

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	! Needed for command editing
libpng14-devel	! PNG Graphics library currently version 14
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
NeXuS	! In the future DISCUS will use this for 3D data

Mandatory development tools:

ccmake, make	
gcc	
gfortran	! At least Version 4.6

Installation:

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

```
mkdir -p $HOME/develop
cp DIFFUSE_CODE_YYYY_MM_DD.tar.gz $HOME/develop
cd $HOME/develop
tar -zxf DIFFUSE_CODE_YYYY_MM_DD.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
```

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:

DIFFEV_MPI, DIFFUSE_PYTHON, DISCUS_CUDA, DISCUS_NEXUS, DISCUS_OMP

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

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

ccmake wants an entry for „CMAKE_BUILD_TYPE“, edit this field and 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

B)

sudo chown -R /usr/local your_user_name
make install

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

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

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

copy pgplot.5.2.tar.gz to /usr/local/src

```
cp pgplot.5.2.tar.gz /usr/local/src
```

unpack the library

```
tar -zxf pgplot5.2.tar.gz
```

Create pgplot directory

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

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

```
cp ~/drivers.list /usr/local/pgplot
```

Create makefile:

```
cd /usr/local/pgplot  
/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:

make

make cpq

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.