



Software Distribution Guide



The *marXperts* Software Distribution Guide

Version 6.0

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1. Supported Operating Systems

The software distribution is available on CD-Rom or DVD. Updates are available via anonymous ftp from:

`ftp.marxperts.de/pub/345`

Due to their size (180 MB), scanner calibration files are not available via FTP. Please contact marXperts for assistance. As by August 2014, most programs comprised in the software distribution run on most flavours of Linux and Mac OS X (Intel versions, 64-bit only). In case of doubt, please consult marXperts.

Most graphical user interfaces rely on X11 and OpenMotif libraries. In particular, on Mac OS X the installation of the Quartz X-server and the "MacPorts" software distribution is required.

Operating system	Suggested home directory (installation path)
Linux kernel ≥ 3.0	/home/mar345
Mac OS X ≥ 10.8	/Users/mar345

2. Environment

The following logical assignments must be set to run certain programs.

Marresearch recommends to use tcsh as the user's default shell. Proper shell initialization files are available for csh/tcsh, but not for bash and related shells.

Variable name	Description	Used by programs
MARHOME	Master directory of distribution	all
MARLOGDIR	Directory for log files	all
MARTABLEDIR	Directory with scanner specific tables	mar345dtb, mar345, scan345, mar345xf
MAR_SCANNER_NO	mar345 scanner serial number	mar345dtb, mar345, scan345, mar345xf
MAR_DTB_NO	dtb serial number	mar345dtb
MARDOCDIR	Directory with documentation	mar345dtb
MARMANDIR	Directory with man pages	mar345, automar
MARHELPDIR	Directory with online help files	mar345, marView

3. Directory Structure

The software distribution directory (\$MARHOME) contains the following subdirectories:

Directory	Contents
bin	Shell scripts for use by some programs
bin/linux/glibc-x.y	Binary executables for several flavours of Linux depending on libc versions
bin/osx86	Binary executables for Mac OS X / Intel versions
bin/x86_64	Binary executables for 64-bit flavours of Linux
man/1	Unformatted man pages for selected programs
man/html	HTML-formatted text of man pages
man/man1	Compressed unformatted man pages
man/doc	ASCII text of formatted man pages, ready for online read (more)
man/pdf	PDF-formatted text of man pages
man/Manuals	PDF-formatted documentation
man/help	Online help files for some GUI's (mar345, marView)
man/mar345dtb	HTML formatted docs for program mar345dtb
log	Log-files for programs mar345dtb, mar345 and scan345
log/log	Up to N versions of mar.log or dtb.log
log/lp	Up to N versions of mar.lp files (statistical output)
log/spy	Up to N versions of mar.spy and dtb.spy files (native controller messages)
log/beam	Up to N versions of dtb.time, dtb.scan and dtb.profile
log/sets	Data collection template files for mar345dtb
log/tv	Up to N versions of martv.log
log/xtal	Directory for saving crystal photos
log/csc	Directory for saving sample changer data
src	Source code for selected programs
tables	Scanner specific calibration and configuration files
Optional:	
ccp4	Latest CCP4 distribution
automar	Latest automar distribution

4. Description of Programs

Name	Docs	Priority	Description
Graphical user interfaces:			
mar345dtb	yes	A	GUI for data collection with mar345-scanner and dtb
mar345	yes	A	GUI for data collection with mar345-scanner without dtb
marstart	-	A	Works together with program mar345dtb and mar345
margrabber	yes	A	Shows crystal on screen as seen by TV-camera in dtb
marView	yes	A	Standalone GUI for data display and inspection
automar	yes	D	GUI for automar processing package (marProcess, marScale)
marmux	yes	D	Stand-alone GUI to operate Xenocs GeniX X-ray generator
Hardware related programs:			
mar345xf	yes	C	Standalone transformation program for spiral images
marsim	yes	D	Simulator for mar345 image plate scanner
dtbsim	yes	D	Simulator for mardtb goniostat
marserver	yes	D	TCP/IP-port multiplier for mar345 scanner and mardtb
scan345	yes	D	Non-GUI data collection program for mar345scanner (not dtb)
modnb	-	D	Modifies header of calibration files
swapnb	-	D	Swaps bytes in calibration file
dtbcmd	-	B	Sends a native hardware command to the dtb controller
dtbstat	-	B	Dumps status information of the dtb controller
dtbdata	-	B	Dumps ionization chamber readings from motor scans of dtb
dtbmess	-	B	Dumps native dtb controller messages
spiral(un)pack	yes	C	(De-)compression of raw spiral images
Other programs:			
catmar	yes	A	Dumps headers of mar345/300 images and calibration files
marcvf	yes	A	Non-GUI image format and manipulation tools (updated)
marcombine	yes	B	Adds up images and produces o/p-file with combined intensities
marshrink	yes	C	Shrinks mar345-formatted images (cut off outer resolution shells)
marheader	-	C	Manipulates headers of mar345-formatted images
marstats	yes	C	Dumps average intensity and sigmas of images
Data processing suite <i>automar</i>:			
marPeaks	yes	C	Spot search
marIndex	yes	C	Autoindexing
marPredict	yes	C	Pattern prediction
marStrategy	yes	C	Calculates optimal data collection strategy
marSurvey	yes	C	Calculates optimal data collection strategy (since end 2004)
marProcess	yes	C	Integrates mar diffraction images
marPost	yes	C	Postrefinement and merging of partials
marScale	yes	C	Scaling of reflections
mar2mtz	yes	C	Conversion of marPost/marScale output into mtz files
scalepackcvf	yes	C	Conversion of scalepack output into SHELX files

Priority codes: A = Essential
B = Helpful, installation recommended

C = Not essential, may be removed
D = Needed only in special situations

5. Documentation

The documentation can be found in directory \$MARHOME/man. Several formats are available:

Directory	Contents
man/1	Unformatted man pages for selected programs
man/html	HTML-formatted text of man pages
man/man1	Compressed unformatted man pages
man/doc	ASCII text of formatted man pages, ready for online read (more)
man/pdf	PDF-formatted text of man pages
man/Manuals	PDF-formatted documentation
man/help	Online help files for some GUI's (mar345, marView)
man/mar345dtb	HTML formatted docs for program mar345dtb
man/mar345	HTML formatted docs for program mar345

The following man pages are available:

Name	Description
mar345dtb	Documentation for program mar345dtb
mar345	Documentation for program mar345
margrabber	Documentation for program margrabber
marView	Documentation for program marView
automar	Documentation for program automar
marserver	Documentation for program marserver
mar345xf	Documentation for program mar345xf
scan345	Documentation for program scan345
marsim / dtbsim	Documentation for program marsim and dtbsim
marcvt	Documentation for program marcvt
marcombine	Documentation for program marcombine
spiralpack	Documentation for program spiralpack
marPeaks	Documentation for program marPeaks
marIndex	Documentation for program marIndex
marPredict	Documentation for program marPredict
marStrategy	Documentation for program marStrategy
mar2mtz	Documentation for program mar2mtz
scalepackcvt	Documentation for program scalepackcvt
mar345_formats	Documentation for program <i>mar345</i> image formats
mar300_formats	Documentation for program <i>mar300</i> image formats
mar345_config_file	Documentation for the configuration file for program <i>mar345</i> (not <i>mar345dtb</i>)

To view the man pages using man, the directory \$MARHOME/man must be in the man page search path. Consult the „man“ man page for further details, since this varies from computer to computer. The GUI's provide „Help“-buttons for additional online information.

When run with the „-h“ command line option, usage information is provided for most of the mar programs, e.g. type:

```
marcvt -h
```

6. Software Installation

6.1 Create a new user account “mar345”

You must be super-user to do this. You can either use a GUI (e.g. *kuser* from the KDE package, *yast1* or *yast2* from the SuSE Linux distribution, or a terminal program like *useradd* or *adduser*.

Suggested home directory: **/home/mar345**
Default login shell: **/bin/tcsh** or **/bin/bash** (highly recommended)

6.2 Login as user mar345

6.3 Copy contents of distribution to home directory

6.3.1 Tar file

If the software distribution has been distributed as compressed tar file (e.g. file *mar345dtb.dist.tgz*), place it into the new user’s home directory and unpack its contents. by just typing:

```
tar xvfz mar345dtb.dist.tgz
```

Note, that the tar file may contain or not contain detector specific data in subdirectory “tables”.

6.3.2 CD-Rom or DVD

If the software distribution has been distributed as compressed tar file (e.g. file *mar345dtb.dist.tgz*), place it into the new user’s home directory and unpack its contents. by just typing:

Insert the CD-ROM in the CD-ROM reader. If there is an automounter, the CD-Rom is going to be mounted automatically (on RedHat usually as */mnt/cdrom*, on SuSE Linux usually as */media/cdrom*). Otherwise, on many systems, users are allowed to mount CD-Roms by just typing:

```
mount /mnt
```

where */PATH* can be */mnt*, */mnt/cdrom*, */mnt/dvd*, */media/dvd* or */media/cdrom*.

If this doesn’t work, the super-user has to do something like:

```
mount -t iso9660 -r /dev/cdrom /mnt (Linux)
```

When successful, the contents of the CD-ROM should be copied into the login directory of the account *mar345*. To do so, as user “*mar345*” type:

```
/PATH/mar_install
```

The installation script chooses reasonable defaults that may be accepted or modified. It is important that the contents of the CD-Rom are really copied to the login directory of the new user since the distribution contains customized startup files (*.cshrc*, etc.) that should reside in the login directory.

7. Setting Up the Ethernet Connection

Program *mar345dtb* communicates with the *dtb* and the *mar345-scanner* through an Ethernet interface. To use program *mar345dtb*, the network must be configured to meet the requirements of the controllers. The *mar345-scanner* has the fixed IP-address 192.0.2.1 and the *dtb* is set to address 192.0.2.3. The host computer Ethernet interface must be set to address 192.0.2.2. Network 192.0.2.x belongs to a pool of addresses that is not assigned to official networks so there should not be any conflict with the outside world.

7.1 Configure a Dedicated Ethernet Card With IP-address 192.0.2.2

To configure an Ethernet card it is most convenient to use the graphical administration tools. On Linux, most system configuration parameters will be taken from files in directory `/etc/sysconfig` which may be edited by hand, but you really need to know what you are doing. It is safer to use graphical administration tools (e.g. *yast2* on SuSE) to do the configuration.

When using 2 Ethernet cards, the primary Ethernet card (`eth0` on Linux, `en0` on Mac) is normally configured as member of your local network and the second Ethernet card (`eth1` or `en1`) should be used to work with the *mar345* and *dtb*. In any case, the following parameters need to be assigned to the network card connecting to the *mar345*-detector and *dtb*:

```
IP-address:      192.0.2.2
Netmask:        255.255.255.0
```

7.2 Add Entries to File `/etc/hosts`

Edit file `/etc/hosts` and add the following lines to the end of the file:

```
192.0.2.1  mar345  scanner
192.0.2.3  dtb     mardtb
```

If you can't find an entry for IP-address 192.0.2.2, also add:

```
192.0.2.2  eth1
```

7.3 Confirm Settings

Configuring the network card normally requires a reboot of the computer. Afterwards, you should be able to access other hosts (e.g. *mar345*) on network 192.0.2. To check network card `eth1` (on Mac: `en1`), type:

```
ifconfig eth1
```

On Linux, this command should come back with something like:

```
eth1      Link encap:10Mbps Ethernet  HWaddr 00:80:C6:FF:EF:08
          inet addr:192.0.2.2  Bcast:192.0.2.255  Mask:255.255.255.0
          UP BROADCAST RUNNING MULTICAST  MTU:1500  Metric:1
          RX packets:0 errors:0 dropped:0 overruns:0
          TX packets:0 errors:0 dropped:0 overruns:0
          Interrupt:12 Base address:0x320
```

The correct routing table can be checked using command:

```
netstat -r
```

On Linux, it should say something similar to:

Kernel IP routing table

Destination	Gateway	Genmask	Flags	MSS	Window	irrt	Iface
193.141.161.0	*	255.255.255.0	U	1500	0	0	eth0
192.0.2.0	*	255.255.255.0	U	1500	0	0	eth1
127.0.0.0	*	255.0.0.0	U	3584	0		

Connect the *mar345*-scanner and/or *dtb* to the Ethernet card and power them up. To check availability on the network, type:

`ping 192.0.2.1` (check availability of *mar345* detector)
or
`ping 192.0.2.3` (check availability of *dtb*)

If the scanner is accessible, ping comes back with:

```
PING mar345 (192.0.2.1): 56 data bytes
64 bytes from 192.0.2.1: icmp_seq=0 ttl=255 time=1 ms
```

If ping comes back with:

`ping: mar345: Unknown host`
or
`ping: dtb: Unknown host`

then, *mar345* and/or *dtb* has not been inserted into file `/etc/hosts` (see above).
If ping hangs with:

```
PING mar345 (192.0.2.1): 56 data bytes
```

or

```
PING dtb (192.0.2.3): 56 data bytes
```

then the reason might be:

- a) the network interface has not been configured correctly
- b) the scanner or *dtb* are not turned or are not yet ready to listen
- c) there is a problem with the Ethernet cable
- d) there is a problem with the hub (check power cable!)
- e) a regular RJ-45 cable has been plugged into the **Uplink** port of the hub
- f) a cross-over cable has been plugged into any but the **Uplink** port of the hub
- g) there is a problem with the scanner or *dtb* itself

7.4 How to connect RJ-45 cables to the hub

A hub allows two or more computers to talk to each other. There are two types of twisted pair Ethernet cables with RJ-45 connectors: regular ones and cross-over cables. Crossed cables must be used to directly connect two computers to each other without a hub in between. I.e. you can use a crossed cable to connect the Ethernet card of your computer and the *mar345*-detector with no hub in between. If there is hub, please note, that most hubs feature 4 or more regular ports and one "Uplink" port. You can connect regular cables to the regular hub ports (i.e. *mar345*-detector, *dtb* and computer). Alternatively, you may use a crossed cable to connect the computer or *mar345* or *dtb* to the "Uplink" port of the hub. All other combinations are not going to work.

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