

## UNIX installation of the DISCUS/DIFFEV/KUPLOT software

### 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  |
| libXmu-devel       |  |
| 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          | ! Can be installed with UBUNTU, may often have to be installed manually, See below |
| Optional Libraries |  |
| Python             |  |
| OpenMP             | ! DIFFUSE needs this for parallel processing                                       |
| mpich              | ! An alternative, OpenMP is preferred  |
|                    | ! DIFFUSE needs this for parallel processing                                       |
| openmpi-dev        | ! 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

As an example, with UBUNTU 16.04 or 18.04 use apt-get to install packages:

```
sudo apt-get install libx11-dev
sudo apt-get install libXmu-dev
sudo apt-get install libreadline-dev
sudo apt-get install libopenmp-dev
sudo apt-get install libopenmpi-dev
sudo apt-get install libopenmpi-bin
sudo apt-get install gfortran
sudo apt-get install c++
sudo apt-get install cmake
sudo apt-get install cmake-curses-gui
```

### Installation:

Download the latest source code archive from GitHub at:

[github.com/tproffen/DiffuseCode/releases](https://github.com/tproffen/DiffuseCode/releases)

The archive is called DiffuseCode-V.M.P.tar.gz, where V.M.P stands for the major Version, the Minor version and the Patch numbers, currently 5.20.0

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

```
mkdir -p $HOME/develop
cp DiffuseCode-5.20.0.tar.gz $HOME/develop
```

```
cd $HOME/develop
tar -xzf DiffuseCode-5.20.0.tar.gz
```

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

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

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

```
cmake ../DiffuseCode-5.20.0/
```

cmake 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 cmake
```

In cmake toggle OFF the options:

DIFFUSE\_PYTHON, DISCUS\_CUDA, DISCUS\_NEXUS, DISCUS\_OMP

In cmake 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 cmake hit the „Enter key“ then type or change text.

cmake wants an entry for „CMAKE\_BUILD\_TYPE“, edit this field and leave it blank.

Once done hit „c“ to configure cmake

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 cmake

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`

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:

```
DISCUS_DIR="/usr/local/bin"; export DISCUS_DIR
DIFFEV_DIR="/usr/local/bin"; export DIFFEV_DIR
KUPLOT_DIR="/usr/local/bin"; export KUPLOT_DIR
MIXSCAT_DIR="/usr/local/bin"; export MIXSCAT_DIR
#
PGPLOT_DIR="/usr/local/pgplot"; export PGPLOT_DIR
PGPLOT_DEV="/XSERVE"; export PGPLOT_DEV
```

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

## PGPLOT Library

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

PGPLOT library needs the files:

libpgplot.a  
libpgplot.so  
grfont.dat  
pgxwin\_server

in the directory under the PGPLOT\_INCLUDE\_DIR entry in ccmake you need the files:

cpgplot.h  
grpckg1.inc  
pgplot.inc  
pgxwin\_server

---

### Manual installation of LIBPGPLOT:

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

```
sudo chown -R your_user_name /usr/local
```

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

I made small adjustments to the PGPlot library to ease the installation on a linux system. Please download pgplot.5.2.3.tar.gz along with the DIFFUSE source code. The following instructions apply to this version.

```
copy pgplot.5.2.3.tar.gz to /usr/local/src
```

```
sudo mkdir -p usrlocal/src  
sudo cp pgplot.5.2.3.tar.gz /usr/local/src
```

unpack the library

```
sudo tar -zxf pgplot5.2.3.tar.gz
```

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
```

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  
export PGPLOT_DIR  
export PGPLOT_DEV
```

Edit your local ".bashrc", 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 pndriv.c. If this occurs, please edit pndriv.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.