose **RETRACT/INSERT CRYO**;
- open/close sample shutter; check the status of the main shutter; get APS ring status
- define the desired beam flux (TRANSMISSION button)
- check the current values of the energy, flux (arbitrary units), transmission (in % of the full beam), detector distance, ADSC state and the status of the beamline software (busy/ready)
- access several functions of the script running on the MASTER computer (MASTER OPS)
- change cold stream parameters (be very careful!) (CRYOJET button)
- read several parameters (to communicate with you support personnel, if requested)
- save or recover the tune state of the beamline, or the current state of the MD2 table
- recover from the shutter errors -WAKE SHUTTER

Robot Operations

Inside the Hutch

Inside the experimental hutch there are two computers, connected to one monitor: use "SCROLL", "SCROLL" and the "down arrow" button on the keyboard to switch between MD2 operation computer and beamline control computer, which is running robotic application script. User should only operate one computer at a time: either inside or outside the hutch.

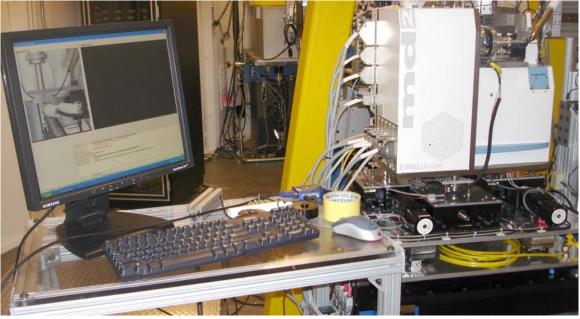


Figure 3. The main working window for all robotic applications INSIDE the hutch

Unload/Load Pucks

1. Remove any mounted crystals on the goniometer, either manually or pressing **DISMOUNT** button.

2. Make sure the MD2 is in "**SAMPLE TRANSFER**" mode and all covers are closed on MD2. Make sure that the BUSY light is dim (not bright red) and **ROBOT READY**.

3. Click on **PARK/SAFE**, select "park gripper" and script will ask you to confirm. Click YES. The robot script will then perform several sanity checks:

* If MD2 is not closed, then the capillary/beamstop will be retracted under the cover.

* Sample on the Goniomter - The sample sensor will detect if there is a pin on the goniometer. If a sample is present, the robot script will ask you to remove the sample or allow the robot to place the sample back in the dewar. If you choose to manually remove, the sample sensor will retract to allow you to reach the pin. The sample sensor may be manually moved– click on "SS PROBE" Once the spindle is unoccupied, and all covers are closed, the robot script will park the gripper.

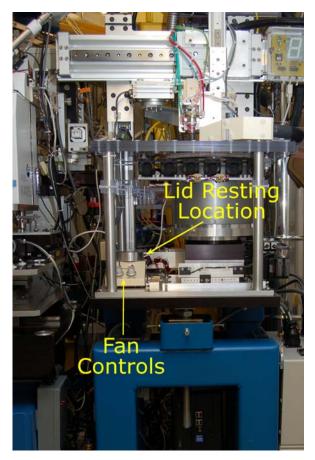
You should wait and NOT touch anything before the gripper stops in Park Position (facing goniometer).

4. Click **UN/LOAD PUCK**. Next a new popup window will appear – select a puck position (A B C D) or CANCEL the operation.

After puck selection, the dewar will rotate that position directly under the opening and allow for

placement of a puck. There are four positions in the dewar: A, B, C, and D. Keep track of which puck goes in which position. After the gripper has been parked, you can access the dewar.

5. Turn off the fan for better viewing. The switch for the fan is on the top of light-yellow box (left figure). Before pucks can be loaded, the lid must be removed and placed in the lid resting location (on the fan control box): see figures below.





6. Remove the puck from the shipping cane. Turn over the puck so that the thick part of the puck is face up. Attach the puck pusher to the puck. Orient the puck so that the notch is facing the center of the dewar. Load your puck into the dewar by lowering into the liquid nitrogen and feeling for engagement of the notch with the pin. It is recommended to slightly tilt the pusher toward the center of the dewar. When the puck is engaged, then it will not move in the dewar and the puck pusher will be perpendicular to the opening of the dewar. The puck will also be seated inside all three pins. Once the puck is engaged, push down with the plunger (of the puck pusher) to separate the two pieces of the puck. Then lift straight up in order to avoid disturbing the pins. Visually check the alignment of ALL pins, use long (and cooled) forceps to place properly tipped over pins.

7. After loading your puck into the dewar, select the next position by first clicking **UN/LOAD PUCK**, confirm, and then choosing the next position. Due to the sanity checks, this step is slow. Repeat steps 3-6, until up to four pucks are in the dewar.

8. Once all your pucks are loaded, replace the lid on the dewar (make sure the pin on the dewar is engaged in the lid) and turn the fan back on.

9. You must cool the gripper before samples can be mounted. Click **COOL GRIPPER**. The gripper should enter the dewar and begin cooling. Once the proper temperature has been achieved, you will be able to select a puck (click A, B, C or D) and a sample (click a number in the puck picture). Now, sample mounting can proceed. It is recommended to mount the first crystal inside the hutch, to check proper alignment of the robot. Once PuckID and Sample# changed color to yellow/cyan – press "MOUNT" button and watch the robot mounting the first crystal.

Now all robot operation should be done OUTSIDE the hutch, using the robot script running on auxiliary computer.

Outside the Hutch

All robot operation can done OUTSIDE the hutch, using either the **XTAL CENTERING** tab (most used robot functions only) or the full robot script running on auxiliary computer – by press tab "**ROBOT LOADER**." You should see the following screen (Figure 5):



Figure 5. "ROBOT LOADER" window for all robot operations

To mount/unmount samples:

- 1. You must cool the gripper prior to mounting your first sample. Press "COOL GRIPPER"
- 2. To mount your first sample click the Puck ID (A, B, C or D), then click the Sample ID (#1-16). The

Puck ID and Sample ID colors will change to red as the robot moves to the sample location. When the dewar move is complete, the Puck ID color will change to yellow and the Sample ID will change to cyan.

Make sure that the BUSY light is green (not bright red), **ROBOT READY** and the status is **DISMOUNTED**

3. Then click MOUNT under Mount Ops. The robot will start mount the selected crystal; Be Patient – it takes ~50 seconds to finish!

When the sample has been mounted, the voice will state, "Ready to Align Sample." At this time, you may align/center your crystal. The robot is still busy doing first de-icing of the gripper and second cooling it. Please do not click anything in the robot window at this time

4. Mount Next Sample. With a sample mounted on the goniometer, you have two choices.

* If you wish to go to the very next sample in the puck, then click **MOUNT NEXT**. The robot will dismount the sample and mount the next sequential sample. When it is complete, the voice will state, "Ready to Align Sample." Be patient – it takes ~115 seconds for this step.

* If you wish to go to new sample in the same puck, then click the Puck ID and then select Sample ID of the desired sample. The puck IDs will change to red, then back to yellow and Sample ID will change to cyan when your selection has been accepted. The robot will dismount the current sample and automatically mount the chosen sample. When the mount is complete, the voice will state, "Ready to Align Sample." Be patient – it takes ~125 seconds for this step.

* If you wish to mount a crystal from a different puck, it is recommended to first click DISMOUNT before selecting your new sample. The robot will return the currently mounted sample to the puck. Once the crystal is dismounted, the BUSY light is green (not bright red), **ROBOT READY**, click the Puck ID and then select Sample ID of the desired sample. The puck IDs will change to red, then back to yellow and Sample ID will change to cyan, then your selection has been accepted. The robot will move to the new location and automatically mount the chosen sample. Be Patient – it takes ~70 seconds to finish! The voice will then state, "Ready to Align Sample."

* The above behavior may be changed by checking "Automount Disabled": in the Maintenance submenu – the crystal will be NOT automatically mounted after new selection. You need to click **MOUNT** to mount the selected crystal.

5. Dismount -This command returns the currently mounted sample to the puck. (duration ~80 sec)

6. **OPTIONS** button will give you the menu with different washing scenarios. The most commonly used are:

POST_WASH to wash the crystal after mounting : it instruct the robot to move the crystal back to the dewar, move it back and forth to remove any ice on the loop surface and mount it back.

WASHING MACHINE – The whole dewar is strongly agitated several times to remove ice from many crystals at once; it is recommended to perform this operation after loading your pucks

ENABLE PRE_WASH – Before mounting every new crystal, the gripper will be agitating up and down with every crystal before mounting.

7. If a long time has passed between sample mounts (such as the duration of a long data collection), **De-Ice Gripper** and then **Cool Gripper** prior to dis-mounting. Ice builds up on the gripper during long intervals and will enter the storage dewar if not removed by de-icing. Ice in the storage dewar is drawn to any crystals present.

8. To move the gripper into a safe state for maintenance (or after finishing the experiment) - click **SAFE GRIPPER**.

General notes for robot trouble-free operations:

Note1: **The robot is SLOOOW** – You can't make it faster: every operation is a set of many instructions and sanity checks, which should be completed before the software can accept a new command. Please be patient, and wait every instruction to be properly finished. Aborting, canceling or just double-clicking may push the system in the delirious state with long recovery time.

Note 2: **Please always watch the status of the robot system**: When the robot is ready for the new operation/command it will display green ROBOT READY status.

Note 3: **Do NOT do anything on MD2 control computer, when the robot is in motion**. This may results in the severe mechanical damage to MD2. Users are liable for all damage to the MD2. Note 4. Double check the video feed on the computer screen above for robot gripper position (it should NOT be protruding into MD2) BEFORE "unlocking" the MD2 computer.

Note 5: Please follow ALL instructions from your support personnel. Any deviations or shortcuts are dangerous and will lead to unpredictable results and/or physical damage of the equipment.

Crystal Centering and Data Collection

XTAL CENTERING is the extension of the centering mode of MD2 software with several robot manipulation tasks.

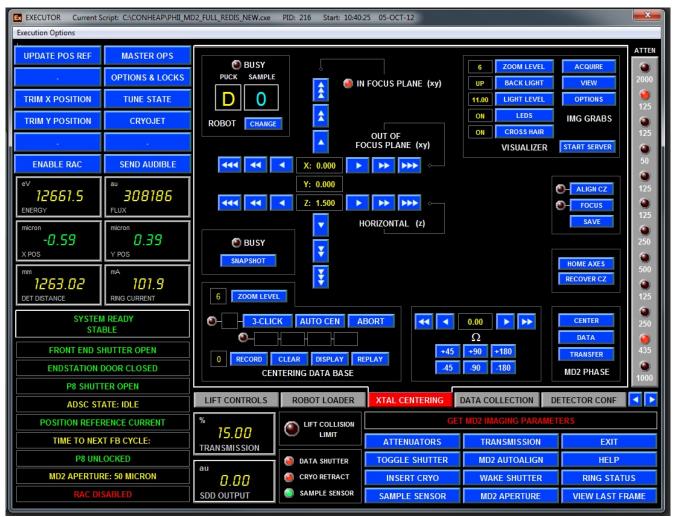


Figure 6. General view of "XTAL CENTERING" tab

There are several embedded operations in this window (from left top corner clockwise):

1. Robot puck ID number (current) and the button to mount next crystal - "CHANGE"; when "BUSY' light is on - the robot is busy doing something, wait before clicking. You can also dismount a currently mounted crystal, wash it, or select pre-washing cycle.

2. Section to control camera zoom, lighting of the crystal, and ability to acquire or view your crystal picture. StartServer button should be used only if the separate visual window is not started automatically (for beamline personnel use only).

3. Button HOME AXES will move all value of the goniometer to the default/zero values; should not be used with mounted crystal: it may move it out of the cold stream.

4. Three button to change MD2 mode: Center(default), Data collection and Sample Transfer

5. Buttons for crystals rotation and input field for a specific phi(omega)-angle.

6. 3-CLICK alignment tools, including alignment for crystal rastering: First, CLEAR the database (if necessary), second do 3-CLICK at the beginning of the raster vector, press RECORD; third, repeat 3-CLICK centering at the end of the rastering vector, and press again RECORD, it should be number 2 in the left box. DISPLAY will show consequently the beginning and the end of the raster vector and REPLAY will repeat two alignment processes. More than two points may be created for complex cases. 3-click alignment should be completely finished, before proceeding to the next operation. ABORT may be used to leave the "3-click" function.

7. Snapshot button to collect snapshots - a snap constructor dialog will appear

8. Buttons for manual movements of the crystal: vertical, horizontal and along the beam (out-focus plane). 1, 10 or 50 microns increments.

DATA COLLECTION tab is used to control ADSC snapshot/data collection parameters.

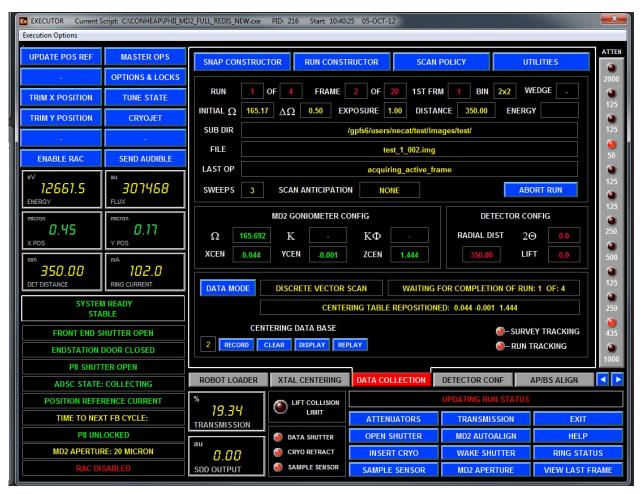


Figure 7. General view of "DATA COLLECTION" tab (with discrete run in progress)

1. **SNAP CONSTRUCTOR** button opens the following dialog window:

SnapShot Con	structor		20777	-	-	-	
Output Fil	e Specificati	on					
© gpfs1	O gpfs2	O gpfs3	© gpfs4	© gpfs5	gpfs6	Select Browse Root	
SubDir	gpfs6/use	rs/run2012_	_3/24IDE/GU	J/Marnett_C	Oct12/images/s	naps Browse	
Prefix	apo89_Imx_7						
FName	apo89_lmx_7_0_003.img Index 3 Reset In						
	Image Binn 1x1 Collect Da On	ining	Paired Or	Snap Acquis	offset 45		
Frame Pa	rameters				Resolution	Limits	
i .	Ω 0.00		$\Delta \Omega$ 1	.00	Edge	2.33 Ang	
Exposu	re 1.00	Di	stance 3	50.00	Corner	1.75 Ang	
5	Transmiss	sion 15.0	0				
	Msg Exe	cute	Up	date	EXIT		

Here you choose all parameters for snapshots. First, you need to define the root directory for your data collection (unless that was not done earlier) - by clicking on "Select Browse Root". It should be the *images* sub-directory below the directory assigned to your group. Next click on "Browse" button and select, or create a new directory, for current project. Confirm by clicking "Update". Next type the file prefix in the corresponding field. Click "Reset Index", if necessary. Select binning mode (1x1 or 2x2) and "Pair Snap Acquisition". When "Paired Snap Acquisition" is ON, two images separated by chosen offset value are collected, and LABELIT/RAPD will autoindex them together with much higher success. Type in starting omega/phi angle, oscillation range, exposure time, detector distance and transmission. Click "Update". Resolution Limits are updated once detector distance is defined and UPDATE is pressed. EXECUTE leads to collection of defined snapshot(s). EXIT closes the dialog window and return operations to DATA COLLECTION tab window.

Note 1: It's VERY important to click "Update" on this window and similar ones for data collection; otherwise

previously collected image(s) may be overwritten.

Note 2: Detector distance should be in the range of 1000 to 125 mm and exposure time should be a multiple of 0.5sec ONLY (use 1 second exposure and change the flux %).

2. **RUN CONSTRUCTOR** - the following dialogs opens, depending on what is selected when DATA MODE was pressed:

2A. (defalt) STATIC ALIGNMENT is for usual data collection; it is much like standard ADSC software RUNs setup:

O gpfs	1	O gpfs2	O	gpfs3	© gpfs4	⊙ gpfs5	gpfst	6 Select	t Browse Root
SubDir	/gpfs	6/users/ne	ecat/test/i	mages/test					Browse
Prefix	test								
Descr	Disci	ete Vecto	r Scan						
		Ima	age Binnin	g	Friedel Flip	ping			
		C) 1x1 (2x2	Off	O On	Wedge 5		
Edit Runs						10.1120			
Run	0	De	lete	Insert A	bove	sert Below	Cor	ργ	Paste
R	un ID	Start	Total	Distance	Energy	Trans	Ω	ΔΩ	Exposure
1	1	1	20	350.00	12661.50	20.00	165.17	0.50000	1.00
2	2	1	20	350.00	12661.50	20.00	205.17	0.50000	1.00
-									
3	3	1	20	350.00	12661.50	20.00	245.17	0.50000	1.00
3 4	3	1	20 20	350.00	12661.50	20.00	245.17 285.17	0.50000 0.50000	1.00
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2
100	12		2778783	10/17/2002220	100 002 0 100 100 000 000 000 000 000 00	1010000000000	A392431, 225, 24	2012/2012/2012/2012/2012	1 - 2 A - 2 - 2

Figure 8. Run constructor dialog

Here you choose all parameters for standard data collection: Every field can be manually edited, as necessary. First, you need to define the root directory for your data collection (unless that was not done earlier) - by clicking on "Select Browse Root". It should be the *images* sub-directory below the directory assigned to your group. Next click on "Browse" button and select, or create a new directory, for current project. Next type the file prefix in the corresponding field. Select binning mode (1x1 or 2x2), and "Friedel Flipping" and corresponding wedge size (if required). Type in Run ID, Number of frames to collect, Detector distance, Transmission, Initial omega/phi angle, Oscillation range, and Exposure time. Repeat for another run ID, if necessary (figure above shows an example of 4 runs of 10 degrees each). Once all values are checked, press "Update" and "Execute". EXECUTE leads to collection of defined run. EXIT close the dialog window and return operations to DATA COLLECTION tab window.

ADSC data collection can be aborted by pressing "ABORT RUN" button on dialog menu or "**ABORT RUN**" button in the middle right area of "DATA COLLECTION" tab – see Figure 7. This operation is slow and several images may be collected, before the run is completely aborted; please wait and do not press any other buttons.

More complicated scenarios are defined when pressing "DATA MODE" button - see menu at right -->

2B. STATIC ALIGNMENT – described above2C. BEST STRATEGY - under development.



2D. **DISCRETE VECTOR SCAN**- discrete data collection all over the predefined vector along your crystal (vector is defined by recording two (or more) points along the crystal on Centering tab window (see above). A new setup window will appear, where you choose the aperture size, zoom view and omega angle for visualization. Next select rastering parameters: Inset - the shift to the right from the leftmost raster vector point for start of data collection. Offset (usually more than aperture size) is the shift along the raster vector for next data set collection. Cycles - number of data sets to be collected. Phi Offset - is the shift of phi/omega angle between different data collection points. Note: for continuous data collection PhiOffset should be equal number of "Frames" number times "Del Omega".



Pressing "GENERATE RUN DATA" will open a graphics window in the top left corner, where you may monitor relative positions of every run along the raster vector. Change Omega values to check the alignment at different orientations. Press RUN and a "Run Constructor" dialog will appear (Fig. 8).

In the "Run Constructor" dialog window you should setup subdirectory for data collection and file prefix (see above), check the correctness of all runs. If there is any mistake, Click "Exit" and go back to "DATA MODE" and make all changes in the "DISCRETE VECTOR SCAN" dialog. If all runs are correct and all values are checked, press "Update" and "Execute". EXECUTE leads to collection of several defined runs along your crystal. EXIT closes the dialog window and return operations to DATA COLLECTION tab window.

Note: The **CONTINUOUS VECTOR SCAN** (described next) provides better protocol to decrease radiation damage, as the crystal is rotated and shifted after every collected image.

2E. **CONTINUOUS VECTOR SCAN** – (sometimes called helical scan) – more advanced mode as compared with "DISCRETE VECTOR SCAN" - continuous data collection all over the predefined raster vector. In this mode the crystal is translated/rotated after EVERY image collected to better spread the radiation decay. This mode is nearly two times slower as compared to "DISCRETE VECTOR SCAN" mode. The following dialog window will appear where you choose the aperture size, zoom view and omega angle for visualization.



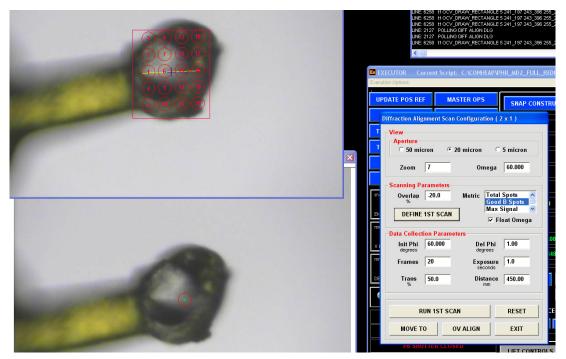
LeftInset and RightInset are offsets from predefined raster vector ends (not zeros - if you want to collect data on a shorted portion of the crystal). They may be negative if you want to extend data collection beyond predefined vector. Omega defines the initial view of the crystal, there are +/-5 and +/-45 degrees rotations buttons.

Next setup all data collection parameters based on the calculated strategy by RAPD (initial omega/phi angle, oscillation range, number of frames, exposure time, transmission and detector distance.

Pressing "GENERATE RUN DATA" will open a graphics window on the left, where you may monitor relative positions of every image point along the raster vector, with all data collection point simulated in red.

Pressing "RUN" will open ADSC data collection dialog which show only one run and it should not be edited (except run number and directory name). Just press "Update" and "Execute" for data collection.

2F ALIGNMENT BY DIFFRACTION - is used to find your crystal in an opaque/non-clear loop: the loop is rastered by a very weak beam and the software analyzes all collected images to find one with the better and stronger diffraction. In the following dialog window you select the necessary parameters:



It is recommended to use 50 micron aperture for big loop and use Omega value corresponding to plane of the loop. The "Metric" parameters are used by DISTIL to recognize best diffraction: "Good B Spots" is the best choice for now. "Overlap" defines the overlap between different search points: use a negative number for a sparse search.

Press "DEFINE 1ST SCAN" and a new window will appear in the top left side, use the left mouse to define a rectangular search box. The final search area will be automatically defined as a convolution of your search box and image centering server oval covering the loop.

Change transmission value to 1% or less and define the desired detector distance. Exposure and DelPhi should be 1 second and 1 degree. Press "RUN 1ST SCAN"; the system will move the loop through all red circles/ellipses and store the corresponding coordinates. After that on ADSC computer the diffraction images will appear. All images are stored in "/gpfs1/users/necat/phi_dfa_1/in" directory and will be deleted after exiting the ADSC tab. The message will appear when the run is complete.

A table with processed results will appear, on which it is possible to select different points and check again the corresponding diffraction (can be also done by making selection in lower left graphics window). Once the region of the best/strongest diffraction is found, pressing "MOVE TO" will center that portion of the loop for subsequent data collection. After that, you may proceed (click EXIT) and scan the orthogonal orientation of the loop, using the "OCCLUDED VIEW".

Now you need to repeat the same procedure in the orthogonal orientation: If successful, the loop will be centered on the best "diffracting crystal" position. Click EXIT to close the Diffraction Alignment dialog. Proceed now to the data collection by pressing **RUN CONSTRUCTOR**

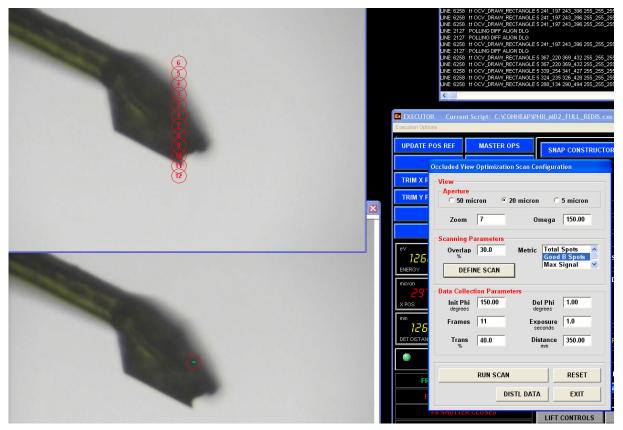
2G. RASTER SNAP

In the dialog window choose the aperture size, zoom and omega angle for specific crystal orientation. Next select rastering parameters: LeftInset and RightInset are offsets from predefined raster vector ends (not zeros - if you want to collect data on a shorted portion of the crystal). Frames - number of snapshots to be collected along the crystal. Select starting angle, oscillation range, exposure, transmission and detector distance.

Pressing "GENERATE RUN DATA" will open a data collection dialog and in a graphics window in the top left corner you may monitor relative positions of every run along the raster vector at the orientation defined by OMEGA value. You may change it for different view, and press again "GENERATE RUN DATA"; once satisfied, click EXECUTE and on ADSC computer you may monitor the incoming images. After the completion of the "raster snap" run another window with simple results will pop-up:

You may analyze (and plot) the results table to find the best portion of the crystal. Or you may select any position of the crystal and press "move to" to center that portion of the crystal.

2H. OCCLUDED VIEW Alignment - With very thin crystals, it is often difficult to visually discern the location of the crystal when in the plane of the loop. First, you need to center at any point in the loop. Second, choose the view corresponding to the plane of the loop (Occluded View), and define a box for scanning. The software calculates a series of points for scanning perpendicular to the plane of view based on user-entered criteria, and then takes snapshots at each point.



A summary of the diffraction metrics are displayed and you can select a point corresponding to diffraction maxima which causes the MD2 x,y,z centering stages step to the selected scan point coordinates. This point can then be entered into the vector database for use in other vector-based scanning methods.

Troubleshooting (in progress)

1. *Lost beam (no flux)* - make sure that all lights are green on PSS panel and there is beam in the ring (check TV screen). If the beam was lost in the ring, after the repair is done APS will announce "shutter permit is enabled" – after that, manually open station A shutter on a PSS panel and wait for 15 minutes for a monochromator to warm up.

If there is a red light "Faults Trips" – call the floor coordinator (2-0101) to inquire about this problem. Call your support beamline personnel if none of the above brings the beam.

2. The most common problem during the MD2 operation is that the program *MD2_comwrapper* is dying either because of lost communications between ADSC and MD2 or because of user error. When MD2_comwrapper is not running the data collection is hindered. Should *md2_comwrapper_server* fails, you should wait ONE minute to *md2_comwrapper_server* autorestart, if not, manually restart

MD2 software: Exit from MD2 control system (Menu-File -> Exit), wait until the window disappears. Kill *MD2_RPC_comwrapper* window, if it is present (check the taskbar). Double click on the desktop icon MD2_APS_v.203, wait until MD2 system is running (2-3 minutes) and *MD2_RPC_comwrapper* window should appear in a while and it should be minimized to the taskbar.

3. *Alarm is sounding* because of liquid nitrogen nose is shifted/bumped. The liquid nitrogen nose is extremely sensitive and should be NEVER moved or adjusted. If the alarm is sounding, locate the crate for MD2 hardware (by the wall on the left side from the MD2) and press the red button (shown by the yellow arrow on the Figure). This button is called "press to reset table drive power". It may be necessary to recover a proper position of the LN2 nose to reset the alarm.

After pressing that red button, an alarm screen on the beamline control "AUXILIARY" computer should be acknowledged by clicking on the alarm window. Remember, you need to press two times "CTRL-CTRL" to switch between master and auxiliary beamline control computers.

4. **ADSC software does not collect any data** after pressing "collect" – may be again the problem of MD2_comwrapper not running , see #2 above. Restarting ADSC software may also help. Next on "auxiliary" computer in the CONSOLE script under "DATA COLLECTION" tab select "UTILITIES" and choose "Restart ADSC system" – a new GUI will start after in a while It may be necessary to check for any ccd daemons still running: Exit ADSC and type "ps –e | grep ccd" and "ps –e | grep det". If you see any ccd/det processes still running –kill them (kill -9 process id#). Now re-start again ADSC software by typing double-clicking on the green icon "AutoADSC" and "Restart ADCS System" from CONSOLE.

5. Alarm is sounding and the detector is moving back because some foreign object went too close to the front of the detector. Report it to your support personnel and disable the alarm on the panel.





6. If any computer is slow or frozen, the corresponding software should be restarted. To close the frozen EXECUTER window, press Execution Options – Abort SCRIPT in the top menu (use *Ctrl-Alt-Del* only as a last resort to kill CONSOLE, (do not send any report to M\$). To start a new CONSOLE script, double-click on the desktop icon called "EXEC_Intel", click on "Execution Option" and choose "Execute Script"

The following software should be always running:

Master beamline computer: EXECUTOR - C:\CONHEAP\md2_phii_full_redis.CXE script. Auxiliary beamline computer: EXECUTOR- C:\CONHEAP\PHII_MD2_FULL_REDIS_new.CXE script;

MD2 operation computer: MD2_comwrapper windows (in the background) and main MD2 window.

7. Restarting the whole MD2 controller – this operation should be done ONLY after receiving authorization from your support personnel. <u>Switching off sequence</u>:

- 1. Exit MD2 Control Program on the PC.
- 2. Go inside E hutch and locate the MD2 control box.
- 3. Press the RED Motion Supply button to stop all motors.
- 4. Wait for 30 secs.
- 5. Press the Main Supply to OFF position.

Switching on sequnce:

- 1. Press the Main Supply to ON position.
- 2. Press the GREEN Motion Supply button to enable all motors.
- 3. Wait for 30 secs.
- 4. Start MD2 Control Software on the PC.

8. Restarting GALIL server

Login to 164.54.212.142 or go inside the hutch and look for the crate behind the detector;

Open a new shell and make sure galil is not running by typing "ps -e |grep galil"

Type "cd /usr/local/galil_rpc_server", type "./galil_rpc_server &"

Check again if galil is running by typing " $ps - e / grep \ galil$ ", close the terminal Master and auxiliary EXECUTOR scripts and ADSC software should be restarted after restarting galil

server.

9. List of running servers (in progress):

Terminal is behind the adsc detector

164.54.212.141 – pc68_rpc_server and utilities_rpc_server

164.54.212.142 – pc68_rpc_server and galil_rpc_server

164.54.212.142 - serial_rpc_server. The KVM switch is behind the monitor

164.54.212.69 (Fig. 8) – pc68_rpc_server 164.54.212.147 – mesa_rpc_, serial_rpc_ and diamond_rpc_server

10. gpfs file system is not responding. -- In an emergency you may collect data directly to the local hard disk on the ADSC computer. Use directory /data/users/your_institution/. Only for a short period of time and your support person should be notified.

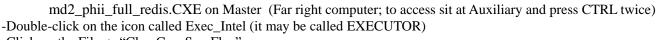
12. Full restart of the control software (only after receiving authorization from your support personnel <u>Shutdown order for full reset on 24ID-E</u>

- ADSC (Far left computer) exit from GUI or type "ccdsys shutdown" at terminal type two commands : "ps -e | grep ccd" and "ps -e | grep det" at terminal kill any remaining ccd/det processes by typing "kill -9 ###" (### = process id, the 1st column of the ps... results)
- PHII_MD2_FULL_REDIS_new.CXE on Auxiliary (3rd from left) press "EXIT" button in GUI (bottom-right button panel,); or "ExecutionOptions"->"AbortScript" Press "File"-> "Exit EXECUTOR"
- ROBOT_E.CXE inside the Hutch (robot computer, KVM switch: "SCROLL", "SCROLL" and the "down arrow") Press "EXIT" button in GUI window (bottom-middle button panel, top-right button) Press "File"-> "Exit EXECUTOR"
- Md2_phii_full_redis.CXE on Master (Far right computer; to access this screen, press the button on KVM switch) Press "EXIT" in GUI window (bottom-right button); or "ExecutionOptions"->"AbortScript" Press "File"-> "Exit EXECUTOR"
- MD2 GUI (MD2 computer ; 2nd from left) Exit GUI by pressing on the Menubar : "File->Exit"; it takes ~90 sec to close
- Comwrapper Server (MD2 computer ; 2nd from left) (This may be stowed in the taskbar) Exit by by pressing "Red Windows X" in upper right corner

Restart order for full reset on 24ID-E

MD2 GUI (MD2 computer ; 2nd from left) -Double-click on icon on desktop "MD2_APS_v.203" -Wait for it to fully start (~2 minutes) -Comwrapper Server window will start in a while; Minimize it to the taskbar.

Robot Server (Inside the hutch) -Double-click on the icon called EXECUTOR (it may be called Exec_Intel) Click on the File -> "ClearConsServFlag", confirm. Don't start any scripts for now.



- -Click on the File -> "ClearConsServFlag"
- -Execute script by pressing on the Menubar : "Execution Options->Execute Script"
- -Wait for it to fully start (~2 minutes); Move the whole window al the way to the right of the monitor

ROBOT_E.CXE inside the Hutch

- -Execute script by pressing on the Menubar ; "Execution Options->Execute Script"
- -Click "OK" on dialog that pops up stating that there is already a Console Server instance running.

PHII_MD2_FULL_REDIS_new.CXE on Auxiliary (3rd from left)

- Double-click on the icon called Exec_Intel
- Execute script by pressing on the Menubar : "Execution Options>>Execute Script"
 - ADSC (Far left computer)
- double-click on green diamond-like icon "AutoADSC"; wait for terminal with green fonts to appear
- On auxiliary computer go to "DATA COLLECTION" tab, select "UTILITIES" and choose "Restart
- ADSC system" a new GUI will start after in a while



