

marresearch



The
mar345 dtb
Software Distribution Guide

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The *mar345dtb* Software Distribution Guide

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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.marresearch.de/pub/345](ftp://ftp.marresearch.de/pub/345)

Due to their size (180 MB), scanner calibration files are not available via FTP. Please contact Marresearch for assistance. As by January 2009, most programs comprised in the software distribution run on most flavours of Linux and Mac OS X (PowerPC and Intel versions). In case of doubt, please consult Marresearch.

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

| Operating system | Suggested home directory (installation path) |
|-----------------------|--|
| Linux kernel >= 2.4.0 | /home/mar345 |
| Mac OS X >= 10.3 | /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 |
| MARHELPPDIR | 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/ppc | Binary executables for Mac OS X / PowerPC versions |
| bin/osx86 | Binary executables for Mac OS X / Intel versions |
| bin/cygwin | Binary executables for cygwin environment on Windows XP |
| 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 | C | GUI for data collection with mar345-scanner without dtb |
| marstart | - | A | Works together with program mar345dtb and mar345 |
| martv | 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 | C | GUI for automar processing package (marProcess, marScale) |
| Hardware related programs: | | | |
| mar345xf | yes | C | Standalone transformation program for spiral images |
| marsim | yes | D | Scanner simulator for programs mar345(dtb) and scan345 for performance tests and/or debugging |
| marserver | yes | D | TCP/IP-port multiplier for mar345 scanner and dtb |
| scan345 | yes | D | Non-GUI data collection program for mar345-scanner (not dtb) |
| modnb | - | D | Modifies header of calibration files |
| swapnb | - | D | Swaps bytes in calibration file. Useful when replacing the data collection computer by one with a different byte-order. |
| 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 |
| log/beam | | | Up to N versions of dtb.time, dtb.scan and dtb.profile |
| marcvt | 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 |
| 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 |
| 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 |
| scalepackcvt | 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 |

The following man pages are available:

| Name | Description |
|--------------------|--|
| mar345dtb | Documentation for program mar345dtb |
| mar345 | Documentation for program mar345 |
| martv | Documentation for program martv |
| 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 | Documentation for program marsim |
| 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** (highly recommended, since no shell initialization file is provided for Bourne shells)

6.2 Login as user mar345

6.3 Copy contents of CD-ROM or DVD

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 /PATH
```

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 /PATH (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 | irtt | 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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