

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

### Preparation:

Install CYGWIN64 or CYGWIN on your computer.

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

|                   |   |
|-------------------|---|
| cmake             | ! Nice make setup                                       |
| cmake-gui         |   |
| gcc-core          | ! Gnu Compiler  |
| gcc-gfortran      | ! Fortran compiler                                      |
| gcc-g++           | ! C++ compiler  |
| make              | ! The gnu make utility                                  |
| libreadline-devel | ! Readline development version                          |
| libreadline7      | ! Needed for command editing, Version 7 or higher       |
| libpng-devel      | ! PNG Graphics library                                  |
| libpng16-devel    | ! PNG Graphics library Version 16 or current highest... |
| libpng16          | ! PNG run time library Version 16 or current highest... |
| libX11-devel      | ! X11 development library                               |
| libX11_6          | ! X11 core library                                      |
| xterm             | ! X-window program                                      |
| xinit             | ! X11 startup   |
| libXm-4           |   |
| libXRes-1         |   |

### 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 |

CYGWIN will install a lot more to resolve dependencies, please be generous.  
Among those check that cygwin includes:

|               |  |
|---------------|--|
| binutils      | ! Basic GNU assembler, linker...           |
| cygwin-devel  | ! Basic Cygwin develop utilities           |
| gccmakedep    | ! Make Dependency tool                     |
| libncursesw10 | ! Terminal display library                 |
| libpng-devel  | ! PNG Graphics library development version |
| libXau6       | ! X11 authority                            |
| libXau-devel  | ! X11 authority development version        |
| libXmu6       | ! X11 miscellaneous utilities              |

## Installation:

### PGPLOT Library

Install the PGPLOT library:

PGPLOT library needs the files:

libpgplot.a  
libpgplot.so  
libcpgplot.a  
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

Its best to keep these in the same directory as the library, "/usr/local/pgplot"

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### Manual installation of LIBPGPLOT:

Place "pgplot.5.2.tar.gz" and "PGPLOT\_PATCH\_RBN.tar.gz" into your home directory

Create /usr/local/src directory:

```
mkdir -p /usr/local/src
```

Create pgplot directory

```
mkdir -p /usr/local/pgplot
```

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

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

Switch to /usr/local/src and unpack the library

```
cd /usr/local/src  
tar -zxf pgplot5.2.tar.gz
```

Switch to /usr/local/pgplot, copy the patch and unpack the patch:

```
cd /usr/local/pgplot  
cp $HOME/PGPLOT_PATCH_RBN.tar.gz .  
tar -zxf PGPLOT_PATCH_RBN.tar.gz  
cp pndriv.c /usr/local/src/pgplot/drivers/
```

If you have a newer version of the PNG library, then copy some png include files into /usr/local/pgplot. Templates from libpng16 are included in the patch.

```
cp /usr/include/libpng16/png*.h /usr/local/pgplot
cp /usr/include/zlib.h /usr/local/pgplot
cp /usr/include/zconf.h /usr/local/pgplot
```

Run makefile with:

```
make
make cpq
make clean
```

If you use the „bash“ then

Edit/create “/etc/profile.d/profile.local” to contain:

```
PGPLOT_DIR=/usr/local/pgplot
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
```

## Installation DISCUS:

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

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

Edit the file "CMakeLists.txt" in the directory DiffuseCode, and have the last line read:

```
#add_subdirectory(suite/prog)
```

Yes, a bug fix, an issue with shared libraries. To be resolved...

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

If you installed the pgplot library as above and created the entries in

/etc/profile/profile.local and in \$(HOME)/.bashrc, the pgplot library should be found correctly. Pay attention to the PGPLOT\_DIR entry, as it tends to remain empty!

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.

`make install`

To clean up, type

`make clean`

Place "CREATE\_DISCUS64.tar.gz" into your home directory, go there and unpack:

```
cd $(HOME)
tar -zxf CREATE_DISCUS64.tar.gz
```

Copy the shell script "kuplot.sh" into the global bin directory:

```
cp $(HOME)/develop/Create_DISCUS64/DISCUS_64_TEMPLATE/bin/kuplot.sh /bin
```

Copy kuplot.exe from /usr/local/bin into /bin as well. Alternatively change the kuplot path in "bin/kuplot.sh".

```
cp /usr/local/bin/kuplot.exe /bin
```

Start a new CYGWIN64 window and you should be able to use discuss, diffev, mixscat simply by typing the corresponding name.

```
discus
diffev
mixscat
```

Start kuplot via

```
/bin/kuplot.sh &
```

Enjoy!

## Prepare Windows installation

place "CREATE\_DISCUS64.tar.gz" into your home directory, go there and unpack:

```
cd $(HOME)
tar -xzf CREATE_DISCUS64.tar.gz
```

Change to the development directory, run the shell script to create a Windows version

```
cd $(HOME)/develop/Create_DISCUS64
./create_discus_64.sh
```

Copy and install the latest DISCUS Software from sourceforge

Use A Windows Explorer to copy the folder:

"C:\cygwin64\home\develop\Create\_DISCUS64\Discus" to

"C:\discus\_installation\_path\Discus"

Replace the Discus folder, do not copy the cygwin...\Discus folder into

"C:\discus\_installation\_path\Discus"

Edit the properties of the kuplot icon, the target should read:

"C:\discus\_installation\_path\Discus\bin\sh.exe" -c './run.sh /bin/kuplot.sh'

instead of

"C:\discus\_installation\_path\Discus\bin\sh.exe" -c './run.sh kuplot'

Use a Windows Explorer to navigate to

"C:\discus\_installation\_path\Discus"

Right click on the "tmp" folder,

Left click on "Properties"

Open the tab "Security"

Below the list of group and user names, left click on "Modify"

Left click on the general "Users" in the list of group and user names.

In the lower panel allow the "modify" access.

All modes below should be set as well, except the bottom most, "Special access rights"

Apply the changes, and leave the window with "OK", same for the "Property window"

The icon should now start kuplot as an X11 application