

Using HXMA CCD for XRD

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1. Introduction

For grazing incidence XRD, GISAXS, or *in-situ* XRD measurement one needs to coordinate control of sample positions (height and angle mostly) and/or sample temperature with data collection including CCD image acquisition. SPEC is popular software for hardware control and data acquisition in synchrotron X-ray diffraction beamlines.

The SX165(previously known as Mar165 or MarCCD) CCD has been used in HXMA for various diffraction measurements. Normally, CCD control through Linux PC will be checked before beamtime by beamline staffs.

Taking CCD image with SPEC can be done by following simple steps described in this document.

- 1) Start marccd software in Linux PC if it is not running already or if it is needed to restart. See “restarting marccd software when EPICS errors occurs.
- 2) Within marccd software start remote control.
- 3) Start MarCCD IOC from the marccd linux PC
- 4) Open MarCCD GUI from beamline PC to set data directory and to monitor ccd status.
- 5) Start SPEC if it is not running already or it is needed to restart SPEC.
- 6) Once SPEC starts, command *ccd_on*, *ccd_setup* will be used to enable and set parameters including CCD image file names.

2. Prepare X-ray CCD camera for spec

MarCCD saves images on local linux PC which control CCD image acquisition.

SPEC can communicate with MarCCD through EPICS and set file name of CCD image. Also SPEC can insert some information to head of CCD image file.

2.1. Prepare EPICS from marccd linux PC

Two steps listed below are required/checked to use CCD through SPEC.
From marccd linux PC

- Software *marccd* (in *marccd* linux PC) should be up and running.

If *marccd* is not running, start *marccd* by double clicking *marccd* icon  in the desktop.

- “Remote Control” in data acquisition in the *marccd* software. Click “start”. Wait 1-2 seconds and click “dismiss”



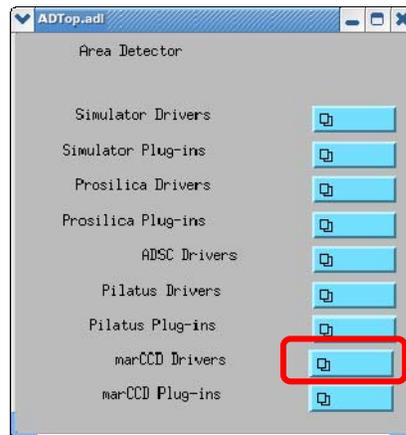
- Starting CCD EPICS IOC by double click icon



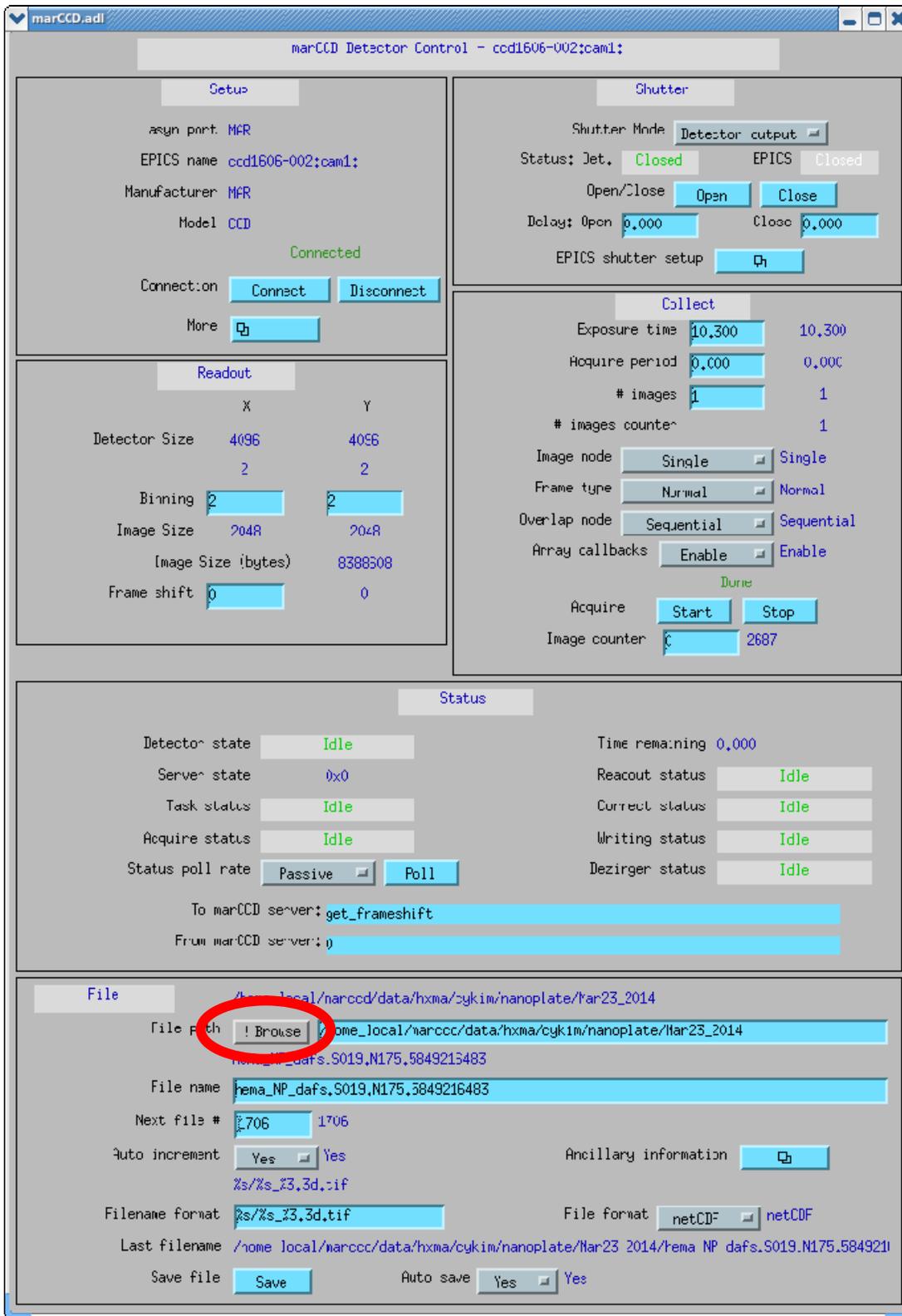
From PC where SPEC is running, double click MarCCD GUI icons

Window shown below will appear.

Select **MarCCD #1 specific** from **marCCD Drivers** button.



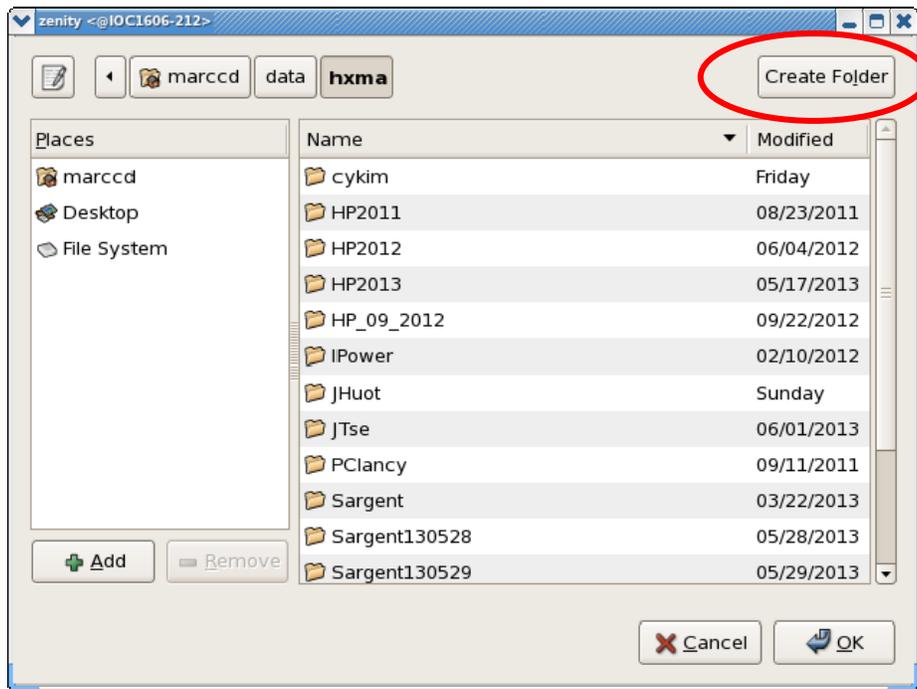
It generates a large additional window of **marCCD Detector Control**.



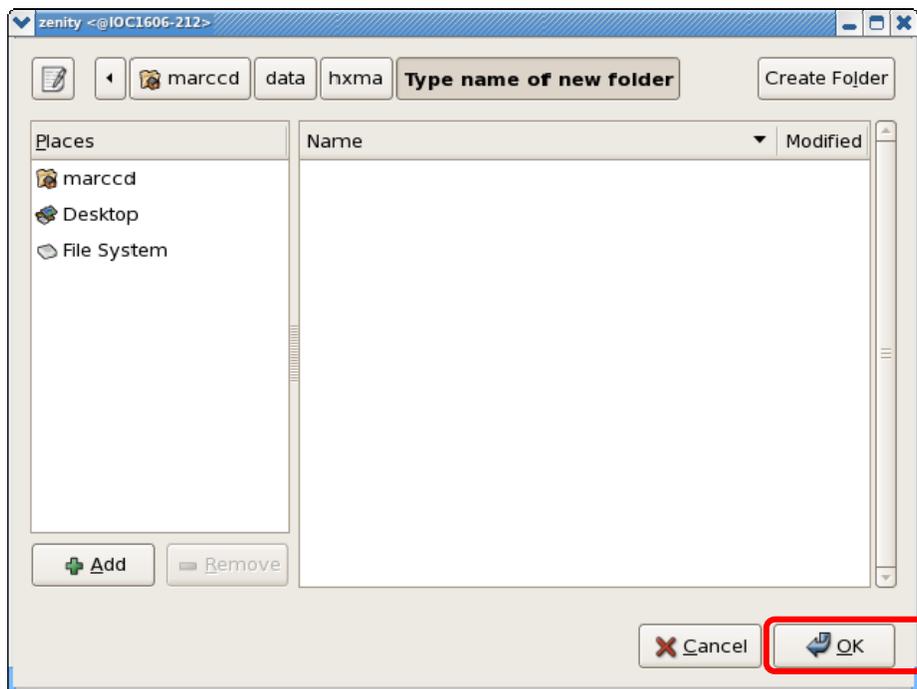
2.2. Making/selecting marCCD image data directory

User can make or select directory where all CCD images will be saved.

Click **!Browse** button in **marCCD Detector Control** window.



Click **Create Folder** will allow user to make new folder.

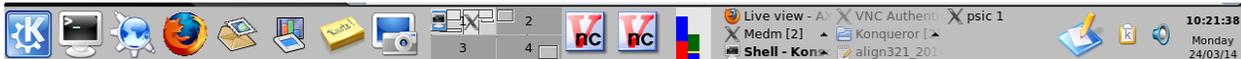


WARNING! Do not use special characters (: or ; or - etc) and no space in the directory name

3. Starting software SPEC

SPEC can be started from any Linux OPI computer at the beamline. It is recommended for user to make new folder for each beamtime (or each project). Typical data folders are under /home/hxma/data .Following example shows how to make a new directory of **testuser** and start SPEC from opi1606-101 PC.

Click **Terminal icon** in the Linux machine to open command line window.



In command line window, make folder where data will be saved and move to that folder.

The command **runPsic** will start SPEC to control sample positions, temperature and data acquisition with CCD and 4 element vortex detector.

```
Shell - Konsole
Session Edit View Bookmarks Settings Help

[hxma@OPI1606-101 ~]$
[hxma@OPI1606-101 ~]$
[hxma@OPI1606-101 ~]$ cd /home/hxma/data
[hxma@OPI1606-101 ~/data]$ mkdir testuser
[hxma@OPI1606-101 ~/data]$ cd testuser
[hxma@OPI1606-101 testuser]$ runP runPsic

                Welcome to "spec" Release 5.07.02-5
                Copyright (c) 1987-2007 Certified Scientific Software
                All rights reserved

(Portions derived from a program developed at Harvard University.)
(Psic based on work done at Argonne National Laboratory,
Materials Science Division [J. Appl. Cryst. (1999) 32, 614-623].)
(Linked with BSD libedit library for command line editing.)

Using "/home/spec/lib" for auxiliary file directory (SPECED).

Getting configuration parameters from "SPECED/psic/config".
Found XIA HSC "v1.4" on "SOCKET:s2e1606-001:4001", 4 of 4 slits responding.
XIA HSC I/O error reading response to !ALL P.
Purported XIA HSC on "SOCKET:s2e1606-001:4003" doesn't respond.
Purported ESP300, unit 0 on "SOCKET:s2e1606-001:4015", is unusable.

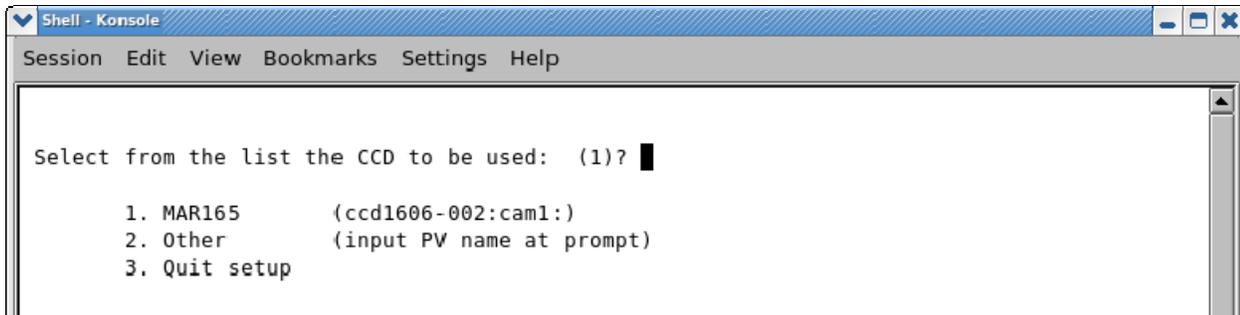
Using psi-circle configuration.
=
spec Hot Line: (617) 576-1610.
Type h changes for info on latest changes.
Browse to http://www.certif.com for complete documentation.
=

Reading file "SPECED/site.mac".

1403.PSIC> █
```

3.1. CCD setup in SPEC

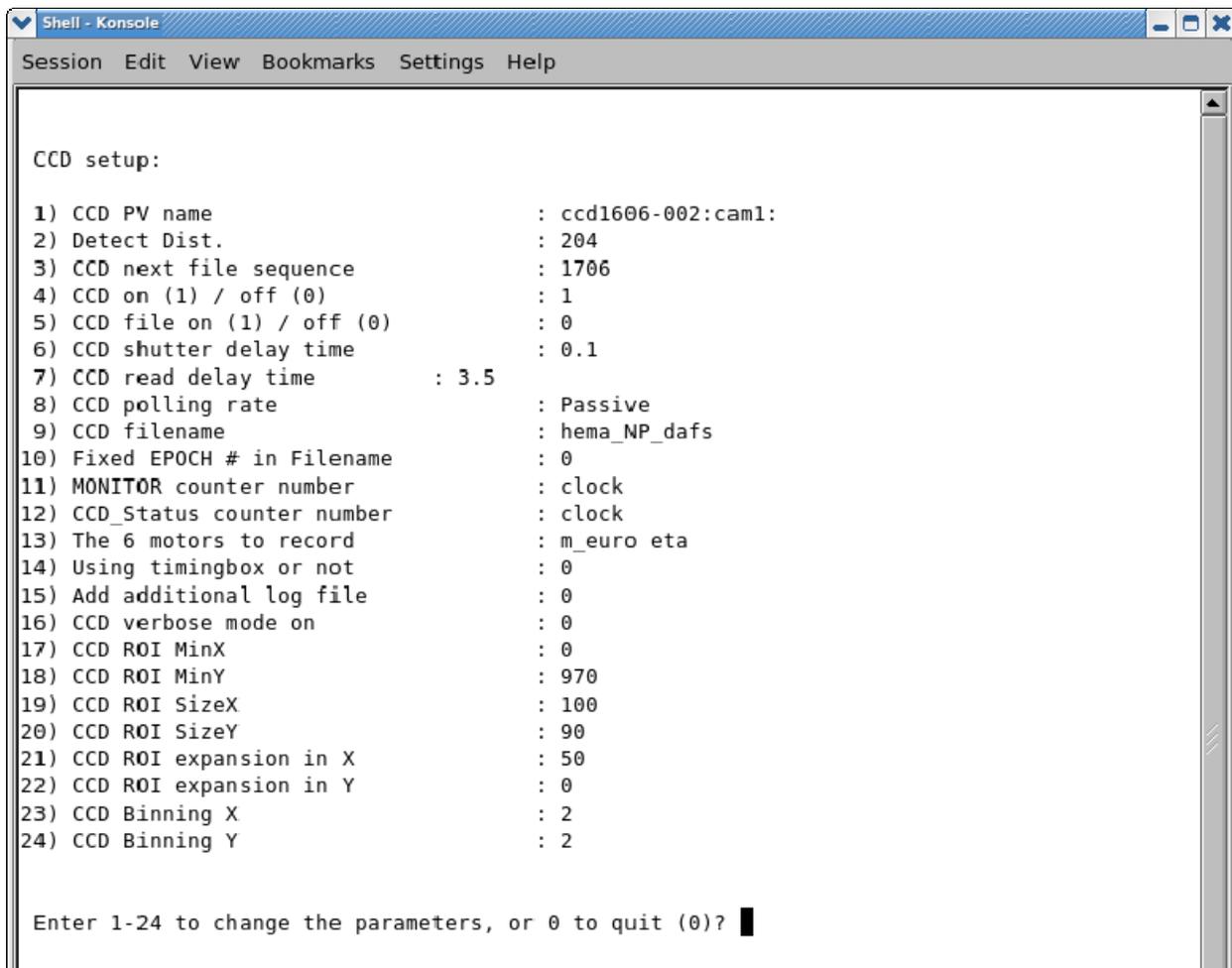
From SPEC type *ccd_setup* to select CCD to use (only one choice for now) and start setup.



```
Shell - Konsole
Session Edit View Bookmarks Settings Help

Select from the list the CCD to be used: (1)? █

1. MAR165      (ccd1606-002:cam1:)
2. Other      (input PV name at prompt)
3. Quit setup
```



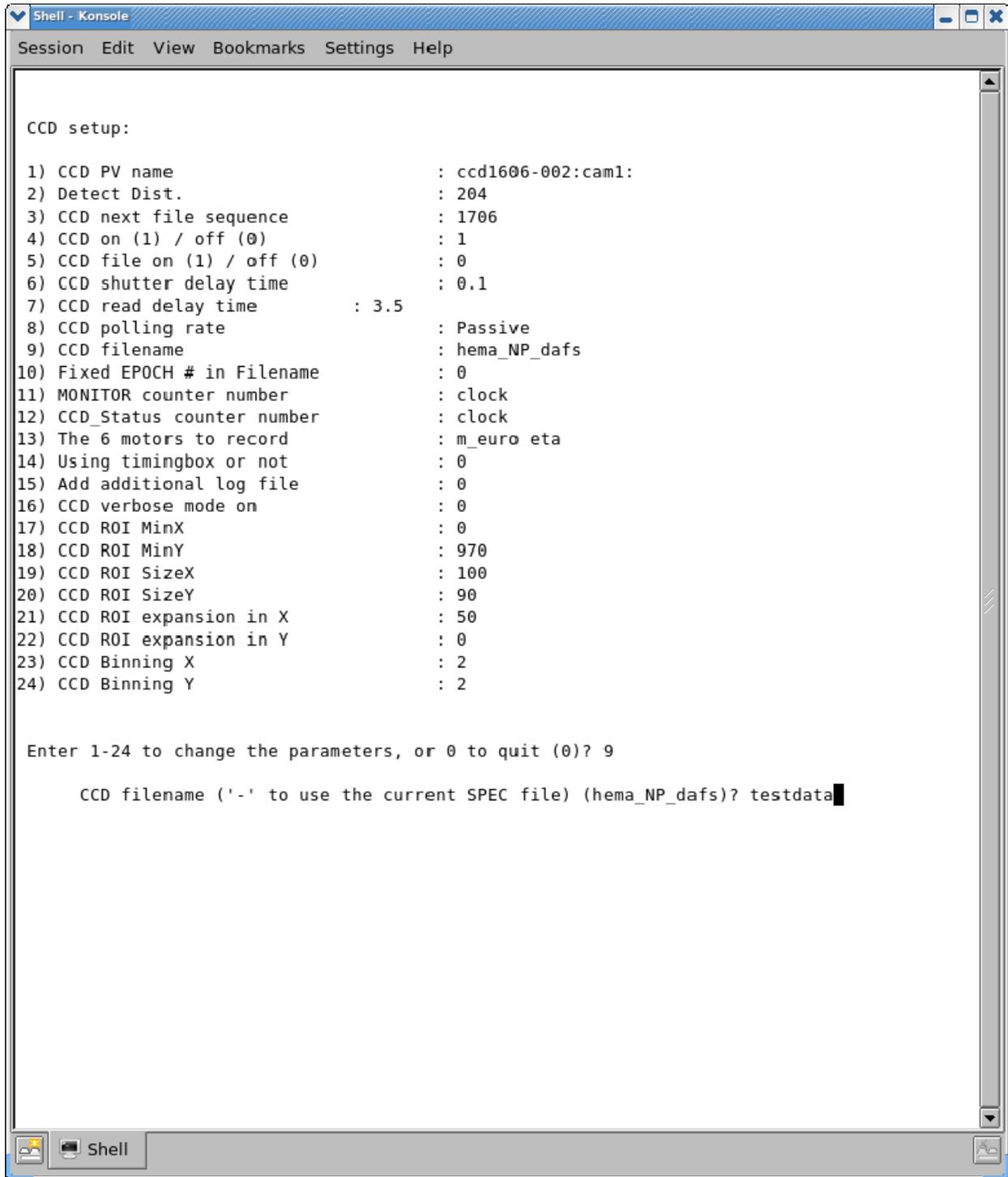
```
Shell - Konsole
Session Edit View Bookmarks Settings Help

CCD setup:

1) CCD PV name           : ccd1606-002:cam1:
2) Detect Dist.          : 204
3) CCD next file sequence : 1706
4) CCD on (1) / off (0)  : 1
5) CCD file on (1) / off (0) : 0
6) CCD shutter delay time : 0.1
7) CCD read delay time   : 3.5
8) CCD polling rate      : Passive
9) CCD filename          : hema_MP_dafs
10) Fixed EPOCH # in Filename : 0
11) MONITOR counter number : clock
12) CCD_Status counter number : clock
13) The 6 motors to record  : m_euro eta
14) Using timingbox or not : 0
15) Add additional log file : 0
16) CCD verbose mode on    : 0
17) CCD ROI MinX           : 0
18) CCD ROI MinY          : 970
19) CCD ROI SizeX         : 100
20) CCD ROI SizeY         : 90
21) CCD ROI expansion in X : 50
22) CCD ROI expansion in Y : 0
23) CCD Binning X         : 2
24) CCD Binning Y         : 2

Enter 1-24 to change the parameters, or 0 to quit (0)? █
```

Type **9** to change CCD filename.



```
Shell - Konsole
Session Edit View Bookmarks Settings Help

CCD setup:
1) CCD PV name           : ccd1606-002:cam1:
2) Detect Dist.         : 204
3) CCD next file sequence : 1706
4) CCD on (1) / off (0)  : 1
5) CCD file on (1) / off (0) : 0
6) CCD shutter delay time : 0.1
7) CCD read delay time   : 3.5
8) CCD polling rate      : Passive
9) CCD filename          : hema_NP_dafs
10) Fixed EPOCH # in Filename : 0
11) MONITOR counter number : clock
12) CCD_Status counter number : clock
13) The 6 motors to record : m_euro eta
14) Using timingbox or not : 0
15) Add additional log file : 0
16) CCD verbose mode on   : 0
17) CCD ROI MinX          : 0
18) CCD ROI MinY          : 970
19) CCD ROI SizeX         : 100
20) CCD ROI SizeY         : 90
21) CCD ROI expansion in X : 50
22) CCD ROI expansion in Y : 0
23) CCD Binning X         : 2
24) CCD Binning Y         : 2

Enter 1-24 to change the parameters, or 0 to quit (0)? 9

  CCD filename ('-' to use the current SPEC file) (hema_NP_dafs)? testdata
```

When modifying filename already typed in, **DO NOT USE** arrow keys to move cursor. Instead **USE** Backspace to delete characters and re-type. SPEC will reject to take filename modified by using arrow keys.

3.2. Enable/disable CCD

SPEC command *ccd_on* will enable CCD image acquisition through spec. Macro *ct* will take CCD image and save it. Any scan will take CCD image and save it at each scan point.

ccd_off will disable CCD. Counting and scanning will be regular one without CCD acquisition.

For sample alignment (height/angle adjustment), usually it is not necessary to take CCD.

3.3. Scan/counting with CCD

> *ccd_on*

Will enable count and any scan macro to take CCD image and saved at each scan point.

CCD files will be saved as

CCD-filename.scan_number.point_number.EPOCH_file_sequence.tif

For example,

> *ccd_on*

> *ct 10*

will expose X-ray 10 seconds and save the CCD image with file name starting with the one specified with *ccd_setup* (*hema_NP_dafs* for example shown above). File name has more terms as explained below.

When scanning,

> *ccd_on*

> *dscan th -1 1 10 2*

will generate 11 CCD files with 2 sec exposure at each scan point.

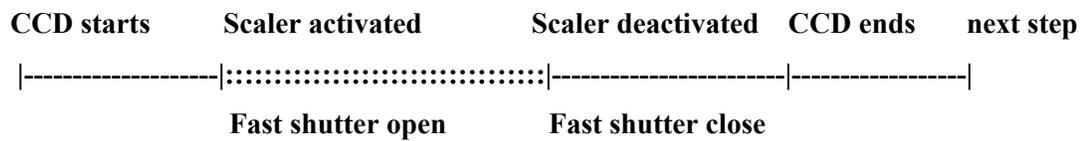
CCD filename might look like **hema_NP_dafs.S003.N012.20776_012.tif** for 12th scan point if “9) CCD filename” was set as “hema_NP_dafs”, and the scan is the third scan and “3) CCD next file sequence” was set to 1 before *dscan* starts.

3.4. Hardware and timing control

Current CCD image acquisition is based on scaler, fast shutter and time delay.

Scaler output is hard wired to the Uniblitz[®] fast shutter so that fast shutter opens only when scaler is activated (counting). If CCD is enabled (*ccd_on*) SPEC takes extra step to give enough time for CCD readout. When counting (*ct* or any scan) starts, SPEC sends command to start CCD. Then, scaler is activated and faster shutter opens. After specified counting time set by SPEC is elapsed scaler

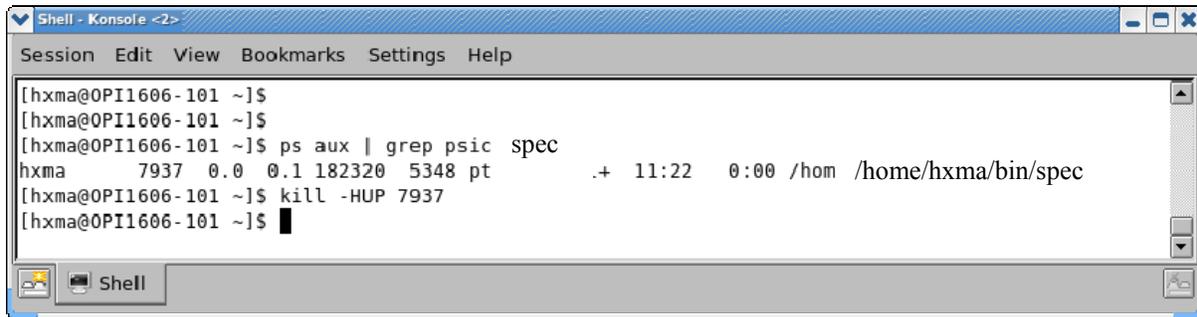
deactivated and fast shutter closes. SPEC waits predefined delay time to move to next point of scan or print counting results.



4 Troubleshooting

4.1 If SPEC window disappears or SPEC hung-up (not responding)

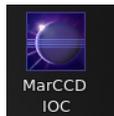
If window where SPEC is running is closed accidentally, the SPEC is still running. If it is in the middle of scan, check whether the scan is on-going. Regular motor motion, activities in scaler, CCD or Vortex GUI is indicator that scan is performing normally. One can wait until scans finishes and attempt normal termination of SPEC.



```
Shell - Konsole <2>
Session Edit View Bookmarks Settings Help
[hxma@OPI1606-101 ~]$
[hxma@OPI1606-101 ~]$
[hxma@OPI1606-101 ~]$ ps aux | grep psic spec
hxma      7937  0.0  0.1 182320  5348 pt      .+  11:22   0:00 /hom /home/hxma/bin/spec
[hxma@OPI1606-101 ~]$ kill -HUP 7937
[hxma@OPI1606-101 ~]$
```

If `kill -HUP` does not work or SPEC hang-up, use `kill -9` but this command is force-quit and hence status of SPEC cannot be saved. For example, recent data file name and recently uploaded macros can be lost. Data are recorded at each scan point, so with forced stop last data point will be lost.

4.2 If MarCCD GUI show white boxes



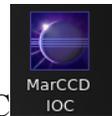
Restart MarCCD IOC from marccd linux PC.

4.3 If MarCCD GUI shows **error** in red font

Quit SPEC by typing Ctrl-D (type **d** while pressing **Ctrl** key) in SPEC terminal.
Quit MarCCD software by close the window.



Restart marccd, remote control, and MarCCD IOC

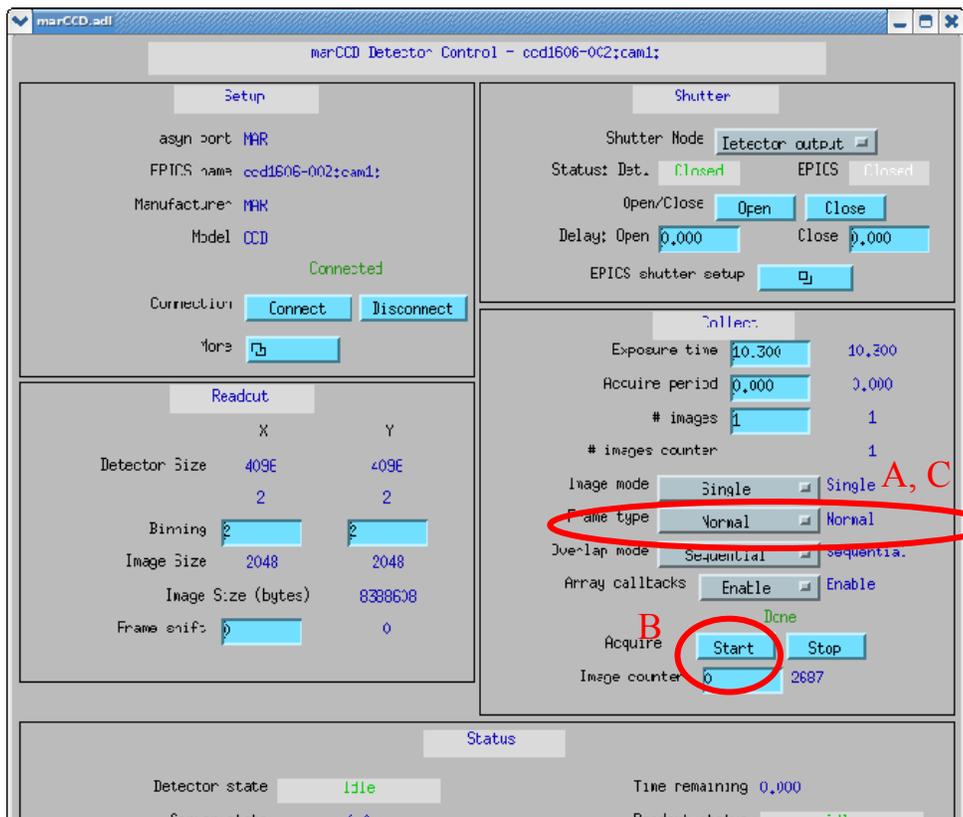
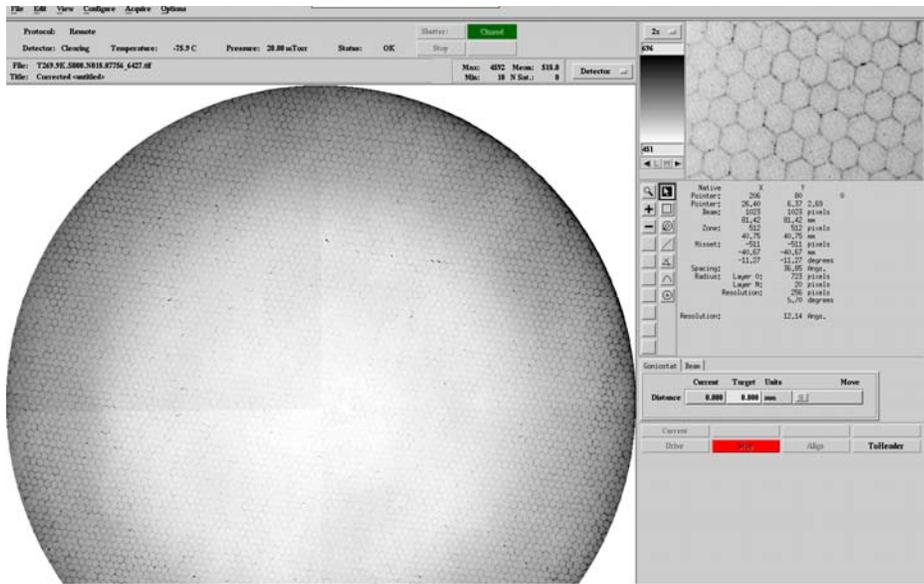


4.4 SPEC complains “UNUSABLE motor”

Quit current SPEC by typing Ctrl-D (type **d** while pressing **Ctrl** key) and restart SPEC.

4.5 See honeycomb pattern in the CCD image

If you see honeycomb pattern in the CCD image it is time to retake background of CCD.



- A. Change Frame type from “Normal” to Background”.
- B. Click “Start”. Wait Detector state become Idle.
- C. Change back Frame type to “Normal”.

After this Background re-taking, first count from SPEC gives unusually short time exposure. Recommend to do one second counting first before you start long exposure counting.

5 Epics control of MarCCD (from HXMA wiki page, too technical)

5.1 Introduction

These are the configuration, startup, and basic usage notes for the MarCCD EPICS control software. The software is based on the **synApps 'areaDetector'** application. This control application connects directly to the MarCCD application and can write image files in TIFF format as per user specification.

These instructions can be found at http://wiki/index.php/HXMA_MarCCD_Detector.

5.2 Quick Start

On the MarCCD workstation, log in as user 'marccd'.

Double-click on the "**MarCCD**" icon.

On the MarCCD GUI, select **Acquire->Remote Control...**

On the Remote Control window, confirm or set the following

Server Environment: NETHOST=localhost

Server Command: /home/marccd/contrib/marccd_server/marccd_server_socket

Server Arguments: 2222

Server Log: /home/marccd/log/remote_server.log

Press **Start** on the Remote Control window, then **Dismiss** the window.

Go back to the data acquisition workstation

Double-click on the "**MarCCD_IOC**" icon.

Double-click on the **MarCCD_GUI** icon.

Select marCCD Drivers->marCCD #1 General, or change settings with marCCD Drivers->marCCD #1 Specific.

Start taking data.

5.3 Usage

Most of the MarCCD EPICS control GUI is informational. The following are the more commonly used controls.

5.3.1 Image Files

The image files are only available in TIFF format, using 16-bits per channel (i.e. 48-bit color/grayscale). The **File format** (not to be confused with **Filename format**) will display "netCDF" and should be ignored.

Note: due to the EPICS version of the controls being named similarly as the vendor's software, there can be some confusion as to whether the EPICS software can write image files. It doesn't do this. It can READ the image files written by the vendor's software for analytical purposes, but it is not set up to re-write it.

5.3.2 Single Shot Exposure

In the **Area Detector** screen, select **marCCD Drivers->marCCD #1 General**. That should launch the general purpose **marCCD Detector Control** window. Alternatively, you can launch the expert controls with

marCCD Drivers->marCCD #1 Specific, which puts most of the controls in a single view with extra status displays.

In the **Collect** section:

Set the **Exposure time** (in seconds)

Ensure the following:

Acquire period is set to 0

images is set to 1

Image mode is set to "Single"

frame type is set to "Normal"

Overlap type is set to "Sequential"

Array Callbacks is set to "Enable"

In the **Readout** section:

Set **Binning** for each axis according to your requirements.

Ensure that **Frame shift** is set to 0

In the **File** section:

In the general control window, press the **Driver file I/O** button. That will launch the files control window. The expert window has the same controls built in.

Set **File path** to the directory you want all of your images saved to.

Set **File name** to the **root name** of the files you want your images saved to.

Set **Next file #** to the starting value you want your sequence of images numbered from.

Set **Auto increment** to "Yes"

Set **Filename format** to a string as follows:

To specify the directory and root part of the file, start with "%s/%s".

To specify the file number, at least use "%d".

You can specify the number of digits with a number between % and d. This really isn't useful unless you also specify zero padding, below.

You can specify zero padding by putting a zero in front of the number, e.g. "%04d", which would result in files numbered "0001, 0002,... 0999, 1000".

Between the filename root and the file number, and after the file number, you can add just about any set of characters.

Since the files are in TIFF format, it is highly recommended that the Filename format end with ".tif".

Examples: assuming you set the File path to /tmp, File name to test, and Next file # to 5:

for a file that you want to look like "/tmp/test-0005.tif", the Filename format should be "%s/%s-%04d.tif"

for a file that you want to look like "/tmp/test05.tif", the Filename format should be "%s/%s%02d.tif"

Set **Auto save** to "Yes"

To actually generate an image, go to the **Collect** section and press **Start**.

The various displays in the **Status** section will inform you of the status of the exposure.

5.3.3 ROIs (Regions-of-Interest)

In the **Area Detector** screen, select **marCCD Plug-ins->ROI #1**. That should launch the **ROI1** window.

Set **Enable** to **Yes**

Set **Callbacks block** to **Yes**

You can examine individual ROI information and modify the ROI's settings with **Individual ROIs** menu.

Set **Use this ROI?** to **Yes**

Make sure **Data type** is set to **UInt16**

Set **Compute statistics** to **Yes**

Set **histogram?** to **Yes** if you are interested in seeing the quasi-distribution of pixel intensities. At first, set the parameters as follows:

Set **Size** to 65535.

Set **Minimum** to 0.

Set **Maximum** to 65535.

Set **ROI start** and **ROI size** as you need. It is **highly** recommended that ROI #1 be set to (0,0) and (2048,2048) respectively, that you pay attention to the **Statistics** section, particularly the **Maximum** reading for overflows.

For multiple ROI information in tabular format select from the **Combined ROIs** menu.

5.3.4 Multiple Frame Exposures

It might be useful to set **Overlap mode** to **Overlap** when doing multiple exposures in succession. This allows an exposure to begin while the previous file is being written. If you do use this feature, AND you do not need ROIs, it would be advisable to set **Array callbacks** to **Disable** if **Overlap mode** is set to **Overlap**. Callbacks will block the overlap feature. If you want reliable ROIs, you have no choice but to keep **Array callbacks** enabled.

5.4 Start-Up

The details of starting up the MarCCD system can be found [here](#).

5.4.1 Hardware

The hardware system is fairly complex. Setup, configuration, and operating instructions should only be performed by experienced personnel, thus are beyond the scope of this document. If the MarCCD workstation, the cryogenics system, or the detector is not powered up, inform the beamline staff.

Regarding the workstation, it is not integral to the operation of the detector hardware. It usually can be rebooted with little or no impact to the detector or cryogenics. **HOWEVER**, the workstation should **NOT** be unnecessarily rebooted. It is still possible to lock up the detector this way.

Finally, the workstation **IS** integral to data acquisition, since it acts as the data and control server for the EPICS control software.

5.4.2 Software

On the MarCCD workstation, log in as user 'marccd'.

Double-click on the "**MarCCD**" icon.

this should launch the MarCCD GUI and a terminal window

the GUI is what users would normally use locally, and can be monitored for remote usage

the terminal window reports the status of the system's hardware.

On the MarCCD GUI, select **Acquire->Remote Control...**

On the Remote Control window, confirm or set the following

Server Environment: NETHOST=localhost

Server Command: /home/marccd/contrib/marccd_server/marccd_server_socket

Server Arguments: 2222

Server Log: /home/marccd/log/remote_server.log

Press **Start** on the Remote Control window.

Dismiss the Remote Control window.

Go back to the data acquisition workstation

Double-click on the "**runMarCCD_IOC**" icon.

There should be a fair amount of text and should end with a prompt such as "ccd1606-002>".

Double-click on the **MarCCD_GUI** icon.

The EPICS control window should appear.

5.5 Shutdown

in the MarCCD IOC window, type exit

in the MarCCD GUI, select Acquire->Remote Control...

Press "Stop".

You will be prompted with "Do you want to abort data collection Immediately?"

Answer "No,..."

Dismiss the Remote Control window

shut down the MarCCD EPICS control GUI (NOT the main MarCCD control GUI). Don't forget to

close the EPICS controls "main" window, also.