The *mar345dtb* User's Guide

Version 10.0

November 17, 2010

By Dr. Claudio Klein, Marresearch GmbH

We are grateful for reports of bugs and are open to suggestions regarding functionality, usability, etc.

Program *mar345dtb* is property of Marresearch GmbH. Usage is restricted to users and customers of Marresearch GmbH.

This manual is divided into the following chapters:

Chapter	Description
Preface	This page ...
Introduction	Functional description of the mardtb/mar345 hardware.
GUI	Usage of the graphical user interface
Image	Usage of the 'Image' section of the GUI
Align	Usage of the 'Align' section of the GUI
Edit	Usage of the 'Edit' section of the GUI
Crystal	Usage of the 'Crystal' section of the GUI
CSC	Usage of the 'CSC' (sample changer) section of the GUI
marµX	Usage of the 'marµX' (X-ray generator) section of the GUI
Input	Description of input files read by the program
Output	Description of output files generated by the program
Appendix	Description of some additional information about specific topics, e.g. a description on how to update the firmware of the *dtb*-controller.
Contents	Table of contents of the documentation
Installation	Instructions on how to install the software
History	History of program changes

The following documents contain additional information related to programs called by program *mar345dtb*.

- ***mar345dtb*** is a Unix man style description of program *mar345dtb*.
- ***martv*** is a Unix man style description of program *martv*.

- ***mar345dtb Software Distribution Guide*** is a PDF-style document describing the structure and contents of the *mar345dtb* software distribution.

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2. Introduction

1.1 The *desktop beamline*TM

1.1.1 Overview

The *desktop beamline (dtb)* is a highly sophisticated goniometer system. Almost all movements are motorized and can be controlled by a host computer. This allows for a detector system mounted onto the *dtb* to be aligned with the beam without user intervention. The *dtb* is capable of finding the beam and refining the optimal position thus yielding the best possible primary X-ray beam intensity. In addition, a beam profile can be obtained and slit apertures can be determined automatically to fit the monochromators properties.

Table 1: *dtb* hardware components

Component	Features
Goniometer	- High precision PHI-axis - Motorized crystal rotation (PHI) - Motorized crystal translation along spindle (z-axis) - Optional crystal x/y-translations for automatic alignment - Optional PHI-swing for mounting cooled crystals
Collimator	- 2 pairs of hor. and ver. slits followed by ionization chambers - Rotary beam shutter - CCD-microscope with viewing direction along X-ray beam - Motorized beamstop
Cardanic cradle	- Positional alignment motors: hor. and ver. translations of entire instrument - Directional alignment motors: hor. and ver. rotations of detector mount coupled to collimator
Detector mount	- Vertical 2-theta arm - Crystal-to-detector translation stage
Others	- Optional motorized cryo-head translation - Optional automatic cryogenic sample changer ("*csc*") - Optional single sample changer ("*ceasymount*")

1.1.2 Motors

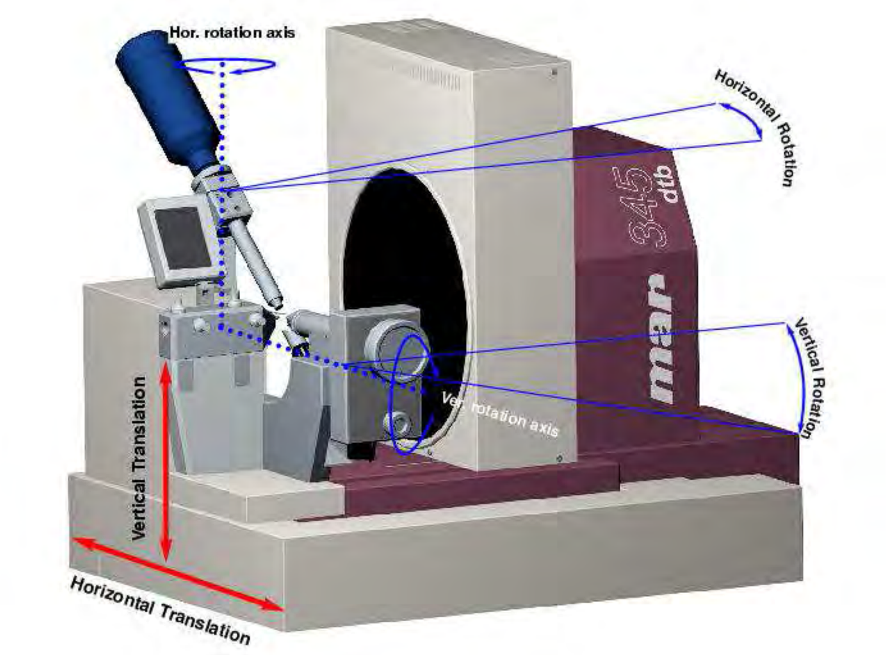
The *dtb* features an expandable number of high precision stepper motors. Most of the motors are driven by a dedicated motor stepper control module which is an autonomous piece of hardware with its own microprocessor (CPU). The motor modules are coupled to a high speed industrial serial bus (CAN-bus). Each module receives commands and sends status information to the CAN-bus. On the CAN-bus, each member is identified by a unique number or "id" in a similar way as computers in a network. The numbers are arbitrary but must be unique. Note, that the main *dtb* controller manages the motors for the PHI-axis, the beamstop and the 2 pairs of slits of the collimator. Those motors don't have their own stepper modules.

The main *dtb* controller is a minicomputer that works as interface between the host computer and the motor modules on the CAN-bus. It features an Ethernet interface to the host-computer and translates commands from the outside world into appropriate signals for the CAN-bus and viceversa. The controller is driven by a real-time operating system and implements the usual TCP/IP-services, i.e. ping, telnet, and ftp. Program *mar345dtb* communicates with the controller using standard Unix sockets on dedicated ports. In program *mar345dtb* the motors are usually referenced by certain abbreviations.

Table 2: *dtb* motors and their names within program *mar345dtb*

Name	CAN-id	Description
SLIT_1_VER	1	Vertical slit in front of 1. ionization chamber
SLIT_1_HOR	2	Horizontal slit in front of 1. ionization chamber
SLIT_2_VER	3	Vertical slit in front of 2. ionization chamber
SLIT_2_HOR	4	Horizontal slit in front of 2. ionization chamber
BEAMSTOP	5	Translation of beamstop along beam
PHI	6	Phi-axis
THETA	11	2-theta arm
DISTANCE	12	Translation of detector along beam
TRANS_VER	13	Vertical translation of dtb (up/down)
ROT_VER	14	Vertical rotation of dtb (up/down). Center of rotation is inbetween 1. and 2. ionization chamber.
TRANS_HOR	15	Horizontal translation of dtb (left/right).
ROT_HOR	16	Horizontal rotation of dtb (left/right). Center of rotation is inbetween 1. and 2. ionization chamber.
XTAL_Z	17	Translates crystal along PHI axis
CHI	18	Optional Phi-swing: rotation of Phi-axis up to + 90 deg.
SERVER	19	Sample changer only: mounts sample on goniometer head
ROTOR	20	Sample changer only: brings sample from carousel close to goniometer
LIFTER	21	Sample changer only: lifts sample out of carousel
PICKER	22	Sample changer only: picks a sample in carousel
CAROUSEL	23	Sample changer only: turns carousel
ACTUATOR	24	Optional: translation for cryo-head
XTAL_X	26	Optional: x-translation of crystal on goniometer head
XTAL_Y	27	Optional: y-translation of crystal on goniometer head

1.1.3 Principles of Operation

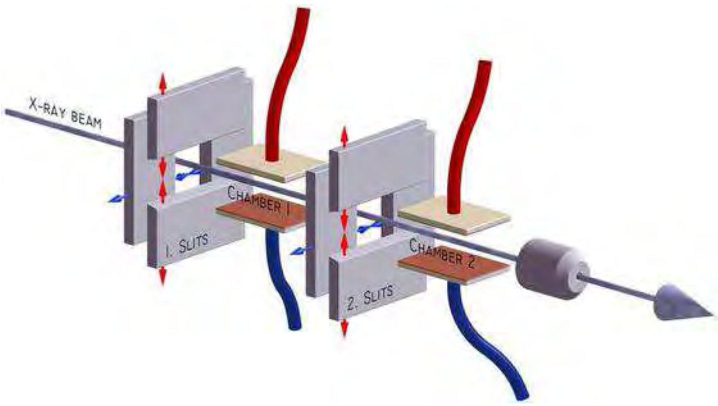


The geometrical setup of the *desktop beamline* is such that a beam passing through the collimator will hit a sample mounted on the goniometer. The cross-hair of a CCD-microscope is centered at the intersection of the primary beam with the sample mounted on the PHI-axis. On the detector translation stage an area detector (CCD, Image Plate) is mounted such that at 2-theta=0 the center of the area detector corresponds to the center of diffraction of the sample.

During the "alignment" procedure the *desktop beamline* drives into a position where the primary X-ray beam passes through the collimation system. To achieve this, 2 motors are required that translate the entire instrument along the beam and 2 motors that rotate the collimator and a frame with the goniometer and detector translation around the beam. The horizontal and vertical axes of rotation are centered at some point close to the first ionization chamber. Within the program the 4 motors are called:

- **TRANS_VER**: motor for translating the instrument in the vertical direction

- **TRANS_HOR**: motor for translating the instrument in the horizontal direction
- **ROT_VER**: motor for rotating the instrument in a vertical plane
- **ROT_HOR**: motor for rotating the instrument in a horizontal plane



In order to understand how the alignment works it helps to have a look at the design of the collimator. It consists of 2 pairs of continuously variable slits followed by an ionization chamber each. The ionization chambers detect the intensity of the primary X-ray beam coming through the slits. The readings of the ionization chamber within the collimator are obtained by constantly digitizing currents as produced by the X-ray beam. For this purpose, each ionization chamber is coupled to a 16-bit ADC with extremely high sensitivity. The range of operation is from weak sealed-tube sources to 3rd generation synchrotron sources. As is usual for ADC's, there is an offset that marks a baseline of the ADC. This offset is adjustable and must be set such that without X-ray beam the readings don't drop to 0. The stability of the ADC readings depends on temperature and humidity, so varying ambiental conditions will have some influence on the readings. See below for more details about how to adjust the ADC offsets.

The alignment procedure usually consists of the following steps:

- **Find beam in the first ionization chamber**:
  The horizontal and vertical translation motors must be moved until the primary X-ray beam passes through the first pair of slits. For this purpose it is helpful to widely open up both slits.

- **Find beam in the second ionization chamber**:
  Once the beam passes through the first chamber, the horizontal and vertical rotation motors must be moved until the primary X-ray beam also passes through the second pair of slits. For this procedure, the first pair of slits can be closed down to < 1.0 mm, but the second pairs of slits again must be opened up. Usually, when aligning the **dtb** from scratch the beam does not go through the second pair of slits right away. Due to an inclination or tilt it is more likely that it hits the second pair of slits and gets swallowed before reaching the second ionization chamber. By driving the rotation motors the intensity readings in the first ionization chambers don't vary too much, since - in first approximation - the rotations are not coupled to the translations. In practice, you will observe some variations, though.

- **Optimize beam in the first ionization chamber**:
  At this stage, you should have some positive readings in both chambers, and it is assumed that only some fine tuning is required. Due to the weight of the detectors the statics of the entire instrument varies when driving the detector translation (**DISTANCE**) or 2-theta stage. Due to the sensitivity of the ionization chambers you will observe a decrease of the readings of up to 20%. In other words: reoptimizing the beam in both chambers is strongly recommended when moving those motors.
  For the optimization the first pair of slits are closed down to the approximate beam size, usually around 0.6 mm for Osmic mirrors. The instrument then determines the maximum of the readings when driving across the beam in the horizontal and vertical plane.

- **Optimize beam in the second ionization chamber**:
  Both pair of slits are closed down, typically to 0.3 mm aperture. Again, the instrument determines the maximum of the readings when driving across the beam in the horizontal and vertical plane.

1.1.4 Remote Control

The remote control unit comes in 3 flavours:

- **"S":** small standard version
- **"M":** extended version for use with automatic goniometer
- **"XL":** extra large version for use with automatic sample changer

1.1.4.1 "S"-Version

The remote control unit features 5 buttons with multiple functionality. The buttons are called "**CRYO, BEAMSTOP, THETA, DISTANCE, CHI**". For all buttons, 3 states are possible and marked by an LED positioned under the button:

1. **Green LED:** task is idle and ready to go
2. **Red LED:** task is active and may be aborted
3. **No LED:** task is NOT available

The buttons work the following way:

1. When pressed while the task is active (red LED), the task will be aborted.
2. When pressed while the task is idle, the corresponding motor drives to position 2 if it is sitting at position 1. Otherwise, if the motor is not sitting at position 1, the motor will drive to position 1.

For **DISTANCE** the typical situation is that the detector sits close to the crystal and you want to drive it out of the way for crystal mounting. Afterwards, you want to drive the detector back to where it was. For this purpose, position 1 should be handled dynamically and position 2 should be set far away from the crystal, e.g. to 400 mm. I.e. when operating the distance via the remote control will move to 400 mm when pushing the DISTANCE button once or otherwise move back to its original position.

For **THETA**, position 1 should be at 0.0 degrees. An alternate position should be set to a relatively small value in order to avoid collisions, e.g. 5 degrees. I.e. the *dtb* is allowed to move in the range 0 and 5 degrees via the remote control.

For **CHI**, position 1 should be at 0.0 degrees. Position 2 should be set to a comfortable position where to mount a crystal. It is **NOT** suggested to set it to 90 degrees since here the CHI arm may collide with the cryo cooler. It is safer to stay below 80 degrees!

The **CRYO** button originally did not have any function, and on some dtbs without a cryo actuator this button has been reassigned to drive the **BEAMSTOP** motor. For instruments delivered before 2004, the button has been called **ADC ZERO** and was used to reset the ADC offsets of both ionization chambers. This functionality has been eliminated in firmware version ≥ 4.0. From version 4.0 on, the "ADC ZERO" button will only operate the beamstop. On instruments with an optional illumination unit, the "BEAMSTOP" button will also operate the paddle and the LED of that illumination unit.

It is possible to reassign buttons of the remote control to take other functions. For more details about how to reassign buttons, to do so, please refer to **chapter "Input: Keywords for dtb"** and to **chapter "Appendix: How to Assign Motors to the Buttons of the Local Motor Control"** .

1.1.4.2 "M"-Version

The extended version of the remote control unit allows for operation of the motors used with the optional automatic PHI axis. In this setup, the dtb is extended by motors for the x- and y-movements of the goniometer head. The remote control unit allows to drive x,y- and z-translations of the goniometer head as well as the PHI axis.

Table 3: Additional buttons on the "M"-version of the remote control unit

Button	Function
X+	Moves crystal to the right if PHI=90 deg. Moves crystal to the left if PHI=270 deg. Moves crystal up if PHI=0 deg. Moves crystal down if PHI=180 deg.
X-	Opposite to X+
Y+	Moves crystal to the right if PHI=0 deg. Moves crystal to the left if PHI=180 deg. Moves crystal up if PHI=90 deg. Moves crystal down if PHI=270 deg.
Y-	Opposite to Y+
Z+	Moves crystal away from PHI-handle
Z-	Moves crystal towards PHI-handle
PHI-X	Moves PHI to either 90 or 270 deg., i.e. a position where an x-translation moves the crystal either left or right.
PHI-Y	Moves PHI to either 0 or 180 deg., i.e. a position where an y-translation moves the crystal either left or right.
Magnet	Activates or deactivates the holding magnet on the goniometer head.

1.1.4.3 "XL"-Version

The extended version of the remote control unit allows for operation of the motors used with the optional automatic sample changer. In this setup, the dtb is extended by motors for the x- and y-movements of the goniometer head and by those to take sample out of the carousel of the sample changer. In addition to the buttons in the "M"-version of the remote control unit, you will find:

Table 4: Additional buttons on the "XL"-version of the remote control unit

Button	Function
CAR-	Decreases the current carousel position by 1 unit
CAR+	Increases the current carousel position by 1 unit
INIT	Initializes all sample changer motors including x,y,z-translations of goniometer head
INIT CAR	Initializes the CAROUSEL and LIFTER.
UNLOAD	Unmounts the sample that is currently mounted on the goniometer head to the selected carousel position.
GIVE/TAKE	GIVE: the vial in the selected carousel position is taken out of the carousel and presented to the user. TAKE: a vial is moved from the presentation position into the carousel position where the GIVE operation has started.

1.2 General Remarks About Program *mar345dtb*

mar345dtb is a highly integrated graphical user interface for collecting data with the *mar345* detector mounted on the *desktop beamline*. The program is fully menu driven and features options for setting up one or more data collection runs. It allows for fully automatic alignment of the instrument with the beam. It also features an area for image display and analysis.

The program is provided as binary executable for Linux. Due to decreasing importance of SGI IRIX and Compaq Tru Unix, support for those architectures is discontinued. The program may run also on Mac OSX, but the TV stream from the crystal cannot be displayed onto the screen from within the application. Hence, usage of the program on OSX is not recommended.

Table 5: Supported architectures and operating system versions

Architecture	Operating system
Linux PC	SuSE >= 8.0, RedHat >= 8.0

1.3 General Remarks About Program *mar555dtb*

Program *mar555dtb* is a derivative of program *mar345dtb*. As far as the goniometer is concerned, it provides the same functionality as program *mar345dtb* and hence, the documentation for that program version is fully valid for program *mar555dtb*. The fundamental difference is that program *mar555dtb* directly interfaces to the *mar555* flatpanel detector instead of the *mar345* image plate detector. While the latter one communicates with the host PC via TCP/IP-sockets, the *mar555* flatpanel detector uses a fiber-optic high speed link. The data read-out time is small compared to the image plage (≤ 2 sec). See the documentation of program *mar555* to learn more about the *mar555* flatpanel detector.

Whereever appropiate, differences in the GUI between program *mar555dtb* and *mar345dtb* will be pointed out.

1.4 Computer Requirements

Program *mar345dtb* needs about 100 MB physical RAM, mainly for transforming incoming images from the detector. Most of the time, however, the program is not very busy and does not consume too much CPU time. For image display and other visualization purposes, a 24-bit color display is mandatory. The program requires a minimum screen resolution of 1280x1024 pixels. The program makes use of large transformation tables, so the minimum program installation requires a disk space of 200 MB. Further components in the current *mar*-software distributions like the *automar*-data processing package may increase the required disk space to 300 MB.

The following specifications are considered as minimum requirements:

Table 6: Computer specifications

Component	Requirement
CPU	Intel or AMD > 1 GHz
Memory (RAM)	>= 256 MB

Component	Requirement
Hard disk	>= 8 GB
Video card	24 bit colors at ≥ 1280x1024 pixels @ > 70 Hz
Network card	Dedicated ≥ 10 MBit/s with IP-address 192.0.2.2
TV card	Optional for displaying crystal on PC. Only supported on Linux. Recommended model: Hauupauge WinTV Express
Peripherals (optional)	DVD or CD-writer (ATAPI or SCSI)
Monitor	19'' or larger, 1280x1024 pixels @ > 70 Hz
Required OS components	X-windows, X11-environment, openmotif libraries v4l-compontents (video for Linux)

Important notes:

- **All computer systems MUST be equipped with an additional Ethernet card.**
- **At installation time computers are expected to be FULLY FUNCTIONAL.**
- **For the *desktop beamline* a video frame grabber is strongly suggested. Marresearch only supports this feature on PCs running Linux.**

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2. GUI

2.1 Basic Concepts

The program has to perform several tasks:

- Allow user input, i.e. setup data collection parameters, analyze images, etc.
- Send commands to the detector (*mar345* Image Plate)
- Receive status information from the detector
- Send commands to the goniometer (desktop beamline)
- Receive status information from the goniometer
- Transform spiral images into Cartesian images (mar345dtb version)
- Display images
- With the optional sample changer: change crystals, center crystals

User input is done via the user interface using text fields, option menues and arrow buttons.

Both the *mar345*-detector and the *desktop beamline* are driven by autonomous mini-computers which communicate with the host computer through an Ethernet interface. They feature a real-time operating system which provides the well known IP services (ftp, telnet, ping, Unix sockets). They come with a defined IP-address: 192.0.2.1 for the *mar345*-detector and 192.0.2.3 for the *desktop beamline*. Program *mar345dtb* talks to the scanner using standard Unix sockets on ports 4441, 4442, 4443 and 4444. In a similar way, the program uses ports 4451 to 4454 to communicate with the *desktop beamline*. An essential requirement for program *mar345dtb* to talk to both the detector and goniometer is a successful "ping" to IP-addresses 192.0.2.1 and 192.0.2.3, respectively. For this purpose, the host computer must be equipped with a dedicated Ethernet card set to IP-address 192.0.2.2. Detector, *desktop beamline* and host computer should be connected to a hub using standard RJ-45 cables.

Transformation and data display requires memory as well as CPU-time. Typically, the program *mar345dtb* keeps the equivalent of 2.5 images in memory. When using images with 3450*3450 pixels, this corresponds to 75 MB. A minimum of 128 MB is therefore recommended for a host computer driving the detector, but 256 MB are actually more appropriate.

Data collection should always have highest priority. However, there is little protection against abuse of the host computer's resources by other processes. In particular, memory consuming data processing jobs can cause drops in performance of the workstation to such a degree that nothing else will work. I/O-operations can be even more critical. This affects network I/O, in particular.

Note: it is not advisable to write data out to an NFS-mounted disk since any problem on the network will affect data collection .

2.2 Environment

The program relies on a couple of predefined environment variables. The environment should best be defined within the shell startup scripts, i.e. files $HOME/.cshrc (C-shell) or $HOME/.tcshrc (TC-shell) or $HOME/.bashrc (Bourne-shell) using the corresponding syntax. The **mar345dtb software distribution guide** gives more details about how the mar software is organized. The official mar345dtb software distributions assumes that the default user's shell is the (t)csh. The following environment variables need to be declared:

Table 1: Environment variables

Variable	Default value	Description
MARHOME	$HOME	Root directory for mar software distribution
MARTABLEDIR	$MARHOME/tables	Location of calibration and configuration files
MAR_SCANNER_NO	000	Three digits serial number for mar345 scanner
MAR_DTB_NO	$MAR_SCANNER_NO	Three digits serial number for dtb.
MARLOGDIR	$MARHOME/log	Location of all log-output files and of data input files. The program *mar345dtb* expects to find subdirectories beam, log, lp, spy and sets. **Very important: this directory must have write permission for the mar345dtb user!**
MARHELPDIR or MARDOCDIR	$MARHOME/doc/	Location of this html documentation

The choice on how to set the environment variables depends on local usage and personal preference. In particular, you will have to decide wether you want to install the software in a location with general read access and no write access. Thus, the software may be installed e.g. in `/usr/local/mar` with subdirectories `tables`, `doc`, `man`, `bin` and `log`. It is essential that the user has permission to write into **$MARLOGDIR** and the following directories thereof:

- $MARLOGDIR/beam
- $MARLOGDIR/log
- $MARLOGDIR/lp
- $MARLOGDIR/spy
- $MARLOGDIR/sets

In cases, where program *mar345dtb* is to be used without mar345 scanner control (e.g. within the marccd software), the environment variable MAR_DTB_NO will be checked first, and only it is not defined MAR_SCANNER_NO will be used.

When using the *mar555* flatpanel detector instead of the image plate scanner, additional environment parameters need to be defined, namely the 3-digit serial number of the detector as MAR555_NO. See the *mar555 man page* for details.

2.3 Command Line Options

mar345dtb can be invoked in a terminal window plainly by typing "`mar345dtb`". The program however understands the command line options given in **Table 2**. Do not run the program in the background and do not use this terminal window for other purposes. The program will send important output to the standard output and you don't want to miss it, although almost all output can also be found in the log file.

At startup, the program will tell you something like:

```
mar345dtb: Version 9.0.0 (Mar 29 2009) by marresearch ...
mar345dtb: Connected to host '192.0.2.3' on port 4451 (COMM)
mar345dtb: Connected to host '192.0.2.3' on port 4452 (STAT)
mar345dtb: Connected to host '192.0.2.3' on port 4453 (DATA)
mar345dtb: Connected to host '192.0.2.3' on port 4451
mar345dtb: Connected to host '192.0.2.1' on port 4441 (COMM)
mar345dtb: Connected to host '192.0.2.1' on port 4442 (STAT)
mar345dtb: Connected to host '192.0.2.1' on port 4443 (DATA)
```

```
mar345dtb: Connected to host '192.0.2.1' on port 4441

=======================================================================
            Program             :  mar345dtb
            Version             :  9.0.0  (Mar 29 2009)
            Scanner S/N         :  001
            DTB     S/N         :  001
            Scanner mode        :  345 mm @ 0.15 mm
            Started on          :  Mon Mar 29 15:10:56 2009
            LOG  file is        :  /home/mar345/log/log/dtb.log.1
            STAT file is        :  /home/mar345/log/lp/mar.lp.1
=======================================================================
```

The program will also tell you if it is able to talk to the detector and to the *desktop beamline*. If environment variables are not set you will be notified.

At startup, the program writes information about connection success or failure into file $MARLOGDIR/mar.message. This message is read and displayed by program *marstart* which is called automatically by program *mar345dtb*. If the program cannot connect to either the detector or the *dtb*, the program *mar345dtb* will be halted. Program *marstart* then offers a choice of either killing process *mar345dtb* or continuing with program *mar345dtb* without network connection.

Note that it takes approx. 1 minute after turning on the *mar345*-detector and/or *desktop beamline* before program *mar345dtb* can talk to them, even if the ping service is available within a couple of seconds time.

After the initializations, the program presents essentially two windows: an image display area and the *mar345dtb* main window with status information and further input buttons.

Table 2: Command line options for *mar345dtb*

Name	Alternative	Arguments	Example	Description
-dtb	**-base**	<string> <number>	-dtb 192.0.2.3 4451	Host name and socket port for dtb.
-mar345	**-scan**	<string> <number>	-mar345 192.0.2.1 4441	Host name and socket port for mar345 scanner.
-marmux		<string> <number>	-marmux 192.0.2.100 502	Host name and socket port for marµX generator.
	--host	<string>	--host 192.0.2.3	Host name to use for the dtb.
-p	**--port**	<number>	-p 4451	Socket port to use for the dtb.
	--admin			Run program in administrator mode.
-c	**--colors**	<number>	-c 32	No. of colors to use for image display.
-d	**--default**	<number>	-d 2300	Default scan mode to use (one of 3450,3000,2400,2300,2000,1800,1600 or 1200).
	--debug	<number>	--debug 16	Debugging flag (undocumented).
-g	**--geometry**	WxH[+x+y]	-g 900x600+320+200	Specifies size [width x height] and location [+x+y] of the main window
	--gear	<N>	--gear 0	Force gear N for exposures. N=0,1,2,3,4 Depends on time and dphi.
-h	**--help**			Print usage summary
-i	**--init**	<number>	-i 11 (=1+2+8)	Hexcode for commands to execute at startup: 0x01 = set time and date inside controllers 0x02 = get firmware version 0x04 = close shutter 0x08 = adjust ADC offsets 0x10 = turn on high voltage 0x20 = lock image plate 0x40 = apply a button mask to the remote control unit 0x80 = tell CSC to operate at cryo conditions 0x100 = tell CSC to operate at room temperature
	+minmax			Prevent user from entering motor target values into user interface that exceed min. and maximum values as provided in the mardtb configuration file.
-n	**--nodisp**			Don't pop up the image display window at start of program.
	--noicon			Prevents usage of color icons (to save colors, see --nodisp).
	--nodtb			Start program without opening connection to *dtb*.
	--no345			Start program without opening connection to detector.

Name	Alternative	Arguments	Example	Description
	--nocsc			Start program without sample changer support (overrides entries in configuratuon file).
	--nomarmux			Start program without marµX support (overrides entries in configuratuon file).
	--novideo			Start program without video support (overrides entries in configuratuon file).
	--print	<string>	--print TASK --print CAN 11	Print additional status block information: TASK = print all changes in task status DIO = print all changes in digital I/O bits ADC = print all ADC value readings ERROR = print all error numbers in status block CAN <number> = print all bits for CAN-motor number
-v	**--verbose**			Increase printed output. No arguments.

2.4 User Interface

The user interface features 2 windows (**Main Window** and a **Status Window**) with a summary of the current activities.

2.4.1 "Main" Window

The main window controls all detector and goniometer functions. It comes in a "notebook" style with a number of pages and subsections. If the first place it consists of two areas:

- menu bar
- notebook containing several pages with tabs for navigation

2.4.1.1 Menu Bar

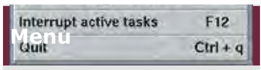
The menu bar allows for opening additional windows. Most of them can be opened either by selecting the corresponding choice with the mouse button or by pressing the corresponding short-cut key. Some of the windows can also be opened by pressing the status buttons or control buttons (see below).

2.4.1.1.1 File Menu

The File menu pops up if the "File" button in the menu bar is pressed or if "**Alt+f**" is pressed while the pointer is in the main window. Most of the choices in the menu (Ctrl+0 to Ctrl+9) will allow to navigate from page to page in order to access specific functions:

Table 3: The "File" menu

Menu	Menu Choice	Shortcut	Description
	**Close**	F1	Closes the main window and pops up the status window
	Status	F2	Pops up the status window
	Image	Ctrl+1	Switches to page for image display
	Edit	Ctrl+2	Switches to page for editing data collection params
	Align	Ctrl+3	Switches to page for dtb alignment
	Motors	Ctrl+4	Switches to page for driving dtb motors
	Initialize	Ctrl+5	Switches to page for initializing dtb motors
	Misc.	Ctrl+6	Switches to page for misc. purposes
	Log	Ctrl+7	Switches to page for log messages
	Crystal	Ctrl+8	Switches to page for crystal display and centering
	CSC	Ctrl+9	Switches to page for sample changer operations
	marµX		Switches to page for marmux generator operations
	Progress	F3	Monitors progress and status of current data collection
	Hardware		Switches to page for monitoring hardware activity
	Optional Header Info		Pops up a window where some values may be edited that go into image file headers

Menu 	Menu Choice	Shortcut	Description
	Administrator		Pops up a window where motor positions can be redefined. Only available when running the program in administrator mode (option --admin)
	Edit configuration file		Calls editor and loads the configuration file
	Reload configuration file		Reload params from configuration file
	Interrupt active tasks		Emergency stop for any activity
	Quit	Ctrl+q	Leave program *mar345dtb*

2.4.1.1.2 Edit Menu

The Edit menu pops up if the "Edit" button in the menu bar is pressed or if "**Alt+e**" is pressed while the pointer is in the main window. The separate chapter **"Edit"** describes this menu.

2.4.1.1.3 Align Menu

The Algin menu pops up if the "Align" button in the menu bar is pressed or if "**Alt+a**" is pressed while the pointer is in the main window. The separate chapter **"Align"** describes this menu.

2.4.1.1.4 Image Menu

The Image menu pops up if the "Image" button in the menu bar is pressed or if "**Alt+i**" is pressed while the pointer is in the main window. The separate chapter **"Image"** describes this menu.

2.4.1.1.5 Video Menu

The Video menu pops up if the "Video" button in the menu bar is pressed or if "**Alt+v**" is pressed while the pointer is in the main window. The separate chapter **"Crystal"** describes this menu.

2.4.1.1.6 CSC Menu

The CSC menu pops up if the "CSC" button in the menu bar is pressed or if "**Alt+c**" is pressed while the pointer is in the main window. The separate chapter **"CSC"** describes this menu.

2.4.1.1.7 Help Menu

The Help menu pops up if the "Help" button in the menu bar is pressed or if "**Alt+h**" is pressed while the pointer is in the main window.

Table 4: The "Help" menu

Menu	Menu Choice	Description
	**Contents**	Calls the WWW-browser and loads file $MARDOCDIR/mar345dtb.htm
	About	Shows current program version

2.4.1.2 Pages

In the following sections the individual pages of the main window will be described in more detail.

2.4.1.2.1 Image

The "**Image**"-page can be accessed by selecting the corresponding choice in the **"File"-menu** or by pressing the "**Ctrl+1**"-keys while the pointer is in the main window. This page is the area where to visually inspect images. The separate chapter **"Image"** describes the functionality of this window.

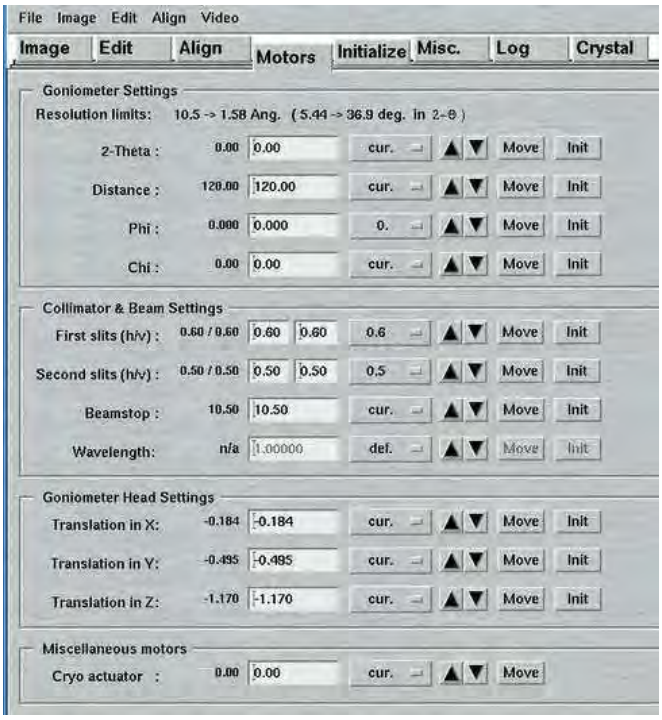
2.4.1.2.2 Edit

The "**Edit**"-page can be accessed by selecting the corresponding choice in the **"File"-menu**, by pressing the "**Ctrl+2**"-keys while the pointer is in the main window. Here, you set all the parameters for one or more data collection runs. The separate chapter **"Edit Data Collection Parameters"** describes the functionality of this page.

2.4.1.2.3 Align

The "**Align**"-page can be accessed by selecting the corresponding choice in the **"File"-menu**, by pressing the "**Ctrl+3**"-keys while the pointer is in the main window. This window is the area where to align the *desktop beamline* with the X-ray beam. The principles of alignment are described in chapter **"Principles of Operation"** of the **Introduction**. The separate chapter **"Align"** describes the functionality of this page.

2.4.1.2.4 Motors



Goniometer Settings

Resolution limits: 10.5 -> 1.58 Ang. (5.44 -> 36.9 deg. in 2-Θ)

2-Theta :	0.00	0.00	cur.
Distance :	120.00	120.00	cur.
Phi :	0.000	0.000	0.
Chi :	0.00	0.00	cur.

Collimator & Beam Settings

First slits (h/v) :	0.60 / 0.60	0.60 0.60	0.6
Second slits (h/v) :	0.50 / 0.50	0.50 0.50	0.5
Beamstop :	10.50	10.50	cur.
Wavelength:	n/a	1.00000	def.

Goniometer Head Settings

Translation in X:	-0.184	-0.184	cur.
Translation in Y:	-0.495	-0.495	cur.
Translation in Z:	-1.170	-1.170	cur.

Miscellaneous motors

Cryo actuator :	0.00	0.00	cur.

The "**Motors**"-page can be accessed by selecting the corresponding choice in the **"File"-menu** or by pressing the "**Ctrl+4**"-key while the pointer is in the main window or by pressing any of the **motor status buttons** in the status window. You can move single motors by pressing one of the motor buttons on the right hand side of the window. The option menues offer several useful choices. The choice "cur." will write the current motor reading into the corresponding text field. Note that the horizontal and vertical slits will both move to the desired positions. If the target position does not differ from the current position, there will be no action.

For most installations, the "**Wavelength**" is not really a movable motor but it can be configured as such.

2.4.1.2.5 Initialize

Drive motor	Use	Initialize	After initialize ...	Target
PHI	☐	Reference	Drive to ...	0.000
CHI	☐	Initialize at NEAR end	Drive to ...	0.000
THETA	☐	Initialize at NEAR end	Drive to ...	0.000
DISTANCE	☐	Initialize at FAR end	Drive to ...	400.000
SLIT_1_HOR	☐	Initialize at NEAR end	Drive to ...	0.400
SLIT_1_VER	☐	Initialize at NEAR end	Drive to ...	0.400
SLIT_2_HOR	☐	Initialize at NEAR end	Drive to ...	0.300
SLIT_2_VER	☐	Initialize at NEAR end	Drive to ...	0.300
BEAMSTOP	☐	Reference	Drive to ...	15.000
XTAL_Z	☐	Initialize at FAR end	Drive to ...	0.000
TRANS_HOR	☐	Initialize at NEAR end	Drive to ...	0.000
TRANS_VER	☐	Initialize at NEAR end	Drive to ...	0.000
ROT_HOR	☐	Initialize at NEAR end	Drive to ...	0.000
ROT_VER	☐	Initialize at NEAR end	Drive to ...	0.000
ACTUATOR	☐	Initialize at NEAR end	Drive to ...	0.000
XTAL_X	☐	Initialize at NEAR end	Drive to ...	0.000
XTAL_Y	☐	Initialize at NEAR end	Drive to ...	0.000

The "**Initialize**"-page can be accessed by selecting the corresponding choice in the **"File"-menu** or by pressing the "**Ctrl+5**"-key while the pointer is in the main window. You can initialize single motors by pressing one of the motor buttons on the left hand side of the window. Otherwise, you can select the "**Use**"-button of the desired motors and press the "**Drive all selected motors**"-button at the bottom of the window to initialize all selected motors. The actual initialization procedure may be followed by another action, typically by driving to a default value.

All motors of the dtb (**see Table 1.2**) can be initialized to a defined (i.e. calibrated) position. The mechanism of initialization may differ from motor to motor, though. Most motors carry sensors (light gaps) at both ends of their translation stages. There are dedicated hardware commands to tell the motors the calibrated positions when driving into these sensors. In principle, all of these motors could be referenced at either the "NEAR" end or the "FAR" end of their translation stage. For some motors, the initialization will be restricted to only one choice via the configuration file (see chapter **Configuration File** in section **Input**). In particular, the **DISTANCE** initialization at the "NEAR" end - close to the crystal - imposes certain risks to drive the detector into some obstacle, e.g. the beamstop, cryostream, etc.. It is therefore useful, to initialize the **DISTANCE** motor at the "FAR" end only, i.e. at the back of the translation stage. Similarly, it does not make too much sense to initialize the 2-theta arm at beyond 30 degrees of rotation but only close to 0!

The **PHI** and **BEAMSTOP** motors have a different way of referencing. They have only one sensor. In the case of **PHI** this sensor sits close to the 0 reading on the hand dial. The sensor for the beamstop sits about 18 mm away from the crystal.

The four slit motors don't have any sensor at all and hence no physical feedback of the correctness of the motor readings. The initialization is done by driving the slits to the minimum. This is physically less than 0.0 mm. Note, that the slits will be slightly open at negative slit readings and will be entirely closed only if they are at 0.00 mm. The exact positions are calibrated in the factory.

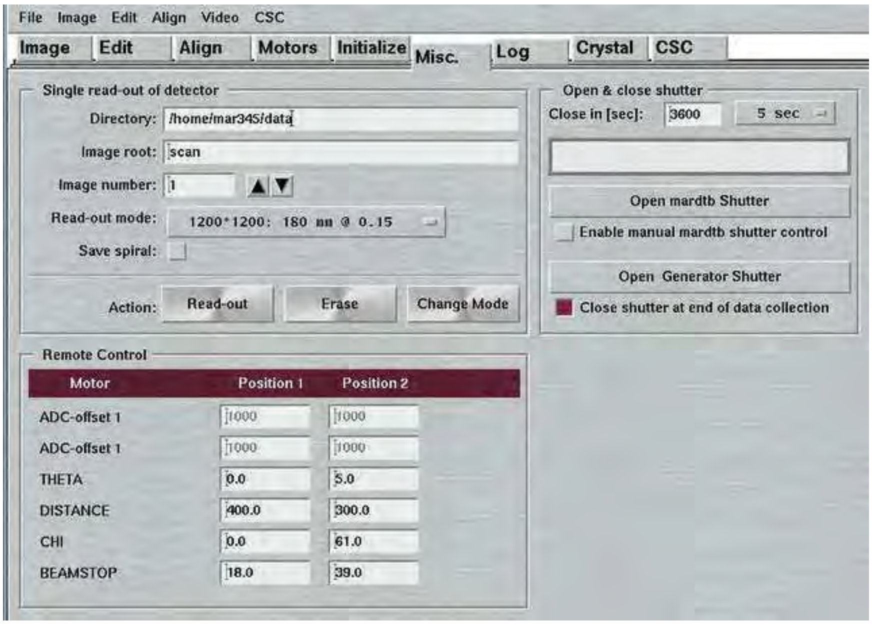
The *dtb*-controller stores all motor positions in static memory, so the motor positions are not lost if the power is cutoff. It is therefore not necessary to initialize the motors regularly. It is only required during installation and after a replacement of the *dtb*-controller. Motors cannot be moved manually except the following:

- PHI
- CRYSTAL (PHI-translation)
- BEAMSTOP
- SLITS (hor. and ver. for ion. chambers 1 and 2)

When moved manually, the motor positions stored by the controller don't coincide any more with the actual positions. For the PHI-axis things are less critical since **the PHI-axis has to be returned to its "locked" state** which is a unique position in the full turn. Otherwise, the PHI-axis will not move properly at all. But for the slits and for the beamstop it will be important, that during data collection they are physically at the correct positions. We therefore recommend:

- **Reference the BEAMSTOP and CRYSTAL translation every time you start working with the instrument. Do this before mounting the goniometer and crystal.**
- **Check SLITS, i.e. check wether the dial readings on the 4 slits correspond to the values of the slits shown in the user interface. If not, manually set the dials to the values displayed by the software.**

2.4.1.2.6 Misc.



Single read-out of detector

Directory: /home/mar345/data

Image root: scan

Image number: 1

Read-out mode: 1200*1200: 180 mm @ 0.15

Save spiral: ☐

Open & close shutter

Close in [sec]: 3600 5 sec

☐ Enable manual mardtb shutter control

■ Close shutter at end of data collection

Remote Control

Motor	Position 1	Position 2
ADC-offset 1	1000	1000
ADC-offset 1	1000	1000
THETA	0.0	5.0
DISTANCE	400.0	300.0
CHI	0.0	61.0
BEAMSTOP	18.0	39.0

The "**Misc.**"-page can be accessed by selecting the corresponding choice in the **"File"-menu**, by pressing the "**Ctrl+6**"-key while the pointer is in the main window, or by pressing the "**Scanmode**"-or "**Shutter**"-button in the status window.

This page offers 3 different functions:

- Single read-out or erase of the detector
- Open/close shutter(s)
- Settings for the remote control unit
- In program *mar555dtb*: parameters dealing with reference images

2.4.1.2.6.1 Single scan

Here, you may select a directory, image name, image number and scanmode and choose an action. You may:

- Scan the plate, i.e. make a single read-out and store data to disk
- Erase the plate, i.e. make a scan without actually storing the data
- Change mode, i.e. drive the scanning head inside the detector to the choosen scanmode and load the

corresponding speed profiles.

This feature is not used very often unless for very special experiments. This is why this window is accessible only via one button. For producing an output file, there is no choice of format. Images will always be produced in the *mar345*-format that is described elsewhere. The output file name follows the same rule as described in the chapter about the data collection.

2.4.1.2.6.2 Shutter

Here, you may manually open the experimental beam shutter of the dtb without having to setup an exposure. It should be noted that for normal users there is little need to do so. When opening the shutter, there will be a clock showing the time elapsed since opening the shutter. The shutter will automatically closed after the time given in the "**Close in [sec]**" text field has elapsed .

Only if the "**Enable manual shutter control**" button is checked, the little switch for operating the X-ray shutter on the *desktop beamline* itself is functional. If this is enabled, the software will loose control over the shutter and won't gain it back until this button is unchecked!

If the option "USE TTL" is set in the configuration file (see chapter **Configuration File** in section **Input**), you will have an option to use the mar345 controller to open or close a generator shutter using the shutter TTL signal of the mar345 scanner. Obviously, the generator shutter has to be wired accordingly. If the hardware is properly connected, you can open and close the generator shutter using the push button. You also have a choice of automatically closing the generator shutter at the end of a data collection. This is a useful thing to do both for safety reasons as well as for increased lifetime of the multi-layer mirrors.

2.4.1.2.6.3 Remote Control

Here, you can select choices concerning the behaviour of the optional **Remote Control**. For these choices to become relevant, the remote control obviously needs to be connected to the *dtb*. The window allows you to provide the following parameters by pressing the **ENTER**-key in the corresponding textfield.

- Alternate positions for driving the 2-theta arm
- Alternate positions for driving the detector distance
- Alternate positions for driving the CHI circle
- Alternate positions for driving the beamstop

The behaviour of the "**Remote Control**"-window can be controlled by keywords in the configuration file (see chapter **Configuration File** in section **Input**). Thus, it is possible to prevent input of values in the textfields.

To provide suitable parameters, an understanding of the functionality of the remote control is required. Please refer to chapter **2.1.4 Remote Control Unit** in section **Introduction**) for more details.

2.4.1.2.6.4 Settings for mar555 detector

Here, you set some parameters that affect the way the detector works, in particular the settings for the way reference images are being taken. For a description of the reference image settings, see the **mar555.key man page**.

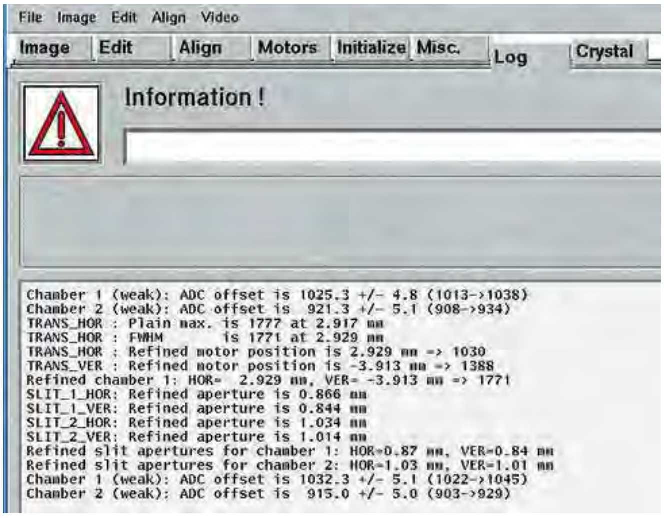
When modifying some of the values, the command will be immediately translated into a detector command according to the following table:

Field	Detector command
Read-outs/reference	SET REFErence *n*
Redo reference after	SET REFErence REDO *n*
... or after N secs	SET REFErence AFTER *n*
Redo for first #	SET REFErence FIRST *n*
Dummy references	SET REFErence DUMMY *n*

When pushing the Read-outs/reference button itself, a reference image will be recorded. Otherwise, the reference image settings given here will apply to a data collection, only.

The parameter DUMMY tells the program to start the procedure with read-outs that will not be used. The argument can be set to **AUTOMATIC** (or a negative value). In that case, the program determines automatically wether there is a requirement to do dummy reference cycles. This depends on the time elapsed since the detector has received a new integration window time, which typically happens at the start of a data collection.

2.4.1.2.7 Log



```
Chamber 1 (weak): ADC offset is 1025.3 +/- 4.8 (1013->1038)
Chamber 2 (weak): ADC offset is  921.3 +/- 5.1 (908->934)
TRANS_HOR : Plain max. is 1777 at 2.917 mm
TRANS_HOR : FWHM       is 1771 at 2.929 mm
TRANS_HOR : Refined motor position is 2.929 mm => 1030
TRANS_VER : Refined motor position is -3.913 mm => 1388
Refined chamber 1: HOR=  2.929 mm, VER= -3.913 mm => 1771
SLIT_1_HOR: Refined aperture is 0.866 mm
SLIT_1_VER: Refined aperture is 0.844 mm
SLIT_2_HOR: Refined aperture is 1.034 mm
SLIT_2_VER: Refined aperture is 1.014 mm
Refined slit apertures for chamber 1: HOR=0.87 mm, VER=0.84 mm
Refined slit apertures for chamber 2: HOR=1.03 mm, VER=1.01 mm
Chamber 1 (weak): ADC offset is 1032.3 +/- 5.1 (1022->1045)
Chamber 2 (weak): ADC offset is  915.0 +/- 5.0 (903->929)
```

The "**Log**"-page can be accessed by selecting the corresponding choice in the **"File"-menu** by pressing the "**Ctrl+7**"-key while the pointer is in the main window, or by selecting the corresponding tab in the main window. All hardware errors and warning as well as some additional information may be written inside the text area of this window. Among others also the final results of alignment procedures ("**Find Beam**", "**Optimize Beam**", "**Shape Beam**") will be printed in this window.

In case of hardware problems, first have a look inside this window to get some history of the problem.

2.4.1.2.8 Crystal

The "**Crystal**"-page can be accessed by selecting the corresponding choice in the **"File"-menu**, by pressing the "**Ctrl+8**"-keys while the pointer is in the main window, or by selecting the corresponding tab in the main window. Here, you set all the parameters for one or more data collection runs. The separate chapter **"Crystal"** describes the functionality of this page.

2.4.1.2.9 CSC

The "**CSC**"-page can be accessed by selecting the corresponding choice in the **"File"-menu**, by pressing the "**Ctrl+9**"-keys while the pointer is in the main window, or by selecting the corresponding tab in the main window. Here, you set all the parameters for one or more data collection runs. The separate chapter **"Cryogenic Sample Changer"** describes the functionality of this page.

2.4.1.2.10 marµX

The "**marmuX**"-page can be accessed by selecting the corresponding choice in the **"File"-menu** or by selecting the corresponding tab in the main window. Here, you set all the parameters for one or more data collection runs. The separate chapter **"Marmux"** describes the functionality of this page.

2.4.1.3 Other Windows

2.4.1.3.1 "Progress" Window

```
Set  Status   Vial   Images      Time Distance Theta   Phi    Delta-Phi Incr.   1. slits    2. slits   Beamstop       Xtal-XYZ      Scanmode     To go  Ending
                     curr./to go [sec]  [mm]  [deg.] [deg.]   [deg.] [deg.]   [mm] [mm]   [mm] [mm]    [mm]      X     Y     Z                [hrs]  time
10  Done      --     1   0/1      10    120     0.0   1.000  1*1.000  0.000   0.60/0.60   0.50/0.50   10.500   0.00  0.00 -1.17  mar1200             Tue 16:22
11  Done      --     2   0/1      10    120     0.0  31.000  1*1.000  0.000   0.60/0.60   0.50/0.50   10.500   0.00  0.00 -1.17  mar1200             Tue 16:22
12  Active    --     3   1/1      10    120     0.0  60.000  1*1.000  0.000   0.60/0.60   0.50/0.50   10.500   0.00  0.00 -1.17  mar1200      00:00  Tue 16:23
13  Queued    --     4   1/1      10    120     0.0  90.000  1*1.000  0.000   0.60/0.60   0.50/0.50   10.500   0.00  0.00 -1.17  mar1200      00:00  Tue 16:24
```

```
Set  Status   Vial   Images     Options                                  Current image name
                     curr./to go Opti/Reopti Erase Photo Thumb Shells Center
 1  Active    --     2   1/1                  y     y     y    -----     /home/cla/data/xtal_002.mar1200
11  Queued    --    91   1/1                        y     y    -----     /home/cla/data/xtal_091.mar1200
```

The "**Progress**"-window can be accessed by selecting the corresponding choice in the **"File"-menu** or by pressing the "**F3**"-key while the pointer is in the main window.

Here, you see the most important parameters of ongoing or programmed data collection runs. The window is opened automatically after pressing the "**Go**" button in the **"Edit Data Collection"-window** and before actually starting with a data collection. Since there is quite a large number of parameters that need to be listed, the window comes in 2 layouts that can be toggled on the fly by pressing the "**Show Filenames**"-button (which then says "**Show Params"**"). On the first page ('Params'), you can see the crystallographic parameters, on the second page ('Filenames') the image file names and some additional options.

The data set that is currently active is marked in "mar" red and white fonts, the queued ones are shown with a lighter background. The ones that are already finished are drawn with a grey background. In this window you will also find the time the data collection needs to complete and the actual ending time.

Table 5a: The columns in the 'Params' section of " Progress"-window

Name	Description
Set	Data set as programmed in the "Edit ..." window.
Status	Either "Active", "Queued" or "Done"
Vial	When using the sample changer, the selected carousel position is shown.
Image curr./to go	No. of current image followed by no. of remaining images out of total no. of images in this set. If set is not active, the current image equals to the starting image.
Time	Exposure time in seconds. When working in DOSE mode, the time will be only approximated.
Distance	The distance detector-to-sample in mm.
Theta	The 2-theta angle in deg.
Phi	The Phi at start of the current image in deg.
Delta-Phi	The no. of oscillations * Delta-Phi in deg.
Phi-inc	Phi-increment in deg., i.e. amount of Phi to be driven inbetween 2 consecutive images.
1.slits	Horizontal and vertical slit apertures in 1. chamber in mm.
2.slits	Horizontal and vertical slit apertures in 2. chamber in mm.
Beamstop	Distance beamstop-to-sample in mm.
Xtal-XYZ	Crystal xyz-translations of the goniometer head in mm
Format & Scanmode	The shown string is the actual image name extension and corresponds to the choices for "Format" and "Scanmode" in the "Edit..."-window.
To go	Time in hrs to terminate this set.
Ending time	Time when this data set completes.

Table 5b: The columns in the 'Filenames' section of " Progress"-window

Name	Description
Set	Data set as programmed in the "Edit ..." window.
Status	Either "Active", "Queued" or "Done"
Vial	When using the sample changer, the selected carousel position is shown.
Image curr./to go	No. of current image followed by no. of remaining images out of total no. of images in this set. If set is not active, the current image equals to the starting image.
Options	Shows selected options of the toggle buttons in the Edit window.
Current image name	Full path name of current image (or first image in set).

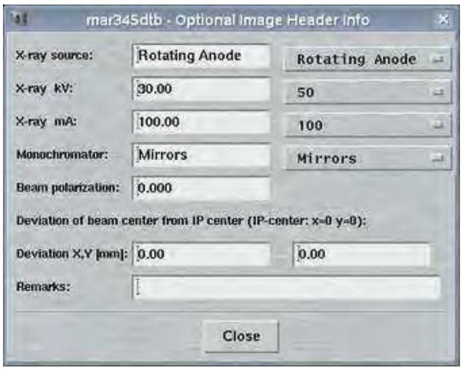
The buttons in the lower part of the window are mostly self-explanatory. Some of the buttons will be made insensitive during certain operations. For instance, during a readout of the detector, the " **Stop NOW**"-button is disabled.

IMPORTANT HINT for using "Stop NOW":
Under certain conditions - e.g. when driving a motor in an endswitch - it is possible that all major action buttons are disabled and you don't seem to have a possibility to go on with your work. In this situation, it usually helps to press the "Stop NOW"-button (or the F12-key) to reenable all buttons instead of restarting the program.

Table 6: The buttons in the "Progress"-window

Name	Description
Go	Start data collection of all programmed sets. This button is enabled only before starting a data collection.
Stop NOW	Immediately abort the exposure or any motor movement.
Stop after IMAGE	Stop data collection of all data sets after finishing exposure and readout of current image. When pressed, this button toggles with "Continue after IMAGE", so there is a chance to revert this action.
Stop after SET	Stop data collection of all queued data sets after finishing the current set. When pressed, this button toggles with "Continue after SET", so there is a chance to revert this action.
Change Params	Returns to the "Edit Data Collection Parameters"-window. This button is enabled only before starting a data collection.
Close	Closes this window. Get this window back with the "**F2**"-key.

2.4.1.3.2 "Image Header Info" Window



X-ray source:	Rotating Anode	Rotating Anode
X-ray kV:	30.00	50
X-ray mA:	100.00	100
Monochromator:	Mirrors	Mirrors
Beam polarization:	0.000	

Deviation of beam center from IP center (IP-center: x=0 y=0):

Deviation X,Y [mm]:	0.00	0.00
Remarks:		

The "**Image Header Info**"-window can be accessed by selecting the corresponding choice in the **"File"-menu** of the main window.

Here, you can provide some information that is going to end up in the headers of images created by the *mar345*-detector. This information is strictly optional and there are no programs that are systematically making use of it. It would be good practice, though, to fill in the fields. A general experience is, that when working with images later you will have trouble to find notes written in a logbook, but it is straightforward to just look into the image header (e.g. with program *catmar*).

2.4.1.3.3 "Administrator" Window

Warning

Redefining motor values can be VERY DANGEROUS!

Do this ONLY if you know very well what you are doing.

Move motors

Motor	Current Position	Target Position
Phi	0.000	0.000

The "**Administrator**"-window can be accessed by selecting the corresponding choice in the **"File"-menu** of the main window.

Here, you can redefine motor positions. This is a dangerous thing to do and normally there should not be a necessity at all to do so. This is why the choice for opening this window only is available when running the program in "administrator" mode. This mode requires to start the program with command line option "--admin".

2.4.1.3.4 "Hardware" Window

dtb Digital IO Bits

Shutter Open :	Off	LCD Enable:	On
Shutter Close:	On	Fan Enable:	On
Beamstop - Reference:	On	Trigger LCD:	On
Phi - Reference:	Off	Ext. Shutter Closed:	On
External 12V:	On	ADC2 High Gain:	On
Local 12V:	On	ADC1 High Gain:	On
Shutter On:	Off	HV On:	On
Shutter External:	Off	Data OK:	On
IO Data 7:	Off	Data Enable:	On

mar345 Status

Erase Lamp - Top:	Off
Erase Lamp - Left:	Off
Erase Lamp - Right:	Off
Laser Status:	Off
Laser Current:	Off
Laser Temperature:	Off
Plate Locked:	Off
Radial Sensor:	Off
Rotation Sensor:	Off

dtb Motor Status

	Warning	Switch1	Quickst	Voltage	Fault	Operat.	Switch2	Ready	Ref -	Ref +	Error	Setpack	Limit	Target	Remote	Refswitch
PHI	☐	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
CHI	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
THETA	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
DISTANCE	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
SLIT_1_HOR	☐	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
SLIT_1_VER	☐	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
SLIT_2_HOR	☐	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
SLIT_2_VER	☐	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
BEAMSTOP	☐	☐	☐	☐	☐	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☐
XTAL_Z	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
TRANS_HOR	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
TRANS_VER	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☒	☐	☒	☒	☒
ROT_HOR	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
ROT_VER	☐	☐	☒	☐	☐	☐	☐	☒	☐	☐	☐	☐	☐	☒	☒	☒
ACTUATOR	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
XTAL_X	☐	☒	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☒	☒	☒
XTAL_Y	☐	☒	☒	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☒	☒	☒

The "**Hardware**"-page can be accessed by selecting the corresponding choice in the **"File"-menu**.

Here, you can look at certain hardware bits in detail. The information presented here reflects the contents of the status block that is periodically sent by the *dtb*-controller to the computer.

The window features 3 areas:

- **dtb Digitial IO Bits**:
  This area looks at some single hardware bits, among others the status of the local X-ray shutter. Note, that for safety reasons the state of the X-ray shutter is controlled by 2 independent sensors: one that checks wether the shutter is open and one that checks wether the shutter is closed. For increased safety, the state "shutter is closed" is true only if both bits "Shutter Close" is "On" (i.e. true) and "Shutter Open" if "Off" (i.e. false).

  On the bottom of this area you will find a button that allows you to toggle the operation of the fan of the cryo exhaust. If the *dtb* is powered on, this fan is turned on as well. With the potentiometer on the fan you can't turn it off completely but only with the help of this button!

- **mar345 Status**:
  This area looks at some information from the *mar345* image plate detector. The entries should be self-explanatory. Watch the bits as they change state during a scan...

- **dtb Motor Status**:
  This area reflects the information of single motor modules on the CAN-bus. Technically, all motors carry a 16-bit status word. Not all of the 16-bits are used. Here you can detect wether a motor hits an end switch, wether a motor is moving at all or wether it is idle. The description of all of the 16 bits would be too much detail.

  Note that the 4 slit motors, PHI and BEAMSTOP behave differently from all others. This is because those motor modules physically sit on the *dtb*-controller card, while all other motors have their own hardware modules.

2.4.2 "Status" Window

The status window monitors all detector and goniometer activity and displays current motor positions, the shutter state, X-ray intensity readings, etc. If the first place it consists of two areas:

- menu bar
- fields displaying status information

2.4.2.1 Menu Bar

2.4.2.1.1 File Menu

The File menu pops up if the "File" button in the menu bar is pressed or if "**Alt+f**" is pressed while the pointer is in the status window. Most of the choices in the menu (Ctrl+0 to Ctrl+9) will allow to navigate from page to page in order to access specific functions:

Table 7: The "File" menu

Menu	Menu Choice	Shortcut	Description
	**Close**	F1	Closes the status window and pops up the main window
	Main	F2	Pops up the main window
	Progress	F3	Monitors progress and status of current data collection
	Quit	Ctrl+q	Leave program *mar345dtb*

2.4.2.1.2 Help Menu

The Help menu pops up if the "Help" button in the menu bar is pressed or if "**Alt+h**" is pressed while the pointer is in the main window.

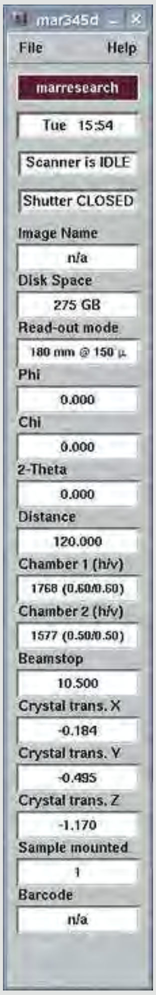
Table 8: The "Help" menu

Menu	Menu Choice	Description
	**Contents**	Calls the WWW-browser and loads file $MARDOCDIR/mar345dtb.htm
	About	Shows current program version

2.4.2.2 Status Fields

Most of the status buttons have double functionality: they display current status (e.g. motor positions) and they can be pushed to pop up additional windows:

Table 9: The "Status"-buttons

Button	Button	Action when pressed	Description
 mar345d File Help marresearch Tue 15:54 Scanner is IDLE Shutter CLOSED Image Name: n/a Disk Space: 275 GB Read-out mode: 180 mm @ 150 µ Phi: 0.000 Chi: 0.000 2-Theta: 0.000 Distance: 120.000 Chamber 1 (h/v): 1768 (0.60/0.60) Chamber 2 (h/v): 1577 (0.50/0.50) Beamstop: 10.500 Crystal trans. X: -0.184 Crystal trans. Y: -0.495 Crystal trans. Z: -1.170 Sample mounted: 1 Barcode: n/a	**marresearch**	none	Shows ending time during data collection
	Mon 15:30	none	Current computer time
	Scanner is IDLE	none	Current dtb or detector action (progress bar)
	Shutter CLOSED	Pops up the "**Misc.**"-page in the main window	Shows current state of experimental beam shutter.
	Image Name	Pops up file selection window	Displays current image name during data collection
	Disk Space	Pops up file selection window	Displays remaining disk space in current data directory
	Scanmode	Pops up the "**Misc.**"-page in the main window	Displays current scan mode of *mar345*-detector
	Phi	Pops up the "**Motors**"-page in the main window	Displays current PHI position
	Chi	Pops up the "**Motors**"-page in the main window	Displays current CHI position (Phi-swing)
	2-Theta	Pops up the "**Motors**"-page in the main window	Displays current 2-Theta position
	Distance	Pops up the "**Motors**"-page in the main window	Displays current distance detector to crystal
	Chamber 1 (h/v)	Pops up the "**Motors**"-page in the main window	Displays current reading of 1. ion. chamber and positions of hor. and ver. slits
	Chamber 2 (h/v)	Pops up the "**Motors**"-page in the main window	Displays current reading of 2. ion. chamber and positions of hor. and ver. slits
	Beamstop	Pops up the "**Motors**"-page in the main window	Displays current beamstop position
	Crystal trans. X	Pops up the "**Motors**"-page in the main window	Displays current position of crystal x-translation
	Crystal trans. Y	Pops up the "**Motors**"-page in the main window	Displays current position of crystal y-translation
	Crystal trans. Z	Pops up the "**Motors**"-page in the main window	Displays current position of crystal translation along Phi-axis
	Sample mounted	Pops up the "**CSC**"-page in the main window	Displays vial no. of currently mounted sample
	Barcode	Pops up the "**CSC**"-page in the main window	Displays barcode of currently mounted sample

If the option "USE TTL" is set in the configuration file or when using the marµX generator within the mar345dtb program, (see chapter **Configuration File** in section **Input**), instead of the "Disk space" field, there will be a status indicator for the generator shutter.

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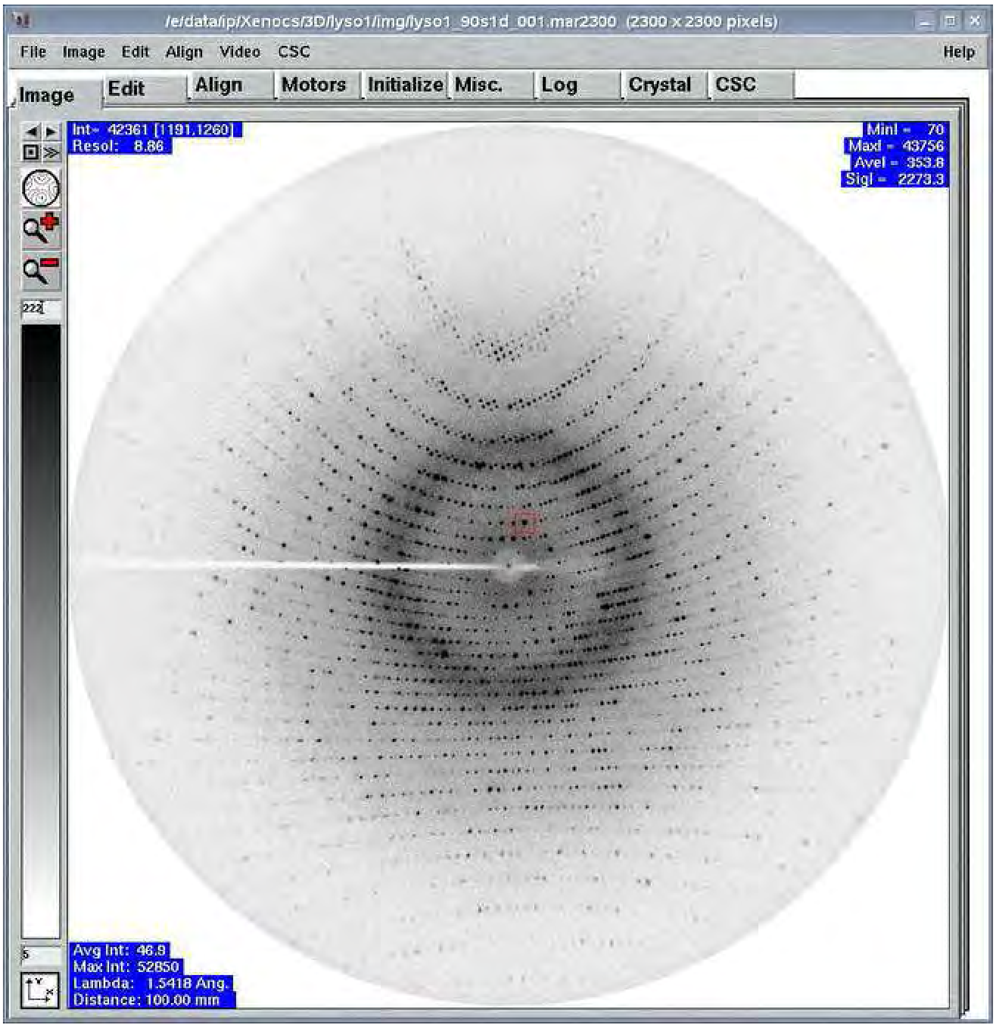
3. Image

3.1 Introduction



Int= 42361 [1191,1260]
Resol: 8.86

Mini = 70
Maxi = 43756
Avel = 353.8
Sigl = 2273.3

Avg Int: 46.9
Max Int: 52850
Lambda: 1.5418 Ang.
Distance: 100.00 mm

The "**Image**"-page can be accessed by selecting the corresponding tab in the main window or by pressing the "**Ctrl+1**"-key while the pointer is in the main window. This window is the area where to visually inspect images. The data display functions are very similar to those used by program *marView* with a couple of restrictions. You can:

- automatically display incoming images during data collection
- manually load images
- adjust color distributions of the image

- integrate areas of the image
- draw cross-sections of the image
- display resolution rings
- zoom in and zoom out
- print an image

The "**Image**"-page features several areas:

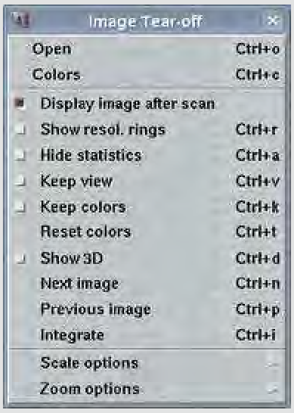
- a menu bar component called "Image" **(see 4.2)**
- a tool box on left hand side of window **(see 4.3)**
- an image display area with some information areas in upper left, upper right and lower left corners **(see 4.4)**

During data collection, incoming images are loaded and displayed automatically, but only if the "**Image**"-page is up or if the **Image menu**-choice **"Display image after scan"** is selected. One should keep in mind, that image display puts load on the computer. During a data collection, it may not really be necessary to keep looking at images if everything proceeds nicely.

3.2 Image Menu

The Image menu pops up if the "Image" button in the menu bar is pressed or if "**Alt+I**" is pressed while the pointer is in the main window. The choices in the menu allow for opening additional windows or accessing special functions:

Table 2: The "Image" menu

Menu	Menu Choice	Shortcut	Description
	**Open**	Ctrl+o	Pops up "**File**"-window
	Colors	Ctrl+c	Pops up "**Colors**"-window
	Close	F1	Takes away "**Display**"-window
	Show resolution rings	Ctrl+r	Toggle display of resolution rings
	Hide statistics	Ctrl+a	Toggle display of some image info in lower left corner
	Keep view	Ctrl+v	Keep same aspect of image and color scheme when loading new images. By default, image colors are recomputed and images are shown to fit in the window
	Keep colors	Ctrl+k	Keep same color scheme when loading new images
	Reset colors	Ctrl+t	Recomputes best color scheme for loaded image
	Show 3D	Ctrl+d	Toggle display of 3-D plots of zoomed areas (for zoom factors > 4)
	Next image	Ctrl+n	Load image with image number increased by 1 unit
	Previous image	Ctrl+p	Load image with image number decreased by 1 unit
	Integrate	Ctrl+i	Integrate the contents of the zoomed area and show results in upper right corner
	Zoom options		See "**Zoom Options**" submenu

The choices in the "**Zoom Options**" submenu affect the way the image looks at zoom factors < 1.0. If one pixel on the monitor corresponds to more than 1 pixel (N pixels) in the image, image colors can be calculated in several ways. Please note, that "N'th" pixel mode is faster than others since it doesn't involve computation.

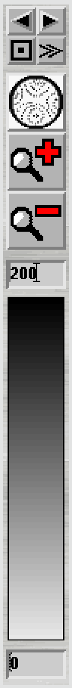
Table 3: The "Zoom Options" submenu

Menu	Menu Choice	Description
	**N,th pixel**	Use every N'th pixel to display colors and ignore others
	Average pixels	Take average value out of N pixel to display colors
	Maximum pixels	Take maximum of N pixel to display colors

3.3 Toolbox

The toolbox on the left hand side of the "**Display**"-window features the following functions:

Table 4: The "Image Toolbox"

Toolbox	Symbol	Description
	◀	Load previous image
	▶	Load next image
	▣	Stop loading images (see next)
	≫	Continuously load images by increasing image number
	◯	Display entire image
	🔍+	Zoom in
	🔍−	Zoom out
	200	Upper limit for distributing grey scales
	0	Lower limit for distributing grey scales

3.4 Image Area

3.4.2 Mouse Button Functions

Within the image area of the "**Display**"-window the mouse buttons have the following functions:

- **Left mouse button:**
  Press the left mouse and drag it to another position in the image. When the mouse button is released a window pops up showing the cross-section through the corresponding part of the image, i.e. a plot of pixel intensities starting at the position where the button has been pressed and ending at the position where the mouse has been released. In the image itself a red line will be drawn describing the trajectory.

- **Middle mouse button:**
  If the area displayed in the window is magnfied (zoom factor >= 1, marked in the upper left corner of the display area), the coordinates of the mouse position and the intensity of the corresponding pixels are displayed in the lower left corner of the display area. Otherwise, the corresponding information is displayed in the upper left corner of the display area and, in addition, a box sized 50x50 pixels centered around that coordinate is integrated. The minimum, maximum and summed intensities are displayed in the upper right corner of the display area. A red box describing the contents of the box is drawn in the image area itself.

- **Right mouse button:**
  If the area displayed in the window is magnfied (zoom factor >= 1, marked in the upper left corner of the display area), the displayed portion of the image is recentered around the coordinate of the mouse position. Thus, one can move around zoomed areas of the image. If zoom factors are smaller, than you can drag the right mouse button. A rectangle will be drawn in the image. If the button is released, the contents of the rectangle will be displayed. Depending of the size of the rectangle the corresponding zoom factor will be used. To increase and decrease the magnfication of the displayed part of the image, use the corresponding buttons with the magnification glass showing the "+" and "-"-sign.

3.4.3 Information Areas

In the corners of the image area of the "**Display**"-window certain information will be displayed, depending on previous actions:

- **Upper left corner:**
  When pressing the middle mouse button in the image area, the [x,y]-coordinate, intensity and resolution of the pixel under the pointer is displayed.

- **Lower left corner:**
  Once an image has been loaded successfully, the most relevant information is displayed here: wavelength, distance, maximum intensity and average intensity. Display of this information may be removed by choosing "**Hide statistics**" in the **Options menu**

- **Upper right corner:**

When pressing the "**Integrate**"-button in the **Options menu** the following information is displayed: number of pixels in x and y, maximum, minimum, average, sum and standard deviation of pixel intensities, average background and mean intensity over background (all relative to the pixels displayed in the image area). The background is calculated from a histogram of intensities of a box of 50x50 pixels around the center of the zoomed area. Pixel values > 1000 are excluded from the histogram. Integration is possible only for zoom factors > 1.

3.5 "File" Window

Directory: /e/data/ip/Xenocs/3D/lyso1/img/

Search Pattern: *

Images:

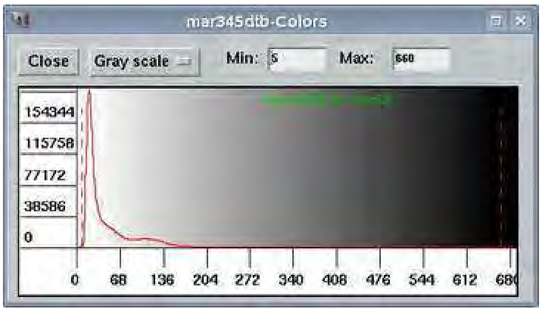
lyso1_90s1d_005.mar2300
lyso1_90s1d_006.mar2300
lyso1_90s1d_007.mar2300
lyso1_90s1d_008.mar2300
lyso1_90s1d_009.mar2300
lyso1_90s1d_010.mar2300
lyso1_90s1d_011.mar2300
lyso1_90s1d_012.mar2300
lyso1_90s1d_013.mar2300
lyso1_90s1d_014.mar2300
lyso1_90s1d_015.mar2300
lyso1_90s1d_016.mar2300
lyso1_90s1d_017.mar2300
lyso1_90s1d_018.mar2300
lyso1_90s1d_019.mar2300
lyso1_90s1d_020.mar2300
lyso1_90s1d_021.mar2300
lyso1_90s1d_022.mar2300

Selected Image: lyso1_90s1d_001.mar2300

The "**File**"-window can be accessed by selecting the corresponding choice in the **"Windows"-menu** or by pressing the "**Ctrl+f**"-key while the pointer is in the display window. This window is used to manually load images.

When the window pops up, the contents of the current working directory are listed in the file area of the window. By double-clicking a file, the corresponding file will be loaded. A single click will transfer the string of the selected file to the **"Selected File:"** area of the window and you will have to press the "**Load**"-button to actually load the image. By pressing the "**List**"-button, the directory is searched and files matching the "**Search Pattern**" are listed. By pressing the "**Follow**"-button a series of image files will be loaded. Image numbers will be continuously increased.

3.6 "Colors" Window



Min: 5

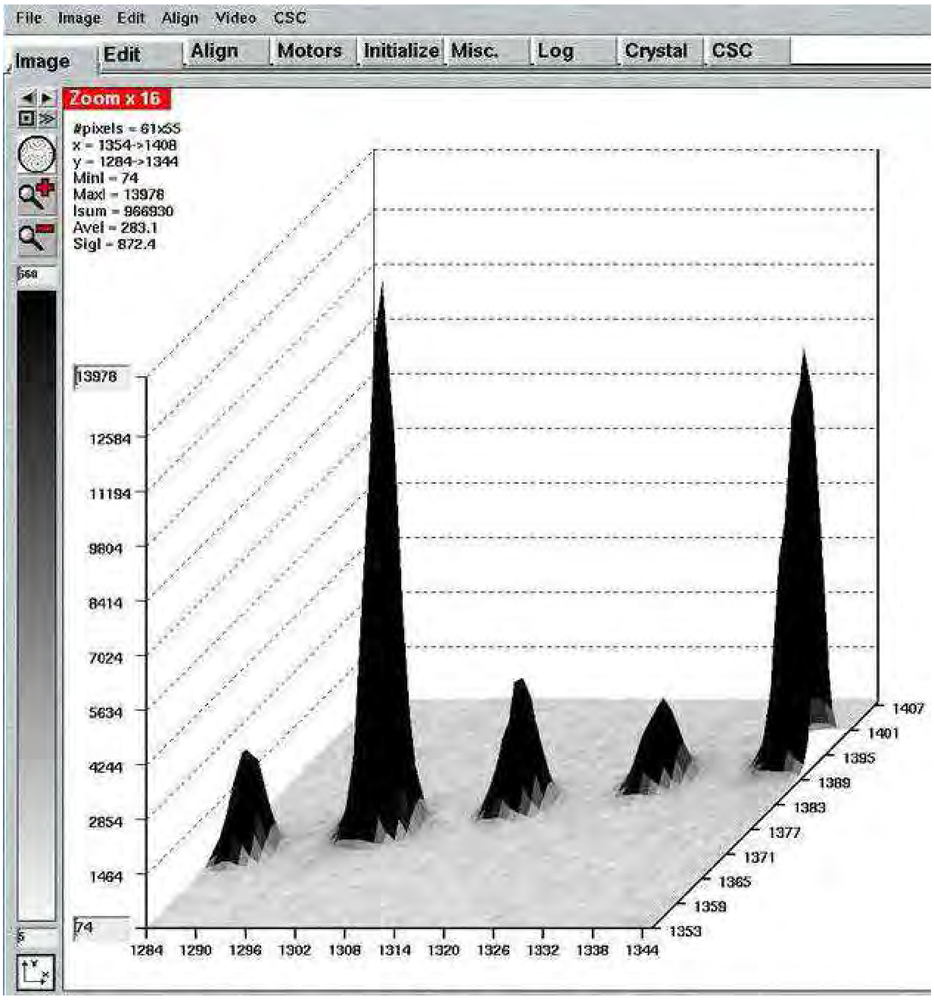
Max: 660

The "**Colors**"-window can be accessed by selecting the corresponding choice in the **"Windows"-menu** or by pressing the "**Ctrl+c**"-key while the pointer is in the display window. This window is used to manipulate image colors.

The continuous red line in the plot shows the frequency of certain pixel values in the entire image, i.e. an intensity histogram. The maximum frequency is normally something like the average background or the "most probable" pixel value. In the histogram, two dashed bars mark the Min and Max values. To change Min or Max, enter values in the corresponding fields (and press RETURN!) or move the left or right bar using the left or right mouse button, respectively, and wait a moment until the image is rescaled accordingly.

When loading an image, the program automatically distributes grey scales in equidistant intensity bins between a minimum (Min) and maximum (Max) value. All pixel values > Max are drawn in black and all values < Min in white. Min usually is 0, but Max is calculated such that 99.998 % of all pixels in the image have intensities <= Max. The Max and Min can be entered in the upper part of the "**Colors**"-window or in the upper (Max) and lower text (Min) text field of the **toolbox** in the "**Display**"-window.

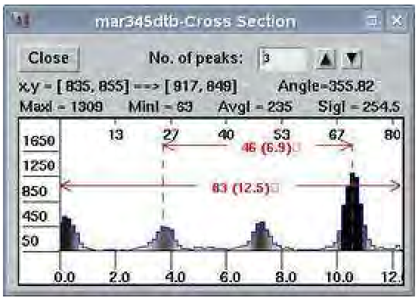
3.7 3-D Plot



```
#pixels = 61x55
x = 1354->1408
y = 1284->1344
MinI = 74
MaxI = 13978
Isum = 966930
AveI = 283.1
SigI = 872.4
```

A 3-D representation of a portion of the image can be obtained by selecting the "**Turn ON 3-D plot**"-choice in the **"Options"-menu** or by pressing the "**Ctrl+d**"-key while the pointer is in the display window. This option works at zoom factors > 4 only. It dumps some statistics of the displayed area in the upper left corner of the display area. The aspect of the peak to be display may be altered by entering a minimum or maximum threshold in the corresponding fields of the vertical axis. As in the regular image area, the right mouse button may be used to recenter the peak. This is a little bit of trial and error but once you get used to it, it works. You may switch between 3-D and regular display any time by pressing `Ctrl+d`.

3.8 "Cross-section" Window



No. of peaks: 3

```
x,y = [835, 855] ==> [917, 849]      Angle=355.82
MaxI = 1309    MinI = 63    AvgI = 235    SigI = 254.5
```

A cross-section through a portion of the image can be obtained by dragging the left mouse button in the image area of the "**Display**"-window. The window features the following elements:

Table 1: The "Cross-section"-Window

Element	Description
No. of peaks	Specifies the number of peaks between two dashed lines in the plot area of the window. Use the arrow buttons on the right hand side of the fextfield to increment or decrement the value by 1. When pressed, the real space cell constant is calculated from the distance between the two dashed lines and the number of peaks. The result is displayed in the message area.
Message area	Shows the coordinates of the start and end of the line, the angle with the base line, maximum, minimum, average and standard deviation of the intensities along the drawn line. When changing the no. of peaks manually, the second line displays the derived cell constant.

Element	Description
Plot: vertical axis	Interpolated intensities
Plot: upper horizontal axis	Length of line in pixel units
Plot: lower horizontal axis	Length of line in mm units
Plot: left dashed line	Marks the beginning of a measured distance. This line can be moved using the **left** mouse button.
Plot: right dashed line	Marks the end of a measured distance. This line can be moved using the **right** mouse button.
Plot: horizontal red lines	Show the total length of the line in pixels (mm) and the distance between the dashed vertical lines.

The pointer can be used to measure distances by setting the red dashed lines to the desired position along the drawn line. This is particularly useful if you want to measure cell constants. The program features a peak finding algorithm which tries to set the bars on top of the first and the last peak of the plot. Inbetween the peaks the program then looks for other peaks and tries to calculate the best inter-peak distances by assuming a harmonic oscillation. The no. of peaks calculated by the program is displayed in the "No. of peaks" textfield. Of course, this value can be modified. The derived cell constants do not take into account any particular setting or symmetry of the crystal but calculates cell constants assuming plain orthogonal axes.

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4. Alignment

4.1 Introduction

The "**Align**"-page can be accessed by selecting the corresponding tab in the main window or by pressing the "**Ctrl+2**"-key while the pointer is in the main window. This window is the area where to align the *desktop beamline* with the X-ray beam. The principles of alignment are described in chapter **"Principles of Operation"** of the **Introduction**. Within this window you can:

- find the X-ray beam from scratch
- reoptimize the X-ray beam
- obtain a 3-D beam profile
- determine appropriate slit apertures
- manually move motors for positioning the *dtb*

The "**Align**"-window features several work areas:

- a menu bar **(see 4.2.1)**
- a status area in the upper quarter of the window **(see 4.2.2)**
- a parameter input area for different tasks in the second quarter of the window **(see 4.2.3)**
- a drawing area where reading readings of both ionization chambers are plotted in the lower half of the window **(see 4.2.4)**

4.2 Work Areas

The dtb features a variety of functions that have to do with moving the alignment motors. Availabel functions are:

Function	Description
Find beam	Find beam from scratch
Optimize beam	Optimize beam assuming that the dtb already sees some beam.
Profile beam	Establish a 3-D beam profile
Shape beam	Determine appropriate beam apertures
Adjust ADC	Readjust the ADC offsets
Manual operation	Move hor. and ver. translations and rotations individually

4.2.1 Align Menu

The **Align**-menu pops up if the "Align" button in the menu bar has been pressed or if "**Alt+a**" is pressed while the pointer is in the main window.

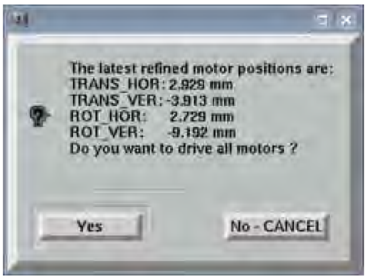
Table 1: The "Align" menu

Menu	Menu Choice	Description
	**Load beam data**	Open beam file and display contents in plot area
	Drive to latest beam maximum	Drives all positional motors to the maximum the latest refined positions

4.2.1.1 Load beam data

This window allows to open and display files that have been created previously and that contain beam profiles, beam scans or beam history. These files are stored by program *mar5dtb* in directory $MARLOGDIR/beam and usually 99 version of either file type dtb.scan.N, dtb.profile.N and dtb.time.N are stored. The number N is configurable (see below). Instead of manually loading single files it is usually more convenient to scroll through previous beam file using the arrow buttons in the drawing area (see below).

4.2.1.2 Drive to latest maximum



The latest refined motor positions are:
TRANS_HOR: 2.929 mm
TRANS_VER: -3.913 mm
ROT_HOR: 2.729 mm
ROT_VER: -9.192 mm
Do you want to drive all motors ?

This window allows to drive directly all translational and rotational motors to the most recent refined positions. A motor position will be treated as refined if it has gone either through the "**Find beam**" or "**Optimize beam**" procedure. This option is very useful if for some reason the motors have been moved manually, or if for instance beam optimization has been started without X-rays.

The refined positions will even be written to a data file and read by program *mar5dtb* at program startup, so the values are available even after program restart.

4.2.2 Status Area

The "**Status Area**" shows the current positions of the motors that have to do with ionization chamber 1 (TRANS_VER, TRANS_HOR, SLIT_1_VER, SLIT_1_HOR) and with ionization chamber 2 (ROT_VER, ROT_HOR, SLIT_2_VER, SLIT_2_HOR), respectively. For both chamber, the current chamber reading is displayed as well. Note, that all components of chamber 1 are colored red and all components of chamber 2 are colored blue. This rule also applies to the intensity plots in the drawing area.

The plot in the right corner of this area is a representation of the motor positions relative to their possible range of translation. It is assumed that all motors have previously been initialized properly. In the plot given above, the red dot stands for the motor positions TRANS_HOR and TRANS_VER (1. chamber) and the blue one for the motors ROT_HOR and ROT_VER (2. chamber). In both cases, the horizontal motor is almost in the center of its range of movement and the vertical motor somewhat closer to the lower end.

The use of this plot is the following: for optimization of the beam it is important that the actual X-ray beam is not too close to one of the limits of the movements. Otherwise, the instrument cannot completely drive over the beam and cannot properly determine the maximum. Even if the movements of the motors are all relatively ample, you may want to stay away from the edges of the movements and ideally end up relatively close to the centers of movements. The graphical representation of the motor positions is much more intuitive than looking at the actual numbers in mm, since this would require you to know where the minimum and where the maximum of the motors are, and this is really too much hazzle.

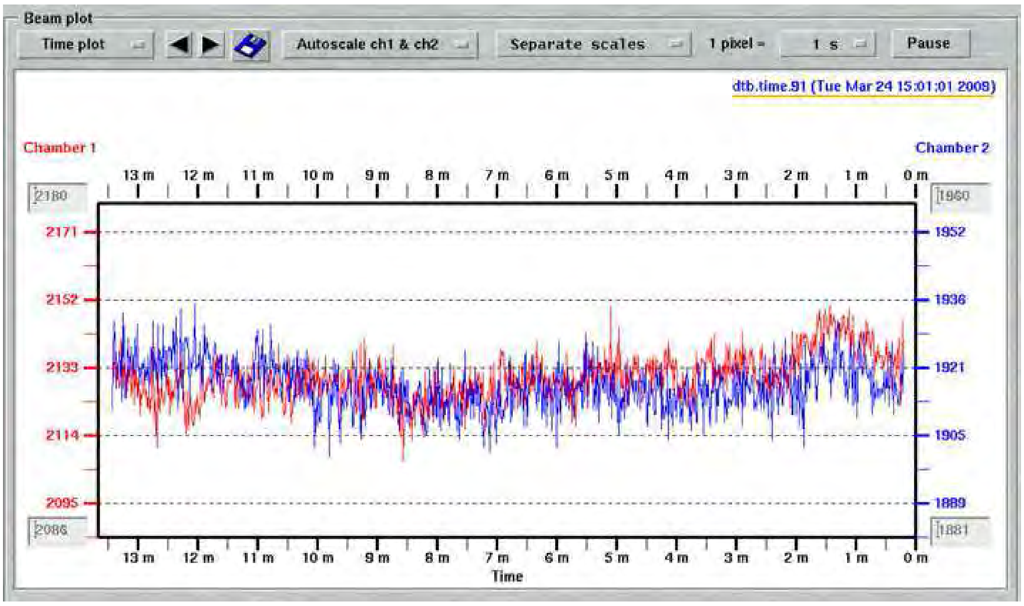
Depending on the current operation, there will be some rectangles drawn around the dots, in particular during the "**Find beam**" and "**Optimize beam**" procedure. These rectangles mark the way the motors are going to move during the procedure. The sizes of the rectangles vary depending on the optional settings for the corresponding tasks (see below).

4.2.3 Input Parameter Area

Chamber	Slit aperture (h/v)		Hor. scan range	Ver. scan range	Speed	Use
First:	0.60 mm	0.60 mm	2.0*slit size	1.0*slit size	10 %	■
Second:	0.30 mm	0.30 mm	2.0*slit size	2.0*slit size	20 %	■

The "**Input Parameter Area**" allows for setting some parameters that affect the behaviour of the individual tasks. Depending on the choosen task, the layout of this area will change. Only the most relevant parameters may be changed, e.g. speed parameters or slit apertures, etc.. See below for more details.

4.2.4 Plot Area



The "**Plot Area**" displays the readings of ionization chambers 1 (red) and 2 (blue). There are 3 different plot types:

- **Time plot:**
  Usually, the *desktop beamline* controller sends status information at a rate of 1/second. The time plot follows the readings over the course of time, i.e. you will see the history of the intensity over some period of time. Many people know this utility from visits to synchrotron sites. On home X-ray sources, you may see instabilities of the generator. If the resulting plot shows a smooth decrease it may also indicate the need of readjusting the ADC offset at some stage. Due to changes in ambiental conditions ADC offsets may drift.

  By default, 1 pixel on the screen corresponds to 1 second. For the width of the "**Align**"-window this corresponds to 14 minutes. By selecting other time units (e.g. 1 pixel = 10 s) you extend the period of time to be displayed. At the largest scale this will be many days.

- **Scan plot:**
  The *desktop beamline* can digitize ionization chamber readings while moving any motor. The time resolution is 154 microsec per digitization! Hence, the mapping of intensity reading to motor position is extremely precise. This utility therefore allows for very accurate determination of X-ray beam maxima and is heavily used during all tasks of automatic beam alignment. During a scan incoming data are automatically scaled and displayed. On the x-axis you will find the positions of the moving motor. See also chapters **Find Beam**, **Optimize Beam**, **Profile Beam** and **Shape Beam** for more details

- **Beam profile:**
  The program allows for establishing a beam profile and display this profile. See chapter **Profile Beam** for more details.

At the top of the drawing area, there is a menu bar where you can select which type of plot you want to look at. For certain plot types, there are additional input options.

Table 2: The "Plot Area" options

Symbol	Plot type	Description
Time plot	All	Choice of type of plottype: time, scan or beam plot
◀ ▶	All	Load previous or next plot (either time, scan or profile). Note, that the name of currently loaded file is displayed in the upper right corner of the plot area. The latest file is written on white background and underlined in orange. Otherwise, the background will be grey.

Symbol	Plot type	Description
💾	All	Save current plot to file. The o/p-file will always be called `beamplot.xwd` and will go to the working directory. Existing beamplot.xwd files will be overwritten without warning. The file format is "**XWD**" (X Windows system window dump file). There are utilities for converting this format into many other image formats (png, jpg), the most useful and popular being the ones from the ImageMagick suite available for all Unix flavours, in particular program *convert*.
Autoscale ch1 & ch2	Time & Scan	Choice of automatic adjustment of scales. By default (autoscale), the y_{min} and y_{max}-values of both red and blue curves are adjusted automatically. Thus, the plot always makes use of the entire drawing range in y. You may provide your own min. and max. values by disabling autoscaling for either chamber 1 and chamber 2 readings.
Separate scales	Time & Scan	Choices for scaling plots for chambers 1 and 2 onto eachother. Usually, the readings in chamber 1 are larger than in chamber 2. Due to automatic adjustment of y-scales, the user may not see the difference. When scaling chamber 2 onto chamber 1 readings, y_{min} and y_{max}-values of chamber 1 readings are used to scale chamber 2 readings. When using separate scales, the blue curve is scaled according to the y-axis scales on the right hand side.
1 pixel = 1 s	Time	Each pixel on the screen corresponds to a defined period of time. By choosing smaller or larger conversion numbers you may shorten or extend the total amount of time to be displayed. Note, that the starting time of the program sets the start of all menu choices. Only if the program stays up for some time, you will see some beam history for the 1 pixel = 30 min choice.
Pause	Time	Disable further updates of plot in TIME mode. Toggles with button **Continue**. Note, that the program keeps updating the beam history internally while pausing the display update.
Zoom x 8	Profile	Zoom factor for displaying the beam profile. With large zoom factors, the beam profile may not fit in the window, but scroll bars will allow to inspect all areas.
Min. & max. for greys: 898 1005	Profile	In the corresponding text fields on the right hand side you may manually enter min. and max. values for distributing grey scales in the beam profile plot. All pixels > **max.** are drawn in black and all pixels < **min.** are drawn in white. All pixels inbetween get some shades of grey.

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4.3 Alignment Tasks

4.3.1 Find Beam

Chamber	Horizontal range		Vertical range		Threshold	Use
First:	25.0 %	75.0 %	Min.	75.0 %	1250	■
Second:	15.0 %	85.0 %	Min.	85.0 %	1250	■

The "**Find Beam**"-tool can be accessed by selecting the corresponding choice in the **"menubar"** or by pressing the "**Alt+f**"-key while the pointer is in the "**Align**"-window.

The purpose of the "**Find Beam**"-procedure is to find the X-ray beam from scratch, i.e. without knowing at all where the beam is going to pass through the 2 pairs of slits. The typical situation is that there is no significant intensity reading in chamber 1 and that the alignment motors will have to move some way to see the beam. For this procedure to work we have to assume that there is only 1 primary beam coming out of the monochromator.

BEWARE:

If there are multiple beams as produced by mirror systems and if the unwanted beams (i.e. polychromatic) are not cut out before entering the collimator of the *dtb*, this procedure has little chances to work

The variable parameters for this procedure are the following:

Table 3: The input parameters for "Find Beam"

Parameter	Description
Horizontal range	Starting and ending position of search box in horizontal direction. The choices are given in percent of the possible movements. The default is configurable (see chapter **Configuration File** in section **Input**). The current choice is visualized by the boxes drawn around the red or blue dots in the plot area of the status area.
Vertical range	Starting and ending position of search box in vertical direction. The choices are given in percent of the possible movements. The default is configurable (see chapter **Configuration File** in section **Input**). The current choice is visualized by the boxes drawn around the red or blue dots in the plot area of the status area.
Threshold	When finding an intensity above threshold, the program assumes that the X-ray beam has been found. This value **MUST** be larger than the ADC offset. A value of twice the ADC offset should be regarded as a suitable condition.
Use	Choice of searching the beam in chamber 1 or chamber 2 only.

The sequence of tasks within the procedure is as follows. Note, that the procedure may be interrupted any time by pressing the "**Stop**"-button.

- Open slits of current chamber to 4.0 mm (wide open).
- Drive horizontal motor to left edge of search box.
- Make a horizontal scan to right edge of search box. Check wether there is some intensity above the given threshold. If there is, continue with next step. If there is not sufficient intensity, move 4.0 mm up (or down) and scan horizontally along next line. Repeat this step until finding a significant peak or until entire search box is covered.
- If previous step succeeded, drive to beam maximum.
- Close horizontal slit until intensity drops below given threshold.
- Make a horizontal scan covering the entire peak found previously with the reduced horizontal slit size and drive to found maximum.
- Repeat the previous 2 steps until hor. slit size is ≤ 0.8 mm.
- Do the same thing (i.e. previous 3 steps) for the vertical slit.

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4.3.2 Optimize Beam

Chamber	Slit aperture (h/v)		Hor. scan range	Ver. scan range	Speed	Use
First:	0.60 mm	0.60 mm	2.0*slit size	1.0*slit size	10 %	■
Second:	0.30 mm	0.30 mm	2.0*slit size	2.0*slit size	20 %	■

The "**Optimize beam**"-tool can be accessed by selecting the corresponding choice in the **"menubar"** or by pressing the "**Alt+o**"-key while the pointer is in the "**Align**"-window.

The purpose of the "**Optimize Beam**"-procedure is to reoptimize the X-ray beam with small slit apertures. It is **important** if not essential that the X-ray beam is already seen in the corresponding chamber, since the movements implemented within this procedure are all relatively small. The procedure is not going to work if the actual beam is not within a fraction of a millimeter from the current motor positions.

NOTE:

Due to the weight of the mounted detectors the statics of the *desktop beamline* varies as soon as the distance translation or the 2-theta stage are moved. This can produce a considerable drop of X-ray intensity in the ionization chambers. A reoptimization is therefore strongly recommded after moving any of these motors.

The data collection menu offers the choice for doing an optimization before starting the data set. It is generally suggested to activate this choice.

The parameters for beam optimization depend on the nature of the X-ray beam, i.e. the type of optics used. As a rule of thumb, for optimizing the first chamber, the slits should be opened to an aperture that corresponds approximately to the beam size at this point. Typical values for Osmic mirrors are 0.7 to 0.6 mm. After refining the first chamber, the slits in the first chamber will be closed down, typically to 0.3 to 0.4 mm and the second chamber should be refined also with small slit apertures. The variable parameters for this procedure are the following:

Table 4: The input parameters for "Optimize Beam"

Parameter	Description
Slit aperture (h/v)	Hor. and ver. slit aperture used for reoptimizing this chamber. The choices are given in mm. The default is configurable (see chapter **Configuration File** in section **Input**).
Horizontal scan range	Range of movement of horizontal motor about current position. The choices are given as function of current slit aperture. A scan range should be choosen such that the scan covers the entire beam and drops down to the baseline at both sides of the peak. Typical values are 2 to 3 * slit size. The current choice is visualized by the boxes drawn around the red or blue dots in the plot area of the status area.

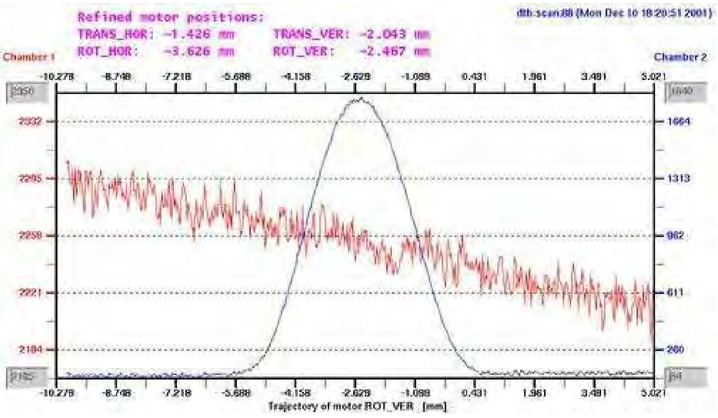
Parameter	Description
Vertical scan range	Range of movement of vertical motor about current position. The choices are given as function of current slit aperture. A scan range should be choosen such that the scan covers the entire beam and drops down to the baseline at both sides of the peak. Typical values are 2 to 3 * slit size. The current choice is visualized by the boxes drawn around the red or blue dots in the plot area of the status area. Note, that the vertical translation (TRANS_VER) is relatively slow compared to all other translations since here the *dtb* has to work heavily against gravity!
Speed	The speeds for doing the scans are not very critical. Slow speeds may make the result a bit more precise. Best to leave at defaults. The choices are provided as percentage of the maximum motor speed. Note, that the vertical translation (TRANS_VER) will always work with 100% speed, regardless of the choice made here. This is because that motor is quite slow anyway.
Use	Choice of optimizing the beam in chamber 1 or chamber 2 only.

The sequence of tasks within the procedure is as follows. Note, that the procedure may be interrupted any time by pressing the "**Stop**"-button.

1. Open slits of current chamber to the given choice (see input parameters). by the horizontal and vertical scan range as provided by the input parameters and is visualized in the status area (see above).
2. Make a horizontal scan to right edge of search box.
3. Go back to refined peak maximum in horizontal plane.
4. Drive vertical motor to lower edge of search box.
5. Make a vertical scan to upper edge of search box.
6. Go back to refined peak maximum in vertical plane.
7. Move the slits back to their original apertures.

Note, that from version 2.2 on the vertical movements will be interrupted by default, as soon as the instrument moves out of the beam. This implies, that the provided vertical scan range may not entirely be covered! This behaviour can significantly reduce the optimization time. It can be turned off by a keyword in the configuration file (see chapter **Configuration File** in section **Input**).

The next figure shows a typical result of an optimization of chamber 2. The actual scan of motor ROT_VER is drawn as blue line. Note, that the red line that marks the readings of chamber 1 shows a slight slope. Ideally the readings in chamber 1 should not be affected when using the rotational motors. In practice, the rotations are not completely discoupled from the translations!


Refined motor positions:
TRANS_HOR: -1.426 mm   TRANS_VER: -2.043 mm
ROT_HOR: -3.626 mm   ROT_VER: -2.467 mm
dtb-scan.88 (Mon Dec 10 18:20:51 2001)

4.3.3 Profile Beam

Slit	Scan range about current position		Slit aperture		Vertical pitch		Profile at
Horizontal:	2.0	2 mm	0.10	0.10 mm			
Vertical:	2.0	2 mm	0.10	0.10 mm	0.05	0.05 mm	Chamber 1

The "**Profile beam**"-tool can be accessed by selecting the corresponding choice in the **"menubar"** or by pressing the "**Alt+p**"-key while the pointer is in the "**Align**"-window.

The purpose of the "**Profile Beam**"-procedure is to get a feeling for the characteristics of the X-ray beam. The procedure eventually comes up with an image of the beam that corresponds to what you see on a fluorescent screen or on an X-ray eye (e.g. *marcam*®) but with more detail. For this procedure to work the first ionization chamber must have been well optimized previously.

NOTE:

The procedure can take quite a while to finish. It consists of a long series of horizontal scans, typically 20 to 40 and some vertical translations inbetween. If you interrupt the procedure, you should use the "Drive to latest maximum" " option to return to the refined positions.

The variable parameters for this procedure are the following:

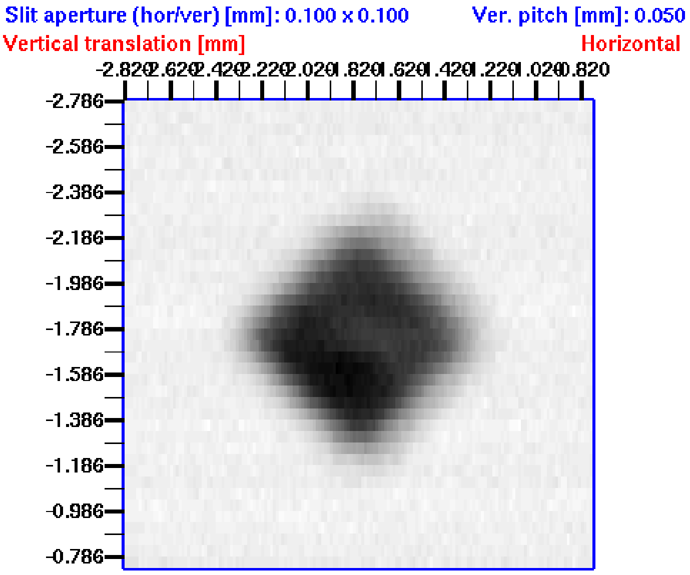
Table 5: The input parameters for "Profile Beam"

Parameter	Description
Scan range about current position	Range of horizontal and vertical movements. The range should be big enough to entirely cover the beam, at least 1 mm. The larger the vertical range, the longer the beam profiling takes.
Slit aperture	Hor. and ver. slit aperture used in chamber 1. The aperture should be rather small, e.g. 0.10 mm.
Vertical pitch	Advance of vertical motors after scanning 1 horizontal line. Should be smaller or equal to vertical slit aperture. Note that the vertical pitch actually determines the time the procedure takes, since the vertical movements are much slower than the horizontal ones.
Profile at	The entire procedure can be done for either chamber 1 or chamber 2.

The sequence of tasks within the procedure is as follows. Note, that the procedure may be interrupted any time by pressing the "**Stop**"-button.

1. Close slits of chamber 1 or 2 to "slit aperture" (see input parameters).
2. Drive horizontal translation to lower left edge of profile box. The profile box is defined by the horizontal and vertical scan range as provided by the input parameters and is visualized in the status area (see above).
3. Make a horizontal scan to right edge of profile box.
4. Drive vertical translation up by "vertical pitch" (see input parameters)
5. Drive horizontal translation back to left edge in order to avoid backlash problems.
6. Repeat previous 3 steps until entire profile box is covered.
7. Go back to original position for horizontal and vertical translations.
8. Move the slits back to their original apertures.

A typical beam profile from an Osmic mirror would look like this:



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4.3.4 Shape Beam

Chamber	Slit aperture for scan	Refine slits	Truncate peak at % of Imax		Speed
First:	0.8 mm	Hor. & ver.	10.0	10 %	30 %
Second:	0.8 mm	Hor. & ver.	1.0	1 %	30 %

The "**Shape beam**"-tool can be accessed by selecting the corresponding choice in the **"menubar"** or by pressing the "**Alt+s**"-key while the pointer is in the "**Align**"-window.

The purpose of the "**Shape Beam**"-procedure is to get a feeling for the size of the X-ray beam as it passes the collimator. For procedures "**Find Beam**", "**Optimize Beam**" and "**Profile Beam**" the translation or rotation motors have to be moved. For "**Shape Beam**", only the slits move! The procedure finishes with a suggestion of slit apertures. It is very useful to know how your beam hits the crystal in order to optimize your experiment. Regardless of the size of the crystal, you should run this procedure every time you are changing something on the X-ray source (mirror alignment, filament change, changes in power and bias settings of the generator, etc.). For this procedure to work both chambers must have been well optimized previously.

NOTE:

For this procedure to work it is essential that all slits are properly initialized, i.e. that the slit apertures as shown by the software corresponds to the dial readings on the hardware.

Usually, the slits in chamber 1 should be used to give the beam its desired shape. The slits of chamber 2 should not truncate the beam any more. The used slit apertures for the experiment depend on the size of the crystal. If the crystal is very small, you may want to cut out some part of the beam which is not going to hit the crystal and only contributes to background.

The variable parameters for this procedure are the following:

Table 6: The input parameters for "Shape Beam"

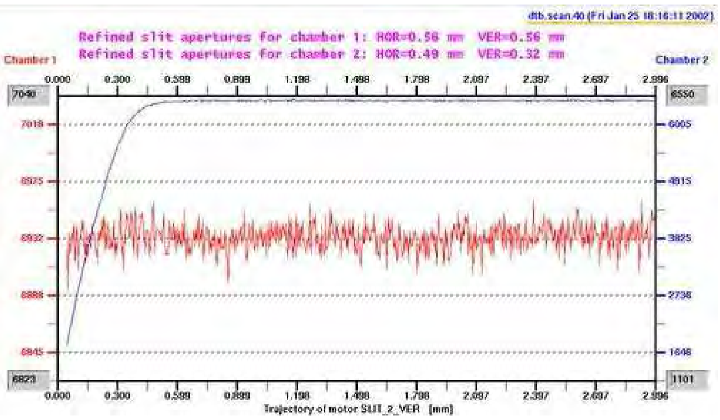
Parameter	Description
Slit aperture for scan	Aperture for slit that stands still during scan. The aperture should be big enough to cover all or most part of the beam, e.g. 0.8 mm.
Refine slits	Choice of refining or horizontal or vertical slit or both or none for this chamber.
Truncate peak at % of Imax	Decision constant were to truncate the beam. Technically, the plots resulting from slit scans are integrated and the percentage given refers to the integrals and not just to the maximum. For chamber 1 you will usually want to cutoff some part of the beam, typically 5 to 10 %. For chamber 2, usually a 1 % cutoff is doing a good job.
Speed	The speeds for doing the scans are not very critical. Slow speeds may make the result a bit more precise. Best to leave at defaults. The choices are provided as percentage of the maximum motor speed.

The sequence of tasks within the procedure is as follows. Note, that the procedure may be interrupted any time by pressing the "**Stop**"-button. Note also, that if you choose to refine slits in chamer 2 only, slits in chamber 1 won't be moved at all but stay where they are.

1. Open vertical slit of chamber 1 to "slit aperture" (see input parameters).
2. Open horizontal slit to 3.0 mm (see input parameters).
3. Make a horizontal slit scan from 3.0 to 0.0 mm.
4. Repeat previous 3 steps for the other slit.
5. Analyze curves and drive slits to their optimized positions.
6. Repeat previous steps for slits in chamber 2.

The next figure shows a typical result of an optimization of chamber 2. The

The next figure shows a typical slit scan of slits in chamber 2 from an Osmic mirror. The actual slit scan is marked with the blue line. The red line is the intensity in chamber 1 and stays on one level during this particular operation.


dtb.scan.40 (Fri Jan 25 18:16:11 2002)

Refined slit apertures for chamber 1: HOR=0.56 mm VER=0.56 mm
Refined slit apertures for chamber 2: HOR=0.49 mm VER=0.32 mm

4.3.5 Adjust ADC

Chamber	Target ADC offset		ADC tolerance		Use	X-ray source
First:	1029	1000	6	5 %	■	
Second:	920	1000	6	5 %	■	Weak source

The "**Adjust ADC**"-tool can be accessed by selecting the corresponding choice in the **"menubar"** or by pressing the "**Alt+a**"-key while the pointer is in the "**Align**"-window.

The purpose of the "**Adjust ADC**"-procedure is to set the baseline of the analogue-to-digital converters (ADC). The ADC's are highly sensitive and show fluctuations, in particular with temperature and humidity variations of the environment. In general, the baseline should be set to a value large enough for the ADC readings to stay in the positive range. The *dtb* controller implements a procedure to set the ADC baseline to a certain target value. The controller also features an electronical gain selector which offers the possibility to switch between strong X-ray sources (synchrotrons) and weak X-ray sources (rotating anodes, sealed tubes). The difference in sensitivity is a factor of approx. 250.

When pressing the "**Measure**"-button, the current ADC offset is actually measured. For this purpose, the slits in the first chamber are closed and the horizontal translation motor moves by approx. 3 mm. The ADC-values without X-rays will then be determined for both chambers. Since in "Weak source" mode the fluctuations can be in the order of +/- 500 counts, for very weak sources like Mo- or Ag-sources it may become important to accurately determine the current ADC offset values before attempting a beam optimization.

NOTE:

This procedure should best be executed with no X-rays at all entering the collimator.

The variable parameters for this procedure are the following:

Table 7: The input parameters for "Adjust ADC"

Parameter	Description
Target ADC offset	Target value for baseline. Suggested values are: 1000 for weak X-ray sources and 20 for strong X-ray sources.
ADC tolerance	This value determines the speed of convergence of the adjustment procedure. Suitable choices are 5 % to 10 % of the target offset.
Use	Choice of adjusting ADC offsets in chamber 1 or chamber 2.
X-ray source	Gain selector for strong sources (synchrotrons) or weak sources (all others). Note that when operating at gain settings of strong sources, the fluctuations of ADC readings also become very small.

4.3.6 Manual Operations

The "**Manual Operations**"-tool can be accessed by selecting the corresponding choice in the **"menubar"** or by pressing the "**Alt+m**"-key while the pointer is in the "**Align**"-window.

This window layout offers the possibility to move motors TRANS_HOR, TRANS_VER, ROT_HOR and ROT_VER individually. Under normal conditions this won't be necessary, but there are certain cases where it can be useful, e.g. if the "**Find Beam**"-procedure fails because there is more than one primary beam entering the collimator. In that case, you will have to decide yourself which beam is the one you want to look at. You should manually drive the translational motors close to that beam and only use the "**Optimize Beam**"-procedure for fine-tuning. Once the desired beam passes through the first pair of slits, the "**Find Beam**"-procedure can be used to catch the beam in the second chamber.

NOTE:

Violating common GUI-programming rules, in the input parameter area the choice +1 mm (and related) below the "Move motor" section will directly produce the action. Usually, option menues are not tied to an immediate action, but for the sake of saving space here we don't stick to this convention.

The variable parameters for this procedure are the following:

Table 8: The input parameters for "Manual Operation"

Parameter	Description
Motor	Choice of driving either hor. and ver. motor. When selected, the "Target Position" field will automatically be updated with the current position of the motor.
Target position	Textfield and menu with prominent choices for desired position.
Speed	Choices are provided as percentage of the maximum motor speed.
Move motor	By pressing the "To target" button the motor will move to the position given in the "Target position" field. By selecting one of the menu choices, the corresponding motor will immediately start driving by a certain amount of mm.
Initialize	Initialize the corresponding motor at one of the end switches.

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PDF files
- Software Distribution Guide

Man pages
- mar345dtb
- martv
- margrabber

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D-22851 Norderstedt /
Germany
Tel. +49 (40) 529 884 0
www.marresearch.com

5. Edit Data Collection Parameters

5.1 Introduction

Directory: /home/cla/data/
Image root: xtal
Image format: mar345
Read mode: 1200*1200: 180 mm @ 0.15

Exp. time: 60 def.
No. of PHI-blocks: 1 def.
No. of images/block: 1 def.
First image number: 1 def.
Oscillations: 1 def.
Δ φ per image: 1.000 def.
φ increment: 0.000 def.

Resolution limits: 10.5 -> 1.58 Ang. (5.44 -> 36.9 deg. in 2-θ)
2-Theta : n/a 0.000 cur.
Distance : n/a 120.000 cur.
Phi : n/a 2.001 cur.
Chi : n/a 0.000 cur.

First slits (h/v) : n/a 0.60 0.600 cur.
Second slits (h/v) : n/a 0.50 0.500 cur.
Beamstop : n/a 10.500 cur.
Crystal translation : n/a -1.768 cur.
Wavelength: n/a 1.00000 def.

☐ Optimize beam before starting set
☐ Optimize after 10 % loss
☐ Erase detector before starting set
☐ Append run number to root
☐ Run shell before optimize
☐ Save crystal photo for each image
☐ Save thumbnail for each image
☐ Run before starting set
☐ Run before starting exposure
☐ Run after ending exposure
☐ Run after completing read-out

Use crystal in vial: unused Unused
Crystal centering: None (leave as is)
☐ Append vial number to root name
☐ Append barcode to root name

The "**Edit**"-page can be accessed by selecting the corresponding tab in the main window or by pressing the "**Ctrl+3**"-key while the pointer is in the main window. Here, you set all the parameters for one or more data collection runs.

The "**Edit**"-page features several work areas:

- a menu bar with various options(see 5.2)

- an area for selecting sets to be programmed (see 5.3)
- a parameter input area for directories, names and formats (see 5.4)
- a parameter input area for exposure settings (see 5.5)
- a parameter input area for goniometer settings (see 5.6)
- a parameter input area for collimator and beam settings (see 5.7)
- a parameter input area for options (see 5.8)
- a parameter input area for external shell commands(see 5.9)
- a parameter input area for sample changer settings(see 5.10)

The window comes in 2 different layouts that can be easily be toggled with a single key stroke (`Ctrl+a`) or by (de-)selecting the choice "**Use advanced features**" in the "**Edit**"-menu of the menubar. The advanced features comprise the following input elements in addition to the "simple" features:

Exposure settings:

- **No. of PHI-blocks:**
  Possibility of setting up a MAD data collection run (see below)
- **Phi increment:**
  Possibility of using a Phi-movement inbetween 2 contiguous images of a data set

Goniometer settings:

- **Chi:**
  Possibility of driving CHI (Phi-swing)

Collimator settings:

- **Slit, beamstop, crystal translations, wavelength:**
  Possibility of using different positions for all motors in this area for each data set.

Options:

- **Shell commands:**
  Option for running external shell commands during a data collection.

Sample changer settings:

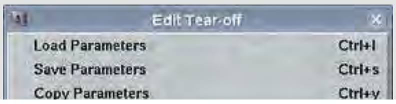
- **Change crystal, center crystal, etc.:**
  When making use of the sample changer, using the "advanced features" is mandatory!

5.2 Edit Menu

5.2.1 Description

The "**Edit**"-menu pops up if the "**Edit**"-button in the menu bar is pressed or if "**Alt+e**" is pressed while the pointer is in the main window. This menu allows for accessing different options that have to do with data collection parameters. The choices are:

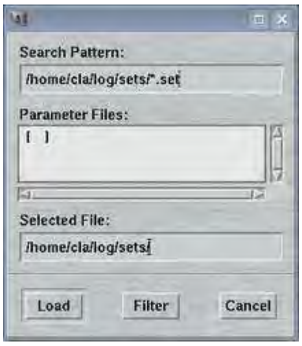
Table 1: The "Edit" menu

Menu	Menu Choice	Shortcut	Description
	**Load Parameters**	Ctrl+l	Opens "**Load parameters**"-window
	Save Parameters	Ctrl+s	Opens "**Save parameters**"-window
	Copy Parameters	Ctrl+y	Opens "**Copy parameters**"-window
	Use advanced features	Ctrl+a	Toggles between "advanced" and "simple" layout of the "**Edit...**"-page
	Use crystal translation		Usually, there is no need to translate a crystal from the "**Edit...**"-page. It can always be done from the "**Motor**"-page. Still, the buttons can be enabled or disabled on the fly.
	Use defaults for THIS set		Updates all parameter fields of current set with default values
	Use defaults for ALL set		Updates all parameter fields of all sets with default values

Menu	Menu Choice	Shortcut	Description
	**Use current positions for THIS set**	Ctrl+u	Updates all motor fields of current set with current motor positions
	Use current positions for ALL sets		Updates all motor fields of ALL sets with current motor positions
	Use current slit aperture for THIS set		Updates slit fields of current set with current slit apertures
	Use current slit aperture for ALL sets		Updates slit fields of ALL sets with current slit apertures
	Use current beamstop position for THIS set		Updates beamstop field of current set with current beamstop position
	Use current beamstop position for ALL sets		Updates beamstop field of ALL sets with current beamstop position

NOTE:
The motor update options are convenient since it can save you a lot of typing. The common situation is that you don't want to have varying slit sizes and you don't move the beamstop inbetween data sets. So those options allow for very easily setting the same parameters for all sets. The option of updating all motor position fields should be used with somewhat more care. Usage of this option implies, that the phi, distance, and 2-theta settings will be updated together with those of the collimator motors. When choosing to **use defaults** for the current or all sets, motor parameters default to the current position.

5.2.2 Load Parameters


Search Pattern: /home/cla/log/sets/*.set

Parameter Files: [ ]

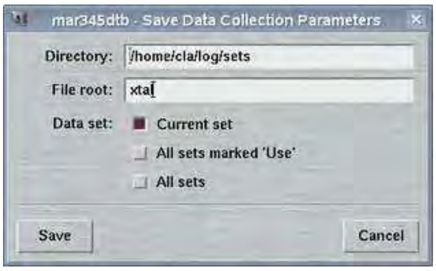
Selected File: /home/cla/log/sets/

The "**Load Parameters**"-window can be accessed by selecting the corresponding choice in the **"Edit"-menu** or by pressing the "**Ctrl+l**"-key while the pointer is in the main window.

This window is used to select a file with data collection parameters. The format of this file is described in chapter **Parameter File** of section **Input**. This feature comes handy for loading parameters typically used for collecting data of a certain sample and saves you lots of typing.

The default place where to store and to load parameter files from is `$MARLOGDIR/sets`

5.2.3 Save Parameters


mar345dtb - Save Data Collection Parameters

Directory: /home/cla/log/sets

File root: xtal

Data set: ■ Current set
☐ All sets marked 'Use'
☐ All sets

The "**Save Parameters**"-window can be accessed by selecting the corresponding choice in the **"Edit"-menu** or by pressing the "**Ctrl+s**"-key while the pointer is in the main window.

This window is used to store parameters from your current program session. You may may either save only the set that is currently in work or all sets at once. The format of this file is described in chapter **Parameter File** of section **Input**.

The default place where to store and to load parameter files from is `$MARLOGDIR/sets`

5.2.4 Copy Parameters

Copy params from current set into set X: 1

The "**Copy Parameters**"-window can be accessed by selecting the corresponding choice in the **"Edit"-menu** or by pressing the "**Ctrl+c**"-key while the pointer is in the main window.

This window is used copy parameters from one data set into another data set. You may either copy parameters from current set into any other or copy parameters from any set into the current. This methods allows for quickly program multiple data sets with almost identical conditions.

5.3 Selecting Data Sets

Use sets: ☑ 1 ☐ 2 ☐ 3 ☐ 4 ☐ 5 ☐ 6 ☐ 7 ☐ 8 ☐ 9 ☐ 10 ☐ 11 ☐ 12 ☐ 13 ☐ 14 ☐ 15
☐ 16 ☐ 17 ☐ 18 ☐ 19 ☐ 20 ☐ 21 ☐ 22 ☐ 23 ☐ 24 ☐ 25 ☐ 26 ☐ 27 ☐ 28 ☐ 29 ☐ 30

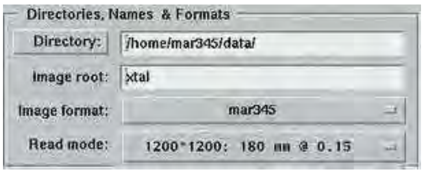
The program allows for programming up to 30 data sets that can be run automatically in sequence. The large blue button in the center of this area tells you which data set you are currently editing. This button has double functionality: by pressing the button on the right hand side you move to next data set, by pressing the button on the left hand side you move to the previous data set. This is identical to pressing the +1 and -1 buttons, respectively. To scroll faster forwards and backwards there are additional buttons that allow you to move on in units of 5 and 10.

For a data set to be actually used you have to explicitely select the corresponding entry in the next 1 or 2 rows. The idea is that you can program a couple of data sets but you don't necessarily want to use them all the time. If there is no data set selected at all and you press the "**Go**"-button, the first data set only is going to be used.

In the configuration file (see chapter **Configuration File** in section **Input**). there is a possibility to restrict the number of programmable sets to 15, which should certainly be enough for home use.

For convenience, you can copy all parameters from one data set into another data set and save some typing. Please refer to chapter **5.2.4 (Copy Parameters)**. You can also load and store entire parameter sets for your current project (chapters **5.2.2 (Load Parameters)** and **5.2.3 (Save Parameters)**. This is useful if you have a particular way of collecting data from a crystal.

5.4 Directories, Names and Formats



Directory: /home/mar345/data/
Image root: xtal
Image format: mar345
Read mode: 1200*1200: 180 mm @ 0.15

The entries of this area are identical for both "advanced" and "standard" layouts. Here is where you specify the place where the images are being stored, the image root names, formats and scan modes.

By pressing the "**Directory**"-button a file selection box pops up. It lists the files in the current directory. If you move up or down the directory tree inside this file selection box, the full directory path is entered automatically into the directory field and saves you from typing.

The "**Image root**" name should be some meaningful string that should allow you to identify your data later on in some way. Usage of blanks or special characters inside the textfield is possible but strongly discouraged.

The "**Image format**" currently allows to choose between 2 output formats: the *mar345* file format and the *cbf* file format. The *mar345* formats have been introduced in 1997 and are supported by all major data processing and display programs (automar, marView, denzo, xdisp, mosflm, xds, fit2d, etc.). The *cbf* file format ("crystallographic binary format") is the definition of a general image data format for the crystallographic community following the CIF-standard as far as headers are concerned. The actual image data are stored using the same compression scheme as used for the *mar345* file format ("pck"). The difference, however, is that the *cbf*-file stores the image data as 32-bit values whereas the *mar345* format uses 16-bit values. Since the data range as produced by the *mar345* detector exceeds 16-bits, intensity values > 65635 are explicitely included in the *mar345*-formatted files together with its address in the 16-bit array. While file sizes in *mar345* and *cbf* formats are almost identical, one has to keep in mind that most images don't contain any intensity data > 65635, so using a full 32-bit array is a waste. On the other hand, with today's computer power and memory equipment those considerations are becoming less important. Note that as by early 2004, still very few programs (e.g. mosflm) actually support the *cbf* format.

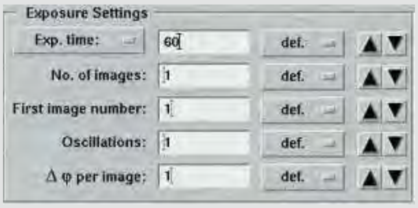
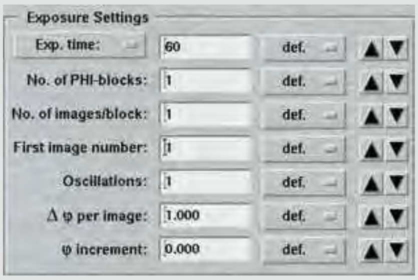
The "**Scan mode**" offers the choices to scan the image plate at 4 differing diameters at 2 differing pixel sizes. The choice for the diameter to be scanned depends pretty much on the diffraction power of the sample. At a given distance, it doesn't make sense to scan the full plate if the diffraction doesn't do it to the edge. Please keep in mind that the larger the diameter the longer the scan process takes and the larger the output files are going to be. Also data processing and data storage takes longer for larger files, so you don't really want to collect only background. As far as the choice for the pixel size is concerned, there are 2 concurring considerations: with 100 micron pixelsize you get somewhat better reflection profiles and also a slightly increased readout efficiency. The price is slightly longer readout times and larger file sizes. In 150 micron mode, the *mar345* detector applies "**double-sampling**", i.e. each transformed pixel is made up of 2 raw spiral pixels. The physical pixel size of the raw spiral pixels is rather 75x150 microns. The benefit is that in 150 micron mode, the real dynamic range is 17-bits (131070), i.e. 2x65635. For strongly diffracting crystals and for synchrotron the 150 micron mode is likely to be more appropriate.

The following table gives an overview of scan times and typical file sizes for all 8 scan modes.

Table 2: Scan modes of *mar345*-detector

IP Diameter [mm]	180		240		300		345	
Pixel size [µm]	**150**	**100**	**150**	**100**	**150**	**100**	**150**	**100**
File size [MB]	0.7	1.4	3.5	4.0	2.2	6.2	3.5	5.9
Readout [sec]	26	34	39	53	56	77	68	96
Total [sec]	34	42	48	62	66	87	80	108

5.5 Exposure Settings

Standard features	Advanced features
 Exposure Settings Exp. time: 60 No. of images: 1 First image number: 1 Oscillations: 1 Δ φ per image: 1	 Exposure Settings Exp. time: 60 No. of PHI-blocks: 1 No. of images/block: 1 First image number: 1 Oscillations: 1 Δ φ per image: 1.000 φ increment: 0.000

The entries of this area differ for "advanced" and "standard" layouts. Here is where you specify the parameters for controlling the exposures.

An exposure consists of the following sequence of actions:

1. Open the shutter
2. Drive Phi over a certain range (Delta-Phi)
3. Close shutter

The time it takes to drive Phi can be either a fixed exposure time or can be controlled by the X-ray dose as read in chamber 2. For an X-ray source with constant flux (i.e. home generators), X-ray dose controlled exposures are not recommended since time control is supposedly more accurate. On synchrotrons, X-ray dose controlled exposures used to be the typical way of collecting data. Recently, with the advent of very high brilliance sources and very stable storage rings, usage of time controlled exposures on synchrotrons may also become more appropriate. This is particularly true for short exposure times (< 10 sec). The choice of X-ray dose controlled exposures is only useful if there is a significant variation of X-ray dose within one exposure, which is going to be unlikely for short exposure times and a rapid completion of data collection. Most other affects can be compensated by the data scaling procedure.

One important feature of the *desktop beamline* is the sophisticated Phi-motor stepper driver with 4 gears. This stepper driver allows for extremely smooth Phi-movements for longer exposures (> 30 sec) and thus enhances data quality. Depending on the given exposure time the program determines a suitable gear to move the Phi-axis. A consequence of this procedure is that the given exposure times may differ slightly from the exposure times the *dtb* eventually uses (but it is guaranteed that the exposure times are identical for all images of one set). For X-ray dose controlled exposures there is only 1 gear regardless of the resulting exposure times.

The "**Exposure time**"-menu allows the choice of using an X-ray dose instead of the actual exposure time. The X-ray dose to be entered is a magnitude that is difficult to handle. Therefore, the program converts the times given in the menu on the right hand side of the textfield into the corresponding X-ray dose units. It is strongly suggested to use this approach to setup the desired X-ray dose. Note, that the *mar555* flatpanel detector cannot be used in DOSE mode! The exposure time is given in seconds. Fractions are possible.

In the "**standard features**" mode, the "**No. of images**" determines how many images will be collected within this set. In the "**advanced features**" mode, this entry is replaced by the "**No. of PHI-blocks**" and "**No. of images/block**". A "PHI-block" is a subset of images contiguous in PHI. If this entry is set to 1, then the "**No. of images per block**" is identical to the entry in the standard features mode. Multiple PHI-block are mulitple subsets of images that differ by a rotation of 180 degrees in Phi. This method is useful for optimizing anomalous differences (e.g. for MAD-data). For 2 PHI-blocks with 50 images each, the data collection program will create 2 subsets of images ("A" and "B") containing 50 images each. The string "_A" and "_B" will be appended to the image root name and each subset starts with the same image number as given in the "**First image number**" field. The difference between subset A and B is a 180 degree rotation in Phi, but within subsets A and B all images are contiguous in Phi.

Multiple "**Oscillations**" are defined as the following sequence of actions during one exposure:

1. Open shutter

2. Move Phi over the desired Delta-Phi range
3. Close shutter
4. Move Phi back to start of exposure and repeat steps 1 to 3

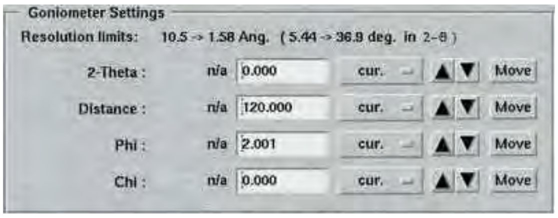
It is not recommended to use multiple oscillations for exposure times < 10 minutes. As far as the image plate is concerned, there are 2 effects that need consideration: the natural decay of stored signal and the accumulation of background on the plate. Both effects are not very critical. A typical decay rate is approx 10% of stored intensity within an hour. Background accumulation depends on the scatter of the sample, in particular the water content. There is also some contribution of cosmic events but this is rather negligible. If there is a choice, it is usually better to reduce the Delta-Phi per image and keep 1 oscillation only rather than increasing the exposure time and using multiple oscillations.

An additional "**advanced feature**" is usage of a "**Phi increment**". This is defined as a Phi movement inbetween 2 images. This can be either a positive or a negative value. To clarify the situation here are 2 examples:

- **Delta-Phi = 1 degree, Phi-increment = 44 degrees**
  1. image ranges from 0 to 1 deg.
  2. image ranges from 45 to 46 deg.
  3. image ranges from 90 to 91 deg.
  etc.
  Useful for accurate data indexing!

- **Delta-Phi = 1 degree, Phi-increment = -0.1 degrees**
  1. image ranges from 0 to 1 deg.
  2. image ranges from 0.9 to 1.9 deg.
  3. image ranges from 1.8 to 2.8 deg.
  etc.
  Useful for data with Phi overlaps!

5.6 Goniometer Settings

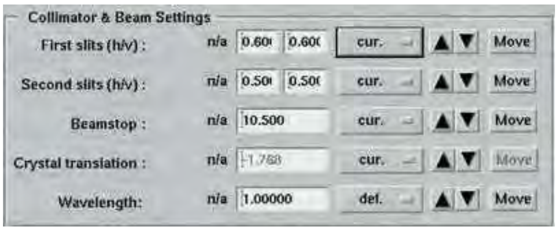


Resolution limits: 10.5 -> 1.58 Ang. (5.44 -> 36.9 deg. in 2-θ)
2-Theta : n/a 0.000 cur.
Distance : n/a 120.000 cur.
Phi : n/a 2.001 cur.
Chi : n/a 0.000 cur.

Here is where you specify the parameters for the detector-to-sample distance, starting Phi and 2-theta position during one data set. From here, you may move the motors directly by pushing the corresponding "**Move**"-button. In the standard layout, there is no option for driving the Chi motor (Phi-swing). In case this was necessary, you have to use the "**Motors**"-page.

Note, that the entries in the textfields do not necessarily coincide with the current motor positions and starting a data collection may therefore produce unexpected movements! It is therefore convenient, to use one of the options in the **Edit menu** for updating the motor positions for this set.

5.7 Collimator and Beam Settings



First slits (h/v) : n/a 0.60 0.600 cur.
Second slits (h/v) : n/a 0.50 0.500 cur.
Beamstop : n/a 10.500 cur.
Crystal translation : n/a -1.768 cur.
Wavelength: n/a 1.00000 def.

This entire area is available only in the "**advanced features**" layout. Here is where you specify the positions of the slits, beamstop and crystal translation to be used within one data set. In the "**standard** featurs" layout there will be no attempt to move any of those motors. If you want to make a crystal movement inbetween two data sets you would therefore have to use the "**advanced features**".

The "**Beamstop**" can be moved inbetween two data sets. A typical use of this feature would be a a data collection at high resolution with the beamstop relatively close to the crystal followed by a data collection of low resolution data. For low resolution data you would move the beamstop and detector further away from the crystal. It would also be helpful to reduce the slit size. In any case, you should confirm first that the beamstop is still going to cover the beam entirely when moving it further away. A primary beam on the image plate takes quite long time and very many scan/erase cycles to be wiped out!

The "**Rel. crystal translation**" entered here is relative to the current position. This is useful, since the absolute position for this motor is rather meaningless. The typical use is that a needle-shaped crystal is moved a fraction of a mm inbetween two data sets to compensate for radiation damage.

The "**Wavelength**" entered here is almost always used only for writing the correct value into the image headers. This is particularly important for synchrotron beam lines and it is very highly recommended to always fill in the appropiate values, since data processing programs may depend on image header values.

5.8 Options

Options

☑ Optimize beam before starting set
☐ Optimize after 10 % loss
☑ Erase detector before starting set
☐ Append run number to root
☐ Run shell before optimize
☑ Save crystal photo for each image
☑ Save thumbnail for each image

For every data set there are couple of options to be selected separately:

Option	Description
Optimize beam before starting set	Optimize chamber 1 and 2 before starting with first exposure. Important, if DISTANCE or THETA has been moved!
Optimize beam after ...	Optimize chamber 1 and 2 during data collection Choice of optimizing after a given amount of images, after a given amount of elapsed time since the last optimization or after a given loss of X-ray intensity in chamber 2 (in percent). Please see note below.
Erase detector before starting set	Before starting with first exposure, the plate is erased. Useful if scanner has been idle for a while.
Append run number to root	In order to avoid creation of identical filenames when collecting multiple data sets, the no. of the data set is appended to the image root name as "_N"
Run before optimize	Runs a shell script (see below) before doing an optimization. The parameters passed are identical to those used with "Run before exposure" (see below). This feature can be used when doing a beamline optimization at a synchrotron using external motors (e.g. for the monochromator).
Save crystal photo for each image	If the PC features a frame grabber card, the program either sends a command to program *streamer* or uses the built-in video support to record a photo of the crystal. The file format is "jpg" and the file name is identical to the image file except the suffix. Place of storage is the subdirectory **photo** of the data directory. The subdirectory will be created automatically if it doesn't exist.
Save thumbnail for each image	With this option, the output data images may be converted into a graphics image and shrinked to thumbnail size. This can be helpful to quickly scan through a data set to check for problems during diffraction. The way this option works is by calling a shell script called *mar2thumb* which may be customized according to user preferences. Please refer to chapter **Thumbnails** of section **Output** for more details.
Save spiral image	Raw spiral images can sometimes be useful for analyzing hardware problems. Note, that raw spiral images need to be transformed and corrected to give a Cartesian image. This choice will be presented only when running the program with option --admin.

NOTE:
It is usually **NOT** recommended to reoptimize during a data collection of one set, since this may have some impact on data quality. The only reason to do so is if the position of the beam is unstable. Please note, that if the X-ray source itself is unstable (i.e. if the beam goes away for some time) a reoptimization carried out at a time when the beam is not present will be counter-productive and severely affect the remaining data collection!

5.9 Using Shell Commands

Options

☐ Optimize beam before starting set
☐ Optimize after 10 % loss
☐ Erase detector before starting set
☐ Append run number to root
☐ Run shell before optimize
☐ Save crystal photo for each image
☐ Save thumbnail for each image
☐ Run before starting set Edit
☐ Run before starting exposure Edit
☐ Run after ending exposure Edit
☐ Run after completing read-out Edit

The "**advanced features**" in addition to the options described in the previous chapter offer the possibility to run a shell command at certain times during data collection. The following choices are available. The corresponding boxes must be checked to activate the option.

By pressing the "**Edit**"-button the "**Edit - Shell**"-window pops up. The way the shell commands work is quite simple. The program *mar345dtb* executes the shell script file `$MARLOGDIR/dtb.csh` and passes parameters from the editing process to that shell script. There are choices for passing the parameters from the parameter input areas to the shell script. The field for "**Custom parameters**" leaves room for any additional parameters you can think of. This method should allow you to execute any function you like by implementing a call to a program or whatever into `dtb.csh`. The program will continue with the next step of data collection after `dtb.csh` has exited. A template for file `dtb.csh` is given in the chapter **dtb.csh** of section **Input**.

The shell command makes use of shell scripts.
Check the buttons if you like to pass params from the
'Edit Data Collection Parameters' window to the shell command!

1.) Custom parameters: optimize

☐ 2.) Use current image name

☐ 3.) Use entries from 'Exposure Setting'

☐ 4.) Use entries from 'Goniometer Settings'

☐ 5.) Use entries from 'Collimator & Beam Settings'

☐ 6.) Use entries from 'Options'

5.10 Sample Changer Settings

Use crystal in vial: unused Unused ▲▼

Crystal centering: None (leave as is)

☐ Append vial number to root name

☐ Append barcode to root name

Here is where you specify the parameters to be used together with a sample changing device. These parameters can only be set when working with the "**advanced features**" layout. The choices are:

Option	Description
Use crystal in vial ...	Select a carousel position for the crystal to collect data with - or choose "unused"
Crystal centering	Choose a method for centering the crystal: ⇨ **None:** don't move xyz-translations ⇨ **Manual:** manually move xyz-translations (and confirm) ⇨ **Automatic:** automatically locate and center crystal after mounting (see chapter **Crystal centering** in section **Crystal**) for details. ⇨ **Automatic with confirmation:** as above but a manual confirmation is required for actually starting with data collection ⇨ **Stored xyz-coordinates:** use stored xyz-positions of given vial (see chapter coordinates of section "Sample Changer") to drive goniometer head ⇨ **Stored xyz-coordinates with confirmation:** as above but a manual confirmation is required for actually starting with data collection ⇨ **Stored xyz-coordinates with shift corrections:** as above but shifts compared to a previously found position of the sample will be computed and corrected for before actually starting with data collection (see chapter **Shift Corrections** in section **Csc**) for details.
Append vial no. to root name	The vial no. of the crystal is appended to the image root name as "_N"
Append barcode to root name	The barcode of the crystal is appended to the image root name as "_STRING".

When choosing to use the barcode as file name component, one can run into the situation that the barcode is not readable in the mounting stage. This is because during mounting there might be some residual liquid nitrogen on the cap or ice crystals that make reading impossible. In consequence, data will be collected with an unknown barcode and images names are not as expected. After data collection, chances for the barcode reader to successfully read the barcode when putting the sample back into the carousel are actually good. If this happens during a data collection, the program will automatically take care to rename the collected images. What happens is that the program writes out and executes a little shell script:

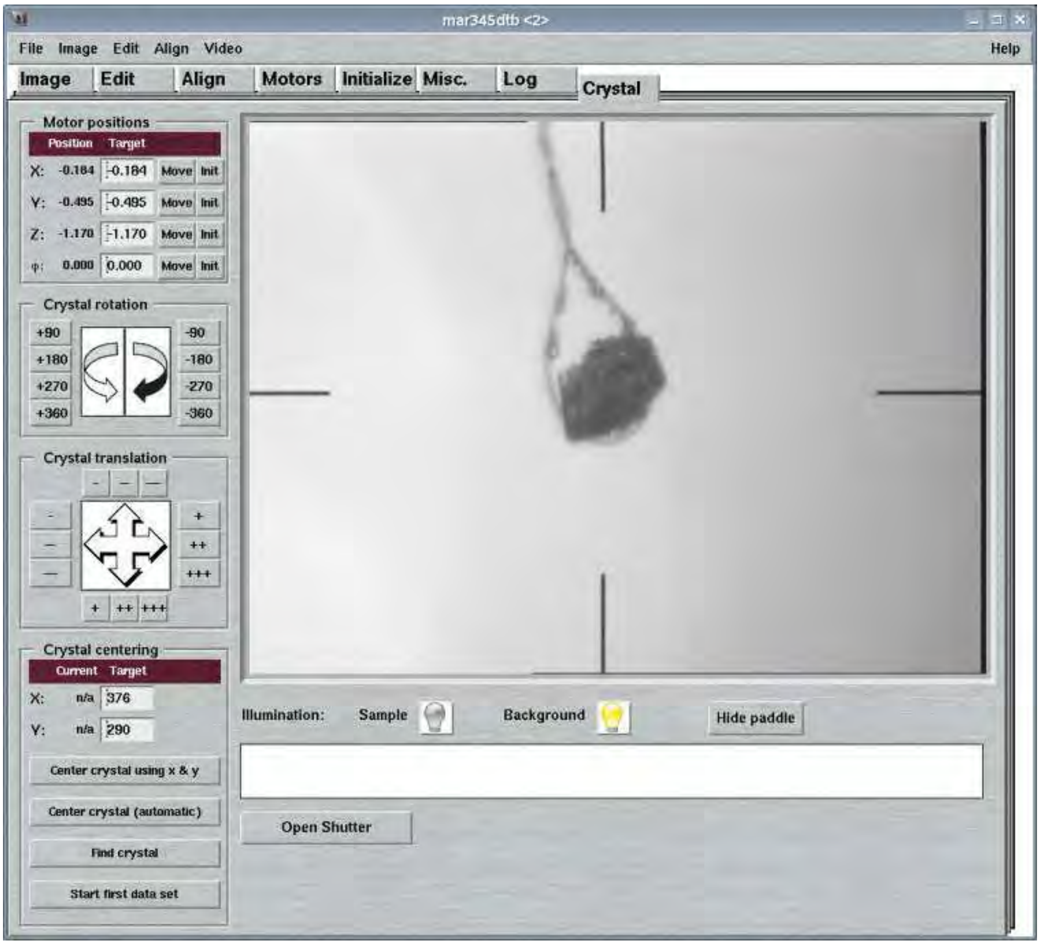
`$MARLOGDIR/csc/setX.vialY.csh`

where **X** is the set number and **Y** is the vial number. This shell script can also be executed manually with the desired barcode as the first command line argument, i.e.:

`$MARLOGDIR/csc/setX.vialY.csh BARCODE`

6. Crystal

6.1 Introduction



Motor positions

	Position	Target
X:	-0.184	-0.184
Y:	-0.495	-0.495
Z:	-1.170	-1.170
φ:	0.000	0.000

Crystal centering

	Current	Target
X:	n/a	376
Y:	n/a	290

The "**Crystal**"-page can be accessed by selecting the corresponding tab in the main window or by pressing the "**Ctrl+9**"-key while the pointer is in the main window. Here, you can display a crystal as seen by the built-in video camera. The crystal can be repositioned and automatically centered.

The "**Crystal**"-page features several work areas:

- a menu bar with various options(see 6.2)
- an area containing the frame grabber outut (video)(see 6.3)
- an area for moving xyz-translations and PHI(see 6.4)
- an area for turning the crystal (PHI rotation) (see 6.5)
- an area for intuitive xyz-translations (see 6.6)
- an area for centering the crystal (see 6.7)

6.2 Video Menu

The "**Video**"-menu pops up if the "**Video**"-button in the menu bar is pressed or if "**Alt+v**" is pressed while the pointer is in the main window. This menu allows for accessing different options that have to do with video. The choices are:

Table 1: The "Video" menu

Menu	Menu Choice	Shortcut	Description
	**TV window**	Alt+t	Displays the video output in a separate window. This is sometimes necessary in order to watch the sample while moving a motor from within another page.
	Show crosshair	Ctrl+h	Displays a digital cross-hair on top of the video layer with coordinates and units taken from configuration file
	Show crystal center	Ctrl+x	Displays a digital cross on top of the video layer at the x,y-coordinates that define the center of the sample
	Zoom x 1	Alt+1	Displays video at 1:1 magnification ratio
	Zoom x 1/2	Alt+2	Displays video at 1:2 magnification ratio
	Zoom x 1.5	Alt+3	Displays video at 1.5:1 magnification ratio
	Zoom x 2	Alt+4	Displays video at 2:1 magnification ratio
	Save Photo	Alt+p	Stores a snapshot in the directory where the program has been started. Output file name is "dtb-XXX.jpg" where XXX stands for a time description string.
	Save Empty Photo		Stores a snapshot as $MARLOGDIR/xtal/empty.jpg It is **very important** that this photo does NOT contain any pin or crystal feature. It must be an empty background image. Otherwise, automatic crystal centering is going to fail! Normally, it is not required to do this explicitely, since the program automatically updates empty images every time a sample is mounted.

NOTE:
As by February 2004, XFree86 (versions 4.3 or smaller) has some serious bugs in the libXv libraries having to do with video output. One of the consequences is, that depending on hardware, the overlay of digital cross-hairs or other digital marks on top of the video output may not become visible. Another reproducible bug is that zooming to magnification ratios > 1 does not work properly. The code of program *mar345dtb* currently ignores these bugs and has implemented some functions as if those bugs didn't exist. A future XFree implementation may fix those bugs.

As by April 2009, the libXv libraries may not work at all as specified, depending on the video card and possibly main board drivers. As a consequence, the native model of XFree/Xorg to display video streams cannot be used at all. It is known that the propietary ATI/AMD video card drivers do not support this model, so none of the ATI cards can be used any more for displaying the built-in video stream. In order to compensate for these limitations, program mar345dtb can be configured to start an external TV-grabber program and "hijack" the window and make it appear to be a built-in screen. Effectively, our choice is a slightly modified version of program tvtime, which is a public TV viewing program. The modified version is called martv and mainly contains possibilities to display a cross-hair and to exchange information with program mar345dtb, in particular for centering issues. Please see chapter **Configuration File** in section **Input**) for more details.

6.3 Video

The video area becomes available on the "**Crystal**"-page depending on settings in the configuration file (see chapter **Configuration File** in section **Input**). This is the place where the output of a frame grabber device is displayed. Brightness and contrast can be altered directly using the slider bars underneath the video window. All other (less variable) settings have to be done from within the configuration file. Please note, that a frame grabber allows exclusive access to only one process. If the "**Crystal**"-page is up, the program tries to access the frame grabber but if another page is up, then the frame grabber is released and other applications may access the frame grabber.

Within the video area, the mouse buttons have the following functions:

- Left hand button: update xy-coordinates in the "**Crystal Centering**"-area
- Middle button: display current xy-coordinates in the upper left corner of the video area
- Right hand button: update xy-coordinates in the "**Crystal Centering**"-area

Note, that xy-coordinates have their origin in the upper left corner of the video area.

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6.4 Motor Positions


Motor positions

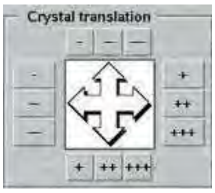
	Position	Target		
X:	-0.184	-0.184	Move	Init
Y:	-0.495	-0.495	Move	Init
Z:	-1.170	-1.170	Move	Init
φ:	0.000	0.000	Move	Init

In this area, motors that have to do with the sample positions can be displayed, moved or initialized. The motors are the xyz-translations of the goniometer head and the PHI-axis.

6.5 Crystal Rotation

In this area, the motor that has to do with the sample rotation (i.e. the PHI-axis) can be moved by 90, 180, 270 or 360 degrees by only pushing the corresponding button.

6.6 Crystal Translation



In this area, the motors that has to do with the sample xyz-translation can be moved. There are 3 choices for the amount of displacement: a large one, a medium one and a short one for fine-tuning. While the upper or the lower buttons will always move the z-translation (either in positive or negative direction), the buttons on the left hand side and the ones on the right hand side move the x or the y-motor in the goniometer head, depending on the current PHI-position. The indicated directions correspond to what will be observed in the video area.

6.7 Crystal Centering

	Current	Target
X:	n/a	376
Y:	n/a	290

This area can be used to reposition a sample, e.g. for centering it with respect to the cross-hair. The xy-coordinates in the upper section correspond to the coordinates of a point in the video area, the origin being the upper left corner. The default center will be taken from the configuration file. A user has 3 choices to update the x and y coordinates:

- Enter desired values manually in the corresponding fields for x and y
- Click the left or right hand side mouse button at the desired position of the video area (see above).
- Let external crystal localization software find xy-coordinates

The push-buttons in this area have the following functions:

Button	Description
Center crystal using x and y	The "target" xy-coordinates are translated into a suitable motion of the xyz-translation motors.
Center crystal (automatic)	Automatically center the crystal. The method is described in more detail in the chapter **Center crystal (automatic)**
Find crystal	Automatically locate the crystal. The method is described in more detail in the chapter **Find crystal**

6.7.1 Find crystal

Automatic crystal finding consists of the following sequence of steps:

1. Shoot a photo and locate crystal in photo, i.e. determine xyz-coordinates of the presumed center of the crystal.
2. Drive goniometer head xyz-translations according to the result of the previous step.

The crystal localization relies on an external program and the command to use within program *mar345dtb* can be specified in the configuration file. It defaults to "*loopfind*" and it gets 3 arguments:

1. $MARLOGDIR/xtal/find.jpg (or some other arbitrary name)
2. $MARLOGDIR/xtal/empty.jpg
3. $MARLOGDIR/xtal/xhair.jpg

The first file is supposed to contain some sample. The second file may not contain any sample, i.e. it must be empty and contain only background. The sample finding algorithm depends on such a background file. Since illumination may vary depending on environmental conditions, the "empty" file is updated each time a sample is mounted. The third file is produced automatically out of the "empty" image and extracts the fixed cross-hair artefacts in the image. This is technically necessary and is used as a mask to leave out invalid pixels in a photo.

The program *loopfind* is implemented as a very simple shell script that passes values to a program called *marloop* that actually does the job of locating the crystal. This program has several possible exit conditions:

1. The sample is located and the program prints x and y coordinates.
2. The photo is empty, i.e. it doesn't contain any significant structure. This means, that if there is a pin with a loop at all, it is completely outside the viewing range of the camera. Typically, this means that the pin is way too short or too much tilted. If it is too short, the only reasonable action is to drive the z-translation.
3. The photo contains a large area - supposedly the pin - but no loop. This implies that the sample has to be moved along z towards smaller values. Please note, that in the current implementation the algorithm may take somewhat long (up to 2 minutes on a 2 GHz processor) to identify this situation.

Within the "**Find crystal**-procedure only the first case is going to automatically produce an action, i.e. xyz-motors are driven according to the obtained xy-coordinates of the sample center.

The progress of the computations and final results will be printed in the white area underneath the contrast slider.

6.7.2 Center crystal (automatic)

Automatic crystal centering is a complex procedure consisting of a series of steps. The program *mar345dtb* implements 3 methods for automatic centering.

The first method (i.e. CSC METHOD 0 in the configuration file) comprises the following sequence of steps:

1. Mount crystal (when chosen as an option of a data collection)
2. Shoot a photo and locate crystal in the photo, i.e. determine xyz-coordinates of the presumed center of the crystal.
3. Drive goniometer head xyz-translations according to the result of the previous step.
4. Drive PHI by a predefined value and repeat the previous two steps
5. Repeat the previous 2 steps for a predefined number of photos

The number of photos and also the phi rotation inbetween the photos is freely configurable. Typically, 4 photos at intervals of 90 degrees in PHI give good results. Also the starting value is configurable (typically at PHI=0). The entire procedure may be repeated over several cycles, but typically 1 cycle of operations should be enough.

The second method (i.e. CSC METHOD 1 in the configuration file) comprises the following sequence of steps:

1. Mount crystal (when chosen as an option of a data collection)
2. Shoot a series of photos at predefined PHI intervals
3. After shooting the last photo, determine xyz-coordinates of the presumed center of the crystal by analysing all photos in single step.
4. Drive goniometer head xyz-translations according to the result of the previous step.

The number of photos and also the phi rotation inbetween the photos is freely configurable. Typically, 9 photos at intervals of 40 degrees in PHI give good results. Also the starting value is configurable (typically at PHI=0). The entire procedure may be repeated over several cycles, but typically 1 cycle of operations should be enough.

The third method (i.e. CSC METHOD 2 in the configuration file) is similar to method 0, in the sense that each photo is evaluated individually. The difference is that there is an additional parameter that comes into play which is a certain tolerance of movements inbetween two successive PHI movements. If the crystal movement drops below that configurable threshold (e.g. CSC METHOD 2 TOLERANCE 0.2) then the centering may be considered as successful. However 4 photos 90 deg. apart will always be shot. If the computed shifts exceed the tolerance, after 360 deg. there will be a phase shift of DPHI/4 in order to increase the likelihood of finding a good pposition from where to shoot photos. So this method comprises the following sequence of steps:

1. Mount crystal (when chosen as an option of a data collection)
2. Shoot a photo and locate crystal in the photo, i.e. determine xyz-coordinates of the presumed center of the crystal.
3. Drive goniometer head xyz-translations according to the result of the previous step.
4. Drive PHI by a predefined value and repeat the previous two steps
5. Repeat the previous 2 steps for a predefined number of photos. If the PHI range covered exceeds 360 deg. and the computed shifts are smaller than a given tolerance the centering is regarded as succesful and the remaining number of photos will not be taken. If the shifts are larger, the PHI movement inbetween 2 successive photos will be diminished.

In cases where a photo is considered as "empty" (i.e. no crystal, loop or pin in the photo), an additional step of z-axis translation will be introduced automatically. It is assumed that the pin may be too short and that a z-axis movement may bring an object into the viewing area of the camera. The advance of the z-axis is going to be one display unit. The procedure will be repeated if the new photo is empty, again. But there is a maximum allowance that is defined on the CSC ZMAX keyword in the configuration file. The value give there should be small enough to avoid a sample to be moved out of the cold stream (2-3 mm).

The opposite situation would be that a pin is too long and that the pin occupies the entire viewing area. Also this situation is handled automatically by moving the z-axis further in. In any case, the z-translation are considered to be intermediate steps and will be done prior to rotating the PHI axis.

It should be pointed out, that the situation of a loop not being within the viewing area of the camera to be a consequence of WRONG mounting of a sample and therefore not necessarily be within what an automatic procedure like the one described here is required to handle.

GENERAL HINT: Success rates of automatic centering will dramatically increase when using appropiate crystal mounting methods. A tiny crystal in a big loop is going to be a pathological case for all crystal centering software. I.e. it is strongly suggested to make use of loops as small as possible!

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Man pages

- mar345dtb
- margrabber

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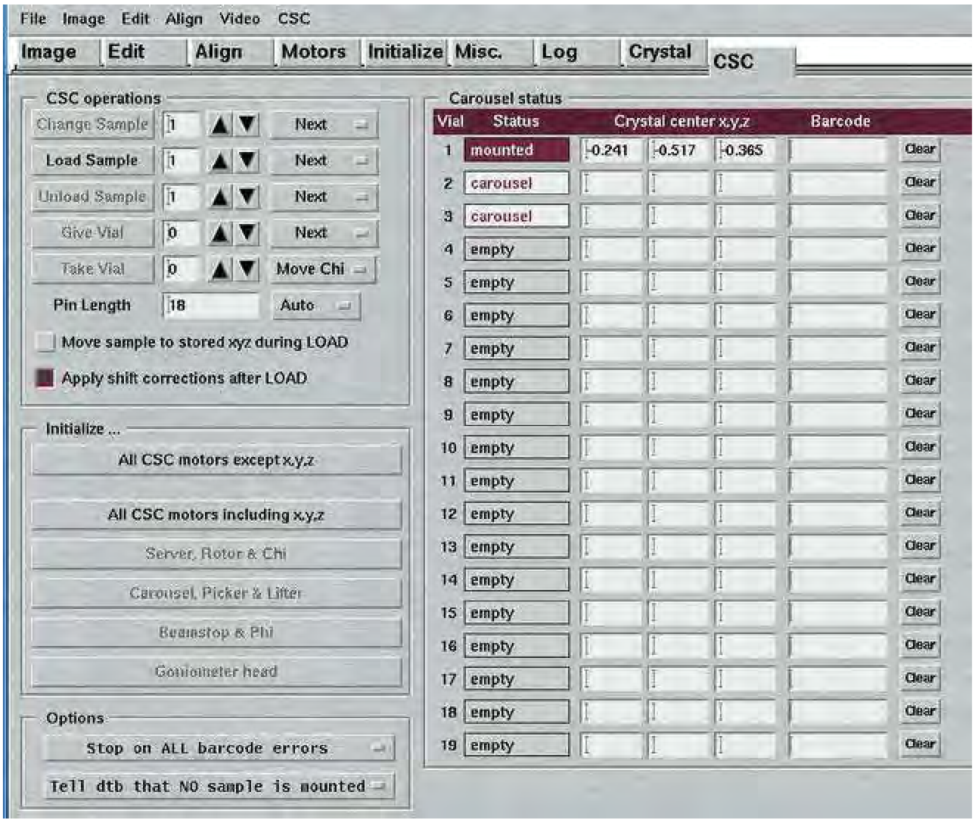
7. CSC (Cryogenic Sample Changer)

7.1 Introduction



Change Sample: 1 — Next
Load Sample: 1 — Next
Unload Sample: 1 — Next
Give Vial: 0 — Next
Take Vial: 0 — Move Chi
Pin Length: 18 — Auto
☐ Move sample to stored xyz during LOAD
☒ Apply shift corrections after LOAD

Vial	Status	Crystal center x,y,z			Barcode	
1	mounted	-0.241	-0.517	-0.365		Clear
2	carousel					Clear
3	carousel					Clear
4	empty					Clear
5	empty					Clear
6	empty					Clear
7	empty					Clear
8	empty					Clear
9	empty					Clear
10	empty					Clear
11	empty					Clear
12	empty					Clear
13	empty					Clear
14	empty					Clear
15	empty					Clear
16	empty					Clear
17	empty					Clear
18	empty					Clear
19	empty					Clear

The "**CSC**"-page can be accessed by selecting the corresponding tab in the main window or by pressing the "**Ctrl+0**"-key while the pointer is in the main window. The page is available only if the configuration file carries the line `CSC USE` (see chapter **Configuration File** in section **Input**). Here, you can access all functions of the optional sample changer.

The "**CSC**"-page features several work areas:

- a menu bar with various options**(see 7.2)**
- an area for performing operations on the sample changer **(see 7.3)**
- an area for initializing the sample changer **(see 7.4)**
- an area containing the status information for 19 samples in the carousel**(see 7.6)**

7.1.1 Principles of Operation

The cryogenic sample changer (CSC) is an extension of the *desktop beamline*. In total, 7 motors are added to the dtb (see chapter **Motors** in section **Introduction**), but they are all driven by the same dtb controller. Changing a sample is a complex sequence of individual motor movements, where one step usually relies on successful completion of a previous step, i.e. it requires exact synchronisation of all participating components. The process of loading a sample, for instance, is a sequence of approx. 30 individual steps. Fortunately, there are only 2 variable parameters for that entire process:

- the vial no. (i.e. carousel position)
- the pin length

The carousel in its current implementation holds 19 samples. It is possible to replace the entire carousel or to replace only single vials in the carousel by new ones. This is described further down in the chapter **CSC Operations**.

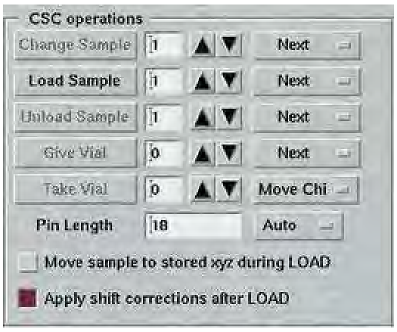
7.2 CSC Menu

The "**CSC**"-menu pops up if the "**CSC**"-button in the menu bar is pressed or if "**Alt+c**" is pressed while the pointer is in the main window. This menu allows for accessing different options that have to do with the sample changer. The choices are:

Table 1: The "CSC"-menu

Menu	Menu Choice	Description
	**Load carousel data**	Loads a sample status file. For details, refer to chapter **Sample Status File** in section **Input**).
	Save carousel data	Saves current sample status in an ASCII-file (see above).
	Clear carousel data	Clears all entries of sample status.
	Release magnet	The magnet holding the loop on the goniometer head is turned off.
	Energize magnet	The magnet holding the loop on the goniometer head is turned on.
	Transfer xyz from mounted sample to Crystal page	This copies the stored xyz-coordinates of a previously mounted sample into the fields for X,Y,Z-translations on the Crystal page. Saves some typing...
	Move sample to stored position	A sample is moved to the previously determined and stored xyz-coordinates. Useful after remounting a sample.
	Unload sample at end of data collection	When checked, the crystal is put back into the carousel after finishing data collection. When unchecked, it stays on the goniometer head.

7.3 CSC Operartions



Change Sample 1 Next
Load Sample 1 Next
Unload Sample 1 Next
Give Vial 0 Next
Take Vial 0 Move Chi
Pin Length 18 Auto
☐ Move sample to stored xyz during LOAD
☑ Apply shift corrections after LOAD

7.3.1 Change Sample

This procedure implies that a sample is currently mounted. This sample is then going to be stored in the carousel and a new sample is mounted from the given carousel position.

Besides providing the desired carousel position, the pin length has to be provided. The pin length plays a critical role at the time when the pin containing the sample is transferred from the SERVER motor onto the goniometer head, since it involves a motion of the z-translation of the goniometer head. from the barcode. The pin length can be obtained from the barcode in those cases where the structure of the barcode really does contain that information. Otherwise, it has to be provided. It should be noted that if the barcode is unreadable the choice for automatically obtaining the pin length from the barcode is an error condition. The consequence is that the samplee in that case will NOT be mounted but stored back in the carousel. It is therefore safer to provide the pin length explicely provided it is known!

7.3.2 Load Sample

This procedure implies that no sample is currently mounted. A new sample is mounted from the given carousel position. The pin length will be considered as described in chapter **Change Sample**.

7.3.3 Unload Sample

The currently mounted sample will be stored in the carousel position that is currently indicated in the status area. The value provided in the text field on the right hand side of the button is meaningless.

7.3.4 Give Vial

The purpose of this operation is to remove a sample from the carousel. It may serve as a component of carousel refill. Please note, that this operation may be carried out while a sample is mounted and even while a data collection is running, i.e. it does not interfere.
The vial from the give carousel position will be taken out of the carousel and presented to the user. The user may grab the vial and transfer it into a transport container or elsewhere.

7.3.5 Take Vial

The purpose of this operation is to insert a new sample into an empty position of the carousel. It is the reverse action of the previous operation. A user inserts a vial (enclosed in a transfer container) in the holding brackets of the SERVER. The vial is then transferred to the given position of the carousel.
Both operations (Give and Take) can also be handled by the remote control unit.

7.3.6 Move sample to stored xyz during LOAD

When remounting a sample that has already been centered on the goniometer head it is useful to use the already known xyz-coordinates that have automatically been stored in the previous centering operation. This will leave the sample at or at least very near its center. Please take care, though, that you turn off this option if you mount a new sample that happens to be in the same carousel position as another sample. The xyz-coordinates of the previous sample will not be valid for the new sample. But the sample changer has no intrinsic knowledge of the fact that the samples have been changed. As by version 5.2, the mar345dtb program does not compare the barcode of the current sample with the one of the previously mounted sample!

7.3.7 Shift Corrections

With the second generation of sample changers, the carousel has been redesigned and makes use of little magnets to keep the vials in place. While this construction is more forgiving to small variations of vial shapes, it allows for more freedom of rotation. The net effect is that it is not longer guaranteed that sample xyz-coordinates that have been determined once, are still valid when the sample is stored back into the carousel and taken out again by the sample changer. Small shifts and rotations may occur that will leave the sample eventually slightly out of the beam after mounting it on the goniometer head.

A special procedure has been implemented to compensate for this mechanical problem. The way it works is the following:

- The sample is mounted onto the goniometer head
- The goniometer head is driven to previously determined xyz-positions
- The picture of the crystal is compared to a picture of the same crystal mounted previously by an external program
- The program computes a correlation factor and suggests shifts
- xyz-translations are adjusted accordingly
- The PHI-axis is driven to a position 90 deg. away and the shifts are recomputed.

All this is being done automatically without user intervention, but only if the box "Use shift corrections" is checked. This checkbox is available only if the configuration file carries a line "CSC SHIFT" (see chapter **Configuration File** in section **Input**).

Usage of this procedure implies that images of the crystal are taken in certain intervals in order to be able to do a comparison later on. Also this is done automatically without necessity of manual intervention.

7.4 Initialize

The sample changer heavily relies on the error-free sequence of a large number of individual tasks. In real life, errors do occur due to various reasons. In most cases it will be necessary to reinitialize the sample changer to recover from a hardware error. The initialization will bring all CSC components back into a known state. The initialization routines work without variable parameters which make them straightforward to use. The initialization is divided into groups of motors which have to be initialized together, since motions or positions of some motors may depend on the ones from other motors:

- SERVER, ROTOR, CHI and barcode-reader
- CAROUSEL, PICKER and LIFTER
- BEAMSTOP and PHI
- Goniometer head translations (xyz)

Usually, an initialization of all CSC-components is the simplest thing to do but there is a choice of only initializing one particular group.

7.5 CSC Options

Stop on ALL barcode errors

Tell dtb that NO sample is mounted

In the options area you can

- specify how the sample changer handles barcodes
- tell the dtb that a particular sample is mounted or that no sample is mounted.

The barcode reader is an important component of the sample changer. It allows for safe identification of the samples, but it also adds security to the instrument and potentially avoids crashes. Let us assume, that a sample is mounted on the goniometer head. You then tell the sample changer to unload the sample and store in the vial in carousel position 5. The sample changer now takes the vial out of the carousel and moves it to the barcode reader. The barcode reader now finds one out of 3 different scenarios:

1. the vial comes without a cap
2. the vial comes with a cap but barcode cannot be read
3. the vial comes with a cap and and barcode can be read

In this particular situation, if the barcode reader identifies a cap (either with or without barcode), the sample changer would produce a crash and lose the currently mounted sample if it would procede with the UNLOAD procedure. The only safe operation in this situation is to put the vial back into the carousel and wait for user action.

To prevent possible crashes, it is therefore generally advisable to choose the option "Stop on CRITICAL barcode errors". The alternative would be to ignore all or to stop also on non-critical errors. A non-critical errors would be the inability to identify the barcode itself. This is something that might happen due to a bad barcode on the cap or due to too much liquid nitrogen floating on the cap. This kind of error should not be regarded as a problem, and therefore it is not recommended to let the sample changer also stop on this error. On the other hand, ignoring all errors is a security risk and has the potential to crash crystals and even to produce hardware crashes.

The second option is to teach the dtb that a certain sample is loaded or that no sample is loaded. When manually removing a sample from the goniometer head or mounting a sample onto the head, there will be no electronical feedback. The controller has to be told explicitely what has been done.

7.6 Carousel Status

Vial	Status	Crystal center x,y,z			Barcode	
1	mounted	-0.241	-0.517	-0.365		Clear
2	carousel					Clear
3	carousel					Clear
4	empty					Clear

The status area shows and stores information about available vials in the carousel. The contents of this window are regularly updated as soon as a bit of information changes, e.g. if a barcode is read or if a new crystal center is found. The window keeps track of the following elements for all 19 samples of the carousel:

Element	Description
Status	One of: "**mounted**", "**carousel**" or "**empty**"
Barcode	Barcode of sample (optional)
Identifier	Optional identification string for the sample
Pin length	Either 14, 16,18,21,24 or 0 mm (with 0=automatic)
Crystal center x,y,z	Positions of xyz-translations of goniometer head

NOTES:

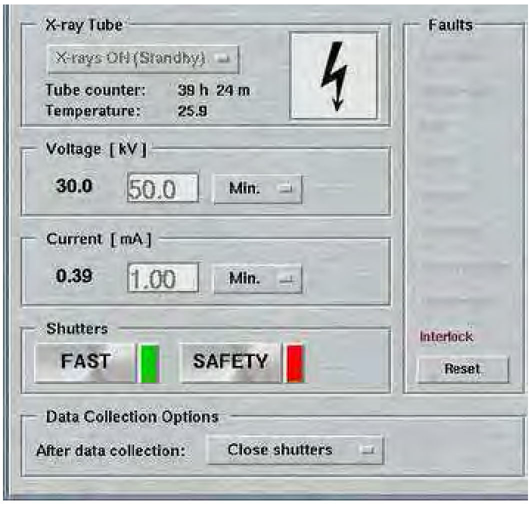
- The barcode will always be updated when loading a sample, i.e. when the vial is on the way to the goniometer head. When inserting a carousel with vials inside, the sample changer will have no knowledge about the barcodes until actually mounting the vial.
- The identifier is an optional component to describe the crystal (e.g. "lysozyme"). It must NOT contain spaces inbetween, but can be left empty. When collecting data, the identifier string is going to be appended to the image name root preceding the barcode string - but only if the option "Append barcode to root name" is selected.
- The pin length may be supplied may be set to 0 only if the barcode contains the pin length.
- The crystal center will be updated automatically as a result of the automatic crystal centering procedure but also if the x,y, or z-translation is moved explicitely.

The sample status will automatically be saved to an ASCII-file called $MARLOGDIR/csc/CSC.csv. It is an Excel-type .csv formatted file. Please see chapter **Carousel File** in section **Output** for details.

Edited on Nov 17, 2010

8. marμX

8.1 Introduction



X-ray Tube: X-rays ON (Standby)
Tube counter: 39 h 24 m
Temperature: 25.9
Voltage [kV]: 30.0 | 50.0 | Min.
Current [mA]: 0.39 | 1.00 | Min.
Shutters: FAST | SAFETY
Faults: Interlock | Reset
Data Collection Options
After data collection: Close shutters

The "**marμX**"-page can be accessed by selecting the corresponding tab in the main window. Here, you can control the marμX generator (Xenocs "GeniX" source).

This page is accessible only if:

- MARMUX USE is given in the configuration file or if the program has been started with command line option +marmux.
- a valid license key has been given on the MARMUX LICENSE keyword in the configuration file.

8.2 License

The license key for using the marμX interface is a computer specific ASCII-string that you may obtain from Marresearch GmbH. For this purpose you may run program 'marlicense' (typically contained in the automar program suite) on the PC where you wish to run program mar345dtb. Program marlicense is going to produce an output file called marlicense.$HOST which you have to maik to Marresearch. If for some reason you don't have access to program marlicense, you can also provide the computer's hostname (as returned by command 'uname -n') and IP-address. In return, you will get a license key that you should put into the configuration file using keyword "MARMUX LICENSE", e.g. like

MARMUX LICENSE license-key

Alternatively, you can set the environment parameter MARMUXKEY in your shell initialization file, e.g. in $HOME/.cshrc as:

setenv MARMUXKEY license-key

Without a valid license, program mar345dtb will not provide the "**marμX**"-page and you cannot run the stand-alone program "**marmux**".

8.3 "Remote Mode" for GeniX Generator

The GeniX micro-focus generator can be controlled by a PC via a TCP/IP-socket interface. To use the generator in "remote mode", pins 5 and 7 on connector X03 on the back of the generator have to be bridged (see the GeniX manual for details). When operating the generator in "remote mode", the local control on the instrument itself is disabled, i.e. you cannot open the X-ray shutters on the instrument and you cannot turn on or off the X-rays. If the "remote mode" is enabled with the proper wiring of the X03 connector, you can still switch to "local mode" by setting the override key on the back of the generator in position "1". This procedure is possible only with X-rays turned off, so you cannot switch on-the-fly from "remote mode" to "local mode".

8.4 Network Setup of GeniX Generator

The controller of the GeniX generator makes use of the industry standard MODBUS/TCP-protocol for communication with a host computer. By default, the GeniX generator IP-address is set to 85.16.44.113 with netmask 255.255.0.0, but for use with the mar345dtb system the IP-address 192.0.2.100 with netmask 255.255.255.0 is used. The generator listens on port 502 for incoming connections. The Ethernet connector of the GeniX generator is located on the back of the instrument just above the main power cable. It is possible to change the IP-address via telnet. To do so, connect to the generator via telnet. If the controller still is in its default configuration, you will have to connect a direct line (cross-over cable) from your PC to the generator and set the PC's network card address to e.g. 85.16.44.1 You may then select to change the IP/Ethernet settings. Usually, it is sufficient to change the IP-address and netmask to fit your local network. The gateway address may be left as is. To save the changes, return to the main menu (R) and select "S" to save. You will be asked for a password. The default password is "USERUSER".

8.5 Operations

There are only 3 useful states of operation of the GeniX generator:

- X-ray OFF
- STANDBY mode
- FULL POWER mode

Hence, from the user interface you select one of the 3 states. Setting the high voltage or current to other than the default values (50 kV, 1.0 mA) is possible, but discouraged. The generator supports a "FAST" and a "SAFETY" shutter. The "FAST" shutter can be disabled on the operation panel of the generator. Depending on availability, the GUI allows for closing the "FAST" and the "SAFETY" shutter and provides a visual feedback of the current status, together with indications of possible hardware faults.

If the high voltage is turned on, in the upper control area on the left hand side you will see a "High Voltage" icon. If the generator is in STANDBY mode or at lower power, the icon will show a white background. At high power, the background turns yellow.

. If X-rays are leaving the generator, i.e. if the HV is on and the generator shutters are open, a yellow "Radiation" icon will show up on the right hand side of the push buttons for the shutters.

In the right hand side of the GUI, well defined hardware faults will be indicated in red fonts.

In the lower area of this page, you have a choice of taking special actions after finishing a data collection. Choose one of:

- Do nothing
- Close generator shutter
- Go into STANDBY mode
- Turn X-rays OFF

In order to increase the lifetime of the tube it is beneficial to let the generator run in FULL POWER mode not longer than necessary. Hence, it is suggested to automatically go into STANDBY mode after data collection. You have to keep in mind, that it does not take longer than 1 minute to go back into FULL POWER mode, so even if you plan to resume work shortly after a data collection has finished it would still make sense to go into STANDBY.

Likewise, if you don't plan to resume work for a couple of hours, you might as well turn off the X-rays at all.

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9. Input

9.1 Overview

Program *mar345dtb* uses the following input files. Some of them are mandatory, others optional.

Table 1: *mar345dtb* input files.

File type	File name	Mandatory	Description
Configuration	$MARTABLEDIR/mar345dtb.cfg or $MARTABLEDIR/config.###	yes	Configuration parameters for *dtb* and detector
Calibration	$MARTABLEDIR/mar2300.### $MARTABLEDIR/mar3450.###	yes	Calibration files for 150 and 100 micron scan modes (for *mar345*-detector)
Parameter	$MARLOGDIR/dtb.dat	no	Saved parameters from "Edit"
Shell script	$MARLOGDIR/dtb.csh	no	Shell script template for executing external commands
Command	$MARLOGDIR/dtb.com	no	Parameter file for triggering an action of the dtb or the scanner
Images	...	no	Image files in several formats
Carousel data	$MARLOGDIR/csc/CSC.csv	no	Saved parameters from "CSC"

denotes a 3-digit serial number and usually is defined as $MAR_SCANNER_NO (or $MAR_DTB_NO if program mar345dtb is used without mar345 support). As of version 9, program mar345dtb tries to read file mar345dtb.cfg as configuration file, in the first place. To be compatible with older versions, if that file is not present, the program falls back to config.###.
The idea is to only add INCLUDE lines to file mar345dtb.cfg and thus separate parameters that are specific to the desktop beamline from those that are specific to the detector. When using program mar555dtb, the corresponding filename is mar555dtb.cfg.

9.2 Configuration File

While all parameters used within program *mar345dtb* are set to reasonable defaults, there are quite a number of parameters that are specific for either a particular model of the *desktop beamline* or the *mar345* image plate detector. Therefore, the program must read in a configuration file for proper function. The configuration file is called `config.$MAR_SCANNER_NO` and resides in directory `$MARTABLEDIR`. If the configuration file doesn't exist, the program can't be started. The file is a keyworded ASCII-file which may be edited. Keep in mind that many of the parameters can be absolutely critical for hardware functions, so for editing you really have to know what you are doing!

9.2.1 Keywords

The configuration file is a keyworded ASCII-file in free format. Lines starting with # or ! are treated as comment lines. Almost all keywords and subkeywords can be truncated to 4 characters. A number of keywords are of general program use, other affect the *dtb* only and others the *mar345*-detector only:

9.2.1.1 General

The following keywords are of general importance to run the program:

USE | IGNORE [options]

There are a number of options that can be turned on (USE) or off (IGNORE):

- **DTB | BASE**
  Try to establish a connection to the *dtb* at program startup.

- **MAR345 | SCANNER**
  Try to establish a connection to the *mar345*-detector at program startup.

- **MAR555 | FLATpanel | TFT**
  Try to establish a connection to the *mar555* flatpanel detector at program startup.

- **AMPTEK**
  AMPTEK is a device that can optionally be fitted to the *dtb* and is used on synchrotron beam lines to choose a proper wavelength for MAD-data collection. This device produces additional restraints of movements for DISTANCE, THETA and CHI (collision protection). If this device is physically present, it it therefore ESSENTIAL to add the line USE AMPTEK to the configuration file.

- **CRYO**
  A cryogenic cooling device can optionally be fitted to the *dtb* and is used on most protein setups. This device produces additional restraints of movements for DISTANCE, THETA and CHI (collision protection). If this device is physically present, it it therefore ESSENTIAL to add the line USE CRYO to the configuration file. The collision parameters depend to a certain extent on the dimension of the cryo-cooler in use. Those can be modified by keyword CRYOPARAM (see below).

- **SPY_MAR**
  Log native *mar345*-controller messages into file $MARLOGDIR/spy/mar.spy.#. This is very important for backtracing hardware problems of the detector.

- **SPY_DTB**
  Log native *dtb*-controller messages into file $MARLOGDIR/spy/dtb.spy.#. This is very important for backtracing hardware problems of the *dtb*.

- **SPY**
  Equivalent to SPY_MAR + SPY_DTB.

- **STATS**
  For each image plate readout ome statistical values of the resulting image (average, sigma of total and of a box of 100x100 pixels in the 10:30 position of the detector) are calculated and the results are logged into the separate output file $MARLOGDIR/lp/mar.lp.#

- **SUMMARY**
  Create a summary file in ASCII format for each collected data set. This file contains all relevant parameters used for collecting this data set: motor positions, exposure times, etc.. Useful for archiving. The file will be created in the current data directory and will be named rootname.#.SUMMARY, where # is a number starting at 1. This number will be incremented automatically if a file of the same name already exists in the data directory.

- **HTML**
  Same as SUMMARY, but file is in HTML format. File name is rootname.#.html

- **AUTOMAR**
  Create a file called rootname.sync that can be used by program marProcess out of the automar suite to process data as they are coming in. Option added in version 5.5.0.

- **DISK**
  Issue a warning message when trying to write data into a disk that is almost full.

- **NFS**
  Issue a warning message when trying to write data out to an NFS mounted disk. Many users may not be aware of potential problems of using NFS mounted disks as data directory. Any problem on the network is going to make the data collection stop, so using NFS directories is definitely not recommended.

- **CENTER**
  Some mar345 image plate detectors suffer from a relatively strong artificial increase of intensities in the inner 5 mm of the IP. This is due to some electronical artifacts in the used controllers. Usually, this is considered as a non-critical problem since this area is mostly covered by the beamstop. However, it is possible to correct for those artifacts by applying a center offset correction. These are additional calibration files that optionally reside in directory $MARTABLEDIR and are called center2300.$MAR_SCANNER_NO and center3450.$MAR_SCANNER_NO. The corrections will be applied with each scanned image, but only if keyword USE CENTER is provided.

- **ERASE**
  Watch erase lamp status and stop data collection if erase lamps fail

- **XRAY**

Watch X-ray intensities as read by the ionization chambers and stop data collection if X-ray intensities drop significantly

- **HARDWARE**
  Make the "**HARDWARE**"-page available as a tab.

- **XTAL**
  Make the "**Crystal**"-page available

- **VIDEO**
  Use the frame grabber output within the "**Crystal**"-page

- **LIGHT or ILLUMINATION**
  Make the Illumination buttons available in the "**Crystal**"-page.

- **CSC**
  Make the "**CSC**"-page (sample changer) available

- **SHUTTER**
  Provides a "Open/Close Shutter" button in the "**Crystal**"-page.

- **TTL**
  Uses the TTL output of the mar345 scanner (at the X25 connector). This signal can be used to operate a generator shutter if wired accordingly. On the "Misc." page of the GUI, you get a button to open and close the generator shutter. You also get a choice of automatically closing the generator shutter at the end of a data collection. **See chapter "Shutter" in GUI ⇒ User Interface ⇒ Main Window ⇒ Pages ⇒ Misc. ⇒ Shutter** for more details.

  Default: USE MAR DTB CRYO SPY ERASE XRAY XTAL VIDEO NFS DISK
  Default: IGNORE AMPTEK ADC STATS CSC HARDWARE LIGHT TTL

DTB | MAR345 | MAR555 [PORT <number>] [HOST <IP-address>] [TIMEOUT <sec>]

Defines the IP-address to which to talk to either dtb and mar345 and the socket ports. The timeout is a time given in seconds after which the program automatically closes and reopens the TCP/IP-sockets to the hardware.
When using the mar555 detector, only USE | IGNORE should be given. All other arguments are meaningless.
Default: DTB PORT 4451 HOST 192.0.2.3 TIMEOUT 30
Default: MAR PORT 4441 HOST 192.0.2.1 TIMEOUT 30
Alternative: MAR555 USE

MARMUX [PORT <number>] [HOST <IP-address>] [INTErval <sec>] [LICENSE <key>] USE|IGNore

Defines the IP-address to which to talk to the marμX generator (typically 192.0.2.100) and the TCP/IP-port (502). The interval is a time given in milliseconds to update information.
The LICENSE key is a computer specific ASCII-string that you may obtain from Marresearch GmbH. For this purpose you need to run program 'marlicense' (typically contained in the automar program suite) on the mar345dtb PC and mail its output to Marresearch. Without a valid license key, the program will automatically set "MARMUX IGNORE". With a valid license, the **page "marμX"** is added to the user interface and the generator can be operated from with the mar345dtb program.
Default: MARMUX PORT 502 HOST 192.0.2.3 INTERVAL 1000 LICENSE none IGNORE

INCLUDE <filename>

Include an entire configuration file to be read by the program. Instead of using a monolithic configuration file, you may split up the configuration parameters into a file containing keywords only for the mardtb and another file with keywords only for the mar345 scanner.
Default: none

EDITOR <command>

Command to use when opening an editor, e.g. for changing the configuration file.
Default: xedit

BROWSER <command>

Command to run html browser for displaying documentation.
Default: firefox

IMAGEVIEWER <command>

Command to use to view graphics image formats (jpg).
Default: display (from ImageMagick suite)

LOOPFIND <command>

Command to use for analyzing a photo for the purpose of automatic centering.
Default: loopfind

MONTAGE <command>

Command to use for assembling several photos taken during crystal centering into a combined graphics file. This command is called from the user interface after the last centering step and the resulting file is automatically shown on the DISPLAY tab.

Default: montagedtb.csh

STREAMER <command>

Command to use to dump video still photos in jpg. The default is to call shell script marstreamer which again calls a special version of program streamer out of xawtv-package.
Default: marstreamer

V4L <command>

Command arguments to use for program *v4lctl* from the V4L (video for linux) interface. If arguments are present, they will be appended to string "v4lctl" and the entire command will be executed before opening the frame grabber device. Please note, that v4lctl will only accept one command per call. If you want to set several parameters via v4lctl, you need to provide several lines starting with keyword V4L.
Default: no arguments

VIDEO (USE|INTERNAL|V4L2)|LIBXV|EXTERNAL|SHMEM|IGNORE [FORMAT] [WIDTH <w>] [HEIGHT <h>] [ORIGIN <x> <y>] [CLASS <name>] [SCALE <x> <y> <z>] [TICK <x> <y>] [FPS <rate>] [AVERAGE <n>] [BRIGHTNESS <value>] [HUE <value>] [CONTRAST <value>] [SATURATION <value>] [RED <value>] [GREEN <value>] [BLUE <value>] [DEVICE <name>] [NO]OVERLAY [NO]CURSOR [GREY|RGB|YUV420|YUYV|AUTO] [INPUT <name>] [NORM <name>] [IDLE <value>]

Settings relevant for the frame grabber output on the "**Crystal**"-page:

(USE | INTERNAL | V4L2) | LIBXV | EXTERNAL | SHMEM | IGNORE
Enable or disable frame grabber handling. With version 8.1, you have a choice of using the built-in video display model or an external program. With version 10.0 the built-in video defaults to the V4L2 interface, while older version made use of the libXvideo interface. While the latter one put the load of displaying the frame grabber data, its functionality depended heavily on the video card driver. For video chips produced by Nvidia or ATI/AMD or Intel in 2010 there are no driver any more supporting this feature. The V4L2 interface, instead, grabs the data from the frame grabber and individually puts them on the screen. This adds some load to the CPU, but is a more reliable approach. The new V4L2 interface should work an older hardware as well as on new hardware. Another benefit of using the new V4L2 interface is that shooting photos now is dealt with much less overhead. Essentially, using 2 TV-cards, one being dedicated for shooting photos now should be obsolete.
Option SHMEM has been added in program version 10.3. In this mode, the program mar345dtb does not grab the frames directly from the video device but rather uses program margrabber to talk to the device. The actual video frames are made available to program mar345dtb via a shared memory segment. There seems to be no obvious benefit from using this approach over the V4L2 option, but it seems as if using the V4L2 option on certain combinations of hardware can produce random problems in the synchronization of the mardtb operations with the mar345dtb program. In those rare cases, using SHMEM can be a useful option.
In any case, in order to display the video stream, the X configuration file (e.g. /etc/X11/xorg.conf) needs to load module "v4l" in the Section "Module".
Before adding V4L2, the only choice to display the TV-stream if the internal interface did not work to use the EXTERNAL mode. While this now should be regarded as obsolete, it is still functional in version 10.x. To use it, you may use either program tvtime or its slightly modified clone "martv" (version ≥ 4). This is a separate program and may be run stand-alone, but when used within program "mar345dtb", it is "hijacked" by the interface, i.e. the mar345dtb program removes all window decorations from the application and pretends that martv/tvtime is an integral part of the mar345dtb program. When using external mode, you must have a "martv.csh" shell script in the binary search path. When using other programs than martv/tvtime you will also have to supply a window class name string with the VIDEO CLASS keyword (see below). The default is to use the INTERNAL built-in video support. Note that VIDEO USE is the same as VIDEO INTERNAL and in program version 10.x the same as VIDEO V4L2. Please also note, that to exchange information between program martv and program mar345dtb, program mar345dtb must be run either as TCP/IP-server or in COMMAND mode. See keyword "COMMAND" and section **Command File"** for more details. Exchange of information is required for (semi-)automatic centering. When using VIDEO EXTERNAL, the video settings light BRIGHTNESS and CONTRAST will become meaningless, since they will be controlled by the external application.

CLASS <name>
When using the VIDEO EXTERNAL video mode you can specify the window class name in order for program mar345dtb to learn which external application is going to display the TV stream. The default is: "TVWindow.tvtime" which is the class name of program martv and tvtime.

OVERLAY | NOOVERLAY
Tells the program that video overlay does or doesn't work on this system. This depends on the video card (driver). If overlay doesn't work, than you won't see the digital crosshair. You can get around that problem by providing NOOVERLAY. For the new V4L2 interface, OVERLAY is the recommended option.

CURSOR | NOCURSOR
Tells the program to use a special cursor on the video output field. On some Linux distributions there might be problems when switching cursors. In those cases, option VIDEO NOCURSOR should be used. Applies only to the VIDEO LIBXV interface.

FORMAT
Default format for output still images. One of JPG, PNG, PPM or PGM.

WIDTH <w>
Width of video frame, typically 768 or 720 pixels.

HEIGHT <h>
Height of video frame, typically 576 pixels.

ORIGIN <x> <y>
Beam center with respect to video image. Coordinates xy have their origin in upper left corner. This needs to be given when using the automatic centering routines with the sample changer or self-centering PHI-axis.

SCALE <x> <y> <z>
Conversion factor for converting x,y and z-pixel coordinates into mm. These values must have been calibrated once for a specific system.

TICK <x> <y>
When painting the digital cross-hair also some tick marks are painted, typically all 100 microns.

FPS <rate>
Frame rate per second. When using the VIDEO V4L2 interface, you may reduce the CPU load by lowering the frame rate from 25 to 20 or 15.

AVERAGE <n>
Form average out of <n> single images before saving them into a file. This is to smooth out some noise and may play an important role in the automatic crystal finding algorithm.

BRIGHTNESS <value>
At initialization of the video output, set brightness to <value>

HUE <value>
At initialization of the video output, set hue to <value>

CONTRAST <value>
At initialization of the video output, set contrast to <value>

SATURATION <value>
At initialization of the video output, set saturation to <value>

RED <value>
At initialization of the video output, set red to <value>

GREEN <value>
At initialization of the video output, set green to <value>

BLUE <value>
At initialization of the video output, set blue to <value>

DEVICE <name>
Name of frame grabber device. It is possible to use 2 frame grabber devices. In particular, for operation with the sample changer, it is advisable. For the VIDEO V4L2 interface it is not required.

INPUT <name>
Frame grabber devices usually come with several interfaces for generating frames. TV-card typically have a an input called "Television" which is the stream from the TV-tuner. They also come with one more input for connecting external video devices. Those input are called Composite0,1,2,3 and S-Video. The dtb camera usually plugs in into one of the Composite inputs, most typically Composite1 which is the default. Used only with VIDEO V4L2.

NORM <name>
Frame grabber devices may generate data using different TV-norms. The most typical in Europe is PAL (768x576 pixels, interlaced) and in the U.S. it is NTSC. For both PAL and NTSC there are some choices (PAL-BG, PAL-DK, PAL-Nc, NTSC-M, etc.). If the image looks strange, try out those choices.

IDLE[time] <value>
Since the V4L2 interface keeps the CPU somewhat busy, while collecting data or doing nothing at the PC it is better to leave the "Crystal" page. This is done automatically after some idle period given in seconds. If the value is 0, the feature will be ignored.

GREY|RGB|YUV420|YUYV|AUTO
Frame grabbers may produce full coloured RGB images with 24 or 32-bits/pixel or somewhat smaller 16-bit color information (YUV420,YUYV) or 8-bit grey-scale images. Since the mardtb camera is black/white only, it does not make too much sense to read full RGB data. This adds unnecessary traffic to the PCI-bus. Therefore, the default is to use GREY as colorspace. This option applies to the VIDEO V4L2 interface only. In version 10.4, the default is 'AUTO' which is going to try first GREY, then YUYV, YUV420 and RGB.

Default: VIDEO V4L2 PNG WIDTH 768 HEIGHT 578 FPS 25 AVE 5 TICK 100 100 SCALE 450 450 DEVICE /dev/video0 INPUT Composite1 NORM PAL IDLE 300 AUTO

THUMBNAIL <command>

Command to use to convert mar data images into graphical thumbnail images.
Default: mar2thumb (shell script)

SOUND <command>

Play sound files when issuing warning, errors, etc. The soundfiles must reside in directory $MARDOCDIR and must be called mar_errorX.wav (X=1,2,3) and mar_warning.wav. The command to use to actually play those sound file must be provided here. If it is left empty, this feature will be ignored.
Default: none

SHOW [NO]RESOLUTION [NO]TOWTHETA

When displaying images, normally only the resolution is shown in Angstroem. In addition (or alternatively) the corresponding 2-theta values may be printed
Default: SHOW RESOLUTION

COLORS <number>

Number of grey shades for image display.
Default: COLORS 64

RETRIES <number>

Number of retries for recovering a hardware problem.
Default: RETRIES 5

STARTUP USE | SKIP [TIME] [SHUTTER] [HV] [LOCK] [VERSION] [ADC] [REMOTE] [CRYO|ROOM] [CYCLE]

Hardware commands to be optionally executed at program startup. To turn off, use SKIP, otherwise USE.

TIME
Synchronize controller time with computer time. This is generally useful.

SHUTTER
Close shutter (for safety reasons). It doesn't hurt!

HV
Turn on high voltage of ion. chambers. The HV is usually turned on, already, but better be sure...

LOCK
Lock image plate. If the plate is locked already, the better!

VERSION
Obtain firmware versions of controllers. This is good to know in certain occasions, but not really essential.

ADC
Adjust ADC using the values given on ADC keyword. This procedure is a bit critical, since you would have to sure that there are no X-rays entering the collimator and you can't be sure about that if the program is not up yet. Therefore it is recommended to skip this step.

REMOTE
Finds out wether the remote control unit is enabled or disabled. Useful, but not essential.

CRYO | ROOM
Assumes that the sample changer operates under cryogenic or under room temperature conditions. This has an impact on some motor movements. With a sample changer attached, the corresponding bit is usually set to CRYO mode and there should not be a necessity to explicitely set or override this bit.

CYCLE
Send the controller a command to automatically send status information every 1000 ms. This is useful in situations where a marCCD software is used simultaneously. Program marCCD disables automatic status sending. This option should not be necessary for normal usage and is not the default.

Default: STARTUP USE TIME SHUTTER HV LOCK VERSION SKIP ADC REMOTE CRYO RROOM

SETS <number>

Number of data sets to be programmed. Either 15 or 30
Default: SETS 30

STATUS [DTB <interval>] [MAR345 <interval>]

<interval> defines the period of time in milliseconds after which a status file `dtb.status` or `mar.status` will be periodically written to directory $MARLOGDIR. This ASCII files contains some information about what the scanner and dtb is currently doing. The purpose for this is to give any other program a chance to exchange information with the mar hardware. A value of "0" means that no status file will be written.
Default: STATUS DTB 0 MAR345 0

COMMAND [<interval>] [PORT <port>] [WRITE <interval>]

<interval> defines the period of time in milliseconds after which an ASCII-formatted command file `$MARLOGDIR/dtb.com` will be periodically checked and parsed. This file may contain commands for either the dtb or the mar345 and is the interface for external programs to interact with the mar hardware. A value of "0" means that no dtb.com file will be checked. If the keyword PORT is supplied commands are read using exactly the same syntax from a TCP/IP-socket on port <port>. In this configuration you may choose to only read from that socket or to write something back. In order to cooperate with the video frame grabber program margrabber, e.g. for point-and-click-centering of a crystal from within program margrabber, it is mandatory to use ports in the range from 9000 to 9010.
If keyword WRITE <interval> is supplied with a positive number, then a status block is sent every <interval> ms to the socket. The format of the status block is described **in chapter "Status File"** in section **Output**). If a negative value is given for <interval>, then the same information that goes into both the scanner and dtb spy files is written to the socket. If the value is 0, then no strings will be written.
Please note, that it is the client program's responsibility to read back information from the socket. If the program mar345dtb sends data to the socket, but the client doesn't read it, the program is going to freeze within short time.
Default: COMMAND 0 PORT 0 WRITE 0

UNITS [STEPS <number>] [SPEED <number>] [ACCEL <number>] [TIME <number>] [MAXTIME <number>] [MULTiple <number>]

With this keyword an additional conversion factor can be applied to convert step units into mm. The hardware doesn't know anything about mm or degrees and deals only with steps and microsteps. The values here are supposed to be constant and are rather of historical importance. Do NOT modify them!
The MAXTIME value only applies to the *mar555dtb* program version. The issue is that the *mar555* detector can be used with relatively short exposure times only. The maximum is 60 sec (60000 msec), but usage of 30 sec or less is strongly recommended. If a positive value in sec is given for MAXTIME, the program will automatically split an exposure longer than MAXTIME seconds into shorter ones by dividing the exposure time by 2 until the resulting exposure time is < MULTIPLE seconds. If only MAXTIME is > 0, and MULTI has not been specified, MULTIPLE is set to MAXTIME. At the same time, the PHI movement for the exposure is divided by 2. On output, the images will automatically be added and averaged to give a single image over with the total exposure time and total PHI range as specified in the GUI. By default, this feature is turned off.
Default: UNITS STEPS 1 SPEED 1 ACCEL 1 TIME 2.5 MAXTIME 0 MULTI 0

WAVELENGTH DEFAULT <lambda> USE|IGNORE INTERN|EXTERN

Wavelength of X-rays. This number will be written into the corresponding section of the resulting images.
Default: WAVELENGTH DEFAULT 1.54178 USE INTERN

WINDOWS [MAIN <x y>] [VIEW <x y [width height]>]

[x,y]-coordinates for main window and display window at program startup. The main window has a fixed size. For the display window also the width and the height can be configured. This allows the program to be fit to any screen resolution (>=1280x1024 pixels) and window manager.
Default: Depends on screen resolution and operating system

VERSION [LOG <N>] [SPY <N>] [STATS <N>] [SCAN <N>] [TIME <N>] [PROFILE <N>] [XTAL <N>] [FIRMWARE <Version>]

The program creates a new version of several log files to be stored in directory $MARLOGDIR and subdirectories log, spy, lp, beam and xtal. Here you specify how many versions you want to keep. Note, that spy files can take quite some disk space, but for keeping track of hardware problems you will want to keep a reasonable number of copies. After reaching version N, the first file (with N=1) will be overwritten.
XTAL only becomes relevant for automatic centering with the sample changer. N sets the number of sample photos that are kept. This might be useful only to find out which samples failed to be centered correctly.
With advent of the sample changer (CSC) major work had to be done to the dtb firmware. Usually the program determines automatically which dtb firmware version is in use but only if keyword STARTUP VERSION is given.
Default: VERSION LOG 99 etc. (all N=99)

9.2.1.2 Keywords for *dtb*

The following keywords affect the *dtb* only:

ADC CHAMBER 1 | 2 [OFFSET <off>] [TOLERANCE <d>] [HIGH|LOW] VARIANCE LOW <dlow> HIGH <dhigh>

Default values for ADC offset adjustment for ionization chambers 1 and 2. <off> is the target offset without X-rays and <d> the tolerance for reaching the target, typically within 10 % of the offset. For each ionization chamber a gain selector can be set to HIGH for weak X-ray sources (rotating anode, sealed tube) or to LOW for synchrotrons. A suitable target offset for HIGH gain is 1000 +/- 20 and for LOW GAIN is 20 +/- 2. Note, that HIGH gain is roughly 300 times as sensitive as LOW gain. The VARIANCE for LOW gain (<dlow>) and HIGH gain (<dhigh>) should reflect the typical fluctuations of the ADC readings (without beam) and are typically +/- 2 for LOW gain and +/- 20 for HIGH gain. These values will play a role in the "**Find beam**" and "**Optimize beam**" procedures. They will decide define suitable thresholds for the start and end of a peak. The program usually expects a peak to be at least above the ADC <off> + 3*<dhigh> (or 3*<dlow>)
Default: ADC CHAMBER 1 OFFSET 1000 TOLERANCE 20 HIGH VARIANCE LOW 2 HIGH 20
Default: ADC CHAMBER 2 OFFSET 1000 TOLERANCE 20 HIGH VARIANCE LOW 2 HIGH 20

INTENSITY [MIN <min>] [WARN <warn>] [DOSEMIN <dose>]

<min> gives the minimum acceptable X-ray reading of chamber 2 during one exposure. If reading is lower than this, data collection stops since it will be assumed that the X-rays went away. To turn this off, enter a negative value. Otherwise, provide a value that is at least twice as large as the intensity reading of the 2. chamber without beam. This reading - of course - depends on the selected gain and the chosen ADC offset. Typically for rotating anode generators running with an ADC offset of 1000, a MIN value of 2000 should be suitable. For operation at a synchrotron with low gain settings and an ADC offset of 20, a MIN value of 30 is suggested.
<warn> gives the allowed variation of X-ray intensity inbetween the start and the end of one exposure in percent. If the variation is larger than this, a warning message is issued and the data collection stops. This is to avoid unnecessary scans if the X-ray generator fails. To turn this off, enter a very large value for <warn>.
<dose> is the minimum intensity required to actually start an exposure when working in DOSE mode. If the intensity is less than <dose>, the exposure will not even be started but waits until the X-ray intensity as measured by the ionization chamber exceeds <dose>.
Default: INTENSITY MIN 2.0 WARNING 50.0 DOSEMIN 0.1

SHUTTER <delay>

Here we enter the delay in mseconds the shutter takes to actually be closed and makes exposure times more accurate. This value has been calibrated in the factory and is specific for a dtb but usually in the range 20 to 40 msec.
Default: SHUTTER 0

FIND CHAMBER 1 | 2 [X <start end> Y <start end> % | MM] [SLIT <hor ver>]

Default parameters for the "**Find Beam**"-procedure of the automatic alignment. The start and end values for X and Y are given either as percentages (subkey "%") of the available driving range (e.g 25 to 75) or in absolute millimeters (subkey "MM") which would be rather inconvenient. The 2 values following the SLIT subkey define the aperture of the horizontal and vertical slits for this procedure.
The method used for doing the beamsearch can be influenced by subkeywords FAST or SLOW on the OPTIMIZE keyword (see below)!
Default: FIND CHAMBER 1 X 25 75 Y 25 75 % SLIT 4.0 4.0
Default: FIND CHAMBER 2 X 15 85 Y 15 85 % SLIT 4.0 4.0

OPTIMIZE CHAMBER 1 | 2 [SPEED <hor ver>] [SLIT <hor ver>] [FIRST <hor ver>] [RANGE <hor ver>] [THRESHOLD <pct>] [SMOOTH <avg>] [FAST | SLOW] [FWHM | MAX]

Default parameters for the "**Optimize Beam**"-procedure of the automatic alignment. The speed values for horizontal and vertical movement are specified separately and are a percentage of the maximum speed.
The 2 values following the SLIT subkey define the aperture of the horizontal and vertical slits for this procedure.
The 2 values following the FIRST subkey define the aperture of the horizontal and vertical slits of chamber 1 used for optimizing chamber 2. The slit apertures to be used depend on the nature of the beam. The defaults

are appropriate for Osmic mirrors but should be decreased for a synchrotron beam.

The 2 values for the RANGE subkey define the default range for horizontal and vertical translation or rotation motors used during the optimization. The values to be entered are supposed to be multiples of the used slit size, typically 3 for a beam produces by a standard generator with standard optics. The range should be increased for very fine beams on synchrotrons when using slit sizes of 0.1 to 0.2 mm.

For values > 1 for the SMOOTH parameter (since version 9) the program computes a running average out of the intensity curve. This is going to remove small spikes and may make the optimization procedure more robust. Very weak peaks are likely to further be reduced by smoothing. Reasonable values for SMOOTH are 3, 5, 7 or 9.

The FAST or SLOW subkeys define the optimization method. In FAST mode (available since version 2.2), vertical movements are interrupted as soon as the instrument moves out of the beam. The decision when beam is going to be lost is marked by subkey THRESHOLD. If the intensity drops below <pct> percent of the seen maximum, the movement is stopped. This speeds up the optimization and also the beamsearch procedure by a factor of 1.5 to 2.

The FWHM or MAX subkeys (since version 9) define wether the motor drives to the absolute max. of the intensity readings (MAX) or to full width half maximum (FWHM) after a scan. For assymetric beam profiles, you can expect a difference of some fractions of millimeters, while for a Gaussian peak the results should be the same. It probably doesn't matter which method you choose, but you should stick to the choice!

Default: OPTI CHAMBER 1 SPEED 10 100 SLIT 0.6 0.6 RANGE 3.0 2.0
Default: OPTI CHAMBER 2 SPEED 20 30 SLIT 0.3 0.3 FIRST 0.3 0.3 RANGE 3.0 3.0
Default: OPTI SHORT THRESHOLD 75 SMOOTH 5 FWHM

MOTOR [options]

MOTOR stands for a particular motor and is any of:

- **SLIT FIRST HOR**
- **SLIT FIRST VER**
- **SLIT SECOND HOR**
- **SLIT SECOND VER**
- **BEAMSTOP**
- **PHI**
- **THETA**
- **DISTANCE**
- **TRANSlation HOR**
- **TRANSlation VER**
- **ROTation HOR**
- **ROTation VER**
- **CRYSTAL Z or CRYSTAL**
- **CHI**
- **SERVER (sample changer/easymount only)**
- **ROTOR (sample changer/easymount only)**
- **LIFTER (sample changer only)**
- **PICKER (sample changer only)**
- **CAROUSEL (sample changer only)**
- **CRYSTAL X (automatic PHI-axis only)**
- **CRYSTAL Y (automatic PHI-axis only)**
- **WAVELENGTH**

The following subkeywords define the specifications of the corresponding motor:

ID <number>: CAN-bus identifier of motor

SPEED <steps/sec>: Max. speed in steps/sec

SLOW <steps/sec>: Speed in steps/sec used for slow movements

FAST <steps/sec>: Speed in steps/sec used for fast movements

STEPS <steps/mm>: Translation of motor steps into mm or deg.

BACKLASH <mm or deg>: Backlash correction in mm or deg. used for accurate motor movements (PHI).

DEFAULT <mm or deg>: Default position in mm or deg.

ACCEL <steps/sec^2>: Acceleration in steps/(sec^2)

TIMEOUT <sec>: Time in sec in which a movement has to be finished before treating it as error

OFFSET <mm or deg.>: A motor offset is only used in very special situations. For CRYSTAL X and Y it defines the deviation of the theoretical PHI position in degrees where the camera view is exactly perpendicular to the axis. For CRYSTAL Y, the theoretical PHI position should be 0 or 180 deg. and for CRYSTAL X it should be 90 or 270 deg. In real life there might be an offset of +/- a couple of degrees.
For ROT_VER, the OFFSET has a different meaning. If the collimator is not perfectly aligned with the camera and the PHI axis, it is possible to compensate for small misalignments by driving the VERTICAL ROTATION motor by a fraction of a mm beyond the found maximum during optimization. This is something that must be obtained experimentally.

MINVAL <mm or deg>: Minimum value in mm or deg. that can be entered within program. Used to restrict movement beyond a certain limit.

MAXVAL <mm or deg>: Maximum value in mm or deg. that can be entered within program. Used to restrict movement beyond a certain limit.

REFERENCE METHOD <number>: Method for referencing this motor (PHI and BEAMSTOP only)

REFERENCE MIN <mm or deg>: Reference position in mm or deg. at NEAR end of movement

REFERENCE MAX <mm or deg>: Reference position in mm or deg. at FAR end of movement

REFERENCE SPEED <steps/sec>: Speed in steps/sec used during referencing

REFERENCE ACCEL <steps/sec^2>: Acceleration in steps/sec^2 used during referencing

For each motor there are additional keywords to define certain properties:

USE | IGNORE: Use or ignore this motor

INTERN | EXTERN: Motor is [NOT] built-in in dtb

ABSOLUTE | RELATIVE : Motor commands are issued as movements to an absolute position or relative to current position

HAS[NO]MIN;: Motor has [does not have] a NEAR end reference switch

HAS[NO]MAX;: Motor has [does not have] a FAR end reference switch

HAS[NO]REF;: Motor has [does not have] a single reference position

[NO]INITMIN : Motor is [NOT] allowed to reference at NEAR end reference switch

[NO]INITMAX : Motor is [NOT] allowed to reference at FAR end reference switch

[NO]INITAUTO: Motor is [NOT] allowed to initialize automatically when reaching a reference switch

[NO]MOD360: Motor positions are [NOT] kept in range 0 to 360 (PHI only)

[NO]CONFIRM: Motor movements must [NOT] be confirmed before driving

REMOTE USE | IGNORE [CHECK] [MASK >mask<] [component options]

Use or ignore remote control. Optional keyword **CHECK** means that the "**Remote Control**"-window cannot be closed until the remote control is explicitely disabled from the software. This option prevents users from accidentally operating the remote control manually while motors are operated from the software.

Optional keyword **MASK** specifies which buttons of the remote control unit can be activated at all. This differs from standard dtb's to the ones that come with sample changer. The sample changer requires an extended remote control unit with buttons to move the carousel etc. The mask to use is a bit mask and is either: 131071 for a plain dtb, 16777215 for a dtbcsc with cryo actuator and 16777214 for a dtbcsc without cryo actuator.

The following **components** are availabe:

ADC

THETA

DISTANCE

CHI

CRYO | BEAMSTOP | PHI

Note that as by early 2002 the CRYO button is not being used and may be reassign to drive either the **BEAMSTOP** or the PHI-motor. It can be handy to drive the beamstop out of the way when mounting the crystal. The beamstop may be moved manually but if this has been done the motor needs to reinitialized afterwards. Alternatively, it can be useful to drive **PHI** to 0.0 with the remote control before mounting a new crystal. The user can make her/his own choice but the instructions in **Appendix: "How to Assign Motors to the Buttons of the Local Motor Control"** . must be followed before the keyword given here is going to take effect.

For each **components**, the following **otions** are available:

ENABLE | DISABLE
Enable or disable this component

EDIT | NOEDIT
(Dis-)allow editing of parameters in the "**Remote Control**"-window

POS1 <value>
Target value for position 1 (meaningless for ADC). Special keyword **POS1 DYNAMIC** means that position 1 will be updated automatically as the corresponding motor moves.

POS2 <value>
Target value for position 2 (meaningless for ADC)

Default: REMOTE IGNORE [component DISABLE NOEDIT]

CRYOPARAM [CRYOSTREAM | XTREME] [DISTANCE <d1> [<d2>]] [THETA <t1> [<t2>]] [WIDTH <w>] [HEIGHT <h>]

The values given for d1 and optionally d2 define the collision criteria when moving the detector along the distance translation and those for t1 and optionally t2 when moving 2-theta. The formulas for driving the motors are as follows:

d_{safe} = d2*tan(2-theta) + d_{min} + d1

t_{safe} = asin [(distance - d_{min} - t1) / t2];

d_{safe} = the shortest distance considered to be safe

t_{safe} = the largest 2-theta angle considered to be safe

d_{min} = min. possible distance (as configured)

d1 = 0.0 for Oxford Cryostream and MSC XTREME

d2 = 240.0 (constant) for Cryostream and 170. for XTREME

t1 = 25.0 for Cryostream and -17.0 for XTREME

t2 = 320.0 for Cryostream and 230.0 for XTREME

For other cryo-cooling devices, it is suggested to modify d1 and t1 and check for collisions. By providing subkeys CRYOSTREAM or XTREME the parameters for the Oxford Cryostream and the Rigaku/MSC Xtreme will be used, respectively.
The width and the height specified here are only relevant for CSC operations. They define the width and height of the actual coldstream and set the allowed limits for automatic centering. I.e. a crystal should not be allowed to move outside the coldstream. The values provided are in mm and default to 8.0 mm
Default: CRYOPARAM DISTANCE 0.0 240. THETA 25.0 320. WIDTH 8 HEIGHT 8

CSC USE |IGNORE AUTO | NOAUTO SHIFT | NOSHIFT INIT_Z | NOINIT_Z [BARCODELEN <N>] [CAP USE|CHECK|IGNORE] [MINHSIFT <N>] [MAXHSIFT <N>] [CORREL <c>] [ZMAX <z>] [METHOD <N>] [PHOTOS <N>] [CYCLES <M>] [DPHI <dphi>] [START <phi0>] [TOLERANCE <mm>]

Option for using or ignoring the sample changer.

USE | IGNORE
Enable or disable marcsc usage.

AUTO | NOAUTO
Enable/disable automatic centering options.

SHIFT | NOSHIFT
Enable/disable automatic xyz-shift correction method. With program version 4.3, a procedure to correct for xyz-shifts after remounting a sample has been implemented. To make use of it, the keyword SHIFT has to be provided. The way it works is described in **chapter "Move Sample to Stored xyz** in section **Csc**). In order to prevent too large movements, a minimum and a maximum shift can be given in pixels. Also, since it is assumed that a particular sample should look quite similar after remounting, the correlation between pictures of the sample when determining xyz and after remounting may be restricted to a value. Typically, correlations should be larger than 0.9 but if pictures don't match the resulting correlation typically is well below 0.5.

INIT_Z | NOINIT_Z
Force or disable initialization of crystal Z axis when initializing the goniometer head or all CSC motors. Forcing the initialization of the Z axis bears the risk to move a sample out of the cold stream.

MAXSHIFT <N>
Max. allowed shift (in pixels) for shift corrections.

MINSHIFT <N>
Min. shift (in pixels) for shift corrections. For shift less than MINSHIFT, the shift will be ignored.

CORREL <N>
Min. correlation for crystal photos from the same crystal. Applies only to shift correction method.

CAP USE | CHECK | IGNORE
For all sample changer operations, one has to specify wether the recognition of a cap is mandatory for ALL operations to complete successfully (CAP USE), only critical ones (CAP CHECK) or none (CAP IGNORE). For CAP USE, all failures to recognize a cap will constitute an error condition.

BARCODELEN <N>
Max. number of characters that barcode encodes

ZMAX <z>
Max. range in mm the dtb is allowed to move the Z-axis during automatic centering. If the number is exceeded, the automatic centering for this sample will be abandoned. The crystal should stay within the cold stream. Therefore, the Z-axis movement should be limited to a reasonable amount (2-3 mm).

TOLERANCE <MM>
When automatically centering a crystal, the adjustments taken from 2 consecutive images at a given Delta-PHI should be fairly small. They should fall below <MM> millimeters, otherwise the centering will be regarded as being unsuccessful. Suitable values should be inbetween 0.1 (default) and 0.3 mm. This option applies only to methodS 1 and 2 (see below).

METHOD <N>
Method used for automatic centering. Must be either 0, 1 or 2. For method 0, the procedure is the following:

Drive sample to starting PHI

Shoot and evaluate photo and apply xyz-shifts

Drive PHI to DPHI and shoot and evaluate another photo

Repeat previous step for N photos

Method 1 differs from method 0 by not evaluating single photos. Instead, a series of N photos is taken in PHI intervals given by DPHI. Only after taking the last photo, the entire series of photos will be evaluated and a set of xyz-movements will be computed.
Method 2 uses the same strategy as method 0, but after going once through 4 photos the program will continue to center the center the crystal until either the desired number N of photos has been reached or if the deviations inbetween 2 adjacent photos drops below a tolerance of MM millimeters. If N has been reached and the last movement was still above TOLERANCE, the centering will be treated as unsuccessful (see above).

PHOTOS <N>

During automatic centering, take N photos at PHI intervales given by DPHI.

DPHI <dphi>
During automatic centering, move PHI by dphi degrees inbetween 2 photos.

START <phi0>
Start automatic centering at the PHI position given by phi0.

CYCLES <M>
During automatic centering, repeat the entire procedure of shooting N photos M times.

CSV [[NO]PIN] [[NO]BARCODE] [[NO]IDENTIFIER]]
Enables or disables optional fields for each sample in the carousel. Usage of barcode strings, crystal identifier strings and the pin lengths is purely optional. Default is CSC CSV NOPIN BAR ID.

Default: CSC IGNORE NOAUTO NOSHIFT NOINIT_Z BARCODELEN 8 CAP USE MINSHIFT 1 MAXSHIFT 350 CORREL 0.8 ZMAX 3.0 METHOD 0 START 0.0 DPHI 90.0 PHOTOS 4 CYCLES 1
TOLERANCE 0.1
CSV NOPIN BARCODE IDENTIFIER

9.2.1.3 Keywords for *mar345*

The following keywords affect the *mar345*-detector only:

IGNORE ERROR <n1> [<n2> [<n3>] [...]]

Most hardware errors will make a data collection stop when encountered. Some hardware errors may, however, not be fatal, and it may be desirable to continue data collection, anyway. Also, some hard- ware errors may not be real. For instance, when the scanners reports that an erase lamp is off during erase, it is possible that only the light sensor is broken but the lamp itself works fine. In such cases, the error number as produced by the hardware can safely be ignored. The error numbers can be looked up in the mar.spy file. There, each message (error or not) has got a unique message number. Up to 20 hardware errors may be ignored but all must go in only one line. If there are multiple "IGNORE ERROR" lines, only the last one will be used.
Default: no errors ignored

MONOCHROMATOR <synchtrotron | mirrors | graphite>

Type of monochromator. This string will be written into the corresponding section of the resulting images.
Default: MONOCHROMATOR MIRRORS

GENERATOR <synchrotron | rotating anode | sealed tube>

Type of X-ray source. This string will be written into the corresponding section of the resulting images.
Default: GENERATOR ROTATING ANODE

GAIN [100u <f1>] [150u <f2>]

Gain for conversion of X-rays into ADC-units for the image plate detector. These gain factors differ between the 100 micron and 150 micron scanmodes due to double sampling in the latter one. The values will be written into the image header and play a role only later during data processing when it comes to a statistically correct estimate of the variances of the reflection intensities. The values provided by *marresearch* are calibrated and scanner specific.
Default: GAIN 100u 1.0 150u 0.65

CENTER USE |IGNORE [MIN <min>]

Choice for using a center correction table during transformation. This implies the existence of files center2300.$MAR_SCANNER_NO and center3450.$MAR_SCANNER_NO in $MARTABLEDIR. Technically, from each pixel in a transformed image a calibrated fixed count is subtracted. By providing a minimum pixel count, pixels will be forced not to drop below a given count (default to 5).

Default: CENTER IGNORE MIN 5

MODE <scanmode> [ROFF <roff>] [ADC <off>] [AADD <a>] [BADD <b>]

Here you specifiy scanner specific values for ADC properties and radial offset corrections for each scanmode (one of 2300, 2000, 1600, 1200, 3450, 3000, 2400, 1800). In particular the ROFF value is really scanner specific and is calibrated during the manufacturing process. The AADD and BADD values are rather dependent on the controller of the detector and have to do with finding an optimal baseline for the ADCs used for digitizing the data. Do NEVER EVER change these values!
Default: MODE ROFF 0 ADC 0 AADD 0 BADD 0

FLAG <number>

The scan command of the *mar345*-detector may be used with some special flags used for debugging. The number can be any hexadecimal combination of the following codes:

0: normal scan

1: scan with laser turned OFF

2: scan with high voltage turned OFF

4: scan with erase lamps turned OFF

9: scan with rotation encoder index line turned ON

16: scan without data transfer

32: scan with ADC offset set to input values

64: scan with profile skipped

128: scan with debug protocol turned ON

256: scan with ADC adjustment turned OFF

Example: FLAG 3 would be a scan with high voltage and laser turned OFF.
Default: FLAG 0

MEMORY <number> MB | KB

The program reads a large calibration file during each scan. To improve reading efficiency, data are read in in larger blocks. Only used in program versions < 2.
Default: MEMORY 1 MB

GAPS <345mm> <300mm> <240mm> <180mm> [TOLERANCE <N>]

The scanning head of the *mar345*-detector is mounted on a translation stage. During a scan the scanning head passes a couple of especially marked positions (gap) that serve as a reference for the correct scanning head positions. The positions are hardwired and scanner specific. For a scan at a certain diameter the positions should always stay the same. The posi tions are given in relative motor steps. The expected tolerance normally is +/- 5 steps. Larger variations of the found "gap" positions may indicate a problem with the scaning head spindle. The observed gaps will be written into image headers, so those values can be verified. If the "GAP" keyword is given and the observed gap for a scan at a certain diameter is not within the tolerance, an error message will be produced and data collection stops. Under normal conditions, the GAP keyword should be left out or the tolerance set to large values, e.g. 99999.
Default: GAPS 89600 78600 63900 49100 TOLERANCE 99999

DATA_INTERVAL <t1> <t2> <t3>

These values are very ciritical program parameters concerning timing of data transfer across the network during scan. <t1> is the timeout in millisec- onds to wait for new data to come in before looking again on the network socket after a block of data has been successfully transformed, <t2> is the time to wait in the case <t1> is a timeout after a block of data has been received and transformed before looking for more incoming data. <t2> is a timeout that occurs if a previous call with a timeout of <t1> has not been successful. <t3> is another timeout that happens only at the end of a scan if there are still some data missing. Most relevant is <t1>. However, these parameters are considered strictly internal and modification will have seri- ous consequences on overall program preformance.
Default: DATA_INTERVAL 3 3 10

9.2.2 Example

The following file listing is a typical configuration file for a *mar345*-detector mounted on the *dtb*:

```
! _____________________________________________________________________________
!
! Configuration file for mar345 S/N 184 and dtb S/N 010
! _____________________________________________________________________________
!
! =============================================================================
! =============================================================================
! ==                                                                         ==
! ==                    Keywords for general program usage                   ==
! ==                                                                         ==
! =============================================================================
! =============================================================================
!
USE        DTB
USE             SCANNER
DTB        PORT  4451   HOST 192.0.2.3 TIMEOUT 0
MAR345     PORT  4441   HOST 192.0.2.1 TIMEOUT 0
MARMUX          PORT  502    HOST 192.0.2.100 INTERVAL 1000 IGNORE
!
INTENSITY MIN 2000  WARN 20.0 DOSEMIN 2.0
!
USE      SPY
USE    STATS
!
USE     HTML
IGNORE  SUMMARY
IGNORE          SHELL
!
IGNORE          TTL
!
COLORS  64
SETS  30
!
BROWSER  firefox
EDITOR          kedit
MONTAGE  montagedtb.csh
SOUND  play
!
!
```

```
! Video params
! ============
!
! VIDEO         V4L2 or LIBXV or  EXTERNAL or IGNORE
!
VIDEO           V4L2 GREY DEVICE  /dev/video0
VIDEO           INPUT Composite1  NORM PAL IDLE 300
VIDEO      BRIGHTNESS 60 CONTRAST 55 AVERAGE 5
VIDEO      WIDTH 768  HEIGHT 576 SCALE 474 474 474
VIDEO      ORIGIN 368  285
VIDEO           OVERLAY JPG
!
THUMBNAIL mar2thumb
LOOPFINDER loopfind
!
! Sample changer params
! ====================
!
CSC             IGNORE
CSC             CAP CHECK BARCODELEN 10
CSC             MAXSHIFT 250 CORREL 0.7 NOSHIFT AUTO
CSC             ZMAX 2.0 XMAX 1.0 YMAX 1.0
!CSC            METHOD 1  CYCLES 1  PHOTOS  8  DPHI 45.0  START 0.0  TOLE 0.3
!CSC            METHOD 0  CYCLES 1  PHOTOS  4  DPHI 90.0  START 0.0  TOLE 0.3
CSC             METHOD 2  CYCLES 1  PHOTOS 12  DPHI 90.0  START 0.0  TOLE 0.3
!
!
! WINDOWS params for Linux:KDE (1280x1024 pixels)
! ===============================================
! WINDOWS         MAIN 1123  0 VIEW 45  0 1070 970
!
! WINDOWS params for Linux:GNOME (1280x1024 pixels)
! =================================================
! WINDOWS         MAIN 1122 22 VIEW 15 22 1095 942
!
! WINDOWS params for Linux:KDE (1680x1050)
! ========================================
! WINDOWS         MAIN 1525  0 VIEW 445  0 1070 1020
!
! WINDOWS params for Linux:KDE (1600x1200)
! ========================================
! WINDOWS         MAIN 1444 0 VIEW 45  0 1392 1174
!
! WINDOWS params for Linux:KDE (1920x1200)
! ========================================
! WINDOWS         MAIN 1765  0 VIEW 585  0 1170 1170
!
! WINDOWS params for Linux:KDE (1920x1080)
! ========================================
! WINDOWS         MAIN 1765  0 VIEW 585  0 1170 1050
!
MONOCHROMATOR Mirrors
GENERATOR Synchrotron
WAVE  DEFAULT 1.000 USE
!
! Log file versions to maintain:
!
VERSIONS        LOG 99  SPY 99 STATS 10 SCAN 99 TIME 99 PROFILE 99
!
! =============================================================================
! =============================================================================
! ==                                                                         ==
! ==                       Keywords affecting dtb only                       ==
! ==                                                                         ==
! =============================================================================
! =============================================================================
!
! ADC values to start with:
!
ADC  CHAMBER 1 OFFSET 1000  TOLERANCE 20 HIGH VARIANCE LOW 2 HIGH 20 EDIT
ADC  CHAMBER 2 OFFSET 1000  TOLERANCE 20 HIGH VARIANCE LOW 2 HIGH 20 EDIT
!
! Initialization commands
!
STARTUP  USE  TIME LOCK VERSION REMOTE
STARTUP  SKIP ADC SHUTTER HV CYCLE
!
! Shutter close delay in [millisec]
!
SHUTTER  25
!
! Find beam params
!
FIND CHAMBER 1  X 25  75  Y  25 75  %  SLIT 4.0 4.0
FIND CHAMBER 2  X 15  85  Y  15 85  %  SLIT 4.0 4.0
```

```
!
! Optimize beam params
!
OPTI CHAMBER 1  SPEED 10 100  SLIT 0.6 0.6                RANGE 2.0 2.0
OPTI CHAMBER 2  SPEED 20  30  SLIT 0.3 0.3 FIRST 0.3 0.3  RANGE 2.0 2.0
OPTI SHORT FWHM  SMOOTH 5
!
! Scaling factors for all motors:
!
UNITS     STEPS 1  SPEED 1  ACCEL 1 TIME 2.5
!
! Slits: Basecon-modul 1-4 (ID = 1-4)
! 1 mm  = 200 fsteps
! V  = 100 fsteps/sec
! A   = 4000 fsteps/s*s
!
SLIT FIRST  VER STEPS 200 SPEED 100 ACC 4000 TIMEOUT 10 DEF 0.4 ID 1
SLIT FIRST  HOR STEPS 200 SPEED 100 ACC 4000 TIMEOUT 10 DEF 0.4 ID 2
SLIT SECOND VER STEPS 200 SPEED 100 ACC 4000 TIMEOUT 10 DEF 0.3 ID 3
SLIT SECOND HOR STEPS 200 SPEED 100 ACC 4000 TIMEOUT 10 DEF 0.3 ID 4
!
SLIT FIRST  VER MIN -0.03  MAX 4.0  SPEED 100 ACC 4000 BACK 0.2
SLIT FIRST  HOR MIN -0.04  MAX 4.0  SPEED 100 ACC 4000 BACK 0.2
SLIT SECOND VER MIN -0.04  MAX 4.0  SPEED 100 ACC 4000 BACK 0.2
SLIT SECOND HOR MIN -0.07  MAX 4.0  SPEED 100 ACC 4000 BACK 0.2
!
SLIT FIRST  HOR INITMIN NOINITMAX HASNOREF ABSOL HASMIN
SLIT FIRST  VER INITMIN NOINITMAX HASNOREF ABSOL HASMIN
SLIT SECOND HOR INITMIN NOINITMAX HASNOREF ABSOL HASMIN
SLIT SECOND VER INITMIN NOINITMAX HASNOREF ABSOL HASMIN
!
! Beamstop: Basecon-modul 5 (ID = 5)
! 0.15 mm  = 1 fsteps
! 1    mm = 6.666
! V  = 2000 fsteps/sec
! A   = 500 fsteps/s*s
!
BEAMSTOP  STEPS 6.6666666 SPEED 100 ACC 500 ID 5
BEAMSTOP  MINVAL 5.0  MAXVAL 45.0 DEFAULT 15.0
BEAMSTOP  REFERENCE 18.6 SPEED 50 SLOW 20 ACC 30000  TIMEOUT 20  METHOD 19
BEAMSTOP  HASNOMIN HASNOMAX  HASREF NOINITMIN NOINITMAX NEGATIVE NOINITAUTO
!
! Phi: Basecon-modul 6 (ID = 6)
! 1 deg = 800 fsteps
! V  = 10000 fsteps/sec
! A   = 20000 fsteps/s*s
!
PHI STEPS 800 SPEED 10000 ACC 20000 BACKLASH -0.5  DEF 0.0 ID 6
PHI     REFERENCE -0.125 SPEED 4000 SLOW 200 ACC 20000 TIMEOUT 180 METHOD 20
PHI     HASNOMIN HASNOMAX HASREF NOINITMIN NOINITMAX NEGATIVE NOINITAUTO
!
! Theta: CAN-modul 1 (ID = 11)
! 1 mm  = 400 fsteps
! V  = 2000 fsteps/sec
! A   = 1000 fsteps/s*s
!
THETA STEPS 400 SPEED 2000 ACC 1000 TIMEOUT 120 ID 11
THETA   MINVAL 0.0  MAXVAL 30.0 DEFAULT 0.0
THETA   REFERENCE MIN -0.115  MAX 30.0  SPEED 2000 ACC 20000 SLOW 500
THETA   HASMIN HASMAX INITMIN NOINITMAX NEGATIVE NOINITAUTO
!
! Distance: CAN-modul 2 (ID = 12)
! 1 mm  = 400 fsteps
! V  = 4000 fsteps/sec
! A   = 4000 fsteps/s*s
!
DISTANCE STEPS 400 SPEED 4000 ACC 4000 DEF 400.0 TIMEOUT 120 ID 12
DISTANCE REFERENCE MIN 75.0  MAX 425.6  SPEED 2000 ACC 20000  SLOW 500
DISTANCE HASMIN HASMAX NOINITMIN INITMAX POSITIVE NOINITAUTO
!
! Vertical translation: CAN-modul 3 (ID = 13)
! 1 mm  = 20000 fsteps
! V     = 800  fsteps/sec
! A     = 2000 fsteps/s*s
!
TRANS VER  STEPS 20000 SPEED 800 ACC 2000 TIMEOUT 333 ID 13
TRANS VER  MINVAL -7.5  MAXVAL 7.5  DEFAULT 0.0
TRANS VER  REFERENCE MIN -7.80  MAX 7.80  SPEED 800 SLOW 500 ACC 2000
TRANS VER  HASMIN HASMAX INITMIN INITMAX POSITIVE NOINITAUTO
!
! Vertical rotation: CAN-modul 4 (ID = 14)
! 1 mm  = 2500 fsteps
! V     = 4000 fsteps/sec
! A     = 2000 fsteps/s*s
!
```

```
ROTAT VER  STEPS 2500 SPEED 3000 ACC 2000 DEF 0.0 TIMEOUT 444 ID 14
ROTAT VER  MINVAL -17.0  MAXVAL 35.0  DEFAULT 0.0
ROTAT VER  REFERENCE MIN -18.0  MAX 37.00 SPEED 3000 SLOW 500 ACC 10000
ROTAT VER  HASMIN HASMAX INITMIN INITMAX POSITIVE NOINITAUTO
!
! Horizontal translation: CAN-modul 5 (ID = 15)
! 1 mm  = 1600 fsteps
! V     = 4000 fsteps/sec
! A     = 10000 fsteps/s*s
!
TRANS HOR  STEPS 1600 SPEED 4000  ACC 10000 DEF 0.0 TIMEOUT 555   ID 15
TRANS HOR  MINVAL -9.8   MAXVAL 9.8  DEFAULT 0.0
TRANS HOR  REFERENCE MIN -10.00  MAX 10.00 SPEED 4000 SLOW 500 ACC 10000
TRANS HOR  HASMIN HASMAX INITMIN INITMAX POSITIVE NOINITAUTO
!
! Horizontal rotation: CAN-modul 6 (ID = 16)
! 1 mm  = 1600 fsteps
! V     = 4000 fsteps/sec
! A     = 10000 fsteps/s*s
!
ROTAT HOR  STEPS 1600 SPEED 4000 ACC 10000 DEF 0.0 TIMEOUT 666 ID 16
ROTAT HOR  MINVAL -33.0   MAXVAL 33.0  DEFAULT 0.0
ROTAT HOR  REFERENCE MIN -34.00  MAX 34.00 SPEED 4000 SLOW 500 ACC 10000
ROTAT HOR  HASMIN HASMAX INITMIN INITMAX NEGATIVE NOINITAUTO
!
! Crystal Z-translation: CAN-modul 7 (ID = 17)
! 1 mm  = 1600 fsteps
! V     = 4000 fsteps/sec
! A     = 10000 fsteps/s*s
!
CRYSTAL Z  STEPS 1600 SPEED 4000 ACC 10000 DEF 0.0 TIMEOUT 777 ID 17
CRYSTAL Z  REFERENCE MIN -20.00 MAX 20.00 SPEED 4000 SLOW 500 ACC 20000
CRYSTAL Z  HASMIN HASMAX NOINITMIN INITMAX NEGATIVE NOINITAUTO
!
! Chi: CAN-modul 8 (ID = 18)
! 1 deg = 437.5 fsteps
! V     = 2000 fsteps/sec
! A     = 10000 fsteps/s*s
!
CHI        USE
CHI        MAXVAL 90.0 DEFAULT 0.0  BACKLASH 0.5
CHI        STEPS 437.5 SPEED 2000 ACC 10000 TIMEOUT 888 ID 18
CHI        REFERENCE MIN -0.00   MAX 90.00 SPEED 1000 SLOW 100 ACC 20000
CHI        HASMIN HASMAX INITMIN NOINITMAX NEGATIVE NOINITAUTO
!
! ============================================================================
! Optional additional motors, e.g. for sample changer ...
! ============================================================================
!
! Crystal x-translation: CAN-modul 9 (ID = 25)
! 1 deg = 20480/360 = 56.888 steps
! 1 mm  = R*sin(x) with R=3.0
! V     = 1000 fsteps/sec
! A     = 5000 fsteps/s*s
!
CRYSTAL X  USE
CRYSTAL X  STEPS 56.888 SPEED 800 ACC 5000 DEF 0.0 BACK 0.0 TIMEOUT 777 ID 26
CRYSTAL X  REFERENCE MIN -1.650  MAX 1.300  SPEED 500 SLOW 500 ACC 3000
CRYSTAL X  INITMIN INITMAX HASMIN HASMAX NEGATIVE NOINITAUTO
CRYSTAL X  OFFSET  0.0
!
! Crystal y-translation: CAN-modul 10 (ID = 26)
! 1 deg = 20480/360 = 56.888 steps
! 1 mm  = R*sin(x) with R=3.0
! V     = 1000 fsteps/sec
! A     = 5000 fsteps/s*s
!
CRYSTAL Y  USE
CRYSTAL Y  STEPS 56.888 SPEED 800 ACC 5000 DEF 0.0 BACK 0.0 TIMEOUT 777 ID 27
CRYSTAL Y  REFERENCE MIN -1.801  MAX 1.300  SPEED 500 SLOW 500 ACC 3000
CRYSTAL Y  INITMIN INITMAX HASMIN HASMAX POSITIVE NOINITAUTO
CRYSTAL Y  OFFSET  0.0
!
! Cryo actuator: CAN-modul 11 (ID = 24)
! 1 mm  = 1600 fsteps
! V     = 4000 fsteps/sec
! A     = 10000 fsteps/s*s
!
ACTUATOR    USE
ACTUATOR    STEPS 1600 SPEED 3000 ACC 10000 DEF 0.0 TIMEOUT 888 ID 24
ACTUATOR    BACKLASH 0.0 MINVAL 0.0 MAXVAL 24.9
ACTUATOR    REFERENCE MIN 0.00  SPEED 3000 SLOW 1500 ACC 10000
ACTUATOR    HASMIN HASNOMAX INITMIN NOINITMAX HASNOREF POSITIVE NOINITAUTO
!
! ============================================================================
```

```
! Remote control settings
! ============================================================================
!
REMOTE     USE
REMOTE     MASK 16777215     ! for csc,  without actuator use: 16777214
REMOTE     ADC      ENABLE NOEDIT
REMOTE     THETA    POS1 0.0     POS2   5.0 ENABLE EDIT
REMOTE     DISTANCE POS1 DYNAMIC POS2 300.0 ENABLE EDIT
REMOTE     CHI      POS1 0.0     POS2  60.0 ENABLE EDIT
REMOTE     BEAMSTOP POS1 18.0    POS2  45.0 ENABLE EDIT
!
! To enable beamstop on button CRYO run the following commands first:
! dtbcmd 103,1,41,5
! dtbcmd 103,1,40,100
! dtbcmd 103,1,39,500
! dtbcmd 103,1,38,-300
! dtbcmd 103,1,37,-120
! These commands need to be given only once and the dtb needs to be rebooted
! afterwards.
!
! =============================================================================
! WARNING WARNING WARNING WARNING WARNING WARNING WARNING WARNING WARNING WARN
! =============================================================================
!
! USE CRYO and USE AMPTEK protect the detector from
! driving into collision. If these keywords are removed while
! the cryo-system INCLUDING cryo-mount (!!!) or AMPTEK are present
! considerable damage to both detector and dtb can be produced.
!
! When setting IGNORE CRYO it is ESSENTIAL to also remove
! the cryo-mount (by removing part of the cryo-stream exhaust).
!
! =============================================================================
!
USE       CRYO
CRYOPARAM OXFORD
! CRYOPARAM XTREME
! CRYOPARAM DISTANCE 0 THETA 25
IGNORE    AMPTEK
!
! =============================================================================
! =============================================================================
! ==                                                                         ==
! ==                     Keywords affecting mar345 only                      ==
! ==                                                                         ==
! =============================================================================
! =============================================================================
!
GAIN            100U 1.00  150U 0.63
!
! Never ever change keywords from here on
!
MODE 2300       ROFF 120     ADC 50 AADD -42  BADD -42
MODE 2000       ROFF 120     ADC 50 AADD -42  BADD -42
MODE 1600       ROFF 120     ADC 50 AADD -42  BADD -42
MODE 1200       ROFF 120     ADC 50 AADD -42  BADD -42
!
MODE 3450       ROFF 120     ADC 50 AADD -42  BADD -42
MODE 3000       ROFF 120     ADC 50 AADD -42  BADD -42
MODE 2400       ROFF 120     ADC 50 AADD -42  BADD -42
MODE 1800       ROFF 120     ADC 50 AADD -42  BADD -42
!
FLAG  0
!
!IP-Diameter:   345mm    300mm    240mm    180mm
!GAPS           89659    78656    63903    49146    (08:49 on 30-Oct-2000)
!
```

9.3 Calibration Files

If used with a *mar345*-detector, program *mar345dtb* requires calibration files. Those calibration files contain flood field correction factors as well as the geometrical information required to transform spiral coordinates into a Cartesian grid system. The file names are:

- `$MARLOGDIR/mar2300.$MAR_SCANNER_NO`
- `$MARLOGDIR/mar3450.$MAR_SCANNER_NO`

These files are very large in size (73 MB and 103 MB, respectively). Every time the scanner reads out the plate this file has to be processed. While most of the file contents are binary data, some part of the header is ASCII. Program *catmar* allows to look into the header.

9.4 Parameter File

Program *mar345dtb* continuously saves parameters whenever they change within the program. When starting the program, the saved parameters are read back so the user always finds the latest changes after quitting a *mar345dtb* session. The parameter file read at startup is called `dtb.dat` and resides in directory `$MARLOGDIR`. If the parameter file doesn't exist, program defaults will be used. The program, however, will always create a new parameter file `dtb.dat`. The parameter file is a keyworded ASCII-file which may be edited.

Parameter files can be created and loaded from within the program. This is useful when working on a project where you always apply the same set of parameters. The parameter files carry the extension ".set" and may be saved using the "**Edit -> Save Parameters ...**" menu option in the main window. The parameters can be read back by using the "**Edit -> Load Parameters ...**" menu option (**also see chapter 6.2** in section **Edit**).

9.4.1 Keywords

The keywords used in the parameter file `dtb.dat` are as follows:

Table 2: Keywords in `dtb.dat`

Keyword	Arguments	Example	Description
SET	N USE|SKIP	9 USE	N is the data set number followed either by string USE or SKIP
DIRECTORY	STR	/data	STR is a string with a path name
ROOT	STR	xtal	STR is a string with image root name
SCANMODE	N	1200	N is one of 8 scanmodes, either 1200, 1600, 1800, 2000, 2300, 2400, 3000 or 3450
FORMAT	mar|cbf	mar	Image output format: either "mar" or "cbf"
COLLECT	TIME|DOSE	TIME	Exposure mode, either TIME or DOSE
BLOCKS	N	1	N is the number of PHI-blocks
NFRM	N	50	N is the number of images per block
FFRM	N	1	N is the first image number
OSCI	N	1	N is the number of oscillations
DPHI	F	0.5	F is the Delta-PHI per image
IPHI	F	0.0	F is the PHI-increment between images
DISTANCE	F	220.0	F is the distance detector-to-sample
PHI	F	45.0	F is the starting PHI angle
CHI	F	0.0	F is the current CHI angle
THETA	F	0.0	F is the current 2-theta angle
WAVE	F	1.54178	F is the current wavelength
BEAMSTOP	F	18.5	F is the current beamstop position
XTAL_Z	F	0.0	F is the relative crystal translation
SLIT1	F G	0.71 0.63	F and G are hor. and ver. slit apertures for chamber 1 slits
SLIT2	F G	0.45 0.43	F and G are hor. and ver. slit apertures for chamber 2 slits
ERASE			Erase plate before starting data collection
PHOTO			Save crystal photo after each image
THUMBNAIL			Produce thumbnails from data images during data collection
SPIRAL			Also create raw spiral images during data collection
OPTIMIZE START			Optimize beam before starting data set
OPTIMIZE	[-]N IMAGE|HRS|MIN|LOSS	30 LOSS	Optimize beam during data collection after given time or after N images or after N percent loss of X-ray intensity. A negative sign preceding N indicates this option to become deselected.
APPEND	[SET] [VIAL] [BARCODE]	SET BARCODE	Append set and/or vial no. and/or barcode (+identifier) to file root on image creation
VIAL	N	14	Carousel position to take sample from
CENT	NONE|MANUAL|XYZ|AUTO [CONFIRM] [SHIFT]	XYZ CONFIRM	Crystal centering method, XYZ and AUTO may be followed by CONFIRM, XYZ may also be followd by SHIFT

Keyword	Arguments	Example	Description
COMOPT	[1][+2][+3][+4][+5]	2+5	Selection of parameters to pass to shell script dtb.csh
COM1/2/3/4/5	STR	sleep 1	Custom argument for shell script dtb.csh

Up to here, the keywords are valid for the "SET" number given on the top. With a new SET keyword, the following keywords will be valid for that new set, so a dtb.dat may contain data for all 30 possible sets and the corresponding entries will be used to update the "**Edit**"-page. A couple of keywords have to be given only once since they are not related to that page:

Keyword	Type	Value	Description
SOURCE	STR	Rotating Anode	STR is the id of the X-ray source as given in the "Header Info"-window
POWER	F G	50.0 100.0	F and G are kV and mA settings of X-ray source as given in the "Header Info"-window
FILTER	STR	Mirrors	STR is the id of the monochromator as given in the "Header Info"-window
CENT	F G	0.0 0.0	Deviations of center coordinates as given in the "Header Info"-window
TRANSLATIONS	F G	-2.048 -1.888	Refined beam positions of motors TRANS_HOR and TRANS_VER
ROTATIONS	F G	-3.241 1.435	Refined beam positions of motors ROT_HOR and ROT_VER
ADVANCED|SIMPLE			Choice of advanced or standard layout for "Edit..."-window
CSC	N1 N2 N3 N4 N5 N6 [NO]SHIFT [NO]STORE	3 2 5 4 4 18	Values to fill in into the "**CSC operation**"-fields on the "**CSC**"-page (Change sample, etc.).
MARMUX	N or STR	1 or TTL	Choice of "Close generator shutter after finishing data collection"

9.4.2 Example

The following example contains parameters for only 1 data set.

```
#======================================================
# Date: Mon Feb 18 19:03:08 2002
# Automatically saved by mar345dtb: DO NOT EDIT!!!
#======================================================
# ----------------------------------
SET        1  USE
DIRECTORY /home/mar345/data/
ROOT       xtal
SCANMODE   1200
FORMAT     mar
COLLECT    DOSE
TIME       10
BLOCKS     1
NFRM       1
FFRM       2
OSCI       1
DPHI       1.000
IPHI       89.000
DISTANCE   350.000
PHI        45.000
CHI        -0.000
THETA      0.000
WAVE       1.541790
BEAMSTOP   10.050
XTAL_Z     0.000
SLIT1      0.710  0.630
SLIT2      0.400  0.400
OPTIMIZE   START
OPTIMIZE   -30 images
ERASE
PHOTO
THUMBNAIL
# ----------------------------------
# --- Shell commands  ---
COMOPT     1+5
COM1
COM2
COM3
```

```
COM4
# --- Optional Header Info ---
SOURCE    Rotating Anode
POWER     50.00   100.00
FILTER    Mirrors
POLAR     0.000
CENT      0.0  0.0
REMARK
# --- Refined X-ray beam positions ---
TRANSLATIONS     -2.048    -1.888
ROTATIONS        -3.261    -2.508
# --- Edit Data Collection in expert mode ---
ADVANCED DATA COLLECTION FEATURES
# --- Crystal translation disabled in Edit ---
XTAL_Z    DISABLED
# --- Sample Changer Settings: Change, Load, Unload, Give, Take, Pin ---
CSC       1 2 1 2 2 18 SHIFT NOSTORE
MARMUX    1
```

9.5 Command File

Program *mar345dtb* may be completely driven by external commands, i.e. all relevant settings and push-button actions can be bypassed. The command interface comes into variants:

- a plain ASCII-file $MARLGODIR/dtb.com with a syntax identical to the **Parameter File** with some extensions.
- a TCP/IP-socket

This ASCII-file interface becomes active, if the configuration file has a positive argument on keyword COMMAND. A typical value would be "COMMAND 1000", i.e. the program would look all 1000 msec for existence of a file dtb.com. If it does exist, it is read and evaluated . If it does contain a command, the file will be deleted (!) and the command will be executed. While the given command is in progress, a new dtb.com may be created, but it will be evaluated only after the previous command has completed - except commands that contain a STOP or ABORT signal. External programs may monitor the progress of the activity either by evaluating the dtb.log, dtb.spy or dtb.status files, all residing in $MARLOGDIR.

The TCP/IP-interface becoms active, if the configuration file has a negative argument on keyword COMMAND. A typical value would be "COMMAND -8678", i.e. the program would listen on UNIX port 8678 for connections. The program allows for multiple connections on the same port. The syntax for commands to be accepted via the TCP/IP-port is identical to the dtb.com file, i.e. ASCII strings will be evaluated. In return, the TCP/IP-socket writes ASCII-strings back to the same socket containing status information. The syntax is the same as used in the dtb.status file. The frequency is approx. 1/sec.

Note, that the command interface can be used together with the GUI but bears a considerable risk of unwanted or unforeseen dtb or mar345 activity. It must be stated that usage of the command interface is beyond the responsibility of *marresearch* and all damage produced by running commands using that command interface are not within our liability!

As stated above, all the syntax of the parameter file is used to modify settings of the data collection parameters, i.e. all parameters belonging to a given "SET" will be used to override the corresponding parameters on the "**Edit**"-pages. The main difference is that the command file in addition to the (optional) keywords of the data collection parameters requires additional lines that actually provide a command to be executed. This line always starts with keyword COMMAND followed by the following arguments:

Table 3: Arguments for keywords COMMAND in `dtb.com`

Arguments	Example	Description
ERASE	ERASE	Erase the image plate
SCAN filename	SCAN /data/lysozyme_001.mar1200	The filename must follow the mar345dtb conventions. The scanmode and format will be taken from the image extension.
CHANGE <mode>	CHANGE 1200	Change the scanmode to: 1200, 1600, 2000, 2300, 1800, 2400, 3000 or 3450.
IPS n1,n2,...	IPS 4,0	Native controller command for the mar345 image plate.
DTB n1,n2,...	DTB 101,0	Native controller command for the dtb.
SHUTTER [OPEN|CLOSE]	SHUTTER CLOSE	Open or closes the shutter (or toggles current state).
MOVE <motor> <value>	MOVE PHI 90.0	Drive <motor> to <value>. The motor must be a string as given in chapter **Motors** in section **Introduction**.
DEFINE <motor> <value>	DEFINE DISTANCE 250.0	Define position of <motor> to be <value>. Beware: this command is VERY CRITICAL and should normally not be used.

Arguments	Example	Description
INIT <motor> MIN|MAX|REF	INIT THETA MIN	Initialize <motor> motor at minimum (near end), maximum (far end) or reference.
OPTIMIZE [FIRST] [SECOND]	OPTIMIZE	Optimization beam in first and/or second chamber. Omitting FIRST and SECOND means using BOTH. COMMAND OPTIMIZE requires additional parameters to be provided on the OPTIMIZE keyword (see below).
FIND [FIRST] [SECOND]	FIND SECOND	Find the beam in first and/or second chamber. COMMAND FIND requires additional parameters to be provided on the FIND keyword (see below).
PROFILE [SLIT <h> <v>] [HOR <hor>] [VER <ver>] [PITCH <val>]	PROFILE HOR 1.5 VER 1.5 SLIT 0.1 0.1 PITCH 0.05	Produce a beam profile covering <hor> mm in HORIZONTAL direction and <ver> mm in VERTICAL direction using slit apertures in chamber 1 of <h> and <v> mm, respectively. The advance per vertical movement will be <valr> mm. If some arguments are missing, the current settings of the GUI will be used.
SHAPE [CHAMBER] 1|2 [HOR|VER <val>] [TRUNCATE <t>] [SPEED <per>]	SHAPE 1 HOR 0.9 TRUNCATE 15 SPEED 20	Produce a beam shape plot for chamber 1 or 2 for the HORIZONTAL or VERTICAL slit, using an aperture for the non-moving slit of <val> mm at a speed of <per> percent . If some arguments are missing, the current settings of the GUI will be used.
ADJUST [CHAMBER] 1|2 [WEAK|STRONG] [[OFFSET] <v>] [TOLERANCE <tr>]	ADJUST CHAMBER 1 OFFSET 1000 TOL 10 CHAMBER 2 OFF 1000 TOL 20	Reset the ADC readings of chambers 1 or 2 to <v> units with a tolerance of <t> units. If some arguments are missing, the current settings of the GUI will be used.
COLLECT [<s1>] [<s2>] [<s3>] ...	COLLECT 3 8 24	Collect data for sets <s1>, <s2>, etc. Please note, that unless the sets are being reprogrammed by the same command file (using the syntax of the dtb.dat file), the current values in the Edit-page of the GUI for the desired set are going to be used.
STOP [AFTER IMAGE|SET] [NOW]	STOP AFTER SET	Stop a data collection after finishing current IMAGE or current SET, or stop a motor movement NOW.
CONTINUE [AFTER] IMAGE|SET	CONTINUE AFTER IMAGE	Undoes the effect of STOP AFTER IMAGE or STOP AFTER SET.
ABORT	ABORT	Immediately stops current activity.
QUIT	QUIT	Makes program mar345dtb shutdown.
CSC {CHANGE <vial>} | {LOAD <vial>} | UNLOAD {GIVE <vial>} | {TAKE <vial>} | INIT | RESET | {MAGNET ON|OFF} | {SAVE <file>} | {READ <file>} |	CSC LOAD 18	Sample changer operations as described in chapter **CSC Operations** in section **CSC**. The commands CSC SAVE and CSC READ will save or read sample status files, respectively.
CRYSTAL FIND |{CENTER [XY] [<x> <y> <z>]}	CRYSTAL CENTER	Triggers a crystal finding or centering procedure as described in chapter **Crystal Centering** in section **Crystal**. While FIND works without further options, CENTER may be followed by xyz-coordinates. If they are omitted, the automatic procedure will be tried.

9.6 Shell Script

Program *mar345dtb* allows to run external commands at certain times during data collection:

- before starting a data set
- before starting an exposure
- after finishing an exposure
- after finishing a detector readout

In all cases, the program relies on the existence of an executable shell script called `dtb.csh` which must reside in directory $MARLOGDIR. If that file doesn't exist, the program will continue immediately with the next step of data collection. Otherwise, the data collection will only continue if the commands in the shell script are finished. The shell script may be edited to add any desired command.

The following listing contains a very simple template for file `dtb.csh`.

```
#!/bin/csh -f
set argc  = $#argv
set NUM  = 2
set cmd  = $1
set LOG  = ( $MARLOGDIR/dtb.csh.log )
while ( $NUM <= $argc )
 set cmd = ( $cmd $argv[$NUM] )
 @ NUM++
end
#
echo "==============================================================" >> $LOG
echo "Time:    `date`" >> $LOG
echo "Command: $cmd"   >> $LOG
echo "==============================================================" >> $LOG
#
# Actual command
#
echo $cmd
sleep 2
#
exit
```

9.7 Images

mar345dtb autodetects image file formats. The program actually looks at contents of files rather than at file names only. *mar345dtb* accepts the following image formats:

Table 4: Image formats accepted by *mar345dtb*

Format	Name suffix	Description
mar345	.marXXXX	Images produced by mar345 detector
cbf	.cbfXXXX	Images produced by mar software in CBF format
image	.image	Original format of 180mm/300mm scanners
pck	.pck	Images of 180mm/300mm scanners, "pck"-compressed.
marccd	.mccd or .####	Images of marCCD detector

9.8 Carousel File

Program *mar345dtb* continuously saves carousel data whenever they change within the program. When starting the program, the saved parameters are read back so the user always finds the latest changes after quitting a *mar345dtb* session. The carousel file read at startup and updated during program execution is called `$MARLOGDIR/csc/CSC.csv`. The format is described in chapter **Carousel File** in section **Output**.

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10. Output

10.1 Overview

Program *mar345dtb* produces a number of output files:

Table 1: *mar345dtb* output files.

File type	File name	Description
Lock file	$MARLOGDIR/dtb.lock	A file indicating that another session of program *mar345dtb* is still active.
Message file	$MARLOGDIR/mar.message	File used at startup by program *marstart*
Log file	$MARLOGDIR/log/dtb.log.N	Log file with slightly more extensive output than printed on the terminal screen (stdout)
SPY file	$MARLOGDIR/spy/dtb.spy.N	Log file with native messages of the *dtb* controller
SPY file	$MARLOGDIR/spy/mar.spy.N	Log file with native messages of the *mar345* controller
Image statistics	$MARLOGDIR/lp/mar.lp.N	Log file with statistical information about produced images
Current params	$MARLOGDIR/dtb.dat	Saved parameters from "Edit"-page
Status file	$MARLOGDIR/dtb.status	Optional status file that is updated regularaly
Carousel file	$MARLOGDIR/csc/CSC.csv	Carousel parameters from "CSC"-page
Beam history	$MARLOGDIR/beam/dtb.time.N	Binary file containing a history of the ionization chamber readings
Motor scan	$MARLOGDIR/beam/dtb.scan.N	ASCII file containing ionization chamber readings as function of a motor positions
Beam profile	$MARLOGDIR/beam/dtb.profile.N	Binary file containing the result of a beam profile determination
Beamplot	$cwd/beamplot.xwd	Screen dump of plot in "**Alignment**"-window saved in X system window dump format
Thumbnails	.jpg	Thumbnail image of data image produced during data collection
Crystal photo	.jpg	Crystal photo in jpg format produced during data collection

File type	File name	Description
Data Images	.marXXXX | .cbfXXXX	Image files in mar or cbf format produced during data collection
Summary (ASCII)	.SUMMARY	ASCII file with current data set parameters produced during data collection
Summary (HTML)	.html	HTML file with current data set parameters produced during data collection
Errors	.ERRORS	List of images that contained some sort of errors during data collection
Empty image	$MARLOGDIR/xtal/empty.jpg	CSC only: latest background picture of goniometer environment without sample mounted
Loop image	$MARLOGDIR/xtal/find.jpg	CSC only: latest picture to be used for automatic crystal finding

denotes a 3-digit serial number and usually is defined as $MAR_SCANNER_NO.

10.2 Lock File

ASCII file `$MARLOGDIR/dtb.lock` will be created at startup of program *mar345dtb*. Existence of this file indicates that a session is or might be active. The file will be deleted by the program when exiting the program. A program crash will leave the file where it is. If the file already exists at program startup, the program will ask you to confirm wether you really want to start another instance of it. The main reason for this procedure is that the *dtb* and the *mar345*-controller reuse the network sockets for talking to the computer, so any attempt to open a new connection to the controllers will make previous connections useless!

10.3 Message File

ASCII file `$MARLOGDIR/mar.message` will be created at startup of program *mar345dtb*. This file reports wether the program is able to establish connection with the controllers. This message file will be read by program *marstart* which presents this information in a window to be acknowledged. In case of failure, the window allows to terminate the current *mar345dtb* process. Program *marstart* is called automatically by program *mar345dtb* and has no other functions.

10.4 Log File

ASCII file `$MARLOGDIR/log/dtb.log.N` will be created at startup of program *mar345dtb*. It contains essentially the same information as printed on the terminal where you run the program.

It is generally a good idea to keep some versions of this file for backtracing hardware problems. The number of file versions to be kept is configurable (keyword **VERSION LOG <max>** in the **Configuration File**). At startup the program determines automatically which version number "**N**" to use. If the current "**N**" exceeds "**max**", N restarts with 1.

The program automatically creates a soft link `$MARLOGDIR/dtb.log` pointing to the current log file `$MARLOGDIR/log/dtb.log.N`, so for looking into the file currently in use you don't have to descend to directory $MARLOGDIR/log and look at the creation dates of all log files.

10.5 Spy Files

At startup, program *mar345dtb* optionally creates ASCII files `$MARLOGDIR/spy/dtb.spy.N` and `$MARLOGDIR/spy/mar.spy.N`. These files contain native controller messages of both the *dtb* and the *mar345*-detector. The controllers produce very detailed information about all hardware processes.

It is generally a good idea to keep some versions of this file for backtracing hardware problems. The number of file versions to be kept is configurable (keyword **VERSION SPY <max>** in the **Configuration File**). At startup the program determines automatically which version number "**N**" to use. If the current "**N**" exceeds "**max**", N restarts with 1.

The program automatically creates a soft link `$MARLOGDIR/dtb.spy` pointing to the current spy file `$MARLOGDIR/spy/dtb.spy.N` and `$MARLOGDIR/mar.spy` pointing to the current spy file `$MARLOGDIR/spy/mar.spy.N`.

Note: the files may become quite large in size. It is therefore advisable to have sufficient disk space!

10.6 Statistics File

At startup, program *mar345dtb* optionally creates ASCII files `$MARLOGDIR/lp/mar.lp.N`. This file contains some statistical information of the images produced during data collection. This file is mostly used for calibration purposes and of little importance for the user.

The number of file versions to be kept is configurable (keyword **VERSION STATS <max>** in the **Configuration File**). At startup the program determines automatically which version number "**N**" to use. If the current "**N**" exceeds "**max**", N restarts with 1.

The program automatically creates a soft link `$MARLOGDIR/mar.lp` pointing to the current file `$MARLOGDIR/lp/mar.lp.N`.

10.7 Parameter Files

Program *mar345dtb* continuously saves parameters whenever they change within the program. When starting the program, the saved parameters are read back so the user always finds the latest changes after quitting a *mar345dtb* session. The parameter file read at startup and updated during program execution is called `$MARLOGDIR/dtb.dat`. The parameter file is a keyworded ASCII-file which may be edited. For syntax, consult chapter **Parameter File** in section **Input**.

Parameter files can be explicitly created from within the program. This is useful when working on a project where you always apply the same set of parameters. The parameter files carry the extension ".set" and may be saved using the "**Edit -> Save Parameters ...**" menu option in the "**Edit**"-page (**see chapters 6.2.3** in section **Edit**).

10.8 Status File

Program *mar345dtb* can be configured to periodically save current status information to file `$MARLOGDIR/dtb.status`. This ASCII-file contains information about motor positions and about progress of current tasks of the detector or *dtb*. The purpose for this is to give any other program a chance to exchange information with the mar hardware.

10.9 Beam History File

At startup, program *mar345dtb* creates the binary file `$MARLOGDIR/beam/dtb.time.N`. This file of fixed size (approx 1 MB) stores information about beam history as plotted in the "**Time**"-plot in the "**Align**"-window. Depending on how long time program *mar345dtb* has been running there may or may not be entries for displaying beam history in the 5, 10 or 30 minute units.

The number of file versions to be kept is configurable (keyword **VERSION TIME <max>** in the **Configuration File**). At startup the program determines automatically which version number "**N**" to use. If the current "**N**" exceeds "**max**", N restarts with 1.

10.10 Beam Scan File

When doing beam scans, i.e. digitization of ionization chamber readings as a function of some motor movement (translations, rotations, slits), program *mar345dtb* creates an ASCII file `$MARLOGDIR/beam/dtb.scan.N` for each scan. This file stores information about current motor positions in a header. The header is followed by a variable number of lines containing readings of chamber 1 and chamber 2, motor position of the moving motor and time (in Unix computer time notation). Stored files can be loaded and displayed in the plot area of the "**Align**"-window.

The number of file versions to be kept is configurable (keyword **VERSION SCAN <max>** in the **Configuration File**). At startup the program determines automatically which version number "**N**" to use. If the current "**N**" exceeds "**max**", N restarts with 1.

10.11 Beam Profile File

Program *mar345dtb* is capable of establishing a beam profile by driving the horizontal and vertical translation motors around the beam at small slit sizes. Beam profiles are stored in binary format as `$MARLOGDIR/beam/dtb.profile.N`. This file stores information about current motor positions in a header. The header is followed by a digital array of data containing normalized chamber 1 readings for a given range of movement in x and y. Stored files can be loaded and displayed in the plot area of the "**Align**"-window.

The number of file versions to be kept is configurable (keyword **VERSION PROFILE <max>** in the **Configuration File**). At startup the program determines automatically which version number "**N**" to use. If the current "**N**" exceeds "**max**", N restarts with 1.

10.12 Beamplot File

All plots displayed in the plot area of the "**Align**"-window can be saved into file `beamplot.xwd` (no other choice of filename) of the current working directory. Existing beamplot.xwd files will be overwritten without warning. The file format is "**XWD**" (X Windows system window dump file). There are utilities for converting this format into many other image formats (png, jpg), the most useful and popular being the ones from the ImageMagick suite available for all Unix flavours, in particular program *convert*.

10.13 mar2thumb: Thumbnail Conversion Script

It is possible to produce data image thumbnails with the help of a conversion program. The command to use can be specified in the configuration file and defaults to "**mar2thumb**" which is a shell script that calls other programs. The shell script shown below calls program **marcvt** to convert a data image into a full size tiff file. The next step is reduction to a suitable thumbnail size and conversion into a compressed graphics format in order to save space. The shell script implies that the called programs (marcvt and convert) are in the executable search path otherwise, the thumbnail creation will fail. The shell script given here will be called during data collection each time an image has been stored on disk. The shell script gets that image file name as argument. The resulting thumbnail will be stored in subdirectory "thumb" of the data directory:

```
#!/bin/csh -f
#
# Parse command line
#
set done  = 0
set v   = 0
set show = 0
```

```
set q  = 50
set p  = 20
set D  = ( none )

while ( $done == 0 )

 switch ($1 )
   case '-o':
   case '-d':
   case '--directory':
 set D   = $2
 set argv  = ( $argv[3-] )
 breaksw

   case '-q':
   case '--quality':
 set q   = $2
 set argv  = ( $argv[3-] )
 breaksw

   case '-p':
   case '--percent':
 set p   = $2
 set argv  = ( $argv[3-] )
 breaksw

   case '-s':
   case '--show':
 set show = 1
 set argv  = ( $argv[2-] )
 breaksw

   case '-v':
   case '--verbose':
 set v   = ( 1 )
 set argv  = ( $argv[2-] )
 breaksw

   case '-h':
   case '--help':
 goto usage
 breaksw

   default:
 set done  = 1
 breaksw
 endsw
end

#
# Remaining arguments on command line?
#
# First argument: complete image name
# Second argument: directory where to store thumbnail
if ( $#argv < 1 ) then
 goto usage
endif
set A = $1
#
# Split path into directory and filename
#
set DIR  = ( `dirname $A` )
set BASE = ( `basename $A` )
if ( $D == 'none' ) then
 set D  = ( ${DIR}/thumb )
endif
#
# Strip off suffix from BASE name
#
set B = ( `echo "$BASE" | awk '{ split( $1, a, "." ); print a[1] }'` )
#
if ( $#argv > 1 ) then
 set D = $2
endif
#
# Check if input file exists
#
if ( ! -f ${A} ) then
 echo "ERROR: Input file ${A} does not exist"
 goto usage
endif
#
# Check if output directory exists
#
if ( ! -d ${D} ) then
 mkdir ${D}
```

```
 if ( ! -d ${D} ) then
  echo "WARNING: Can't create output directory ${D}. Using current one"
  set D = ( . )
 endif
endif
#
# Convert mar image into tiff file and deposit in directory D
#
if ( $v == 1 ) then
 echo "Transform $A info tiff in: ${D} "
 marcvt -v -tiff --force $A -o ${D}
else
 marcvt -tiff --force $A -o ${D} > /dev/null
endif
#
# Convert uncompressed tiff files with N x N pixels into something smaller
# using standard Unix tools, e.g. convert from the ImageMagick package
#
cd ${D}
set IN = ( ${B}.tiff )
set OUT = ( ${B}.thumb.jpg )
if ( $v == 1 ) then
 echo "Converting ${IN} info ${OUT} "
endif
if ( -f ${IN} ) then
 convert -quality $q -geometry ${p}% ${IN}  ${OUT}
 echo "          Thumbnail: $OUT"
else
 echo "ERROR: marcvt didn't work on file ${A}"
 goto usage
endif
/bin/rm -f ${IN}
if ( $show == 1 ) then
 display ${OUT}
endif
exit
#
#
#
usage:
 echo "Usage: mar2thumb [OPTIONS] input_mar_image [output-directory]"
 echo "Options:"
 echo "       -h  --help              show usage"
 echo "       -v  --verbose           show messages                [dont]"
 echo "       -s  --show              display thumbnail            [dont]"
 echo "       -q  --quality N         quality for jpg              [50]"
 echo "       -p  --percent N         shrink original to N percent [20]"
 echo "       -d  --directoy D        output directory             [thumb]"
 EXIT
```

10.14 Data Images

mar345dtb produces images in 3 formats during data collection. See chapter **6.4 Directories, Names and Formats** of section **Edit** for more details about file formats.

Table 2: Image formats produced by *mar345dtb*

Format	Usual extension	Description
mar345	.marXXXX	Images in mar345 format
cbf	.cbfXXXX	Images in CBF format
spiral	.sXXXX	Raw spiral images

10.15 ASCII Summary File

During data collection, the program optionally produces an ASCII file containing all relevant information about parameters of the current data collection. The file will be saved into the current data directory and is called "**Image root**".N.SUMMARY. N is a number starting at 1 and is incremented if the file already exists. This file is useful for keep track of what has been done during the current data collection.

10.16 HTML Summary File

Same as the ASCII summary file, but in html format.

10.17 Automar Sync File

ASCII file that may be used by program marProcess to synchronize with processing. When configured (option 'USE AUTOMAR' in configuration file), the program writes a file rootname.sync into the current data directory. During data collection, this file is being updated with every image. Program marProcess can make use of this file to determine how many images to process. The syntax follows the requirements of the marProcess control files. See the automar documentation for further details.

10.18 Errors File

If an image has been recollected during a data collection because of some hardware problem, there will be a file written to the data directory containing the number of the images affected by an error. The file is called "**Image root**".N.ERRORS where N is a number starting at 1 and is incremented if the file already exists.

10.19 Images used for Crystal Finding

When using the sample changer, there is an option of automatically finding a crystal after it has been mounted. The method requires 2 images: one that contains an object ("**find.N.jpg**), i.e. a crystal to be located, and another that provides an empty background ("**empty.jpg**). Since the illumination of the sample is a critical parameter, the background file will be updated every time a new sample is mounted. This is done automatically by the mar345dtb program without user intervention. The images will be stored in directory $MARLOGDIR/xtal.

When calling the automatic crystal finding routines from within the program, the program **loopfind** will be executed. This program is called with 3 arguments:

1. $MARLOGDIR/xtal/find.N.jpg
2. $MARLOGDIR/xtal/empty.jpg
3. $MARLOGDIR/xtal/xhair.jpg

Please note, that N is a number running from 1 to 99 (configurable). I.e. after 99 versions have been created the photos will be cyclically overwritten.

For reasons of flexibility **loopfind** is a shell script that calls the program to actually do the work (typically program **marloop**):

```
#!/bin/csh -f
#
# Set some defaults
#
set N           = ( $#argv )
set dir         = ( ${MARLOGDIR}/xtal )
set skip        = ( )
set F1          = ( )
set F2          = ( )
set F3          = ( )
set done        = 0
set verb        = 0
set method      = 0
#
if ( $N < 1 ) then
        goto USAGE
endif
#
#
# Command line args
#
while ( $done == 0 )

        switch ( $1 )
# Verbosity
                case '-v':
                case '-verb':
                        @ verb++
                        set argv = ( $argv[2-] )
                        breaksw
# Method
                case '-m':
                case '-method':
                        set method = $2
                        set argv = ( $argv[3-] )
                        breaksw
# Directory
                case '-d':
                case '-dir':
                        set dir = $2
                        set argv = ( $argv[3-] )
                        breaksw
# Help
# Help
                case '?':
                case '-h':
                case '-help':
                        goto USAGE
                        breaksw
# Skip
                case '-s':
                case '-skip':
                        set skip = ( "-skip" )
                        set argv = ( $argv[2-] )
                        breaksw
#
```

```
#       End of cases
#
                default:
                        if ( ${F1} == '' ) then
                                set F1 = $1
                                if ( ${F1} == '' ) then
                                        set done = 1
                                else
                                        set done = 0
                                endif
                        else if ( ${F2} == '' ) then
                                set F2 = $1
                                set done = 0
                        else if ( ${F3} == '' ) then
                                set F3 = $1
                                set done = 0
                        else
                                set done = 1
                        endif
        endsw
end
#
# End of command line
#
if ( ${verb} > 0 ) then
        echo "Input file 1: ${F1}"
        echo "Input file 2: ${F2}"
        echo "Input file 3: ${F3}"
        echo "Directory   : ${dir}"
        echo "Method      : ${method}"
        echo "Skip        : ${skip}"
endif
#
# Argument is a filename containing crystal photos
#
if ( $N < 2  || ${method} == 1 ) then
        if ( ! -f ${F1} ) then
                goto USAGE
        endif
#
        cd ${dir}
        lis2txt FIND.lis XC.in
        if ( -f XC.log ) then
                /bin/rm XC.log
        endif
        XCentering XC.in XC.log
        if ( -f XC.log ) then
                CosFit -i XC.log -l CF.log
                echo ======================================================================
                if ( -f CF.log ) then
                        awk '{print "Result:    ", $2, $3, $4, $1}'  CF.log
                else
                echo "Result:    error in CosFit"
                endif
        else
                echo "Result:    error in XCentering"
        endif
        echo ======================================================================
#
# Arguments are: 1. xtal photo 2. empty photo 3. xhair photo
#
else if ( ${F1} != '' && ${F2} != '' && ${F3} != '' ) then
        echo "Running marloop"
        marloop ${skip} $1 $2 $3
else
        echo "ERROR running marloop "
        goto USAGE
endif
#
exit
#
USAGE:
echo "usage: loopfind   FIND.lis | find.N.jpg   empty.jpg  xhair.jpg"
exit
```

10.20 Carousel File

Program *mar345dtb* continuously saves carousel data whenever they change within the program. When starting the program, the saved parameters are read back so the user always finds the latest changes after quitting a *mar345dtb* session. The carousel file read at startup and updated during program execution is called `$MARLOGDIR/csc/CSC.csv`. The parameter file is a ASCII-file in Excel-type format using 8 columns:

1. **Vial no.:** 1 to 19
2. **Status:** one of "carousel", "mounted" or "empty"

3. **Barcode:** barcode on sample, e.g "A18B0001"
4. **Identifier:** arbitrary sample identification string, e.g "lysozyme"
5. **Pin:** Pin length in mm, either 14,16,18,21,24 or 0
6. **x y z:**Positions of xyz-translations of goniometer head where the crystal is located

All columns are separated by a colon (;). It is legal to leave a column empty, e.g. if the barcode is unknown or the xyz-coordinates are not yet determined.

During operation, the corresponding fields will be updated automatically. A barcode is usually updated in the loading process of a sample. The xyz-coordinates will be updated as a result of an automatic or manual centering process of a mounted sample. The identifier is an additional string that does not have further relevance for the program, but may help to identify samples.

All fields may be edited by hand, even the status field. When replacing an entire carousel manually, the information stored in the "**Carousel status**"-area of the "**CSC**"-page will become void. All positions should either be cleared by choosing menu option "**Clear carousel data**" in the "**CSC**"-menu of the main window. Otherwise, it is possible to manually compose a carousel file using the syntax as described above, deposit that file in directory $MARLOGDIR/csc and load the file using option "**Load carousel data**" in the "**CSC**"-menu of the main window.

The following contains an example of the contents of CSC.csv file:

```
! Generated by program mar345dtb on Fri Feb 27 11:09:59 2004
! and contains current settings of the mar CSC carousel
!
! Vial ; Status ; Barcode ; Identifier ; Pin ; x ; y ; z
1;carousel;B18A0153;Trypsin;18;-0.337;0.970;-4.713
2;mounted;A18B0020;Lysozyme;18;0.482;0.228;-3.460
3;empty;A18B0026;Myoglobin;18;0.482;0.228;-3.460
...
```

Edited on Nov 17, 2010

11. Appendix

11.1 *dtb* Firmware Upgrade

This chapter describes the procedure for upgrading the application software and operating system RTOS within the dtb controller.

11.1.1 Firmware Distribution

The firmware distribution contains two components: the application software (APPL) and the operating system (RTOS). The operating system RTOS is likely to be a stable distribution and in the an update of the RTOS is going to happen with low frequency. The application software is the part of the controller firmware that handles the details and is likely to undergo more frequent updates.

11.1.1.1 Apllication Software (APPL)

The following files form part of the application software. For firmware version ≥ 4.0:

- DTB4xx

For firmware versions ≤ 3.5:

- APPLLOAD
- APPLLOAD.LOC
- APPLLOAD.NET
- CANBIO.SR
- DTBH.SR
- IO.SR
- LOAD.BAT
- MAIN.SR
- MESSAGE.CSV
- SERVER.SR
- STEP.SR

11.1.1.2 Operating System (RTOS)

The following files form part of the operating system RTOS:

- sys36v#.fld

The # denotes the version number. As by November 2002, the current version number is "40".

11.1.2 Application Software Update

In the following section, red text denotes user commands. Text printed in green is the expected output on the terminal screen. Please do the following and note that strings are case sensitive:

- **Telnet into dtb.**
  In a terminal window, type:

```
telnet 192.0.2.3
```

```
Username: esd
```

There will be no prompt for a password but an immediate login. The output on the screen at login will look like this:

```
WD=/R1/HOME
XD=/
/R1/HOME/PROFILE--:  wrong command
```

⇨ **Add directory /R4 to the binary path.**
Type:

```
CXD /R4
```

The output on the screen will look like this:

```
WD=/R1/HOME
XD=/R4/-
```

11.1.2.1 Update Procedure for Firmware Version ≥ 4.0

⇨ **Reboot dtb without loading application.**
In the telnet session, type:

```
REBOOT NOAPPL
```

Wait about 15 seconds for the dtb controller to reboot, then telnet again into the dtb as described above (sections 1 and 2) using username "esd" with no password.
In the telnet session, on the command prompt, type command:

```
CXD /R4
memadd
```

⇨ **FTP the dtb firmware from subdirectory APPL of the distribution into directory /ED in the dtb.**

Do the following on your host computer:

```
cd APPL    (i.e. go to subdir. APPL of this distribution)
ftp   192.0.2.3
    Username:  esd_ftp
    Password:       <RETURN>        (i.e. no password)

passive         (SuSE  only) (i.e. toggle use of passive transfer mode)
epsv4  (SuSE  only) (i.e. toggle use of EPSV/EPRT commands)

    cd /ED        (i.e. go to directory /RF/BIN)
    binary           (i.e. use binary transfer mode)
    prompt           (i.e. turn off prompting)
    put DTB4xx          (i.e. copy file DTB4xx from directory APPL into /ED)
                        ('xx' denotes the version number)
```

⇨ **Burn application software into flash.**

Telnet into the dtb as described above (sections 1 and 2) using username "esd" with no password.
In the telnet session, on the command prompt, type command:

```
CXD /R4
APPUPD /ED/DTB4xx
```

BEWARE:

xx in DTB4xx gives the version number, e.g. DTB425.
This procedure takes approx. 1 minute to complete.
Do NOT switch off the dtb while APPUPD has not completed.
If you do so, restart the entire procedure with the first step.

⇨ **Reboot dtb.**

You may either power cycle the instrument or type the following command in the telnet session:

```
REBOOT FULL
```

11.1.2.2 Update Procedure for Firmware Version ≤ 3.5

- **Get disk /R2 from the flash memory and put it into RTOS memory as directory /RF.**

Type:

```
editappl
```

The output on the screen will look like this:

```
EDITAPPL: start
>> #SRAM : NO_BAD BLOCK(S)

>> DISCMOVE/0084: (terminate)
EDITAPPL: done.
```

Keep this session open.

- **FTP the dtb firmware from subdirectory APPL of the distribution into directory /RF/BIN in the dtb.**

Do the following on your host computer:

```
cd APPL    (i.e. go to subdir. APPL of this distribution)
ftp   192.0.2.3
    Username:  esd_ftp
    Password:       <RETURN>        (i.e. no password)

passive         (Linux only) (i.e. toggle use of passive transfer mode)
epsv4  (Linux only) (i.e. toggle use of EPSV/EPRT commands)

    cd /RF/BIN    (i.e. go to directory /RF/BIN)
    binary           (i.e. use binary transfer mode)
    prompt           (i.e. turn off prompting)
    mput *           (i.e. copy all files from directory APPL into /RF/BIN)
```

BEWARE:

Make sure that all files are transferred in uppercase! If you are getting errors while transferring files into the controller the most likely reason is that the storage area inside the controller is full due to multiple versions of the desired files. By giving the "DIR" command in the FTP session you may want to check that there is only one version of file APPLLOAD (and not another one named "applload"). In that case, the safest thing to do is to power cycle the controller and start all over again!

- **Burn application software into flash.**

In the telnet session, on the /RF/-> prompt, type command:

```
saveappl
```

BEWARE:

This procedure takes approx. 1 minute to complete.
Do NOT switch off the dtb while saveappl has not completed.
If you do so, restart the entire procedure with the first step.

The output on the screen will look like this:

```
SAVEAPPL: Please wait until "all done" appears.
SAVEAPPL: Clearing Bank 1...9 and saving /R2...
SAVEAPPL: Clearing Bank 1...9
```

```
>> CLEARFLASH/0086: (terminate)
SAVEAPPL: Clearing Bank 1...9 done.
SAVEAPPL: SAVING /R2 ...

>> MOVETOFLASH/0087: (terminate)
SAVEAPPL: SAVING /R2 ...done
SAVEAPPL: all done.
```

- **Reboot dtb.**

  You may either power cycle the instrument or type the following command in the telnet session:

  ```
  system_reset
  ```

- **Restore variables and reboot.**

  After reboot, telnet into the dtb and type command:

  ```
  PARA_DEFAULT 0
  ```

  There will be no feedback for this command. Afterwards, reboot again.

11.1.3 Operating System Update

In the following section, red text denotes user commands. Text printed in green is the expected output on the terminal screen. Please do the following and note that strings are case sensitive:

- **Transfer operating system into dtb via FTP.**
  FTP the RTOS operating system from subdirectory RTOS of this distribution into directory /ED in the dtb. Do the following on your host computer:

  ```
  cd RTOS                         (i.e. go to subdir. RTOS of this distribution)
  ftp   192.0.2.3
       Username:  esd_ftp
       Password:       <RETURN>        (i.e. no password)

  passive         (Linux only)    (i.e. toggle use of passive transfer mode)
  epsv4  (Linux only)    (i.e. toggle use of EPSV/EPRT commands)
       cd /ED            (i.e. go to directory /ED)
       binary           (i.e. use binary transfer mode)
       prompt           (i.e. turn off prompting)
       mput *           (i.e. copy all files from directory RTOS into /ED)
  ```

  In your terminal window, you should see something similar to:

  ```
  binary
  200 TYPE Command ok, Type set to IMAGE.
  dtb:/R3>
  dtb:/R3>
  dtb:/R3> cd /ED
  250 Requested fileaction okay, completed.
  dtb:/ED> mput *
  local: sys36v10.fld remote: sys36v10.fld
  200 PORT Command ok.
  150 Opening data connection for sys36v10.fld (192.0.2.2,30682).
  100% |*************************************|   497 KB  111.49 KB/s    00:00 ETA
  226 Closing data connection. Successful.
  509870 bytes sent in 00:04 (107.40 KB/s)
  ```

  After file transfer, check contents of directory /ED by typing "DIR" in the FTP session. You should see something similar to:

  ```
  dtb:/ED> dir


  200 PORT Command ok.
  150 File status ok; about to open data connection (192.0.2.2,30681).
  -rwxrwxrwx  1 esd rtos            1     -- 00:09 tmp03
  -rwxrwxrwx  1 esd rtos       509870     -- 00:09 sys36v10.fld
  lrwxrwxrwx  1 esd rtos            0           :   LIB
  226 Closing data connection. Successful.
  ```

- **Telnet into dtb.**

In a terminal window, type:

```
telnet  192.0.2.3
Username: esd
```

There will be no prompt for a password but an immediate login.
The output on the screen at login will look like this:

```
WD=/R1/HOME
XD=/
/R1/HOME/PROFILE--:  wrong command
```

➪ **Add directory /R4 to the binary path.**

In the telnet session, type:

```
CXD /R4
```

The output on the screen will look like this:

```
WD=/R1/HOME
XD=/R4/-
```

➪ **Burn new RTOS into flash.**

Type:

```
sysupd /ED/sys36v10.fld  USER-RTOS
```

BEWARE:

This procedure takes approx. 2 minutes to complete.
Do NOT switch off the dtb while sysupd has not completed.
If you do so, restart the entire procedure with first step.

The output on the screen will look like this:

```
/ED/->sysupd /ED/sys36v10.fld  USER-RTOS

USER-RTOS booted.
SYSUPD: USER-RTOS booted.
SYSUPD: Flash USER-RTOS.

>> LOAD/0025: (terminate)
SYSUPD: FLLOAD loaded.
SYSUPD: Please wait until "all done" appears.
SYSUPD: REWIND  /ED/sys36v10.fld  OK.
SYSUPD: Clearing Bank 101 ... and flashing rtos-image...
SYSUPD: Clearing Bank 101 ...

>> CLEARFLASH/0026: (terminate)
SYSUPD: Clearing Bank 101 ... done.
SYSUPD: Flashing rtos-image (bank  101 ...) /ED/sys36v10.fld (wait 2 min)
FLLOAD: File loaded: /ED/sys36v10.fld          Addr 00000000 > 00042840
SYSUPD: Flashing image done. Ok.
SYSUPD: all done.
```

➪ **Reboot dtb.**

After an RTOS update you MUST power cycle the dtb. It is NOT sufficient to do a soft reset only!

⇦ ⇧ ⇩ ⇨

11.1.4 List Firmware Versions

In a terminal window, type:

```
telnet  192.0.2.3
Username: esd
```

There will be no prompt for a password but an immediate login. On the command prompt (/R1/HOME>) type:

```
version
```

In the command ouput, the entry "SOFTWARE VERSION" (see below) corresponds to the current version of the application software (here 3.3) The line "RTOS-IMAGE-NO." gives the current version of the operating system (here 10). A typical output looks like this:

```
/R1/HOME>version


SOFTWARE-VERSION :      3.30
  DTB-NO. :         0
  CONTROLLER-NO. :        16
  RTOS-IMAGE-NO. :        10
  RTOS-IMAGE-NAME:P:\rtos\cmdfiles\base360\sys36v10.cmd
       created at:Mon Nov 12 18:21:53 2001
/R1/HOME>
```

⇦ ⇧ ⇩ ⇨

11.1.5 Update of Disks R2, R3 and R5

In certain situations it might become necessary or useful, to update user data on one of the internal disks of the controller. The following table summarizes the available partitions, their contents and the name of the command procedure to use for updating the information.

Partition	Name	Contents	Update Commands
/R2	TEST	Batch files, etc.	edittest/savetest
/R3	CONF	Configuration files, etc.	editconf/saveconf
/R5	TOOL	Some system tools	edittool/savetool

The most likely thing to do is an update of partition /R3 that contains instrument specific configuration data for certain motors or hardware components like the barcode reader. In the following example we will assume that we want to update disk /R3. For updating disks /R2 or /R5, the commands editconf/saveconf must be replaced by edittest/savetest or edittool/savetool, respectively.

In the following section, red text denotes user commands. Text printed in green is the expected output on the terminal screen. Please do the following and note that strings are case sensitive:

- **Telnet into dtb**
  In a terminal window, type:

  ```
  telnet 192.0.2.3
  Username: esd
  ```

  There will be no prompt for a password but an immediate login. The output on the screen at login will look like this:

  ```
  WD=/R1/HOME
  XD=/
  /R1/HOME/PROFILE--:  wrong command
  ```

- **Add directory /R4 to the binary path.**
  Type:

  ```
  CXD /R4
  ```

  The output on the screen will look like this:

  ```
  WD=/R1/HOME
  XD=/R4/-
  ```

- **Copy disk /R3 into temporary RAM**
  Type:

  ```
  editconf
  ```

  The output on the screen will look like this:

  ```
  /R1/HOME>editconf
  EDITCONF: start
  >> #SRAM : NO_BAD BLOCK(S)

  >> DISCMOVE/007F: (terminate)
  EDITCONF: done.
   :  (terminate)
  ```

- **FTP the desired file from the computer into the dtb.**
  Let us assume that you want to place a file called STATP.033 into directory /R3 of the dtb. After the previous step using command "editconf", the entire disk /R3 has been copied to disk /RF including the

entire directory tree. Do the following on your host computer:

```
  ftp   192.0.2.3
      Username:  esd_ftp
      Password:       <RETURN>        (i.e. no password)

  passive         (SuSE  only) (i.e. toggle use of passive transfer mode)
  epsv4  (SuSE  only) (i.e. toggle use of EPSV/EPRT commands)

      cd /RF        (i.e. go to directory /RF/BIN)
      binary           (i.e. use binary transfer mode)
      put STATP.033         (i.e. copy file STATP.033 from current dir. into /RF)
  quit
```

Burn /RF into flash.
In the still open telnet session, type command:

```
saveconf
```

The output on the screen will look like this:

```
/RF/->saveconf
RTOS-DIRECTORY DEVICE  /RF/
**FREE**       115  BC_CONF.TLP      2  BC_CONF.033      2  CONF/            1
IO_CONF          1  PARA/            1  RC/              1  STATP.TLP        3
STATP.033        2
Temp. RAM-Disk /RF found. Continue!
SAVECONF: Please wait until "all done" appears.
SAVECONF: Clearing Bank 6...9 and saving /R3...
SAVECONF: Clearing Bank 6...9

>> CLEARFLASH/0083: (terminate)
SAVECONF: Clearing Bank 6...9 done.
SAVECONF: SAVING /R3 ...


>> MOVETOFLASH/0084: (terminate)
SAVECONF: SAVING /R3 ...done
SAVECONF: UNMOUNT temp. RAM-Disk /RF
SAVECONF: all done.
```

BEWARE:
Regardless if you are using commands edittest, editconf or edittool, there will always be a temporary copy of disks /R2, /R3 or /R5 in directory /RF. You should always take good care not to use the "wrong" save command which may copy /RF back into the wrong place. I.e. a combination of commands edittest/saveconf or similar MUST BE AVOIDED!

11.2 How to Assign Motors to the Buttons of the Local Motor Control

The **Local Motor Control** features 5 buttons with multiple functionality. There are 4 motor buttons ("**CRYO, THETA, DISTANCE, CHI**") and the "**ADC ZERO**"-button. As by 2002 the CRYO button is not being used and may be used to drive either the **BEAMSTOP** or the **PHI**-motor. It can be handy to drive the beamstop out of the way when mounting the crystal. The beamstop may be moved manually but if this has been done the motor needs to reinitialized afterwards. Alternatively, it can be useful to drive **PHI** to 0.0 with the **Local Motor Control** before mounting a new crystal.

In any case, the *dtb*-controller needs to know which motor to talk to before the buttons can be used. By default, no motor is assigned to the CRYO button. To use the CRYO button to drive either BEAMSTOP or PHI, add a corresponding line to the configuration file **(see chapter "Keywords for dtb" in section "Input"**). Before starting program *mar345dtb*, you must set a couple of parameters with the help of program *dtbcmd* that allows to send single hardware commands to the *dtb*-controller.

In order to use motor **BEAMSTOP**, please do the following:

Command	Description
dtbcmd 103,1,41,5	Assign BEAMSTOP motor to CRYO button
dtbcmd 103,1,40,100	Set speed for BEAMSTOP motor to 100 steps/sec.
dtbcmd 103,1,39,500	Set acceleration for BEAMSTOP motor to 500 steps/sec*sec.
dtbcmd 103,1,38,-300	Set position 2 for BEAMSTOP motor to 45 mm
dtbcmd 103,1,37,-120	Set position 1 for BEAMSTOP motor to 18 mm

In order to use motor **PHI**, please do the following:

Command	Description
dtbcmd 103,1,41,6	Assign PHI motor to CRYO button
dtbcmd 103,1,40,10000	Set speed for PHI motor to 10000 steps/sec.
dtbcmd 103,1,39,20000	Set acceleration for PHI motor to 20000 steps/sec*sec.
dtbcmd 103,1,38,-144000	Set position 2 for PHI motor to 180.00 deg.

Command	Description
dtbcmd 103,1,37,0	Set position 1 for PHI motor to 0.0 deg.

If you don't have a CHI axis you may also reassign the CHI button to either BEAMSTOP or PHI. To do so, use the same sequence of commands as described above. The only difference will be the third argument (41 to 37) which will have to be replaced by the given value -5, i.e. 36 to 32.