McStas installation instructions

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Abstract

This document describes installation of the McStas package, including some information on installing other required pieces of software.

The text below is also included as a chapter in the McStas manual.

1 Getting McStas

The McStas package is available in various distribution packages, from the project website at http://www.mcstas.org/download.

- `McStas-1.11-i686-Win32.exe`
  Self-extracting executable including essential support tools. - Refer to section 3.
- `McStas-1.11.dmg`
  Mac OS X disk image for PPC and Intel machines. Please follow the instructions in the README file in the disk image.
- `mcstas-1.11-i686.deb`
  Binary Debian GNU/Linux packages for 32 bit Intel/AMD processors, currently built on Debian stable. Tested to work on Ubuntu and Debian systems. - Refer to section 4.1
- `mcstas-1.11-i686-unknown-Linux.tar.gz`
  Binary package for Linux systems, currently built on Debian stable. Should work on most Linux setups. - Refer to section 4
- `mcstas-1.11-src.tar.gz`
  Source code package for building McStas on (at least) Linux and Windows XP. This package should compile on most Unix platforms with an `ANSI-c` compiler. - Refer to section 4

2 Licensing

The conditions on the use of McStas can be read in the files `LICENSE` and `LICENSE.LIB` in the distribution. Essentially, McStas may be used and modified freely, and copies of the McStas source code may be distributed to others. New or modified component and instrument files may be shared by the user community, and the core team will be happy to include user contributions in the package.

3 Installation on windows

As of release 1.10 of McStas, the preferred way to install on Microsoft Windows is using a self-extracting `.exe` file.
The archive includes all software needed to run McStas, including perl, a c-compiler, PDL, PGPLOT, a vrml viewer and Scilab 4.0. (Use PGPLOT or install Matlab if possible, since support for Scilab will eventually end.)
Installation of all the provided support tools is needed to get a fully functional McStas. (The option not to install the tools is included for people who want to upgrade from a working, previous installation of McStas.)
The safe and fully tested configuration/installation is to install all tools, leaving all installation defaults untouched. Specifically you may experience problems if you install to non-standard locations.
Simply follow the guidance given by the installer, pressing 'next' all the way.
To use grid and cluster computing, you will need an SSH client. McStas is configured to use PuTTY.
For MPI (parallelisation) on Windows, we advice you to install MPICH2 from Argonne National Laboratory including development libraries before installing McStas. Also, your `mpiexec.exe` must be on the `PATH`. You may have to customize the `mpicc.bat` script from the McStas distribution with the proper C compiler and MPI library path.
If you experience any problems, or have some questions or ideas concerning McStas, please contact peter.willendup@risoe.dk or the McStas mailing list at neutron-mc@risoe.dk.

4 Installation on Unix systems

Our current reference Unix class platform is Ubuntu Linux, which is based on Debian GNU/Linux. Some testing is done on other Unix variants, including Fedora Core, SuSE and FreeBSD.

WARNING: The 'dash' shell which is used as /bin/sh on some Linux system (Including Ubuntu 8.04) makes the 'Cancel' and 'Update' buttons fail in mcgui. Possible solutions are:

- If your system is a Debian or Ubuntu, please run the command `dpkg-reconfigure dash` and say 'no' to install dash as /bin/sh (See section 4.1)
- If your /bin/sh is dash, please install bash and manually change the /bin/sh link to point at bash.

4.1 Debian class systems

As of release 1.11, we provide a Debian binary package (32 bit package for Intel/AMD). We have tested that the package works properly on Ubuntu and Debian systems. To install it, please perform the following tasks:

1. Download the package from `http://www.mcstas.org/download`
2. As root, issue the command
   `apt-get install perl perl-Tk gcc libc6-dev libg2c0 pdl bash`
3. Optionally, as root, issue the commands
   `apt-get install openssh-client openssh-server`
   `apt-get install mpich-bin libmpich1.0c2 libmpich1.0-dev`
   to benefit from MPI and SSH grid parallelization
4. As root, issue the command
   `dpkg-reconfigure dash`
   and say 'no' to install dash as /bin/sh.
5. As root, issue the command
   `dpkg -i mcstas-1.11-i686.deb`. This later step may be replaced by a ./configure; make; make install procedure after extraction of the Mctas tarball (see below)

Updating your operating system to a new release *may* in some cases require you to re-install McStas following the procedure above. We hope to make a so-called *apt repository* available in the future, which will ensure automatic upgrade of McStas in case of a new release.

4.2 Other Linux/Unix systems

To get a fully functional McStas installation on Unix systems, a few support applications are required. Essentially, you will need a C compiler, Perl and Perl-Tk, as well as a plotter such as Matlab, Scilab or

PGPLOT (Using Scilab is not recommended and support will eventually end). In the installer package, we supply a method to install PGPLOT and related perl modules - see step 3 below.
On Debian and Ubuntu systems, the needed packages to install are `perl-tk, pdl, gcc, libc6-dev`
(On Ubuntu you need to enable the 'universe' package distribution in the file
`/etc/apt/sources.list`.)
We also recommend to install octaga vrml viewer from
http://www.octaga.com/download_octaga.html.
Additionally, MPICH, OpenMP (gcc-4.2 or icc or pgcc), openssh, Octave/Gnuplot, HDF and NeXus libraries may be installed, to enhance McStas clustering method and data formats.

4.3 Configuration and installation

McStas uses autoconf to detect the system configuration and creates the proper Makefiles needed for compilation. On Unix-like systems, you should be able to compile and/or install McStas using the following steps:

1. Unpack the sources to somewhere convenient and change to the source directory:
   `gunzip -c <package>.tar.gz | tar xf -`
   `cd mcstas-1.11/`
2. Configure McStas:
   `./configure` or `./configure --with-nexus --with-cc=gcc-4.2`
3. Optionally build/install PGPLOT (as superuser - build dependencies are pdl, g77, libx11-dev, xserver-xorg-dev, libxt-dev on Ubuntu):
   `make install-pgplot && ./configure`
4. Build McStas (only in case of the `mcstas-1.11-src.tar.gz` package):
   `make`
5. Install McStas (as superuser):
   `make install`

The installation of McStas in step 5 by default installs in the `/usr/local/` directory, which on most systems requires superuser (root) privileges.

4.4 Specifying non-standard options

To install in a different location than `/usr/local`, use the –prefix= option to configure in step 2. For example,

./configure –prefix=/home/joe

will install the McStas programs in /home/joe/bin/ and the library files needed by McStas in /home/joe/lib/mcstas/.
On 64-bits systems, you may have to use: ./configure –with-pic before installing PGPLOT with: make install-pgplot
To enable NeXus format in mcformat, you need the NeXus and HDF libraries, and have to use: ./configure –with-nexus
To specify a non standard C compiler (e.g. gcc-4.2 or icc that support OpenMP), you may use e.g.: ./configure –with-cc=gcc-4.2
To enable a non standard C compiler to be used with MPI, you may have to edit your mpicc shell script to set e.g.: CC="icc", or redefine the 'cc' to point to your prefered compiler, e.g.: ln -s /usr/bin/gcc-4.2 /usr/bin/cc

In case ./configure makes an incorrect guess, some environment variables can be set to override the defaults:

- The CC environment variable may be set to the name of the C compiler to use (this must be an ANSI C compiler). This will also be used for the automatic compilation of McStas simulations in mcgui and mcrun.
- CFLAGS may be set to any options needed by the compiler (eg. for optimization or ANSI C conformance). Also used by mcgui/mcrun.
- PERL may be set to the path of the Perl interpreter to use.

To use these options, set the variables before running ./configure. Eg.

```
setenv PERL /pub/bin/perl5
./configure
```

It may be necessary to remove configure's cache of old choices first:

```
rm -f config.cache
```

If you experience any problems, or have some questions or ideas concerning McStas, please contact peter.willendup@risoe.dk or the McStas mailing list at neutron-mc@risoe.dk.

5 Finishing and Testing the McStas distribution

Once installed, you may check and tune the guessed configuration stored within file

- `MCSTAS\tools\perl\mcstas_config.perl` on Windows systems
- `MCSTAS/tools/perl/mcstas_config.perl` on Unix/Linux systems

where `MCSTAS` is the location for the McStas library.

You may, on Linux systems, ask for a reconfiguration (e.g. after installing MPI, Matlab, ...) with the commands, e.g:

```
cd MCSTAS/tools/perl/
sudo ./mcstas_reconfigure
```

On Windows systems, the reconfiguration is performed with the `mcconfig.pl` command.

The `examples` directory of the distribution contains a set of instrument examples. These are used for the McStas self test procedure, which is executed with

```
mcrun --test # mcrun.pl on Windows
```

This test takes a few minutes to complete, and ends with a short report on the installation itself, the simulation accuracy and the plotter check.

You should now be able to use McStas. For some examples to try, see the examples/ directory. Start 'mcgui' (mcgui.pl on Windows), and select one of the examples in the 'Neutron Sites' menu.