UNIX style installation of the DISCUS/DIFFEV/KUPLOT/DISCUS_SUITE software with CYGWIN

Preparation:
Install a basic CYGWIN64 or CYGWIN on your computer. To be found at "www.cygwin.com"

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
gccmakedep	! Make Dependency tool
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	
zlib-devel	! gzip compression
openmpi	! DIFFUSE needs this for parallel processing
libopenmpi-devel	! DIFFUSE needs this for parallel processing

Optional Libraries
Python
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
libncursesw10	! Terminal display library
libpng-devel	! PNG Grahics library development version

libXau6 ! X11 authority
libXau-devel ! X11 authority development version
libXmu6 ! X11 miscellaneous utilities

Once the installation is finished, you will have a linux system running on your computer. Double click the cygwin icon and a simple text window will open up. Within the window a right-click on your mouse allows you to set options like foreground and background colors, the font size etc.

See the UNIX section for a very short introduction.

Installation:

Quick Installation

Copy the current DISCUS_INSTALLATION_CYGWIN.tar.gz to your home directory

cp /cygdrive/c/Users/your_name/Downloads/DISCUS_INSTALLATION_CYGWIN.tar.gz $HOME

If necessary adjust the source path...

Unpack this archive:

```
cd $HOME
tar -zxf DISCUS_CYGWIN.tar.gz
```

This will create a directory DISCUS_INSTALL.
Copy the current source code archive into this directory

```
cd $HOME/DISCUS_INSTALL
cp /cygdrive/c/Users/your_name/Downloads/DIFFUSE_CODE_2016_0608.tar.gz .
```

Install PGPLOT by running the shell script pgplot_cygwin.sh:

```
./pgplot_cygwin.sh
```

If all libraries were installed properly this will -hopefully- run without errors.
As I do not want to mess with your system files, please edit manually the file "/etc/profile.d/profile.local". If this file does not exist, copy the file profile.local into the /etc/profile.d folder.:

```
cp $HOME/DISCUS_INSTALL/profile.local  /etc/profile.d/
```

If the file exists, then add the following lines the end of the file:

```
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 "$HOME/.bashrc", add at end:

```
source /etc/profile.d/profile.local
```

See the section editor further down with hints on editing a file within unix.

To ensure that these environment variables are set, start a new cygwin terminal.

Now go back to the DISCUS_INSTALL directory and start the main discus installation:

```
 cd $HOME/DISCUS_INSTALL
./install_discus    DIFFUSE_CODE_2016_1028.tar.gz
```

The argument to the script install_discus.sh must be the current Source code archive.
This should install the programs discus, kuplot, mixscat, discus_suite into the directory /usr/local/bin
you can start the stand alone programs DISCUS and DIFFEV by typing their name in small letters at any prompt:

```
discus
```

To start kuplot or the recommended suite type :

```
discus_suite.sh
kuplot.sh
```

Best define an alias within your $HOME/.bashrc:

```
alias discus_suite=/bin/discus_suite.sh
alias kuplot=/bin/kuplot.sh
```

Enjoy !

If errors might occur, try to check with the more detailed instructions on the following pages.

Editors:

If you do not feel comfortable with the unix editor “vi”, you can actually use your favorite Windows based editor program like wordpad or notepad++. Do NOT use OpenOffice or other text processing utilities. If you use wordpad, keep in mind that this is a Windows type program which does not entrust you with any intelligence of your own and usually attempts to add an extension “.txt” to the file. You do not want this to happen. Something like notepad++ or similar editor programs do a much better job.

If installed under the default path you will find all of the cygwin stuff at:

c:\cygwin or
c:\cygwin64

You user files will be in the folder “home” and then your Windows account name. Your home directory will therefore be:

c:\cygwin64\home\YOUR_NAME

with YOUR_NAME properly replaced.

Notepad++ does recognize the presence of hidden files i.e. files that start with a dot : “.”

System files will be in all of the other folders, be careful!

UNIX:

Important Unix commands

• man <command>
  Display informationen(=manual) for command <command>
• info <command>
  Display informationen for command <command>, modern version
• ls
  List the content of a directory
• cd [<PATH>/]<dirname>
  Change into another directory
• cp <from> <to>
  copy a file from to
• mkdir [<PATH>/]<dirname>
  create a new directory
• rmdir [<PATH>/]<dirname>
  removes a directory
• rm <name>
  removes a file called <name>.

Warning: Unix usually does NOT ask: ”do you want to do this?, are you sure?, do you really want to do this?” ! What’s gone is gone!
Most of the commands offer many more options. Just try it out, in many cases a parameter ”- help” will give a short summary of the available options.

Examples

ls -a	List all files, that includes hidden files
ls -l	list a long listing that includes many details
ls -R	list recursively into sub directories as well

Unix offers many possibilities to work in a flexible manner with file names:

*	character string of any length
?	exactly one character
[a-z,A-Z]	a character from interval a-z or A-Z. You may provide a single interval as well, and also a range of numbers.

Examples

ls *.mac	List all files that end in ".mac"
ls data.0[0-9]1	List all files called data.001, data.011, to data.091 files called data.002 etc. are omitted

If you start a program that will open its own window, it is often convenient to add a space and then the ”&” sign after the command name as in: ”emacs &”. This allows you to continue to use the command line window from which you started the program, which would otherwise be blocked by the program.

More detailed installation instructions.

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”

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 cpg
make clean
```

Copy grfont.dat into /usr/local/bin as well:

```
cp /usr/local/pgplot/grfont.dat /usr/local/bin
```

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
```

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

Its best to toggle DIFFEV_MPI on, but this requires MPI to be installed.

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 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.

```
make install
```

To clean up, type

```
make clean
```

Go back to the installation source directory DISCUS_INSTALL

```
cd $HOME/DISCUS_INSTALL
```

Copy the shell scripts “kuplot.sh” and “discus_suite.sh” into the global bin directory:

```
cp kuplot.sh /bin/
cp discus_suite.sh /bin
```

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

```
discus
diffev
mixscat
```

Start kuplot via

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

Alternativley create an alias within your $HOME/.bashrc:

```
alias kuplot=/bin/kuplot.sh
alias discus_suite=/bin/discus_suite.sh
```

Enjoy!

Prepare Windows installation (for development team only)

place “CREATE_DISCUS64.tar.gz” into your development directory, go there and unpack:

```
cd $HOME/develop
tar -zxf 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
```

Use Inno setup to create the distribution.