# marccd

Version 0.3.15 (LINUX)

**Manual Version 0.0**

by
Christine R.A. Muchmore

Copyright MarUSA, Inc.

# Contents


| | Page |
|---|---|
| Getting started | 1 |
| Turn Detector on | 1 |
| Reboot Detector Controller and Start Cooler | 2 |
| Just Turn Cooler on | 3 |
| Collect Single Frame | 4 |
| Save the Single Frame | 5 |
| Collect Data Set | 6 |
| Stop a Data Collection | 8 |
| Size of Data Frames | 8 |
| Collecting Data with the MarCCD System | 9 |
| Status | 9 |
| Resolution | 9 |
| Pixel Size | 10 |
| Distance | 10 |
| 2 theta offset | 10 |
| Tables | 10 |
| Synchrotron or Rotating Anode | 15 |
| Multi Read | |
| Time/Dose Mode | |
| Tools to Set Up Optimal Data Collection | |
| Single Frame | |
| Large Oscillation or Phi Slicing | |
| Oscillation Range | |
| Exposure Time/Dose | |
| Strategies | |
| Simple Data Set | |
| Inverse Beam Experiment | |
| MAD Data | |
| Starting the Data Collection | |
| Stopping/Interrupting the Data Collection | |
| Data Storage | |
| Size of Frames | |
| Formats | |
| Archive Commands | |

Detailed Description of the MarCCD Program 16
Command Line Options 16
The Main Panel 17
Detector Status 18
Display Status 20
Zoom Window and Colour Scale 20
Toolbox 22
Pull-Down Menus 26
File 26
Load Data Frames 26
Save Displayed Data Frame 27
Save Displayed Image 28
Print 28
Quit 29
Edit 29
Copy to 29
Byte-Swap Frame 29
Bin Frame 29
Unbin Frame 30
View 30
Show Header 30
Color Scheme 30
Scaling 30
View Direction 31
Coordinates 31
Values 31
Rendering 31
Configure 32
Detector 32
Goniostat 37
Acquire 39
Single Frame 39
Data Set 42
Remote Control 48
Display 48
PEAKS File 48
TROIDINF File 48
SPOTLIST File 48
REFLECTIONS File 48
Filter 49
Plot 49
Reduce 49
Test 50
Options 50
Output File Format 50

Frame Math 51

Hardware
- MarCCD Detector head
- MarBase, remote Control and TV Monitor
- Cooler&Detector Controller Crate
- Computer
- Setup and Checking Connections
- First Start

Theory of Operation

Trouble Shooting
- Table of Symptoms&Fixes 52
- Procedures for Fixes and Checks 57

FAQ

# Getting Started

If the MarCCD detector is on, the controller and the cooler are running, the software has been started and the user only needs to get started taking pictures, skip to page ?.

**To turn on the detector system:**

The big beige box on rollers provides access to the internal main power switch through an opening in one of the side panels. Reach in and turn the power switch inside on. The switch is lit up red when the power is on.

Log into the computer controlling the MarCCD:
`user: marccd`
`password: marccd`

The working directory should be `/home/marccd` .
To start the MarCCD software type:
`marccd <return>`

The main marccd window will appear on the screen:

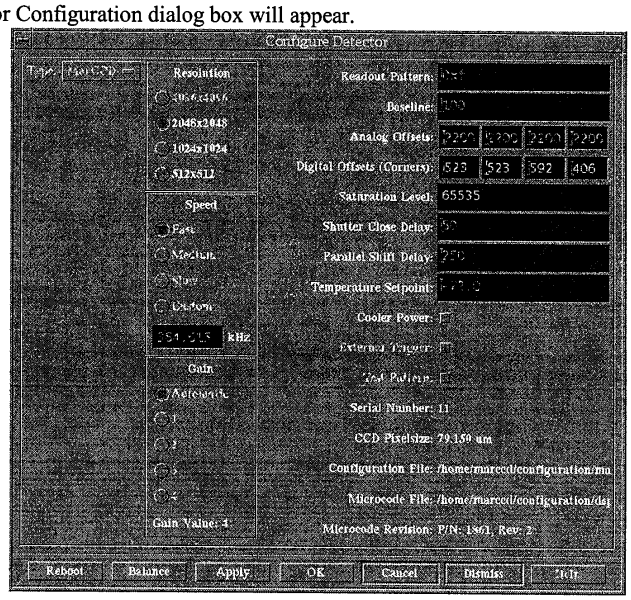
Remark: Detailed explanations of all panels including the main marCCD panel are supplied in the third section of this manual.

If the detector was turned off since the last time this software was run, the camera controller needs to be rebooted. This is not necessary if the detector has been running while just the software was stopped and restarted.

General:
Use Dismiss, Cancel or OK buttons rather than closing windows from window frame.
Use Apply button to accept and save changes.

**To reboot the detector controller and to turn the cooler on:**
(This is not necessary if the detector has been running while just the software was stopped and restarted.)
Use the left mouse button to choose from the pull-down menus on top:

Click on Configure
Detector
The Detector Configuration dialog box will appear.

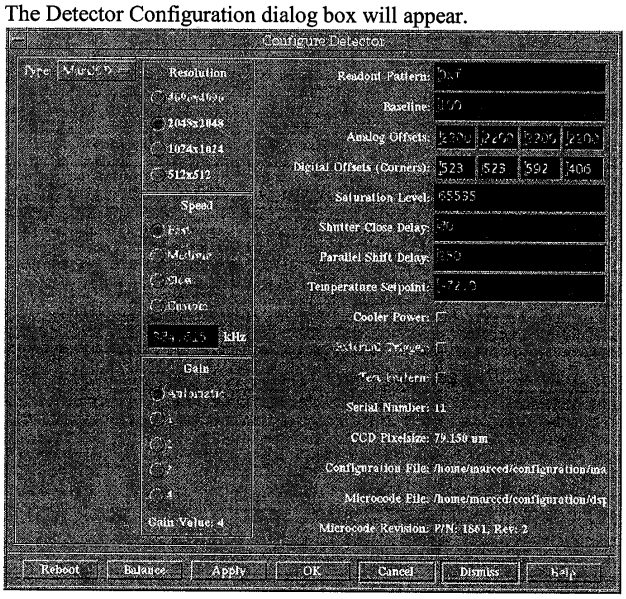



⇒ Click on "Reboot" - wait for OK.
⇒ Click on Cooler Power to show a checkmark (✓)
⇒ Click on "Apply", cooler will turn on about 40 seconds after this button was clicked, but the detector status should change to "Cooler ON" immediately.
⇒ Click on "Dismiss".

**To just turn the cooler on:**
If the MarCCD software is running and the detector status panel does not show any "???" but the Status is "Cooler OFF", then the cooler should be turned on by this procedure.

Use the left mouse button to choose from the pull-down menus on top:

Click on Configure
Detector
The Detector Configuration dialog box will appear.

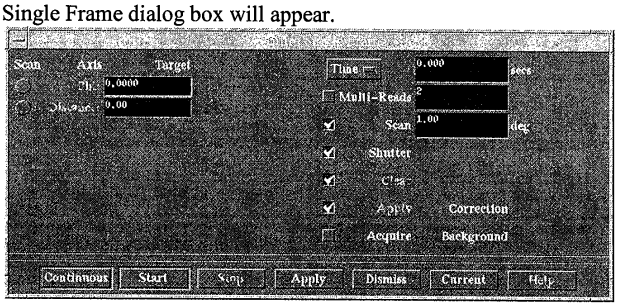



⇒ Click on Cooler Power to show a checkmark (✓)
⇒ Click on "Apply", cooler will turn on about 40 seconds after this button was clicked, but the detector status should change to "Cooler ON" immediately..
⇒ Click on "Dismiss".

It takes 2-4 hours to cool the detector from room temperature to optimal operating temperature.

**To take a single exposure:**
Use the left mouse button to choose from the pull-down menus on top of the main marCCD window:

Click on Acquire
Single Frame
The Acquire Single Frame dialog box will appear.




*Top left:*

- Scan for Phi (top left of panel) should generally be on.
- Under "Target" type in the phi angle for a still or the start of an oscillation.

*Top right, going down:*

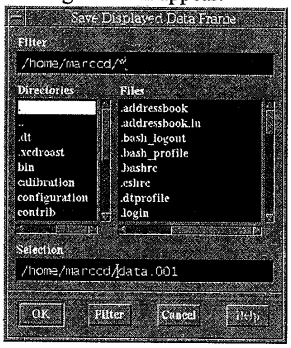
- Choose Time on the pop-up button, type desired exposure time into the window next to the Time/Dose button.
- Check Multi-Reads only if the exposure time is long (longer than several minutes - this depends on the source, signal strength and other conditions).
- If Multi-Reads is checked, enter the number of reads per frame into the box next to the button, usually 2.
  This feature essentially splits the exposure into sections, with read-outs between them. The sections are then used to eliminate "zingers" (cosmic rays causing spots on the frame that are not part of the diffraction pattern). At synchrotrons this feature should not be used because the exposures are very short.
- Click on the Scan button to show a checkmark (✓) for an "oscillation" picture, no checkmark for a "still" picture. For an "oscillation" picture type the phi range into the box on the right.
- Click the shutter button to show the checkmark (✓) to give the software shutter control.
- Usually "Acquire Background" should not be checked.
  When checked, this will cause a read-out of the detector without prior x-ray exposure, to determine the background, which will then be subtracted from the diffraction image. If "Acquire Background" is **not** checked, the software will *still take a background frame* if there is a special reason (no background frame stored, or the stored frame is too old, etc.).

Once all this data is entered to your satisfaction, go to the bottom row of buttons.
⇒ Click "Apply" to accept all the settings.
⇒ Click "Start" to take the frame (Actually, "Apply" is implied in "Start".).
⇒ Click "Dismiss" if you wish to get rid of the panel. The exposure will continue.
⇒ To abort an exposure click on "Stop".

Above the top right corner of the data display area in the main marccd window is pop-up menu button. Use the left mouse button to choose "Detector" (rather than "Background" or "Scratch") from this menu. Once the exposure is completed, the frame will be displayed under "Detector".

Frames collected via the "Acquire Single Frame" dialog box are **not** automatically written to a file.

**To save the displayed frame:**
Click on File
Save Displayed Data Frame
The Save Displayed Data Frame dialog box will appear.



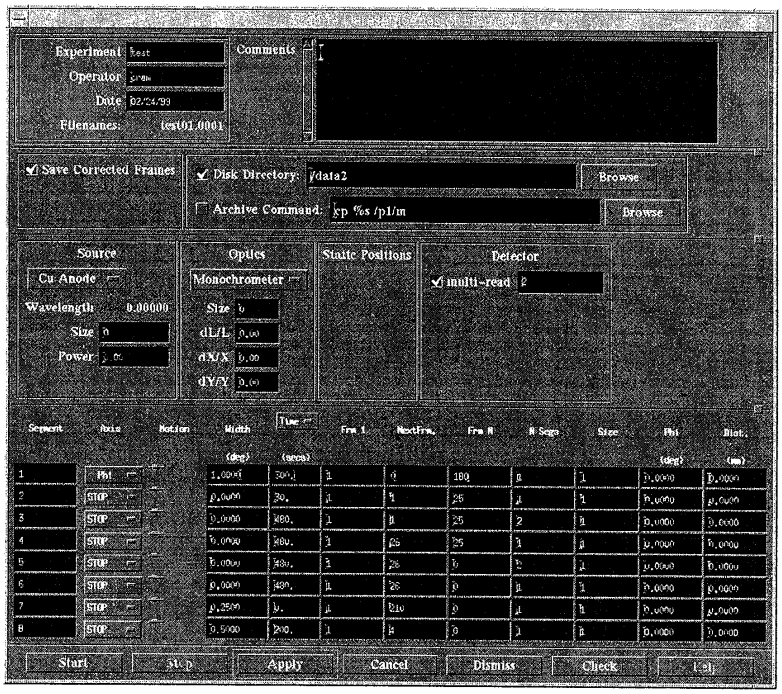

- Type the desired file name, including path, into the box on the bottom.

⇒ click on "Save"

Remark:
Do not use "Save Displayed Image". The "Save Displayed Image" option saves a picture of the current display in 8-bit TIFF format for other purposes than data processing, it does not save the actual data frame.

**To collect a data set:**
Remark: This is just the simplest example for collecting a data set. Please read section two of this manual for more sophisticated methods to collect your data.

Use the left mouse button to choose from the pull-down menus on top of the main marccd window:
⇒Click on Acquire
Data Set
The Acquire Data Set dialog box will appear.




*Top third (Data set Information, File Deposition)*

- Fill in the information on the top - this will be recorded in the header of the frames. The string typed into the "Experiment" box will be used to compose the filenames for the data written to disk.
- Click the button by "Save Corrected Frames" to show a checkmark (✓).
- Click the button by "Disk Directory" to show a checkmark (✓) and in the adjacent box, type in the entire path for the directory in which the data frames should be written.

- Click the button next to “Archive Command” to show **no** checkmark.

*Middle third (Experimental Conditions)*

- With one exception (see below), the information under "Source", "Optics", "Static Positions" and "Detector" will be recorded in the headers of the frames and is not used in any other way during data collection. Filling in the correct information at this point will simplify record keeping.

- The exception is "multi-read" under the "Detector" heading. If this button shows a checkmark (✓) each exposure will be split into several detector readouts to facilitate the removal of "zingers" (cosmic rays causing unwanted spots in addition to the diffraction pattern from the crystal). Enter the desired number of readouts per exposure in the adjacent box, usually 2. This feature should only be used in case of long exposure times (over several minutes) and is almost never recommended when collecting data at a synchrotron.

*Bottom third (Protocol)*

These instructions are for collecting one simple data set. To set up more complicated strategies and for explanations of all the options and features available here, read the detailed description of this dialog box in section ?.

To collect just one data set, type only in the top row of boxes.

- Name the Segment "1".
- Under "Axis" choose "Phi" by clicking the button.
- "Motion" should be set to "Scan".
- Under "Width" type in the oscillation angle in degrees, for example 0.1 for "phi-slicing" or 2.0 for "large oscillation images". Obviously, these numbers depend on the crystal and the type of experiment.
- Choose "Time" on the Time/Dose button, then type in the exposure time in seconds.
- Under "Frm1" type in the number you wish to give the first frame of this data set, usually 1.
- Under "Next Frm" type in the frame number at which you wish to start this data set, usually 1.
- Under "Frm N" type in the total number of frames to collect.
- Under "Nsegs" type in 1.
- If "Nsegs" is 1, then it does not matter what is given for "Size", type in 1, for example.
- Under "Phi" type in the starting Phi position for the frame listed as "Next Frm".
- Under "Dist" type in the desired crystal-to-detector distance in mm.
- If "Nsegs" is 1, then it does not matter what data is in all subsequent rows of this table.

*Action*

Once all the data is typed in correctly

⇒ click on "Apply" in the bottom row of buttons.

⇒ Next, click on the "Check" button in the bottom row. A dialog box will pop up and offer comments on the data collection setup. This is useful for spotting typos and/or mistakes.

⇒ If everything looks right, click on the "Start" button in the bottom row.

The instrument will now drive to the distance and starting phi requested and start the data collection.

To get rid of the data collection dialog box:
⇒ click "Dismiss" in the bottom row of buttons.

**To stop the data collection at any point:**
*Go back into the "Acquire Data Set" menu.*
(Click on Acquire, Data Set, the "Acquire Data Set" dialog box will appear.)
⇒ click on the "Stop" button on the data collection dialog box to abort after the current frame is finished.

**Size of Data Frames:**
Unless the user chooses to change the binning, each data frame from a MarCCD (133mm or 165mm option) is 8392704 bytes in size, a little over 8 MB.
The files are not compressed.

The MarCCD software will check for disk space and warn the user if there is not enough disk space for a data set about to be started. If the disk space runs out during the data collection (either because there was not enough space to begin with, or because other data was written to the same disk in the meantime), then MarCCD will pop up a dialog box with a warning and keep on trying to write the last collected frame. It will not go on to the next frame in the data set until it has successfully saved the previous data frame.

# Collecting Data with the MarCCD System

## Status

To start collecting data, the MarCCD software should be running, the detector status panel should show the temperature to be close to the optimal temperature (see description of Configuration => Detector panel on page ?), the pressure should be below 1 Torr and the Status should read "Cooler ON".
There should be X-rays (check ionization chambers, page ?) and the slits should be set appropriately for the experiment (page ?).
Please refer to the First Start (page ?), or the Getting Started (page ?) sections of this manual if any of these conditions are not met.

## Using the Acquire Single Frame Menu

This can be used to orient the crystallographer in reciprocal space such that a data set can be started at the most appropriate place in reciprocal space or such that a specific wedge of reciprocal space can be targeted.
For protein crystals, two or three 1° oscillations about 30° apart in phi are often used for this purpose.
In some cases all that is needed is a first rough estimate of cell dimensions, in which case one might only require one oscillation image.
It is possible to take still or oscillation exposures and the exposure can be set either in seconds (time) or in kHz, which is a unit of dose in this case (see below).
If it is known that the crystals decay very quickly (in a few exposures) it may be advantageous to start a data set "blindly" (using the "Acquire Data Set" panel) without first using this panel to optimize phi and exposure setting.

## Resolution

The word "resolution" is used for two very separate phenomena in this context.

The first is what is often referred to as the "resolution of the diffraction data" (d-spacing, number of orders etc.), ultimately limited by the sample quality. Throughout this manual "resolution" refers to this phenomena.

The second is the ability of the X-ray detector to resolve features in the measured diffraction pattern, i.e. how close can two spots be together and still be recognized as separate spots. This depends on the detector, specifically the pixel size and the point spread function in case of CCD type detectors. When collecting crystallographic data with MarCCD detectors, the data collection should be set up to give at least 8 pixels between the centers of the closest spots (i.e. longest cell edge). Of course this value can vary for individual experiments because

variations in X-ray beam size/quality and crystal size/quality will change the size of the diffraction spots themselves.

**Pixel Size**
The pixel size varies slightly between individual detectors. The exact pixel size for the detector at hand can be found in the Configure => Detector panel (page?).
For the 165mm diameter MarCCD the pixel size is approximately 0.08mm, for the 133mm diameter MarCCD model the pixel size is approximately 0.064mm. Both of these values are for the standard readout of 2048x2048 pixels per frame. To resolve large unit cell edges (X-Ray Crystallography) one should allow for at least 8 pixels between Bragg Maxima. If the diffraction spots are large, one might decide to leave 10 pixels between Bragg Maxima. The Tables on page ? provide examples for both cases.

**Distance**
The sample-detector distance can be set anywhere between 30mm and 430mm. The user should check carefully, that the detector will not hit the beam stop when driven very close to the crystal. This is best done by approaching the short distance in steps.

Generally the user will know best how to decide on the optimal sample-detector distance for data collection. The following list is not meant as a complete discussion of all factors, it merely a short summary of effects:

*Shorten sample-detector Distance or decrease wavelength of X-rays:*
Resolution of data at detector edge gets better.
Long cell edges (Crystallography) are not resolved as well.
Absorption of X-rays by air decreases.

*Lengthen sample-detector distance or increase wavelength of X-rays:*
Resolution of data at detector edge gets worse.
Long cell edges (Crystallography) are resolved better.
Absorption of X-rays by air increases.

**2-Theta Offset**
When the 2-theta angle is increased, the resolution of data at the edge of the detector will become better, without effecting the ability to resolve long cell edges (Crystallography).
On the older MarCCD systems the 2-theta offset is in form of blocks under the detector. The detector is in the 2theta= 0.0 position when all three blocks are inserted under the detector. As blocks are removed, 2-theta increases.

Generally the user will know best how to balance the choices of wavelength, sample-detector distance and 2 theta to measure the desired data.

**Example Tables**
The tables on the following pages can be used as a rough guide to aid the user in choosing good settings for a data collection.

**No** block removed, Detector diameter= **165.00mm**, Wavelength= **1.00Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 0.87 | 70.02 | 0.00 | 37.5 | 46.9 |
| 70.0 | 1.19 | 49.69 | 0.00 | 87.5 | 109.4 |
| 110.0 | 1.58 | 36.87 | 0.00 | 137.5 | 171.9 |
| 150.0 | 2.01 | 28.81 | 0.00 | 187.5 | 234.4 |
| 190.0 | 2.46 | 23.47 | 0.00 | 237.5 | 296.9 |
| 230.0 | 2.92 | 19.73 | 0.00 | 287.5 | 359.4 |
| 270.0 | 3.38 | 16.99 | 0.00 | 337.5 | 421.9 |
| 310.0 | 3.86 | 14.90 | 0.00 | 387.5 | 484.4 |
| 350.0 | 4.33 | 13.26 | 0.00 | 437.5 | 546.9 |
| 390.0 | 4.81 | 11.94 | 0.00 | 487.5 | 609.4 |
| 430.0 | 5.28 | 10.86 | 0.00 | 537.5 | 671.9 |

**One** block removed, Detector diameter= **165.00mm**, Wavelength=**1.00A**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 0.82 | 75.19 | 45.94 | 37.5 | 46.9 |
| 70.0 | 1.03 | 58.34 | 23.89 | 87.5 | 109.4 |
| 110.0 | 1.28 | 45.90 | 15.74 | 137.5 | 171.9 |
| 150.0 | 1.57 | 37.11 | 11.68 | 187.5 | 234.4 |
| 190.0 | 1.88 | 30.85 | 9.27 | 237.5 | 296.9 |
| 230.0 | 2.20 | 26.27 | 7.68 | 287.5 | 359.4 |
| 270.0 | 2.53 | 22.80 | 6.55 | 337.5 | 421.9 |
| 310.0 | 2.86 | 20.11 | 5.71 | 387.5 | 484.4 |
| 350.0 | 3.20 | 17.97 | 5.06 | 437.5 | 546.9 |
| 390.0 | 3.54 | 16.23 | 4.54 | 487.5 | 609.4 |
| 430.0 | 3.89 | 14.79 | 4.12 | 537.5 | 671.9 |

**Two** blocks removed, Detector diameter=**165.00mm**,Wavelength=**1.00Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 0.79 | 78.27 | 64.18 | 37.5 | 46.9 |
| 70.0 | 0.94 | 64.15 | 41.53 | 87.5 | 109.4 |
| 110.0 | 1.13 | 52.72 | 29.41 | 137.5 | 171.9 |
| 150.0 | 1.34 | 43.93 | 22.46 | 187.5 | 234.4 |
| 190.0 | 1.57 | 37.25 | 18.07 | 237.5 | 296.9 |
| 230.0 | 1.81 | 32.14 | 15.09 | 287.5 | 359.4 |
| 270.0 | 2.06 | 28.16 | 12.93 | 337.5 | 421.9 |
| 310.0 | 2.31 | 24.99 | 11.31 | 387.5 | 484.4 |
| 350.0 | 2.57 | 22.43 | 10.0 | 437.5 | 546.9 |
| 390.0 | 2.83 | 20.33 | 9.03 | 487.5 | 609.4 |
| 430.0 | 3.10 | 18.57 | 8.20 | 537.5 | 671.9 |

**No** block removed, Detector diameter=**165.00mm**, Wavelength=**1.5418Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 1.34 | 70.02 | 0.00 | 57.8 | 72.3 |
| 70.0 | 1.83 | 49.69 | 0.00 | 134.9 | 168.6 |
| 110.0 | 2.44 | 36.87 | 0.00 | 212.0 | 265.0 |
| 150.0 | 3.10 | 28.81 | 0.00 | 289.1 | 361.4 |
| 190.0 | 3.79 | 23.47 | 0.00 | 366.2 | 457.7 |
| 230.0 | 4.50 | 19.73 | 0.00 | 443.3 | 554.1 |
| 270.0 | 5.22 | 16.99 | 0.00 | 520.4 | 650.4 |
| 310.0 | 5.94 | 14.90 | 0.00 | 597.4 | 746.8 |
| 350.0 | 6.68 | 13.26 | 0.00 | 674.5 | 843.2 |
| 390.0 | 7.41 | 11.94 | 0.00 | 751.6 | 939.5 |
| 430.0 | 8.15 | 10.86 | 0.00 | 828.7 | 1035.9 |

**One** block removed, Detector diameter=**165.00mm**, Wavelength=**1.5418Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 1.26 | 75.19 | 45.94 | 57.8 | 72.3 |
| 70.0 | 1.58 | 58.34 | 23.89 | 134.9 | 168.6 |
| 110.0 | 1.98 | 45.90 | 15.74 | 212.0 | 265.0 |
| 150.0 | 2.42 | 37.11 | 11.68 | 289.1 | 361.4 |
| 190.0 | 2.90 | 30.85 | 9.27 | 366.2 | 457.7 |
| 230.0 | 3.39 | 26.27 | 7.68 | 443.3 | 554.1 |
| 270.0 | 3.90 | 22.80 | 6.55 | 520.4 | 650.4 |
| 310.0 | 4.42 | 20.11 | 5.71 | 597.4 | 746.8 |
| 350.0 | 4.94 | 17.97 | 5.06 | 674.5 | 843.2 |
| 390.0 | 5.46 | 16.23 | 4.54 | 751.6 | 939.5 |
| 430.0 | 5.99 | 14.79 | 4.12 | 828.7 | 1035.9 |

**Two** blocks removed,Detector diameter=**165.00mm**,Wavelength=**1.5418Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 1.22 | 78.27 | 64.18 | 57.8 | 72.3 |
| 70.0 | 1.45 | 64.15 | 41.53 | 134.9 | 168.6 |
| 110.0 | 1.74 | 52.72 | 29.41 | 212.0 | 265.0 |
| 150.0 | 2.06 | 43.93 | 22.46 | 289.1 | 361.4 |
| 190.0 | 2.41 | 37.25 | 18.07 | 366.2 | 457.7 |
| 230.0 | 2.78 | 32.14 | 15.09 | 443.3 | 554.1 |
| 270.0 | 3.17 | 28.16 | 12.93 | 520.4 | 650.4 |
| 310.0 | 3.56 | 24.99 | 11.31 | 597.4 | 746.8 |
| 350.0 | 3.96 | 22.43 | 10.05 | 674.5 | 843.2 |
| 390.0 | 4.37 | 20.33 | 9.03 | 751.6 | 939.5 |
| 430.0 | 4.78 | 18.57 | 8.20 | 828.7 | 1035.9 |

**No** blocks removed, Detector diameter= **133.00mm**, Wavelength= **1.000Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 0.92 | 65.72 | 0.00 | 46.9 | 58.6 |
| 70.0 | 1.35 | 43.53 | 0.00 | 109.4 | 136.7 |
| 110.0 | 1.86 | 31.15 | 0.00 | 171.9 | 214.8 |
| 150.0 | 2.41 | 23.91 | 0.00 | 234.4 | 293.0 |
| 190.0 | 2.98 | 19.29 | 0.00 | 296.9 | 371.1 |
| 230.0 | 3.56 | 16.13 | 0.00 | 359.4 | 449.2 |
| 270.0 | 4.15 | 13.84 | 0.00 | 421.9 | 527.3 |
| 310.0 | 4.74 | 12.11 | 0.00 | 484.4 | 605.5 |
| 350.0 | 5.33 | 10.76 | 0.00 | 546.9 | 683.6 |
| 390.0 | 5.93 | 9.68 | 0.00 | 609.4 | 761.7 |
| 430.0 | 6.52 | 8.79 | 0.00 | 671.9 | 839.8 |

**One** blocks removed,,Detector diameter=**133.00mm**, Wavelength=**1.000Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 0.84 | 72.90 | 45.94 | 46.9 | 58.6 |
| 70.0 | 1.10 | 54.32 | 23.89 | 109.4 | 136.7 |
| 110.0 | 1.41 | 41.55 | 15.74 | 171.9 | 214.8 |
| 150.0 | 1.76 | 33.02 | 11.68 | 234.4 | 293.0 |
| 190.0 | 2.13 | 27.16 | 9.27 | 296.9 | 371.1 |
| 230.0 | 2.51 | 22.97 | 7.68 | 359.4 | 449.2 |
| 270.0 | 2.90 | 19.86 | 6.55 | 421.9 | 527.3 |
| 310.0 | 3.29 | 17.46 | 5.71 | 484.4 | 605.5 |
| 350.0 | 3.69 | 15.57 | 5.06 | 546.9 | 683.6 |
| 390.0 | 4.09 | 14.04 | 4.54 | 609.4 | 761.7 |
| 430.0 | 4.49 | 12.78 | 4.12 | 671.9 | 839.8 |

**Two** blocks removed, Detector diameter=**133.00mm**, Wavelength=**1.000Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 0.80 | 76.86 | 64.18 | 46.9 | 58.6 |
| 70.0 | 0.98 | 61.42 | 41.53 | 109.4 | 136.7 |
| 110.0 | 1.20 | 49.44 | 29.41 | 171.9 | 214.8 |
| 150.0 | 1.44 | 40.59 | 22.46 | 234.4 | 293.0 |
| 190.0 | 1.71 | 34.07 | 18.07 | 296.9 | 371.1 |
| 230.0 | 1.98 | 29.19 | 15.09 | 359.4 | 449.2 |
| 270.0 | 2.27 | 25.45 | 12.93 | 421.9 | 527.3 |
| 310.0 | 2.56 | 22.51 | 11.31 | 484.4 | 605.5 |
| 350.0 | 2.86 | 20.16 | 10.05 | 546.9 | 683.6 |
| 390.0 | 3.16 | 18.24 | 9.03 | 609.4 | 761.7 |
| 430.0 | 3.46 | 16.64 | 8.20 | 671.9 | 839.8 |

**No** blocks removed, Detector diameter=**133.00mm**, Wavelength=**1.5418Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 1.42 | 65.72 | 0.00 | 72.3 | 90.3 |
| 70.0 | 2.08 | 43.53 | 0.00 | 168.6 | 210.8 |
| 110.0 | 2.87 | 31.15 | 0.00 | 265.0 | 331.2 |
| 150.0 | 3.72 | 23.91 | 0.00 | 361.4 | 451.7 |
| 190.0 | 4.60 | 19.29 | 0.00 | 457.7 | 572.2 |
| 230.0 | 5.50 | 16.13 | 0.00 | 554.1 | 692.6 |
| 270.0 | 6.40 | 13.84 | 0.00 | 650.4 | 813.1 |
| 310.0 | 7.31 | 12.11 | 0.00 | 746.8 | 933.5 |
| 350.0 | 8.22 | 10.76 | 0.00 | 843.2 | 1054.0 |
| 390.0 | 9.14 | 9.68 | 0.00 | 939.5 | 1174.4 |
| 430.0 | 10.06 | 8.79 | 0.00 | 1035.9 | 1294.9 |

**One** block removed, Detector diameter=**133.00mm**, Wavelength=**1.5418Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 1.30 | 72.90 | 45.94 | 72.3 | 90.3 |
| 70.0 | 1.69 | 54.32 | 23.89 | 168.6 | 210.8 |
| 110.0 | 2.17 | 41.55 | 15.74 | 265.0 | 331.2 |
| 150.0 | 2.71 | 33.02 | 11.68 | 361.4 | 451.7 |
| 190.0 | 3.28 | 27.16 | 9.27 | 457.7 | 572.2 |
| 230.0 | 3.87 | 22.97 | 7.68 | 554.1 | 692.6 |
| 270.0 | 4.47 | 19.86 | 6.55 | 650.4 | 813.1 |
| 310.0 | 5.08 | 17.46 | 5.71 | 746.8 | 933.5 |
| 350.0 | 5.69 | 15.57 | 5.06 | 843.2 | 1054.0 |
| 390.0 | 6.31 | 14.04 | 4.54 | 939.5 | 1174.4 |
| 430.0 | 6.93 | 12.78 | 4.12 | 1035.9 | 1294.9 |

**Two** blocks removed, Detector diameter=**133.00mm**, Wavelength=**1.5418Å**

| distance | resolution, 2 theta at detector edge | | effective 2 theta offset | resolved cell edges 10 pixels | 8 pixels |
|---|---|---|---|---|---|
| mm | Å | degrees | degrees | Å | |
| 30.0 | 1.24 | 76.86 | 64.18 | 72.3 | 90.3 |
| 70.0 | 1.51 | 61.42 | 41.53 | 168.6 | 210.8 |
| 110.0 | 1.84 | 49.44 | 29.41 | 265.0 | 331.2 |
| 150.0 | 2.22 | 40.59 | 22.46 | 361.4 | 451.7 |
| 190.0 | 2.63 | 34.07 | 18.07 | 457.7 | 572.2 |
| 230.0 | 3.06 | 29.19 | 15.09 | 554.1 | 692.6 |
| 270.0 | 3.50 | 25.45 | 12.93 | 650.4 | 813.1 |
| 310.0 | 3.95 | 22.51 | 11.31 | 746.8 | 933.5 |
| 350.0 | 4.40 | 20.16 | 10.05 | 843.2 | 1054.0 |
| 390.0 | 4.86 | 18.24 | 9.03 | 939.5 | 1174.4 |
| 430.0 | 5.33 | 16.64 | 8.20 | 1035.9 | 1294.9 |

## Synchrotron or Rotating Anode

Certain issues need to be considered when setting up a data collection and they vary based on the type of experiment, sample quality and character of X-ray beam.

# Detailed Description of the MarCCD Program

## Command Line Options

The user should be logged into the computer controlling the MarCCD detector and the Marbase as "marccd". To start the software one only has to type

```
marccd <return>
```

However, several options can be invoked from the command line. Typing

```
marccd -h <return>
```

will produce the following listing:

```
Usage: /home/marccd/bin/linux/marccd [X11 options] [-hrvV]
   -h  Show this help message.
   -r  Startup in remote mode.
   -v  Output version and exit.
   -V  Verbose (debug) mode.
```

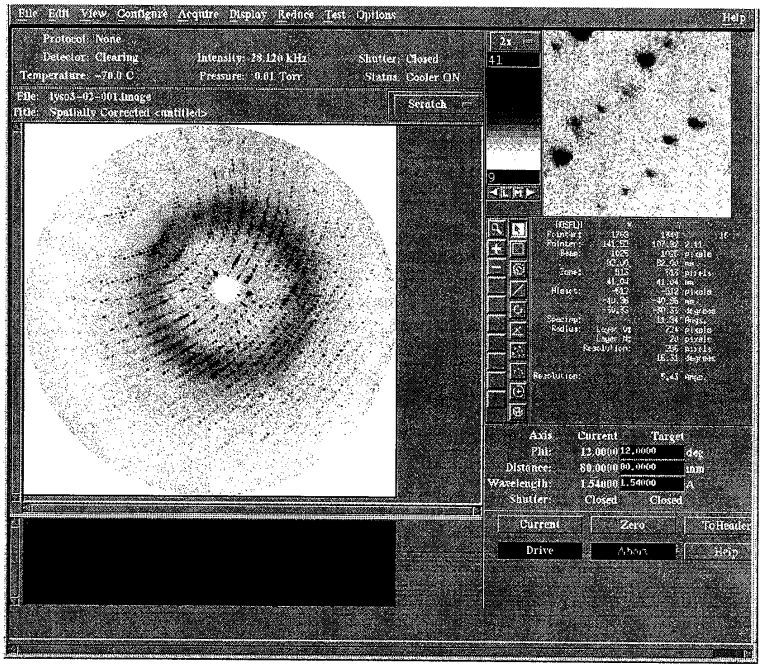
The -r option (remote mode) is used by customers who wish to run the...
The -v option is just a quick method to find out which version of marccd is currently installed.
The -V option may be used in certain cases of trouble shooting.
The not mention -d flag over-rides the DISPLAY variable.
The not mentioned -name flag runs the program with a different name attached (i.e. -name bigmarccd will invoke all the "bigmarccd*..." options and choices from the file Marccd.

In addition to these options, typing -xrm on the command line facilitates passing on commands to the x-resource manager (X11).
This has to be of the format marccd -xrm "name*option:choice"
name: marccd or bigmarccd. The program runs under this "name", the chosen option only applies when this "name" is used. I.e. changing the program to the name "bigmarccd" instead of "marccd" would then use all the options chosen for name=bigmarccd.
There is also a class associated with the program, Marccd. This is never changed. It causes the file Marccd to be read.

To find possible options and choices, look in Marccd and in /mar/sw/marccd/source/resource.c.

## The main marccd panel

This panel displays data frames, the current status of the MarCCD detector, current status of the Marbase and provides tools to closely examine data frames as well as tools to drive the Marbase.




The top row of buttons produces various pull-down menus which in turn offer other functional panels. These buttons and subsequent panels are described in detail in section ?? of this manual.

*Status Window*

Between the top row of buttons and the large data frame display area, the current status of the detector is described.

**Protocol:**

| | |
|---|---|
| None | when the data collection is idle, |
| Single Frame | when a single frame is in progress, started from "Acquire Single Frame", |
| Remote | when the detector is under remote control; |
| Data set | when a data set is in progress, started from "Acquire Data set", in this case the segment and type of data frame (see "Acquire Data set, page??) are given on the same line after the Protocol definition; |

**Detector:**

| | |
|---|---|
| Clearing | when the detector is idle, |
| Exposing | when the detector is integrating with the shutter open |
| Reading | when the detector is being read out |
| Integrating | when the detector is integrating with the shutter closed; |

**Intensity:**

The intensity is reported in kHz, which corresponds to the reading from the ionization chamber in the Marbase and is thus directly proportional to X-ray photons per second. In other words, this value is directly proportional to the intensity of the X-ray beam.

Note that the choice of chamber and the gain of the ionization chambers in the Marbase can be changed by the user, either on the Marbase itself or via the remote control (see the "hardware" section of this manual). The value displayed on the Marbase and Remote Control is also displayed here.

However, when data is collected in "Dose" mode (page ??) the software always uses the reading from ionization chamber 2 and locks the ionization chamber controls to display chamber 2. The current gain setting still applies.

**Shutter:**
Can be "Open" or "Closed". If the marccd software is not controlling the shutter, this will read "Unknown".

**Temperature:**
The current temperature of the detector head in °C. This should be close to -70°C for data collection. Each detector has a factory-determined optimal temperature for operation, which is loaded as the set temperature upon starting MarCCD. The cooler will automatically keep the detector to this set temperature. Most detectors operate best between -65°C and -90°C. A detector that is warmer than the ideal operating temperature will simply produce noisier images.

**Pressure:**
This is the pressure inside the detector head in Torr. This value should always be less than 1 Torr when the detector is cold.
A pressure of 2 Torr or higher at room temperature indicates that the detector requires routine maintenance (page?).

**Status:**

| | |
|---|---|
| Cooler ON | Everything is functioning well and the cooler is running. |
| Cooler OFF | Everything is functioning well and the cooler is turned OFF.<br>(turn it on/off via the "Configure Detector" panel, see page ??) |
| No Response | The computer cannot communicate with the detector controller. |
| Check Cables! | The computer communicates well with the detector controller<br>but the detector controller cannot communicate with the detector. |

*Frame Title Bar and Frame Display Pop-Up Menu:*

**Pop-up menu:**
Choose between several display locations:

| | |
|---|---|
| Detector | the last image read from the detector will be displayed, |
| Background | the currently stored (and used) background image will be displayed, |
| Scratch, Scratch1-3 | locations to be used to display data frames that have been previously |

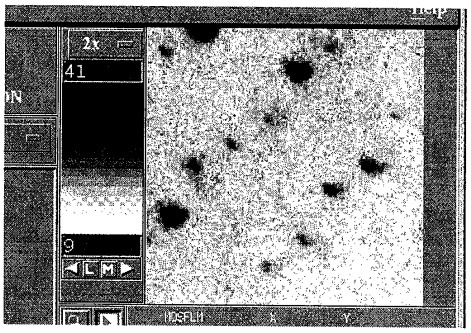
collected. Data frames can be loaded into these locations via the "File, Load Data Frame" menu, see page ??).

If the display is set to a location that does not have a data frame loaded, the main frame display window will show the marccd logo in large letters. If the display is completely monotone, a blank frame is displayed.

**File:**
Name of the currently displayed file.

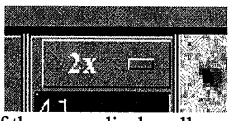
**Title:**
Title from the header of the currently displayed file.

*Zoom Window and Color Swatch/Contrast&Brightness Control:*



**Zoom Window:**
An area from the large display window is shown enlarged in this field. The magnified area within the data frame is chosen by clicking the left mouse button in the desired location in the main frame display window.

**Magnification pop-up menu:**

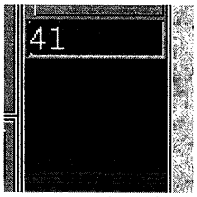



This pop-up menu to the top left of the zoom display allows the user to choose the magnification. When it is set to 32, the actual integers stored for each pixel will be displayed in the zoom window.

**Greyscale for both display areas:**
All settings in this area apply to both the main display and the zoom display.
The choice of colour versus black&white, negative/positive and view directions is made via the "View" pull down menu, described on page ??.

On top of the box showing the colour spectrum in use is a dialog box containing a number. This is the integer number stored for each pixel. Any pixel with this value or higher will be displayed in the colour at the top of the display spectrum. On the bottom of the colour spectrum is another dialog box. Any pixel with a value equal or less to what is in this box will be displayed in the colour at the bottom edge of the colour spectrum. To enter a value into either box by hand, use the mouse to click in the box, then type in the desired value, then hit return.

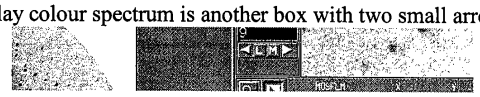
Example:



Top box reads 41, colour at top edge of spectrum is black => all pixels with a value of 41 or greater will look black in the display (both the large display and the zoom window).

The bottom dialog box reads 9, the bottom edge of the spectrum is white => all pixels with values of 9 or less will be displayed in white.

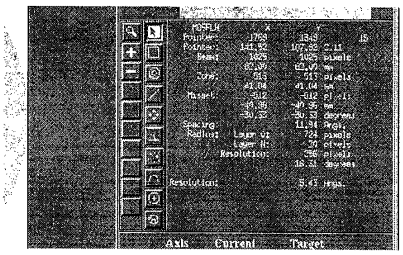
Also below the display colour spectrum is another box with two small arrow buttons:



If the arrow button pointing to the large data frame display window is clicked, the values for the top and bottom pixel values in the spectrum dialog boxes are automatically adjusted appropriately to view the large display area. If the arrow button pointing to the zoom display is clicked, the values in the top and bottom dialog boxes of the colour spectrum are automatically adjusted for viewing the zoom box.

The colour spectrum itself can be adjusted via the mouse by positioning the mouse in the spectrum, holding the left button down and then moving the mouse. If the mouse is moved vertically the brightness is adjusted. By moving the mouse horizontally the contrast is adjusted.

## *Tool Bar:*




***Explain information in table, how coordinate convention is changed etc. Insert pictures of this table and poss. Graphs at the aprobriate tools.***

There are two sets of buttons.

**The left column of buttons perform miscellaneous functions:**

Zoom

If this button is clicked on, the area displayed in the zoom window will be outlined by a box in the main display window. As the zoom area is re-located by clicking with the mouse, this box is moved accordingly. The box can also be dragged (with the right mouse button) to reposition the zoomed area. The zoom display will update when the mouse button is released.

Forward

A click on this button automatically loads the next frame of a data set into the current display. An error message is displayed if such a frame cannot be found.
The filename is determined from the name of the displayed frame. The frame number is assumed to be the rightmost numerical part of the name.

Backward

A click on this button automatically loads the previous frame in a data set into the current display. An error message is displayed if such a frame cannot be found.
The filename is determined from the name of the displayed frame. The frame number is assumed to be the rightmost numerical part of the name.

**The right column of tool buttons:**
If any button in this column is clicked, it causes the previously selected tool to be turned off. While the arrow tool is active, the table to the right of the tool buttons shows the position of the cursor in the display window and other information related to the position:

Pointer

When this button is clicked all other tools are turned off.

Area of Interest Box

When this button is clicked, the user can draw a box anywhere in the main display window or zoom window to get statistics about the area in the box displayed in the table to the right of the tool buttons.

To draw the box, hold down the middle mouse button and drag. To move the box, position the mouse in the center of the box and drag the box by holding down the right mouse button while moving the mouse. To change the size of the box, position the mouse on the edge of the box, hold down the right mouse button and drag.

The displayed statistics are defined as:

Layer Lines

This tool provides rings defining a zero layer and an n'th layer circle in a diffraction pattern from a three dimensional crystal.

The zero layer ring will always go through the current beam position. To move this beam position, either grab and drag the cross on the zero layer ring with the right mouse button, or move the beam position with the beam tool (?).
To reposition the center of the zone, grab the larger circle with the right mouse button and drag. The mouse will be attached to the center of the circles but the cursor will not appear in the center of the circles.
The table to the right of the tool buttons will display the following information:

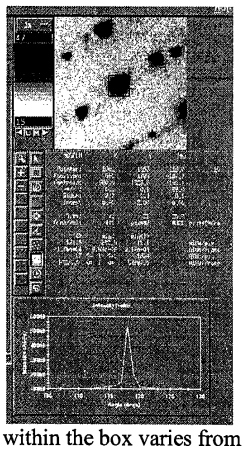
Histogram
This tool allows the user to draw a line in the display and then inspect a plot of the intensities along this line. The plot will appear under the table to the right of the tool buttons.

Spot Statistics
This button is currently not used.

Angle
This tool measures the angle between two lines. To draw the angle, use the middle mouse button to draw align - a short horizontal line will automatically appear attached to the user-drawn line. Use the right mouse button to drag the end of the horizontal line to the desired position. The table to the right of the tool buttons will now display:

This button is currently not used.

Profile
This tool allows the user to examine the profile of a spot in the phi direction.
When this button is clicked, a dialog box appears. The user is asked to type in the number of frames to be used, with the currently displayed frame at the center of the stack. Note that the currently displayed data frame will be lost unless it is already saved to disk.
Once "OK" is clicked, the frames surrounding the currently displayed frame will be loaded. A small box can be positioned in the display via the middle mouse button. This is best done in the zoom window. The right mouse button can grab the edges of the box and change the box size. The middle mouse button will move the center of the box to wherever it is clicked in the display. The area within the small box is used for the plot displayed under the table and tool buttons.



This plot shows how the intensity within the box varies from frame to frame. This tool would be used to examine spot profiles in order to decide on the oscillation range for phi when a data collection is to be set up.

Beam, Resolution

This tool allows the user to define the beam position, by dragging the center of the circle with the right mouse button. The new beam position will be shown in the table to the right of the tool buttons.

Crystal Parameters

This button is currently not in use.

*Goniostat Window:*

This window sometimes changes into a graph window when certain tools are in use. To get back to the goniostat window turn all tools off by clicking on the arrow button in the tool bar.

insert picture, write up description and use.

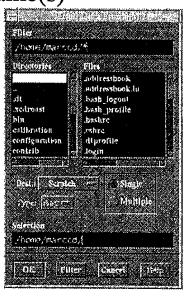
*Log Window*

Messages from the software will be listed in this window.
Say more???

*Pop-Up Menu Bar in Main marccd Window:*

File

==> Load X-ray Data Frame(s)




This panel is used to read previously collected data frames which have been saved to disk into marccd.

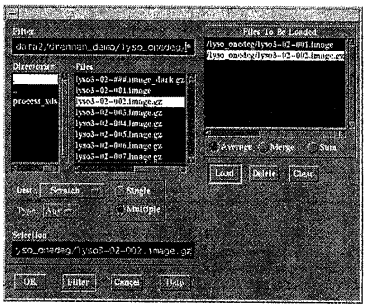
The top dialog box is used for the "Filter" function. Type a directory and partial filename into this box, use the standard wild card characters (*, ?, etc.). Once the "Filter" button on the bottom of the panel is clicked, the large two center boxes will list the directory and all files matching the description given in the top box.

Clicking on a file name in this list will copy that filename to the bottom dialog box. Alternatively, the filename can be typed into the bottom dialog box.

From the pull-down menu choose a destination for the file, i.e. "Scratch" or "Background" etc.
Note that whatever is in the destination location will be lost once you load a new file into that location. When in doubt, use the "Save Displayed Data Frame" option first.

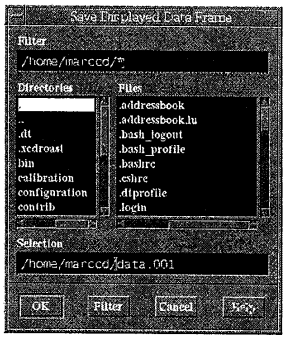
Once the OK button is clicked, the file listed in the bottom dialog box will be loaded into the location chosen by the pull down menu. When the display is set to the chosen location the data frame is displayed. In case "Scratch" is selected as destination location, the display automatically switches to "Scratch" when the file is loaded.

***Insert multi-option.....***




File

==> Save Displayed Data Frame




This panel allows the user to save the currently displayed data frame to a file. A frames saved via this panel can subsequently be loaded back into the marccd software and can also be processed by the usual data processing methods.

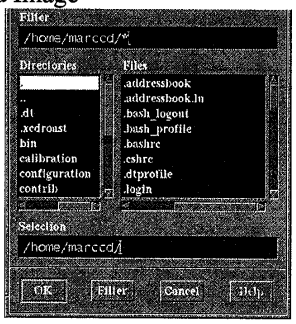
The top dialog box is used for the "Filter" function. Type a directory and partial filename into this box, use the "*" character as a wild card. Once the "Filter" button on the bottom of the panel is clicked, the large two center boxes will list the directory and all files matching the description given in the top box.

Clicking on a file name in this list will copy that filename to the bottom dialog box. Alternatively, the filename can be typed into the bottom dialog box or a chosen filename can be edited here.

Once the OK button is clicked, the frame currently displayed by the marccd software will be written to the filename given in the bottom dialog box. A warning is given, if such a file already exists.

File

==> Save Displayed Image




This panel allows the user to save the currently displayed data frame as an image file. Note that the image file thus created is not a data frame that can be read by subsequent data processing programs. This file is an 8-bit TIFF file of the image as it is displayed (256 grey levels). It can be read by image manipulation/display programs such as *xv*, Photoshop etc.

The top dialog box is used for the "Filter" function. Type a directory and partial filename into this box, use the "*" character as a wild card. Once the "Filter" button on the bottom of the panel is clicked, the large two center boxes will list the directory and all files matching the description given in the top box.

Clicking on a file name in this list will copy that filename to the bottom dialog box. Alternatively, the filename can be typed into the bottom dialog box or a chosen filename can be edited here.

Once the OK button is clicked, the image currently displayed by the marccd software will be written to the filename given in the bottom dialog box. A warning is given, if such a file already exists.

File

==> Print  Ctrl+P

If set up properly, this feature produces a postscript file of the graph window. For making graphs see the Tool Window section of this manual (page?).
Simply let go of the mouse button on this field or type Ctrl+P on the keyboard.

File

==> Quit Ctrl+C

This is the recommended method to stop the marccd software. Simply let go of the mouse button on this option or type Ctrl+C on the keyboard. A dialog box will appear to ask for confirmation.

Edit

==> Copy to

Several "Copy to" options may be turned off in the distributed software.
These commands are useful for moving data frames from one buffer within the marccd software (i.e. "Detector", "Scratch", "Background" etc.) to another. Clicking on "Copy to" will produce a sub-menu of destinations. Note that any frame stored in the destination buffer will be written over. Use the "Save Data Frame" option first when in doubt.
To execute, simply click on the desired "copy to" destination. The currently displayed data frame will be copied to the new location.

Edit

==> Byte-Swap Frame

This option will swap bytes of the currently displayed data frame and display the result. The marccd is usually controlled from a PC running Linux. Thus, all data frames would usually be small endian byte order.
In combination with the Load/Save Data Frame functions under File on the main panel this may be used to create swapped frames or view frames that have the wrong byte order for some reason.

Edit

==> Bin Frame

This function will bin the requested number of pixels into one pixel.
When the mouse button is released on this option, a dialog box pops up. Type in how many pixels should be binned into one.

If only one number (n) is given the binning will be square (nxn). If two numbers are given (n m), the first number is the binning in the fast (horizontal) direction (binning will be nxm).

This option will operate on the currently displayed data frame and the unbinned data will be lost unless saved to disk first.
Example: A 2048x2048 pixel data frame is displayed. Choose 2x2 binning. The data frame has now 1024x1024 pixels. Each new pixels has the average intensity value of the 4 pixels that were binned into it.

Note that information will be lost if a data frame is binned and subsequently unbinned.

Edit

==> Unbin Frame

This function will split each pixel into the requested number of pixels, unbinning into 4, 16, 64 pixels if possible. However, no additional data is available, thus all pixels will have the same value as the original binned pixel.

Note that information will be lost if a data frame is binned and subsequently unbinned, but unbinning a data frame and then re-binning it will produce a binned file identical to the original.

View

==>Show Header

This option produces a display with the text stored in the header of a data frame. It is easy to check exposure time, phi angle etc. by this method.

View

==>Color Scheme

Users may choose their favorite display mode, black&white negative or positive or colour display.

View

==>Scaling

Formula to assign all possible 65535 data values to N possible display colours (N is usually 128, depending on colours available on the Xserver). The following describes the available options, with min and max corresponding to the smallest and largest value stored for any pixel in the data frame and X representing the value to be assigned to a color.

Linear:
Linear assignment of all values between the minimum and maximum value in the dada frame to the colors 0 to N-1.

$$\text{Colour} = N(X - \text{min}) / (\text{max} - \text{min})$$

Log:
This option offers a log mapping. When chosen, a dialog box will pop up, asking the user for a value for $\gamma$.

$$\text{Color} = N (\log \gamma(X-\text{min})/(\text{max}-\text{min})) / \log \gamma$$

View
==>View Direction

Any data frame can be displayed as if viewed from the X-ray source or into the beam. Simply let the mouse button go on the desired option.

View
==>Coordinates

Several options are given for the convention of the coordinates within the displayed data frame.
The effect of changing this setting is on all coordinate values in any tool display on the right side of the main marccd window.

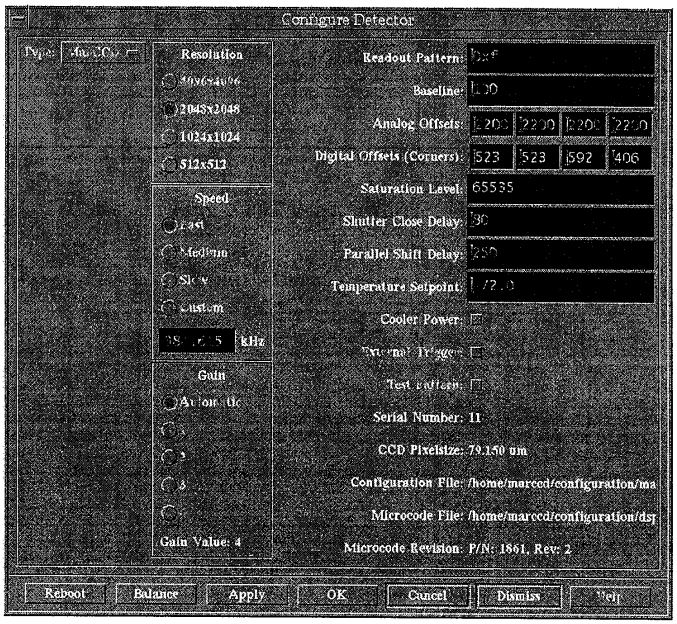
View
==>Values

The choices Decimal, Hexadecimal, Octal and Binary effect the display of pixel values in the zoom window, when the maximum zoom is chosen. The default is decimal numbers.

View
==>Rendering

These options determine how a 2048x2048 frame will be drawn in a 1024x1024 or 512x512 display window, if necessary:
When more than one pixel value must be represented by one pixel in the display, the pixels can be sampled or averaged. Averaging is safer since less information is lost, hence this is the default

Configure
==> Detector




*Parameters on the left:*

**Type**
This cannot be changed by the user. It should read "marCCD", unless the software couldn't find the detector, then it may read "None". Default is "marCCD".

**Resolution**
Normally the MarCCD detector is read out at highest resolution (2048x2048 pixels). The user may elect lower resolution, in which case the pixels on the CCD chip will be binned into groups of 4 (or 16). This would speed up the read out, reduce the size of the files containing the frames, and increase the dynamic range (because there are now 4 (or 16) wells on the CCD chip contributing to each pixel in the finished data frame), but each frame would have only 1024x1024 (or 512x512) pixels for the same size detecting surface. The corresponding change of pixel size is reflected on the lower right half of the Configure/Detector panel as soon as "Apply" is clicked.
Highest resolution (unbinned) is recommended (less than 5 sec readout time, very low readout noise), thus 2048x2048 is the default.

**Speed**
This is preset to the fastest Speed possible and cannot be changed by the user. It is set to the default value: Fast.

**Gain**
In most cases the Gain is set to Automatic, in any case this is preset to the optimal value and cannot be changed by the user. It is set to the default value: Automatic.

*Parameters on the right half:*
These parameters all pertain to the treatment of the signal delivered by the chip. For each pixel a signal in the range of 0 to about 100mV is received on the readout channel in question from the chip. On each channel this is amplified to a signal varying between 0 and 10V, followed by an analog offset (specific for each channel) such that the signal going into the A/D converter lies between -5V and +5V. The A/D converter produces a digital signal of the range 0 to 65535. At this point the signal is converted to "a number" and could be stored. However, the digital offset (specific for each channel) is subtracted from each pixel and the baseline value (identical for all four channels) is added. The effect is, that all four quadrants have the same baseline value corresponding to a mean of zero, regardless of the differences in the signal level from the chip or analog and digital offsets between channels.
Obviously, once the system has been calibrated and installed, it is important that the hardware configuration is not changed. For example, if the system was calibrated with channel A from the detector going through the A/D converter A, channel B going through A/D converter B etc.(as determined by the cables going from the detector head to the controller), then the detector must always be set up this way for use as well. Likewise the A/D cards in the controller may not be switched or the calibration will no longer be optimal.

**Readout Pattern**
This refers to which channels should be used to read out the chip. For the 4-channel CCDs this should be set to 0xf, causing the system to use all four channels for maximum readout speed (the option to read out on less than four channels is disabled in the distributed software). The default for four-channel detectors is 0xf, for others it varies.

The prefix 0x indicates that the number which follows is hexadecimal. However, the marccd software currently always interprets the following number as hexadecimal, regardless of the prefix. To avoid confusion the prefix 0x should be used at all times.

The four readout channels of the CCD chip are numbered by bits:
1 refers to the top left read-out channel (output connector A on the back of the detector),
2 refers to the top right (output connector B),
4 refers to the bottom left (output connector C),
8 refers to the bottom right (output connector D).

The hexadecimal number describing the readout pattern is the sum of numbers corresponding to the channels to be used. They should not be changed from factory default. Non-standard values may require cabeling changes to work as expected.
Examples:

| | |
|---|---|
| all four channels read out: | 1+2+4+8=15, hexadecimal: f |
| read out only on channel 2 (B) and 4 (C): | 2+4=6 , hexadecimal: 6 |
| read out on channels 4 (C) and 8 (D): | 4+8=12 , hexadecimal: c |

Thus to read from only the two channels on the right, enter 0x6 into the window, to read out only the two channels on the bottom enter 0xc and so on.
Diagonal combinations or combinations of three channels are not permitted.

**Baseline**
This number is also read in from the default parameter file. It is usually set to 100.0 and is added to each pixel after the digital offset is subtracted. This value should not be changed, the default is 100.

**Analog Offset**
These values should be read from the default parameter file and not be changed by hand. Default values are 2200 for all four A/D converters, the four numbers are usually identical.

The leftmost number refers to the A/D converter card furthest away from the controller board, the rightmost number to the A/D converter closest to the controller board. This is independent of how the jumpers are set on the A/D boards. The numbers set here should bring the lowest signal to the lowest end of the voltage range of the A/D converter, i.e. these values can have an effect on the dynamic range.

**Digital Offsets (Corners)**
Also factory preset and should always be read from the defaults file.
The four numbers refer to the four corners of the CCD chip: first number corresponds to top left, second number to top right, third number to bottom left, fourth number to bottom right. Normal values are 300 to 600. The four numbers may differ from each other.
These numbers may change if a "balance" is performed. To get back to the default numbers, reboot the camera controller and load the defaults.

**Saturation Level**
All values greater than this number will be marked as saturated (65535). The default is 65535.

## *Small buttons on the right half:*

**Cooler Power**
Click this button to toggle the cooler on/off, then click the "Apply" button to execute.
The default is "OFF" but the cooler should be "ON" for normal operation.

**External Trigger**
If this button is checked, the detector will only be read out if an external signal is received on the aux. input of the CCD controller (black box in the cooler cabinet).
The expected signal is usually set to TTL, i.e. the rising edge of a positive 5V pulse triggers a detector read-out.
A set of jumpers internal to the CCD controller allows this to be set to OPTICALLY ISOLATED OPEN COLLECTOR INPUT. The default is OFF.
In most cases this button should be off, i.e. the detector should be read under software control.

**Test Pattern**
If this button is on, then a test pattern will be generated whenever the detector is read. The test pattern contains all values required to check that no bits are missing in the images.
The default is OFF.

*Information on the lower part of the right half:*

**Serial Number**
This number must agree with the detector serial number.

**CCD Pixel Size**
The exact value varies between individual detectors.
The pixel size will change if one chooses a different resolution and then click either on "Apply" or "OK".
The change is, of course, due to the binning of physical pixels into larger pixels for lower resolution.

**Configuration File**
This file must exist and agree with the serial number of the detector. It contains the default parameters needed to run each detector properly.

**Microcode File**
This code may be customized for each detector and the serial number must match the detector serial number.
The file must exist.
The version number may be different from .1 .

**Microcode Revision**
This number is currently a composite of a part number and a revision number. It is used to check whether the controller is currently running the same microcode version that marccd is expecting.

*Buttons on bottom:*

**Reboot**
This When this button is clicked, the system will reboot the camera controller. In older versions of marccd a box appears, offering the choice to either reload the current parameters or to load default parameters upon rebooting. These parameters are customized for each detector. Given a choice, the user should choose to load the default parameters.

**Balance**
When this button is clicked the detector chip is read out twice (removal of zingers) and proper digital offsets for each A/D converter is calculated to produce the same final intensity range on all 4 channels.
The 4 channels are then read out a third time to produce an image that demonstrates the effect of the new offsets visually.

**Apply**
When this button is clicked the currently showing data in the window is read and/or acted upon.
The user should click this button or the "OK", after setting "Cooler Power On", causing the program to actually turn the cooler power on. Likewise, if the Resolution is to be changed one has to first choose the resolution and then click this button or the "OK" button for the change to take effect.

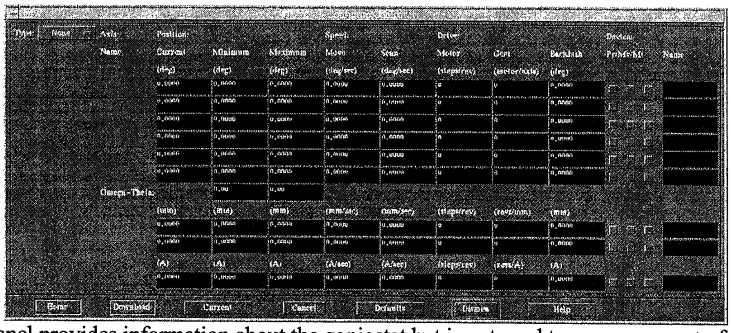
**OK**
When this button is clicked the currently showing data in this window is read and/or acted upon and the window closes. It does the same as clicking the "Apply" button,followed by the "Dismiss" button.

**Cancel**
When this button is clicked the window will close without accepting any changes made after the last "Apply" click. If the window is subsequently re-opened it will not show any changes made after the last "OK" or "Apply" click.

**Dismiss**
When this button is clicked the window will close without storing or acting upon any new data entered after the last "Apply" click. However, if the window is subsequently re-opened the new data will still be visible as typed in.

Configure

==> Goniostat



This panel provides information about the goniostat but is not used to move any part of the goniostat.
If movement of the goniostat is desired, the main MarCCD panel or the "Acquire" panels should be used.

*Top left button:*

**Type**
The correct network type for your local setup should be chosen here. Normally the default should be adjusted at the time of installation of the MarCCD such that this need never be changed. Possible network types are marSCSI (Mar300 type SCSI controller), marNETVL (mar ethernet base controller) or NONE.

*Large table occupying most of this control panel:*

**Axis, Name:**
This Refers to a motor of the goniostat that can be driven by the user via other control panels. Available are: Phi, Omega-Theta and the Distance.

**Position:**
The Current position of the motor in question, as well as the maximum and minimum positions can be found here The current value will change whenever the motor is driven via the main MarCCD panel or the "Acquire" control panels.

**Speed:**
The speed for driving to a new position and the scan speed for the motor in question are listed here. These values are factory pre-set and should not be changed.

**Drive:**
Technical details for the motor listed in the leftmost column are provided under this heading: steps per revolution, gearing information and the backlash in degrees.

**Device:**
These buttons determine whether these axis appear in other menus:
Pr = Pre-set
Mv = Movable (Software will allow changes in position.)
Mt = Motor (Software can actually drive axis to new position)

**Name:**

*Buttons on the bottom row:*

**Home**
When this button is clicked the goniostat will automatically drive to the limits to find the maximum/minimum distance again. This button is used when there is reason to believe that the current value for the distance is incorrect.

**Download:**
Downloads new values to controller.

**Current:**
Uploads current values from controller.

**Cancel:**
Cancel any changes that have been made since last download.

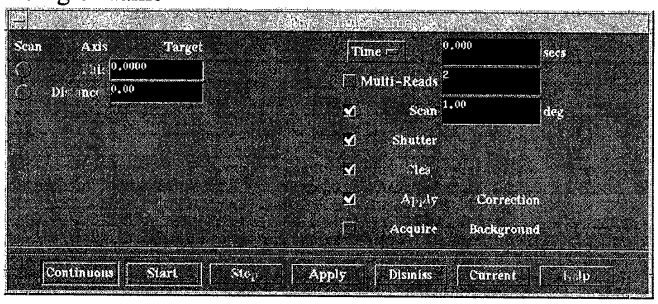
**Defaults:**
Reload defaults.

**Dismiss:**
Close window.

**Help:**

Acquire

==> Single Frame




This dialog box is designed to collect one single exposure at a time. Obviously, this is useful to determine whether a crystal diffracts well enough to start an entire data collection.
Data frames collected with this "Acquire Single Exposure" control panel are NOT automatically saved to disk. To preserve these frames use the "Save Displayed Data Frame" option under "File" in the main MarCCD control panel, see section ??.

*Left part of this panel:*

**Scan:**
This determines which axis will be scanned during an exposure.
Most MarCCD systems only allow a phi-scan and these buttons cannot be toggled on/off by the user.

**Axis:**
This just lists the axes corresponding to the "Scan" buttons on the left.

**Target:**
Type in the position for a still exposure or the starting position for an oscillation exposure.

*Right part of this panel:*

**Time/Dose:**
Use the mouse to choose either time (in seconds) or dose (in kHz) for the unit to define the exposure per rotation angle.
The time option is what is mostly used in crystallography, simply enter the exposure time in seconds in the box to the right of this button if "Time" is chosen.
The "Dose" option is a useful feature at synchrotron sources. It uses ionization chamber 2 of the Mar goniostat to adjust exposure time such that all frames will have the same radiation dose.

If the Mar remote control for the slits and ionization chambers is set to chamber 2, the MarCCD panel will show the current reading of this chamber on top (It will show chamber 1 when the remote is set to chamber 1 but chamber 2 is the one used for the dose option). Multiply this value by the intended exposure time (seconds) and type the result into the box to the right of the "Dose" button. If several frames are taken with this same value then they will all be exposed to the same amount of radiation, adjusted for any decay in the synchrotron beam.

*Small toggle buttons on the right half:*

These buttons turn the described option on when they show a checkmark (✓). Use the left mouse button.

**Multi-Reads:**

This is used to remove "zingers" ( cosmic rays causing spots on the frames that are not diffraction spots from the crystals). The number of sections are typed into the box to the right of this button.

This option is usually desired for long exposure times(over 4 minutes). It is generally not useful at synchrotrons because of the short exposure times. The default setting is OFF, if it is turned on by the user, the number of reads defaults to 2 unless explicitly changed.

**Scan:**

Click to show a checkmark if an oscillation picture is to be taken and type the desired oscillation range into the box to the right of the button. Click this button to show NO checkmark when a still picture is to be taken.

If the button shows no checkmark, it does not matter what is typed in the box to the right.

**Shutter:**

In almost all cases this button should show a checkmark to enable shutter control. Turn this off to take a dark exposure (i.e. check for radiation leaks around the shutter) by unchecking this box. Default is ON.

**Clear:**

This button should show a checkmark and is usually disabled in the distributed MarCCD software. The detector is actually continuously cleared if it is not busy integrating (i.e. during the X-ray exposure) or reading out data. Since the CCD chip continuously integrates it will accumulate a few electrons (from various sources) in the wells, even if not exposed to X-rays. This is the case for all CCD and IP detectors. To assure reproducible data this accumulation should be cleared before an X-ray exposure is measured. Default is ON.

**Apply Correction:**
This button is set to a checkmark and disabled. All data frames are automatically corrected according to factory calibration. This includes flood field, spatial correction and dark field subtraction. Default is ON.

**Acquire Background:**
A background image is always subtracted from the collected data frame. If this button is clicked to show a checkmark, a new background image will be collected prior to the exposure. If no current background image is available, one will be collected, no matter how this button is set.

*Active Area (Bottom row of big buttons):*
Click these buttons with the left mouse button to take action once data has been entered into this panel.

**Continuous:**
Continuously repeats acquiring the requested frame until stopped via the "Stop" button. None of the frames collected by this option will be written to disk, they will just be displayed if the display is set to "Detector".
This option can be used to make any kind of adjustment e.g. To the beam, the beamstop or crystal) while the same diffraction image is sampled repeatedly.

**Start:**
This will start the requested single exposure (just once) and display it when done.

**Stop:**
This button will stop a current exposure or stop a "continuous" single exposure which may have been started with the "Continuous" button.

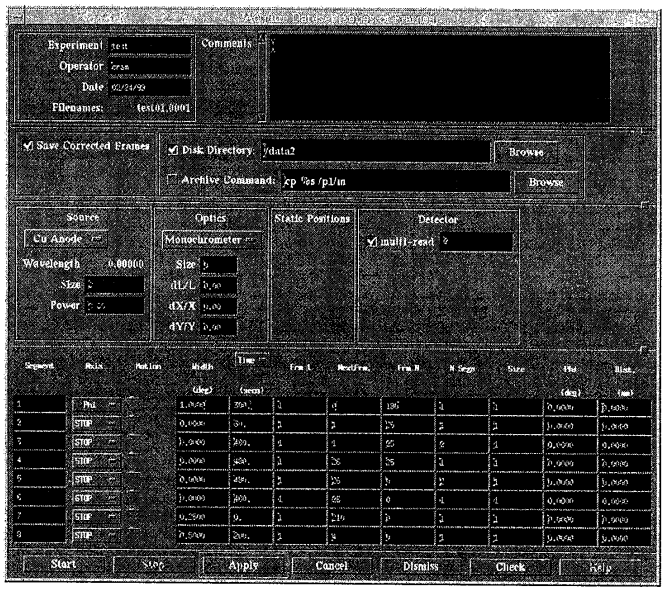
**Apply:**
When this button is clicked, all data will be accepted as typed and update the entire panel.

**Dismiss:**
Clicking on this button will close this panel.

**Current:**
If the goniostat has been moved from a different control panel, then the actual current values of the positions will be loaded into the "Acquire Single Frame" panel.

**Help:**

Acquire
==> Data Set




*Top of panel:*

**Experiment:**
Type in a name for the data set to be collected. This text string will be used to name the frame files, with an extension to number the frames. This will also be written to the headers of the data frames. A sample is displayed under "Filename": the segment number will be substituted for "%" and the frame number for "#". There is no default, this entry is required.

**Operator:**
This information will be written to the headers of the data files. It is for note keeping purposes only, default is NONE, this is not a required entry.

**Date:**
Date and time will also be written to the logfile and data frame headers. Default is none.

**Filenames:**
This line shows the name that will be given to the data frames. This name can be changed by typing in the "Experiment" box and then clicking on the "Apply" button on the bottom of the panel.

**Comments:**
This is for bookkeeping purposes. The information typed in here will be recorded in the headers of all data frames.

*Small buttons:*

**Save Corrected Frames:**
In most MarCCD distributions this is locked to show a checkmark (✓), since there is usually no reason to collect a data set but not save the data. The data files that will be written to disk are flat-field and spatially corrected and the background has been subtracted. They are ready to be interpreted by all popular data processing packages.
Given the option, the user should click this button to show a checkmark. The default is ON.

**Disk Directory:**
This button should be clicked to show a checkmark (✓), and then the path for the directory to write data frames should be typed into the box. Alternatively the left mouse button can be used to select the proper directory via the browse feature. The default is ON and the current working directory (no entry).

**Archive Command:**
If the data is not to be processed soon, or to be stored for transport (synchrotrons), this button can be clicked to show a checkmark (✓), and an archive command can be typed into the adjacent box. Use the left mouse button to select a destination via the browse feature.
An example archive command would be tar ....

*Middle portion of the panel:*

**Source:**
This information is written to the file headers and does not have any effect on the data collection.
**CuAnode/Synchrotron/Mo Anode:**
Use the left mouse button to select the X-ray Source. If a different target than Cu or Mo is used on a rotating anode, select "synchrotron" and enter the proper wavelength under "Static Positions".
**Wavelength:**
This simply states the current wavelength. To change this value, use the "CuAnode/Synchrotron/MoAnode button and the "Static Positions" block.

**Size:**

**Power:**
Type in the mA*kV setting of the rotating Anode in use, or the ring current of the synchrotron.

**Optics:**
This information is to written to the file headers but has no effect on the data collection.

**Nickel/Nickel Mirror/Monochromator:**
Use the left mouse button to choose the most appropriate description of the optics. At a synchrotron one would choose "monochromator".

**Size:**
Type in the thickness of a Ni filter, size of a mirror, etc. or leave blank.

**dL/L:**
Dispersion

**dX/X:**
Crossfire (divergence)

**dY/Y:**
Crossfire (divergence)

**Static Positions:**
The current position of the goniostat and wavelength should be displayed here.

**Detector:**
Except for the "Multi-read" button, the information under the "Detector" heading is only written to the file headers and has no effect on the data collection.

**2Theta:**
This is usually zero. The value cannot be changed here. The 2theta listed here will be recorded in the file headers.

**Distance:**
This value should agree with the crystal to detector distance for data collection. It can be changed under the "Static Position" heading. The distance will be recorded in the file headers with the value shown here.

**Multi-read:**
This small button can be clicked with the left mouse button to show a checkmark (✓). This facilitates the removal of "zingers". Zingers are spots on the X-ray image that are not caused by crystal diffraction but rather by random cosmic rays. When exposure times are short (less than a few minutes) the Multi-read" option should be turned off. Type the number of reads for each data frame into the box to the right of the button.
If Multi-reads is turned on, the number of reads is usually set to 2, since that is sufficient to remove zingers. Any higher number would further increase the dynamic range but also extend the time the entire data collection takes and worsen the signal/noise ratio.

*Data collection table in the bottom half of the panel:*
This control table offers a lot of flexibility in experiment design. An example for a very simple data collection is given in the "Getting Started" section of this manual.
Using the Segment options it is possible to set up several data collection runs (i.e. "Segments") at the same time and then have the software automatically execute one after the other. Alternatively, the software can collect a number of frames of one Segment, then a number of frames from another, eventually return to the first segment to take another batch of frames. This type of pattern, to collect a few frames from each segment in turn, is set up using the Nsegs and Size columns in this table. Thus, an inverse beam experiment can be designed to collect one or more frames of the first segment, then turn the crystal 180 degrees in phi and collect the equivalent frame(s) from the second segment. This may be done to collect the Friedel Mates close together in time (crystal decay, beam variation). Ultimately Mar software should communicate with beamline software at synchrotrons to also change the wavelength for separate segments (MAD experiments).

**Segment:**
In this column each individual data set is given a Segment Number. Usually one would number those sequentially starting from the top. Simply type the number into the box. This number will be included in the data file names from this Segment.

**Axis:**
Use the left mouse button to select:
**Phi:**
The phi angle will scan through the oscillation range given in next to last column of this table. The starting phi for each frame is automatically calculated from the starting phi of the segment and the number of frames within each Segment that have already been collected.

**Skip:**
No action is taken, the program will move on to the next segment.

**Stop:**
The data collection will stop.

**Motion:**
Only one option (Scan) is given here.

**Width:**
Type in the width of the oscillation angle for all frames in each segment.

**Time/Dose:**
Use the left mouse button to select the unit that defines the exposure:
**Time:**
Set the exposure time (in seconds) for all frames in each Segment by typing the number of seconds into the box.

**Dose:**
The reading from the second ionization chamber on the Mar base is used to adjust the exposure time to a constant dose throughout the data set.
On top of the main MarCCD panel the currently chosen (by the remote control box for the slits) ionization chamber is displayed. Once "dose" is chosen this will be locked to chamber 2. If an exposure time of 10sec seems adequate at the current beam intensity, then read the current value for Chamber 2 from the top of the main MarCCD control panel (in units of kHz/sec), multiply by 10 seconds and type the result in for "dose". If the x-ray beam now decays during data collection (synchrotrons), the exposure time will automatically extended, such that all frames receive the same X-ray dose.

**Frm1:**
Type in the number that should be given to the first frame in each segment. Usually this is one, but in some cases the user may have a reason to start the numbering at a different value. Do not change this when resuming an interrupted data collection.

**NextFrm:**
Type in the frame number of the next frame to be collected within each segment. This is useful if the data collection was interrupted and should be restarted. If the interruption was accomplished via a "Stop" or "Abort" from the MarCCD software, then this data collection panel is automatically updated to the proper "NextFrm". However, sometimes it is wise to change this number by hand and retake the last frame before the interruption (i.e. when a synchrotron beam dumped and it is not certain that the last frame was fully exposed). If this table was not updated by the software after an interruption, then check the frames written to disk and retake the last one by entering the appropriate number here.

**FrmN:**
Type in the total number of frames to be collected in each segment.

**NSegs:**
If a "1" is typed in here, the program assumes that no other data collection Segments are to be considered until all frames of this segment are complete. If Nsegs is set to 1, it does not matter what is entered into the "Size" column, the segment will be completed before the program moves on to the next Segment.
Any number larger than 1 in the Nseg column tells the program how many segments are tied together in this experiment. If there is a "3" in this column, then the software will collect "Size" frames from this segment and then collect the "size" number of frames from the next two segments before returning to the starting segment for another batch of "size" frames.

**Size:**
Type in the number of frames to collect in the Segment before moving on to the next Segment.

**Phi:**
Type in the starting angle for the first frame (Frm1) of the Segment in degrees.

**Dist:**
Type in the crystal to detector distance in mm of the Segment.

*Active Area (Buttons in the bottom row of the panel):*
These buttons cause immediate action when clicked with the left mouse button. It is possible to click the "Check" button before starting a data collection. Naturally, "Check" will not catch all mistakes, but it can save the user a lot of time, sometimes just by finding a typing error.

**Start:**
Starts the data collection. It does an automatic "Save" and "Check".

**Stop:**
Stop the data collection. When this button is clicked a dialog box pops up, offering to let the current frame finish. It is recommended to finish the current frame.

**Apply:**
When this button is clicked the program reads and accepts the new information in the panel.

**Cancel:**
When this button is clicked, everything in the panel reverts to the settings at the last "Apply" click.

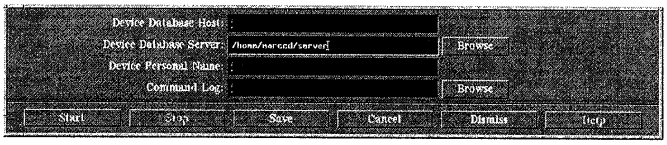
**Dismiss:**
Closes the window, after asking whether changes should be saved.

**Check:**
When this button is clicked the program checks the data collection set up to make sure it is feasible and offers suggestions in a dialog box that pops up. This check is also done automatically whenever a data collection is started.

**Help:**
???

Acquire

==> Remote Control

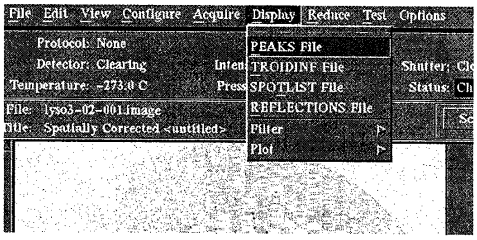



This is customized for a few particular synchrotron installations and not a generally available feature.

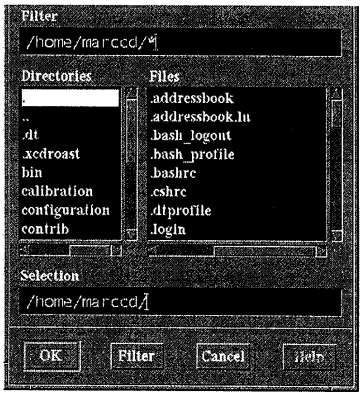
Display

==> PEAKS File
TROIDINF File
SPOTLIST File
REFLECTIONS File

These options are not implemented so far (04/08/99). They are intended for future interaction with data processing software.




Any of these "File" options bring up a panel to load the file (next page):




The top dialog box is used for the "Filter" function. Type a directory and/or partial filename into this box, use the "*" character as a wild card. Once the "Filter" button on the bottom of the panel is clicked, the large two center boxes will list the directory and all files matching the description given in the top box.

Clicking on a file name in this list will copy that filename to the bottom dialog box. Alternatively, the filename can be typed into the bottom dialog box.

Once the OK button is clicked, the file listed in the bottom dialog box will be loaded into the location chosen by the initial choice in the "Display" pull-down menu.

Display
==>Filter
Plot

These options are not implemented yet (04/08/99). They are intended for interfacing with data processing packages.

Reduce
==>???
This option is not implemented as of 04/08/99. It is intended for use with data processing.

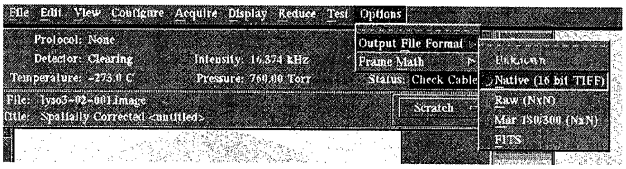
## Test

==>???

This option is not implemented as of 04/08/99. It is intended for use with data processing.

## Options

==>Output File Format




**Unknown**
Cannot be chosen by the user.

**Native (16 bit TIFF)**
This option should almost always be used. The standard MarCCD data frames are essentially in 16 bit TIFF format, with a header at the beginning. The header contains information about the data frame and it's history.

The full header, as written to the file, is a TIFF header. The initial 1024 bytes are a minimal TIFF header with a standard TAG pointing to the image data and a private TIFF TAG pointing to this header structure. As written by mmx/marccd, the frame_header structure always begins at byte 1024 and is 3072 bytes long making the full header 4096 bytes.

Immediately following the header is the image - it is of arbitrary size defined by the header fields nfast, nslow and depth. The stored data frame is always with the origin in the upper left corner and view direction from the source. The file `header.doc` in the `documentation` directory supplied with the MarCCD software should be consulted for more detailed information on the MarCCD frame format.

**Raw (NxN)**
With this format option no header is written and the frame is written out as Nx by Ny integers (2 byte).Nx and Ny are the numbers of pixels across the detector in the x and y direction respectively.

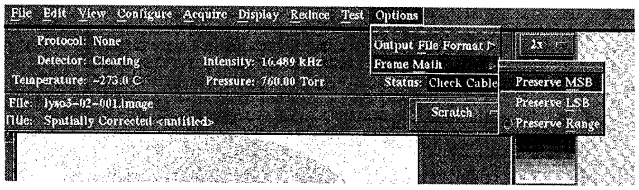
**Mar 180/300 (NxN)**
Frames will be written in the same format as packed frames from Mar180 or Mar300 IP Scanners. Except that the number of pixels will be the actual number of pixels and not one of the fixed numbers allowed in a true mar300 frame.

**FITS**
Flexible Image Transport System File, a format commonly used by astronomers and various image processing software.

## Frame Math

The setting under this menu has an effect on many options under the "Edit" menu and , most importantly, on the correction of frames during data collection. The user should usually not change this setting, it should be set to "Preserve Range" for data collection.

In general, arithmetic with 16-bit pixel values will result in 17-bit values. These options tell the program how to store the result in the final 16-bit pixel.




==>Preserve MSB

If any mathematical operation is performed on a frame, the resultant value for each pixel will have the most significant bit preserved.

==>Preserve LSB

If any mathematical operation is performed on a frame, the resultant value for each pixel will have the lest significant bit preserved.

==>Preserve Range

If any mathematical operation is performed on a frame, the resultant values for the pixels will be truncated to within the range of 0 to 65535.

# marccd service manual

| problem/symptom | probable cause | fix |
|---|---|---|
| ***Streaks, vertical***<br>Example: An image of a crystal diffraction pattern shows long vertical streaks starting/ending at diffraction spots. | ***Shutter problem:***<br>The shutter remains open after the detector has stopped integrating (i.e. exposure is finished) and starts to read out. | Lubricate with graphite or WD-40 into brass bushing around shutter shaft.<br>Toggle shutter manually (the switch is on underside of base, close to the detector side edge of the phi-motor housing). If this does not help, call Mar-USA for instructions. |
| ***Blank zone, horizontal stripe in center***<br>It looks as if the Image has been cut in half horizontally and the two halves have been shifted apart by the width of the blank zone. | ***Shutter problem:***<br>Shutter opens and closes before the detector starts integrating. | |
| ***Noise***<br>High background noise in images. | ***Experimental Setup:***<br>Air scatter, fibers in beam, diffuse scatter...<br>***Temperature:***<br>The detector is not cooled to the proper operating temperature. | Check the beam path and crystal mount.<br><br>Check the pressure (detector status window within main marccd software window). |
| ***Pressure***<br>The pressure reported in the detector status window is higher than 1 torr when the detector is cold or higher than 2 torr when warm. | ***Vacuum decayed:***<br>The vacuum in the detector chamber is probably not good enough to allow cooling the detector to the optimal operating temperature. | Follow the procedure for re-evacuating the CCD chamber (page 6 of this section). |
| ***Temperature***<br>The detector will not cool below -30 or -40°C.<br><br>Detector will not cool below 0°C. | ***Vacuum decayed:***<br>The pressure in the detector chamber is too high.<br><br>***Moisture in the system.*** | Follow the procedure for re-evacuating CCD chamber (page 6 of this section).<br><br>Call Mar-USA for service. |
| ***Question marks:***<br>The main marccd window has question marks for the temperature and pressure readings. | ***Lost Communication:***<br>The controller has lost communication with the detector. | Check:<br>1) Power to controller is on.<br>2) All switches are on.<br>3) Cable connectors are OK.<br>4) Fuses are not burned out. |

| | | |
|---|---|---|
| ***No update of status window***<br>The information on the status window in the main marccd window does not change even though data is being collected properly. | **Bug** | Restart software. |
| ***Blank image*** | ***Experimental setup:***<br>No X-rays?<br><br>***Shutter problem:***<br>Does not open?<br><br>***Background image:***<br>A frame with large values for all pixels is stored as background. Automatic subtraction of this faulty background produces an all-zero image. | Turn X-rays on.<br><br>Check shutter manually, make sure all cables are hooked up properly.<br><br>Collect new background frame. |
| ***No Response***<br>(Message in detector status window): | ***The controller*** (black box in cooler cabinet) ***cannot communicate with the detector head.*** | Check all cables, especially power to detector head and the SCSI-like cable between the controller and the detector head. |
| ***Cooler won't come on***<br>***or***<br>***Cooler turns off on it's own.*** | ***Intentional Delay:***<br>There is about a one-minute delay after asking for cooler power via software before the cooler actually comes on. This is to prevent damage from rapid power-cycling of the cooler.<br>***No power:***<br>The power to the cooler is not on?<br><br>***Time-delay relay bad.*** | Click the check box next to "cooler power" in the "Configure Detector" window to show a check mark. ***Then click on "Apply"*** and wait about one minute.<br><br>Check power cables, switch on the power strip inside the cooler cabinet and the power switch on the compressor itself.<br>Call Mar-USA for replacement parts. |

| | | |
|---|---|---|
| ***Goniostat does not move or moves incorrectly***<br><br>***The "Configure Detector" window contains nonsense numbers.*** | ***Communication problem and/or corrupt goniostat file.*** | Follow goniostat reset procedure on page?. |
| ***"Could not open file..." error message*** | ***Permissions wrong.*** | Type<br>chmod 666 filename (return) |
| ***One or more quadrants of the images are missing.*** | ***Not all readout-channels are working.*** | Check cables between Detector controller (black box inside cooler cabinet) and detector head. |
| ***The images look as if they have been cut into 4 quadrants and re-assembled wrong.***<br><br>quadrants mixed up | ***Cables*** between Detector head and controller are ***mixed up.*** | The four color-coded cables between the 4 readout channels on the detector head and the black controller box inside the cooling cabinet have to connect A (on detector) to A (on controller), B (on detector) to B (on controller), C to C, D to D. |
| ***Shutter: won't open***<br>***or***<br>***Shutter: won't close*** | | Exercise shutter manually via the switch on the bottom of the Marbase below the detector-side edge of the phi-motor housing. If that does not help, call Mar-USA for instructions. |
| ***Phi axis does not turn*** | ***Preload on Phi-axis bearings is too tight.***<br><br>***Contact between gears is too loose or too tight.*** | Refer to section ? of this manual. |
| ***Beam stop missaligned*** | ***The direct beam should not damage the MarCCD detector.*** | To align the beam stop, refer to section ? of this manual. |

| | | |
|---|---|---|
| ***"weak beam"*** | Rotating Anode:<br>***Not at full power.***<br><br>Rotating Anode or Synchrotron:<br>***Slits completely closed or base is missaligned.***<br><br>***Beam conditioning optics are out of alignment.*** | Slowly turn power up on the rotating anode.<br><br>Open slits (0.4mm or as desired).<br>Re-align base as described in section ? of this manual.<br>Refer to alignment procedure for your optics. |
| ***The detector has run against a limit switch and cannot be backed off.*** | ***Limit switch is depressed.*** | Try to initialize from the marccd software to both the near and the far end.<br>If it does not work, reach in and push the limit switch open while driving the detector away from it. |
| ***The shadow of the mylar-type beam stop holder is visible in the images.*** | ***Beam stop holder is pulled out.*** | Push the bottom part of the beam-stop holder towards the crystal position. Make sure it does not interfere with the goniometer head in any phi position. |

**The temperature and/or pressure readout in the software show "???".**

This means that the detector controller is either not running at all or not communicating with the computer running the MarCCD software.
Usually this is fixed by rebooting the detector controller. To do this, choose "Detector" from the "Configuration" menu and then click on the "Reboot" button on the bottom of the Configure Detector panel. A dialog box will appear informing you that the default settings will be loaded upon rebooting the detector controller. Click on "OK". The detector controller itself (in the large gray box on wheels that also contains the cooler) will beep twice upon rebooting.
*After rebooting the cooling needs to be turned back on as soon as possible.* To turn the cooling on, click the cooler button to show a check mark (√) and then click on the large "Apply" button. The cooling will come on about 40 seconds after the "Apply" button was clicked.

**The cooler is on but the detector temperature readout does not go down.**

When starting from room temperature, it takes about 2 hours before the temperature starts to drop faster. The ideal temperature for data collection may not be reached for 3-4 hours. This is because the entire fiber optics taper is cooled and a solid block of glass this size takes a while to cool to such low temperatures.
If the temperature does not go down in 3-4 hours, the pressure inside the detector may be too high. At room temperature the pressure should usually be less than 1 Torr, anything above 2 Torr may make cooling difficult. See the section on re-evacuating the detector, page ?.
If the temperature goes down for a while but then actually starts to go back up slightly while the cooler is running, it may help to stop the cooler (turn "Cooler Power" off in Configure=>Detector panel, then click on "Apply) and restart it after about an hour.
A drastic measure (only if the temperature is RISING while cooler is ON) is to raise the "set" temperature to 30°C and actually warm the detector up a little bit. This can only be done in "Expert Mode" in the "Configure => Detector" panel, by typing "30.0" into the ?? box and the clicking on "Apply". Leave the detector at 30°C for about one hour, then change the set temperature back to the normal value and try cooling again.

**"Vac" Light on the detector is on.**

The light labeled "vac" indicates that the pressure is high enough to justify pumping down the chamber.

**Cooler not running:**
If the "Temperature" and/or "Pressure" read "???", the problem is communication. See page ? on rebooting the detector controller.

The cooler can only be turned on via the MarCCD software. This is done from the “Configure => Detector” panel: Click on the “Cooler Power” button to show a check mark (√), then click on “Apply”.
If the cooler does not come on within minutes of turning it on from the software, then the problem is almost certainly a fuse or circuit breaker.

The first to check is the "circuit breaker" switch - it is on the opposite side of the cabinet from the pressure gauge. You will need to take the other outer cover off of the cabinet.

REMEMBER TO UNPLUG THE COOLER BEFORE CHECKING FUSES!!
Then, there are two fuses (1A) in the power entry module in the cooler itself - where the power cord enters.

Then, unfortunately, there are two 10A fuses inside the cooler box itself. Checking/changing these is rather cumbersome and has been changed on later models (serial numbers here?). You must remove the panel that holds the circuit breaker switch.
REMEMBER TO UNPLUG THE COOLER BEFORE REMOVING THE CIRCUIT BREAKER!
The fuses are BEHIND the circuit breaker. It is usually easiest to remove the two screws holding the circuit breaker into its bracket so that you can see/reach the fuses.

**Procedure for re-evacuating CCD chamber:**

Tools needed:

1) 3 mm hex key
2) vacuum pump capable of 0.1 Torr (0.01 Torr is better)
3) vacuum hose with clamp or fitting to attach to a 1/4" OD tube (~ 6mm).
4) Actuator for marCCD systems with external valve.

*For all marCCD detectors:*

- Turn the cooling power off: in the Configure Detector menu in the marccd software, click on the "cooling power" button to show NO check mark and then click on "Apply".

*The following steps apply to marCCD systems with INTERNAL vacuum valves only:*

- Switch off power to electronics/cooler crate. You can leave the software running with the configure/detector dialog box up.
- Write down the order in which the blue analog cables are hooked up. They have colour-coded ends for this purpose.
- Remove the electrical cables (6 cables) from the detector head. LEAVE the cooling hoses ATTACHED!
- Remove the 4 socket head cap screws holding the cylindrical cover on the back of the detector and remove the cover by sliding it back over the cooling hoses.
- You should be able to see the brass vacuum fitting at the bottom of the detector and the green valve handle. Attach the vacuum hose to the fitting and secure it with a clamp. You may need to dismount the detector in order to reach the fitting. In this case, the best place to put the detector is on the floor, standing on its front. It is perfectly safe to handle the detector by the cooling tubes on the back.
- Reconnect the two larger (power and control) cables. It is NOT necessary to reconnect the 4 blue analog cables.
- Switch on power to the electronics/cooler.
- Reboot the detector controller from the Configure/Detector window.

*The following steps apply to marCCD detectors with EXTERNAL vacuum valves only:*

- Remove the black vinyl cover from the vacuum port (labeled "VAC PORT") at the back of the detector head.
- Attach the vacuum pump via the vacuum hose and secure it with the hose clamp.
- Remove the plastic cover from the vacuum valve at the back of the detector head (labeled "VAC VALVE").
- Gently attach the actuator to the valve, do not turn it yet.

*The following steps apply to all marCCD detectors:*

- Check that you get a reading of temperature and pressure.
- Switch on the vacuum pump.

- Slowly turn the valve handle to open the valve while watching the pressure reading in the software. Verify that the pressure starts to go DOWN when the valve is opened. If it goes UP, then CLOSE THE VALVE IMMEDIATELY and verify/improve the vacuum connection to the pump and try again.
- Open the valve fully and allow to pump until the pressure is reasonable. The pressure increases approximately 0.1 Torr/week. It is possible to pump the chamber to 0.01 Torr, but that will only increase the lifetime of the vacuum by about a week and may not be worth the effort. 0.1 to 0.2 is usually good enough. A short vacuum hose will improve the speed of pumping. With a 25cm hose I can usually bring the vacuum to 0.1 Torr in 5-10 minutes and to 0.01 within 20-30 minutes.
- When satisfied with the vacuum, close the valve, disconnect the hose, and switch off the pump. Check that the vacuum is still OK!

*For marCCD systems with internal vacuum valves*

- Switch off the power to the electronics.
- Disconnect the power and control cables.
- Replace the cover. replace the 4 screws.
- If you dismounted the detector, then remount it now.
- Reconnect all 6 cables. The color code of should be used to verify that the cables are connected properly. Top to bottom on the detector is ABCD. On the controller ABCD is left to right. Connect A to A, B to B, ... etc... (use note made earlier)
- Switch on power to the electronics/cooler.
- Reboot the detector controller from the Configure/Detector window.

*For all marCCD detectors:*

- Enable cooling and click OK or Apply.
- Verify that the cooler comes on. The detector temperature should begin to drop within 10-15 minutes, although occasionally it will take 1 hour to get started. It should reach operating temperature in about 2 hours.

## When the marCCD detector is not being used.

It is recommended that, for short-term periods of inactivity (say less than 1 month), the detector be left operating with the cooler running and the detector at operating temperature. If possible, the detector should remain connected to the workstation with the marccd software running, which will keep a log of the temperature and pressure within the detector head. This log is helpful if a problem develops during this time.

For longer periods of disuse, the detector can be shut down. It is not necessary to shut it down, but, since the detector head is likely to require routine refresh of the vacuum before it is put back into service after a long shutdown, it may be easier to simply shut it down at the beginning of storage.

## Shutting down the marCCD detector.

Before powering down the detector, it is a good idea to quit the marccd program because the program will start to complain and may act sluggishly when the detector stops operating. After stopping the software, the CCD133 and CCD165 detectors may be shutdown by simply turning off the lighted red power switch located at the bottom of the cooler/electronics cabinet.

## Storing the marCCD detector.

When the detector is not to be used for some time, it may be necessary to store the detector.

It is strongly recommended that the cooling hoses remain attached between the detector head and the cooler. If the cooling hoses must be disconnected it is important that all open ends of the hoses and the fittings on the detector head and/or the cooler be capped! A set of caps is supplied in the detector toolkit for capping the hoses at one end and capping the detector head cooling ports. Capping the fittings prevents moisture from entering the system and refrigerent gas from escaping.

If the hoses are to be disconnected, the detector head must first be warmed to room temperature. If the detector is too cool when the hoses are disconnected, then excess gas will be partitioned into the detector head and this gas will expand as the detector continues to warm after disconnection. This will cause the gas to reach too high a pressure and the overpressure relieve valve will open, venting gas to the surrounding environment. The temperature of the detector head can be monitored in the marccd software – it should reach at least +10C before disconnecting the hoses. If the temperature readout is unavailable (no power, or no computer), then it is sufficient to

allow the detector head to warm for 90 minutes after the cooling is stopped before disconnecting the hoses.

## Shipping the marCCD detector.

The marCCD detector does not need to be serviced in normal operation and most problems that may appear can be addressed by the user or by a Mar service person working on-site. If the detector does need to be returned to the factory for service, it should be properly packed. It is very unlikely that the entire system will be shipped, but rather only the detector head and/or the detector electronics chassis.

If the detector head is to be shipped, it is very important that it be packed properly. It is strongly recommended that the original shipping carton for the detector head be saved so that it can be reused for shipping. This carton is specially designed to protect the fragile (and most expensive) components – the CCD chip and fiber-optic taper. If this box is not available, please contact Mar USA for a new shipping carton.

Before placing the detector head into the shipping box, check that the cooling gas supply and return lines are capped as described above under "Storing the marCCD detector". Unplug the heater cable that runs from the rear of the detector head to the front window retainer ring. Carefully coil this cable and/or tape it to the side of the detector. Failure to unplug the power cable before packing may result in damage to the connector when the detector is placed in the box.

If possible, cover the detector with a static free plastic bag. Then place the detector into the box and into the bottom half of the foam packing material. Check that the detector fits <u>into</u> the foam, particularly at the large end, so that the detector cannot slide out of the foam cradle. Place the top half of the foam cradle over the detector and push it down firmly at the front, taking special care that the large end of the detector also fits <u>into</u> the top half of the foam. Close and seal the inner box with tape before closing and sealing the outer box.

The detector electronics chassis can be dismounted from the cooler/electronics cabinet to be shipped. Disconnect all cables from the rear of the chassis. Remove the two M6 screws and washers from the front panel. Slide the chassis forward until it locks in place, then depress the green button on each slide-rail and pull the chassis further forward until it comes completely free of the rails. The chassis does not contain any particularly fragile components. Nonetheless, it should be properly packed in a sturdy box with sufficient padding to prevent damage to the corners and to the connectors. The controller chassis is quite heavy, so be sure that the packing is strong enough to not become damaged nor deformed during shipment.

In the unlikely event that the entire detector system is to be shipped, including the cooling unit, then the cooler/electronics cabinet should be shipped in the original shipping container. If this is not available, please contact Mar USA for a new container.