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”
During the basic installation, please accept all defaults of the Cygwin installer.
See the section **Detailed Cygwin Installation** for a step to step guide

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.

Detailed Cygwin Installation
In order to install a suitable Cywin please do:

Download setup-x86_64.exe from the Cywin site at https://www.cygwin.com/
I recommend to store setup-x86_64.exe in a local folder say
Documents\CYGWIN_SETUP.
Execute setup-x86_64.exe
For the available choices during the installation, please take the defaults:

Source:	Install from Internet	
Root Install Directory:	c:\cygwin64	
Local Package Directory	Documents\CYGWIN_SETUP	Make it identical to setup-x86_64.exe location
Internet Connection	Use System Proxy settings	
Download site	any site with fast connection; ftp or http does not matter	
Select packages	Initially do not select anything that deviates from the defaults	

Despite the various internet sites, the post processing of cygwin tends to be very slow.
So once you get to the
z/perpetual
0p_000_autorebase.dash
screen, please be patient.

The DISCUS_SUITE compilation requires several additional libraries beyond the default, 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:

Execute setup-x86_64.exe
On the Select Packages screen select the View: Category

To select the required packages, the most efficient way, is probably to search for them in the Search input icon. Cygwin will display categories where the text that you entered into the search icon is found. With this please select:

Search string	Category	Select packages:	
cmake	Devel	cmake	! Nice build environment
		cmake-gui	! Nice gui for cmake
gcc-core	Devel	gcc-core	! Basic GNU compilers
gcc-fortran	Devel	gcc-gfortran	! Fortran compiler
gfortran	Libs	libgfortran4	! Fortran
gcc-g++	Devel	gcc-g++	! C++ compiler
make	Devel	make	! The gnu make utility
gccmakedep	Devel	gccmakedep	! Make Dependency tool
readline	Libs	libreadline-devel	! Readline development version
		libreadline7	! Should be in state “Keep” by now
			! Needed for command editing,
			! Version 7 or higher

Search string	Category	Select packages:	
png	Libs	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	Libs	libX11-devel	! X11 development library
libX11	Libs	libX11_6	! X11 core library
xterm	X11	xterm	! X-window program
xinit	X11	xinit	! X11 startup
dejavu	X11	dejavu-fonts	! True type fonts
zlib	Libs	zlib	! gzip compression
openmpi	Libs	openmpi	! Basic OpenMPI
		libopenmpi40	! DIFFUSE needs this for parallel
			! processing
		libopenmpi-devel	! DIFFUSE needs this for parallel
			! processing
ssh	Net	openssh	! Secure shell
zip	Archive	zip	! Compression
		unzip	! Reverse compression
ghostscript	Graphics	ghostscript	! Ghostscript interpreter
rgb	X11	rgb	! RGB data base

Optional Libraries

Python	! Make sure that you install Python 3.* only
	! Forget about Python2.* There are nasty incompatibilities between
	! Python2 and Python3.
NeXuS	! In the future DISCUS will use this for 3D data

Once all these packages have been installed, you are ready for the DIFFUSE_CODE installation itself.

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.

Make sure you start a new Cygwin64 Terminal after the installation of Cygwin has finished.
At the first time use, the bashrc files will be copied to your home directory. Please close the Cygwin terminal and open a new one again to ensure that paths and environment variables are properly set.

Installation:

One touch installation

Make sure you start a new Cygwin64 Terminal after the installation of Cygwin has finished.
At the first time use, the bashrc files will be copied to your home directory. Please close the Cygwin terminal and open a new one again to ensure that paths and environment variables are properly set.

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 called DIFFUSE_INSTALL.
Copy the current source code archive into this directory
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 5.29.0

```
cd $HOME/DIFFUSE_INSTALL
cp /cygdrive/c/Users/your_name/Downloads/DiffuseCode-5.28.0.tar.gz .
```

Install everything including the PGPLOT library by running the shell script install_discus_suite.sh:

```
./install_discus_suite.sh DiffuseCode-5.29.0.tar.gz
```

Close Cygwin and restart, as a line has been appended to the file '.bashrc' to define the PGPLOT environment variables.
Start the discus_suite with

```
discus_suite.sh
```

Alternatively, if and only if you do not need graphics, you can also run

```
discus_suite.exe
```

If you prefer a Linux like environment, that has access to X-windows, start the shell script /bin/xenv_suite.sh. Within this run suite_discus.exe or any other x-program.

```
/bin/xenv_suite.sh
```

The advantage of this X-terminal like environment is that you can start the discus_suite as a parallel process. See the DIFFEV manual for full details. To run a parallel (refinement) process type within the xterm, created by suite_discus.exe A possible command within the x-terminal might be:

```
mpiexec -np 4 discus_suite_parallel.exe -macro refine.mac
```

For Cygwin, we compile two versions, discus_suite.exe and discus_suite_parallel.exe. As the startup of MPI seems to be slow on many Windows versions, the non-parallel version can be used for many applications and will be much faster at startup. Unfortunately this requires to have the second version discus_suite_parallel.exe with a different name.

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

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

Enjoy !

In the unlikely event that errors might have occurred, try to check with the more detailed instructions on the following pages. Ensure that cygwin is exactly installed as detailed on the last 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 does 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 information (=manual) for command <command>
• info <command>
  Display information 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 that is defined within ccmake as the variable: PGPLOT_INCLUDE_DIR 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:

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 called DIFFUSE_INSTALL.

Change to this directory and unpack the archive DIFFUSE_CODE_pgplot.tar.gz

```
cd $HOME/DIFFUSE_INSTALL
tar -zxf DIFFUSE_CODE_pgplot.tar.gz
```

You will now have two new directories: pgplot and src/pgplot. Move these to their correct locations:

```
mv pgplot /usr/local
mv src/pgplot usr/local/src/
```

Switch to /usr/local/pgplot and for a standard installation run make:

```
cd /usr/local/pgplot
make
make cpg
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
```

The following instructions are needed only if you want to change graphic drivers.
If you want to add additional graphics drivers, edit the file drivers.list in /usr/local/pgplot and then make the makefile:

```
cd /usr/local/pgplot
vi drivers.list
/usr/ocal/src/pgplot/makemake /usr/local/src/pgplot/makemake linux gfortran_gcc
```

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
```

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 DiffuseCode-V.M.P.tar.gz to a suitable directory and unpack:

```
mkdir -p $HOME/develop
cp DiffuseCode-V.M.P.tar.gz $HOME/develop
cd $HOME/develop
tar -zxf  DiffiseCode-V.M.P.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 DIFFUSE_INSTALL (see one touch installation)

```
cd $HOME/DISCUS_INSTALL
```

Copy the shell scripts from SHELLS into the global bin directory:

```
cp SHELLS/* /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 &
```

Alternatively 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)

In addition to the components for a CYGWIN installation, we need installed in addition installed:

Search string	Category	Select packages:	
ssh	Net	openssh	! Secure shell
zip	Archive	zip	! Compression
		unzip	! Reverse compression
Xm4	X11	libXm4	! ?
paper	Libs	libpaper1	! Paper handling
		libpaper-common	! Paper handling
ghostscript	Graphics	ghostscript	! Ghostscript interpreter
gsm	Libs	libgsm1	!? Speech recognition?
rgb	X11	rgb	! RGB data base

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.