

UNIX installation of the DISCUS/DIFFEV/KUPLOT/REFINE software
Version 5.99.19 and later

1. Installation:

1.1. One touch installation

Download the installation script **bbb_install_script.sh** from the DiffuseCode download site at:
<https://github.com/tproffen/DiffuseCode/releases/>.

Run this script, if necessary adjust the source path...

```
chmod u+x $HOME/Downloads/bbb_install_script.sh  
$HOME/Downloads/bbb_install_script.sh
```

The script will ask for the type of installation (globally for all users into /usr/local/bin or locally into \$HOME/bin). If the script needs to install packages you will be asked for your password. If you do not have sudo rights, please ask your local administrator for help with the first installation. On a LINUX distribution I recommend to install the discus_suite globally.

The script will create a local installation directory \$HOME/DIFFUSE_INSTALL. For future work with the DISCUS_SUITE I suggest to use a different directory for your macros and data.

Once the installation is finished, open a new terminal/konsole and type

```
discus_suite
```

Enjoy!

Future updates can be run via the script **bbb_install_script.sh** or simply from within the discus_suite with the command command ‘**update**’, to be issued at the top level.

Occasionally, an operating system update might mess up the links to dynamically linked libraries. In this case the pre-compiled version is likely not working for you any longer. To force a fresh compilation, change to your home directory and run the install script with optional parameters:

```
$HOME/Downloads/bbb_install_script.sh code=git install=local
```

The full scope of the optional parameters is:

code=pre	! Use a precompiled DISCUS version
code=git	! Use the current source code released at GitHub
code=archive.tar.gz	! Use the archive called “archive.tar.gz”, often something like ! DIFFUSE_CODE_v.6.06.00.tar.gz
install=fetch	! Get the latest installer from GitHub
install=local	! Use the current installer
install=archive.tar.gz	! Use the archive called “archive.tar.gz”, often something like ! DIFFUSE_INSTALL_local.tar.gz
prepare=libraries	! Install and update libraries
prepare=none	! Skip the check for new libraries

UNIX installation of the DISCUS/DIFFEV/KUPLOT software

Version 6.00

This step by step installation should really no longer be needed. If the installation according to step 1.1. fails on your Linux system, please drop us a mail and we'll look into the issues.

1. Preparation:

The compilation requires several libraries, especially their development versions, not all of them may be installed automatically. Especially Ubuntu leaves off many development versions.... Some of these libraries might be present on your system with different version numbers or slightly different names/paths, please be flexible:

libX11-devel	! X11 development library
libm	! Usually installed
libreadline6-dev	! Needed for command editing
libpng16-devel	! PNG Graphics library currently version 16 ! The current version is 16, but older versions seem to work fine ! as well
libpgplot	! Might already be installed, Best left off, as the installation script ! does provide a version and installs it. ! See below
OpenMP	! DIFFUSE needs this for parallel processing
openmpi-dev	! DIFFUSE needs this for parallel processing

Optional Libraries

Python	
mpich	! An alternative, OpenMP is preferred ! DIFFUSE needs this for parallel processing
NeXuS	! In the future DISCUS will use this for 3D data

Mandatory development tools:

cmake, ccmake, make	
gcc	

gfortran	! At least Version 4.6
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As an example, with UBUNTU 16.04 or 18.04 or later use apt-get or simply apt to install packages:

```
sudo apt-get install build-essential
sudo apt-get install libx11-dev
sudo apt-get install libxmu-dev
sudo apt-get install xterm
sudo apt-get install fonts-dejavu
sudo apt-get install libreadline-dev
sudo apt-get install libopenmpi-dev
sudo apt-get install openmpi-bin
sudo apt-get install gfortran
sudo apt-get install g++
sudo apt-get install lib hdf5-dev
sudo apt-get install cmake
sudo apt-get install cmake-curses-gui
sudo apt-get install curl
```

```
sudo apt-get install chrpath  
sudo apt-get install psmisc  
sudo apt-get install ghostscript  
sudo apt-get install qpdfview  
sudo apt-get install jmol
```

As of Ubuntu 18.04 Open Java should be installed with the default system installation.

2. Individual manual Installation:

Download the latest source code archive from GitHUB at:

github.com/tproffen/DiffuseCode/releases

The archive is called DiffuseCode-vV.M.P.tar.gz, where V.M.P stands for the major Version, the Minor version and the Patch numbers, currently 6.00.00

Copy the source code archive to a suitable directory and unpack:

```
mkdir -p $HOME/develop  
cp DiffuseCode-v5.99.13.tar.gz $HOME/develop  
cd $HOME/develop  
tar -zxf DiffuseCode-v5.99.13.tar.gz
```

create a „build“ directory, and change to build directory:

```
mkdir -p $HOME/develop/DiffuseBuild  
cd $HOME/develop/DiffuseBuild
```

execute ccmake with source code directory as parameter.
ccmake should open a graphical interface:

```
ccmake ..DiffuseCode-v5.99.13/
```

ccmake operates mostly via one letter commands, the main are:

- c for configure
- e exit the message screen
- g to generate the make files and exit ccmake

In ccmake toggle OFF the options:

DIFFUSE PYTHON, DISCUS CUDA, DISCUS NEXUS, DISCUS OMP

In ccmake toggle ON the options:

DIFFEV MPI

press „t“ to toggle to advanced mode. Go down with cursor and inspect pgplot settings
they should point to the directory in which the pgplot library is found:
/usr/local/pgplot OR may be: /usr/local/lib64/pgplot

The pgplot library need at least the following files in this directory:

grfont.dat
libcpgplot.a or libpgplot.so

libpgplot.a or libpgplot.so

pgxwin_server

Especially if you use a pgplot installation provided by the linux system, these files might be in different directories. It might be best to create a directory

/usr/local/pgplot

and to copy these files into this directory or to create symbolic links within this directory that point to the actual files.

To edit an entry within ccmake hit the „Enter key“ then type or change text.

ccmake wants an entry for „CMAKE_BUILD_TYPE“, edit this field ad leave it blank.

Once done hit „c“ to configure ccmake

You will get an info screen with hopefully no error messages.

If errors are listed, type „e“ and then „q“ and fix the error

If no errors occur hit „e“ to leave the info screen

Hit „g“ to generate the actual make files and to exit ccmake

then you need to compile the program, type without options

make

If this worked out without error messages you can install DISCUS, DIFFEV etc.

Our default installation directory is /usr/local/bin thus you can:

A) do it with „sudo“

B) Change the ownership of /usr/local to your own account:

A)

sudo make install

sudo cp suite/prog/discus_suite /usr/local/bin

B)

sudo chown -R /usr/local your_user_name

make install

With UBUNTU the style B) seems to create issues with other packages and is discouraged.

To clean up type

make clean

for the on-line help to work, a couple of environment variables should be set:

PGPLOT_DIR=“/usr/local/pgplot“; export PGPLOT_DIR

PGPLOT_DEV=“/XSERVE“; export PGPLOT_DEV

PGPLOT_FONT=“/usr/local/pgplot/grfont.dat“; export PGPLOT_FONT

define these within \$HOME/.bashrc.local if a „bash“ is used.

4. PGLOT Library

With Ubuntu the PGLOT library can be installed using the package manager but needs fine tuning. On other systems you might have to install the PGLOT library locally.

PGLOT library needs the files:

libpgplot.a
libpgplot.so
grfont.dat
pgxwin_server

in the directory under the PGLOT_INCLUDE_DIR entry in ccmake you need the files:

cpgplot.h
grpckg1.inc
pgplot.inc
pgxwin_server

Manual installation of LIBPGLOT:

Make /usr/local your own, or proceed throughout with sudo. This is best on an UBUNTU system, as a change of ownership seems to interfere with other packages and their updates.... Changing the ownership is not an issue with SuSe

NOT on UBUNTU: sudo chown -R your_user_name /usr/local

INSTALL x11-dev, libreadline6, libpng, libpng-dev

I made small adjustments to the PGLOT library to ease the installation on a linux system. Please use the archive

https://github.com/rneder/DiffuseSuplement/releases/v.1.0.0/DIFFUSE_CODE_pgplot.tar.gz from GITHUB along with the DIFFUSE source code. The following instructions apply to this version.

copy DIFFUSE_CODE_pgplot.tar.gz to your home directory and unpack:

```
cp DIFFUSE_CODE_pgplot.tar.gz $HOME  
tar -zxf DIFFUSE_CODE_pgplot.tar.gz
```

You will have a good template for the pgplot installation within the directory `pgplot`. See the directories `pgplot` and `src/pgplot` after you unpack `DIFFUSE_CODE_pgplot`.

For a fully manual installation do:

```
sudo mkdir -p /usr/local/src  
sudo cp -r src/pgplot /usr/local/src
```

Create pgplot directory

```
sudo mkdir /usr/local/pgplot  
cd /usr/local/pgplot
```

Copy your drivers.list to /usr/local/pgplot

```
sudo cp /usr/local/src/pgplot/drivers.list /usr/local/pgplot
```

Edit drivers.list and uncomment any driver you need. The DISCUS_SUITE needs at least
NUDRIV
PSDRIV 1 to 4
PNDRIV 1
XWDRAV 1 and 2

Create makefile:

```
cd /usr/local/pgplot  
sudo /usr/local/src/pgplot/makemake /usr/local/src/pgplot linux gfortran_gcc
```

ONLY if you have the older version pgplot.5.2.tar.gz, do the following instead:

```
cd /usr/local/pgplot  
sudo /usr/local/src/pgplot/makemake /usr/local/src/pgplot linux f77_gcc
```

Edit makefile

change line 25 and 26 to:

25: FCOMPL=gfortran
26: FFLAGC=-ffixed-form -ffixed-line-length-none -u -Wall -fPIC -O

48: Remove "-lf2c"

Copy line 875(?), change to
pndriv.o:

Exit makefile

run makefile with:

```
sudo make  
sudo make cpg  
sudo make clean
```

If you use the „bash“ then

edit /etc/profile.d/profile.local to contain:

```
PGPLOT_DIR=/usr/local/pgplot  
#PGPLOT_DEV=/XSERVE  
PGPLOT_DEV=/XWINDOW
```

```
PGPLOT_FONT=/usr/local/pgplot/grfont.dat  
export PGPLOT_DIR  
export PGPLOT_DEV  
export PGPLOT_FONT
```

Edit your local ".basrc", add at end:
source /etc/profile.d/profile.local

Alternatively you can of course edit your local .bashrc.local .

Note on current releases of png_dev libpng16 and later. As the file pngconf has been modified, you might get an error while compiling file pndrv.c. If this occurs, please edit pndrv.c in the folder drivers and comment lines 225 to 233.

Finally run one or more of the pdgemo programs to verify that the installation proceeded properly. Sometimes, if graphics libraries are missing, the PGPLOT make file seems to quietly turn off the corresponding driver in drivers.list. In this case verify that you have installed the required graphics libraries, especially in their “devel” version. Make sure you edit drivers.list again before compiling the pgplot library.