

## MACOS 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.

Install XCode, XQuartz and Homebrew

### One touch installation

Open a terminal. Click on the magnifying glass and enter **terminal**.

Copy the current DISCUS\_INSTALLATION.tar.gz to your home directory

```
cp Downloads/DISCUS_INSTALLATION.tar.gz $HOME
```

If necessary adjust the source path...

Unpack this archive:

```
cd $HOME
tar -zxf DISCUS_INSTALLATION.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 Downloads/DiffuseCode-5.29.0.tar.gz .
```

We will need a C and Fortran compiler, the PGPLOT plotting library, the PNG library and the cmake program to build large projects. To install all these packages once, run the shell script **macos\_brew\_discus\_suite\_pgplot.sh**. For future updates of the DISCUS\_SUITE you will not have to repeat this step. Install all of these packages including the PGPLOT library:

```
cd $HOME/DIFFUSE_INSTALLATION
sudo ./macos_brew_discus_suite_pgplot.sh
```

Install the DISCUS\_SUITE itself by running the shell script install\_discus\_suite.sh:

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

The install\_discus\_suite.sh script will place the sources into **\$HOME/develop/** and **\$HOME/develop/DiffuseBuild**. The compiled programs will be in **/usr/local/bin**. Feel free to adjust paths.

The following steps do not seem to be absolutely necessary:

In order to use the PGPLOT library, you need the following environment variables:

See the files in **DIFFUSE\_INSTALL/SHELL** for templates. You can write the following lines for

example into `/etc/profile.d/profile.local`, or into `$HOME/.bashrc.local`.

```
PGPLOT_DIR="/usr/local/pgplot"; export PGPLOT_DIR
PGPLOT_DEV="/XSERVE"; export PGPLOT_DEV
PGPLOT_FONT="/usr/local/pgplot/grfont.dat"; export PGPLOT_FONT
```

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

## Open issues

The build in ‘manual’ command currently does not work. Look up the manual in the directory `/usr/local/share/`

Manual files are

```
suite_man.pdf
discus_man.pdf
diffv_man.pdf
kuplot_man.pdf
package_man.pdf
```

from within the `discus_suite` you can look at each of these manual files with the command:

```
system open /usr/local/share/suite_man.pdf
system open /usr/local/share/discus_man.pdf
system open /usr/local/share/kuplot_man.pdf
system open /usr/local/share/diffv_man.pdf
system open /usr/local/share/package_man.pdf
```

To run an interactive plot, please install Jmol and the proper MACOS java run time environment.

## Individual manual 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 5.29.0

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

```
mkdir -p $HOME/develop
cp DiffuseCode-5.29.0.tar.gz $HOME/develop
cd $HOME/develop
tar -zxf DiffuseCode-5.29.0.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-5.29.0/
```

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 MACOS 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. See the file [macos\\_brew\\_discus\\_suite\\_pgplot.sh](#) for a template for the symbolic link.

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:

**sudo make install**

To clean up type

**make clean**

for the on-line help to work, a couple of environment variables should be set:

```
PGPLOT_DIR="/usr/local/pgplot"; export PGPLOT_DIR
```

```
PGPLOT_DEV="/XSERVE"; export PGPLOT_DEV
```

```
PGPLOT_FONT="/usr/local/pgplot/grfont.dat"; export PGPLOT_FONT
```

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

## PGPLOT Library

With MACOS the manual installation currently is an issue. Please try

```
brew install homebrew/X11/pgplot
```

See the file [macos\\_brew\\_discus\\_suite\\_pgplot.sh](#) for a template to create the necessary symbolic links.

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
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

Alternatively you can of course edit your local .bashrc.local .

Finally run one or more of the pdgemo programs to verify that the installation proceeded properly.