MACOS installation of the DISCUS/DIFFEV/KUPLOT software
Version 5.31.

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 5.29.1

```
cd $HOME/DIFFUSE_INSTALL
cp Downloads/DiffuseCode-5.29.1.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
./macos_brew_discus_suite_pgplot.sh
```

As some steps in this macro are run as “sudo”, the script macos_brew_discus_suite_pgplot.sh will ask you for your password.
Install the DISCUS_SUITE itself by running the shell script install_discus_suite.sh:

```
sudo ./install_discus_suite.sh   DiffuseCode-5.29.1.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.

JMOL Installation

The discus_suite has build in capabilities to plot a crystal structure interactively. For this the program jmol which is a java program is used. Compared to other CIF file viewers it is super fast. If you want to use these capabilities please:

Download and install JDK Java Development Kit from the most recent JDK download site, currently:

https://www.oracle.com/technetwork/java/javase/downloads/jdk8-downloads-2133151.html

select MAC OS X x64 and download. On you MAC click on the Download icon and click on the jdk dmg icon to start the JDK installation. Follow the instructions on the screen.

Download Jmol from

http://jmol.sourceforge.net/download/

follow the Download link. Select a binary, either as zip or tar file. This should start an automatic download of a MAC installation file. Upon your download unpack the archive and you should have in your Downloads directory a directory called

Downloads/jmol-14.29.29

The exact name will of course depend on the jmol version that you download.
Go to the DIFFUSE_INSTALL directory

```
cd $HOME/DIFFUSE_INSTALL
```

run the jmol preparation script

```
sudo ./jmol_prepare.sh   jmol-14.29.29
```

Make sure that the parameter to the script is the name of the jmol installation that you downloaded into Downloads and that the jmol directory is in the Downloads folder. The script will create a folder JMOL in your home directory and copy the jmol run script into /usr/local/bin
As I cannot copy the Jmol.jar file into /usr/share/java (MAC does protect this directory rather strictly) the file Jmol.jar needs to be referenced via an environment variable.
The script looks for either of .bashrc or .bash_login or .bash_profile or .profile. It will then add a line source $HOME/.profile.local to the end of the file .bashrc, .bashrc_login, .bashrc_profile or .profile. It furthermore adds a file .profile.local I to your home directory which the environment variable JMOL_HOME is set.
If you now open a new terminal, the command jmol should start the Jmol program. If this works, the following discus_suite macro will successfully display your crystal structure:

```
plot
  program jmol
  outfile   any_nice_name.cif
  select all
  run plot:inter
exit
```

Individual manual Installation:

Download the latest source code archive from GitHUB at:
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 5.29.1
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 ccmake with source code directory as parameter.
ccmake should open a graphical interface:

```
ccmake ../DiffuseCode-5.29.1/
```

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:
DIFFUSE_PYTHON, DISCUS_CUDA, DISCUS_NEXUS, DISCUS_OMP

In ccmake 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 ccmake 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.
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.