marXperts

Software Distribution Guide

The
marXperts
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1. Supported Operating Systems

The software distribution is available for purchase or for members of the marXperts Software Club via:

http://www.marxperts.com/club

Due to their size (180 MB), scanner calibration files are not available online. Please contact marXperts for assistance. As by February 2019, 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	/opt/mar (previously: /home/mar345)
Mac OS X >= 10.8	/opt/mar

2. Environment

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

We recommend to use bash as the user's default shell as this is the default shell for all modern Linux and Mac distributions. A proper shell initialization files is available for bash. Files for csh/tcsh and related shells are not maintained any more.

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/x86_64	Binary executables for 64-bit flavours of Linux
bin/linux/i386	Binary executables for 32-bit flavours of Linux
bin/osx86	Binary executables for Mac OS X / Intel versions
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
mardtb	yes	A	GUI for data collection with Dectris dectectors and mardtb
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
marmus	yes	D	Stand-alone GUI to operate Incoatec IuS 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 multiplyer 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
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
marstats	yes	C	Dumps average intensity and sigmas of images
Data processing suite *automar*:			
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   C = Not essential, may be removed
                  B = Helpful, installation recommended   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/mardtb	Documentation for program mar345dtb/mardtb
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 *mar345* image formats
mar300_formats	Documentation for program *mar300* image formats
mar345_config_file	Documentation for the configuration file for program *mar345* (not *mar345dtb*)

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 Copy contents of distribution to directory /opt/mar

You must be super-user to do this. Create directory /opt/mar with command:

mkdir /opt/mar

If the software distribution has been distributed as compressed tar file (e.g. file mar345dtb.dist.tgz), place it into/opt/mar and unpack its contents. by typing:

cd /opt/mar; tar xvfz mar345dtb.dist.tgz

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

If the software distribution has been distributed on DVD or CD-Rom, insert the media in the DVD reader and copy the contents 1:1 into directory /opt/mar. With PATH being the full actual mount path for the media, use a command similar to:

cd /PATH; tar cvf - . | (cd /opt/mar; tar xf -)

Please note, that when copying data from a DVD or CD-Rom, all files will have read-only permission, since DVDs and CD-Rom are read-only media.

Please note also, that all files in /opt/mar now probably belong to user root, which is fine, since you do not really want regular users to override files of the distributions. However, ownerships of the files do not really matter. Everything that lives in /opt/mar does not have to be writable.

6.2 Create a new user account, e.g. user "mar345"

You must be super-user to do this. You can either use a GUI (different names on different Linux distributions) or a terminal program like *useradd* or *adduser*.

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

Note: it is not mandatory to create the username "mar345". Any other username will work. It is essential, however, that every user wanting to use the mar345dtb software obtains the proper environment (see below).

6.3 Login into new user account

Open a terminal window and modify the shell initialization file (.bashrc). Add the following lines to its end:

if [-e /opt/mar/mar-env.sh]; then
        . /opt/mar/mar-env.sh
fi

These lines will load file mar-env.sh containing the required environment parameters to run all mar programs. One important feature of the mar-env.sh script is that it creates a new directory $HOME/log and copies the contents of directory /opt/mar/log of the software distribution into that directory. If $HOME/log already exists, this step is skipped.

7. Updating an existing mar345dtb software distribution

If a mar345 scanner has been at the factory, it will usually be recalibrated before being returned to the customer. A new calibration will make the previous scanner calibration files invalid and care must therefore be taken, to delete old scanner calibration files from your software distribution and to always use the latest one.

The scanner will always be returned from a factory calibration with media (CD-Rom, DVD) containing the new calibration data and fresh executables. Make sure that you keep the media in a safe place. You will have to copy at least the calibration files from the media to your existing software distribution. The media will also allow you to clone the software to another PC. If for some reason your existing PC dies the contents of the media are all you need for reinstalling the mar software. Of couse, it does not contain a Linux distribution, so it assumes that the PC comes with a working Linux distribution.

Scanner calibration files are not provided on the web site, but are only available on media. It is therefore the customer's responsibility to keep the distribution media in a safe place. It is also highly advisable to make backups from time to time of the software distribution on your hard disk, at least of the the calibration files in $MARTABLEDIR (/opt/mar/tables or /home/mar345/tables, respectively). It may save you time and money to restore the software in case of a breakdown.

In order to update your existing software, you MUST copy at least the following scanner calibration files:

tables/mar2300.XXX
tables/mar3450.XXX

where XXX denotes the serial number of your scanner. The files on the media should replace the ones in directory $MARTABLEDIR (/opt/mar/tables or /home/mar345/tables, respectively).

Please note, that your existing software configuration files contained in directory $MARTABLEDIR might differ from the files contained on the media. This is because we do not necessarily have the latest version of your configuration files because they might have been modified after installation. It is therefore advisable to keep a copy of the existing files before overwriting them.

If you want to also update the executables please make sure that the executables on the media are compatible your current Linux distribution. Current compilations of the software will not necessarily be compatible with Linux distributions installed 5 years ago. On the media you will find executables for 64-bit and 32-bit flavours of Linux distributions, that should be compatible with a large variety of distributions, our favourites being Ubuntu and CentOS. As compilation systems we typically use the Ubuntu LTS-series (long-term-support) dating 2-3 years back.

For plainly copying the entire software distribution from the CD-Rom mounted on /PATH to your hard disk with the mar345dtb software distribution residing in directory /opt/mar or /home/mar345, go to the directory where the media is mounted (here: /PATH) and copy he entire contents of the media into /opt/mar (or /home/mar345, respectively). Make sure, that you actually are allowed to write into the target directory /opt/mar (or /home/mar345), otherwise you will get lots of error messages.

cd /PATH; tar cf - . | (cd /opt/mar; tar xvf -)

The "tar" command is going to overwrite any existing file. It preserves the date of the files on the media. Since all data on read-only media are read-only, the file permissions of the files copied to the disk will also be "read-only", which is okay. If you want to make files and directories in your home directory also writable, do the following:

chmod -R +w /opt/mar

8. 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.

8.1 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**

8.2 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

8.3 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

8.4 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.