MACOS installation of the DISCUS/DIFFEV/KUPLOT software
Version 5.99.

1. Preparation:
The compilation requires several libraries, especially their development versions, not all of them may be installed automatically.

Currently these are Xcode, Command Line Tools, Xquartz, Homebrew, gcc, cmake , libpng and ghosscript. The installation file currently DIFFUSE_INSTALL-v5.99.13.tar.gz contains a shell script

macos_brew_discus_suite_pgplot.sh

which will install all these packages. This step needs to be carried out only once. For later updates of the discus_suite you can skip this step.

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

Copy the current DISCUS_INSTALL-v5.99.13.tar.gz to your home directory

```
cp Downloads/DISCUS_INSTALL-v5.99.13.tar.gz $HOME
```

If necessary adjust the source path...

Unpack this archive:

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

This will create a directory called DIFFUSE_INSTALL.
Execute the shell script:

macos_brew_discus_suite_pgplot.sh

The installation will require administrator rights to install. Once everything is installed, restart your computer to ensure that all processes are properly updated.

If this step worked fine, jump to the section **2. One touch installation**. Otherwise see the section on further details.

2. One touch installation

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

Copy the current DISCUS_INSTALL-v5.99.13.tar.gz to your home directory

```
cp Downloads/DISCUS_INSTALL-v.5.99.13.tar.gz $HOME
```

If necessary adjust the source path...

Unpack this archive:

```
cd $HOME
tar -zxf DISCUS_INSTALL-v.5.99.13.tar.gz
```

This will create a directory called DIFFUSE_INSTALL.
Copy the current source code archive into this directory
The archive is called DiffuseCode-vV.M.P.tar.gz, where V.M.P stands for the major Version, the Minor version and the Patch numbers, currently 5.99.13

```
cd $HOME/DIFFUSE_INSTALL
cp Downloads/DiffuseCode-v5.99.13.tar.gz .
```

2.1 Preparation

If the steps in **1. Preparation** were done, you can skip this paragraph. 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:

```
cd $HOME/DIFFUSE_INSTALL
./macos_brew_discus_suite_pgplot.sh
```

As some steps in this macro require administrator privileges please run this from an administrator account. Once the installation is done, restart your computer.

2.2 DISCUS Installation

Install the DISCUS_SUITE itself by running the shell script install_discus_suite.sh:

```
sudo ./install_discus_suite.sh   DiffuseCode-v5.99.13.tar.gz
```

or alternatively

```
./install_discus_suite.sh   DiffuseCode-v5.99.13.tar.gz
```

If run with sudo the install_discus_suite.sh script will place the compiled programs into /usr/local/bin and they will be available to all users of the MAC, if run without sudo the programs will be in $HOME/bin as a private installation.

Feel free to adjust paths. Once the installation is finished, please check the file $HOME/.profile.local. Due to MAC specifics, there might be multiple lines within thus file. Please remove any multiple occurrences of a line. Close the terminal to ensure that all paths are set properly. At a new terminal you should be able to run the suite with the command

```
discus_suite
```

Enjoy!

3. 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:

Go to AdoptopenJDK

https://adoptopenjdk.net

Choose and download OpenJDK11. This will download the file

OpenJDK13U-jdk_x64_mac_hotspot_11.0.4.pkg

Or a similar version wit slightly different version numbers. Once the file download is complete, click on the package file to start the installation. Follow the on-screen instructions

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 check if the archive has been unpacked automatically, if not unpack the archive and you should have in your Downloads directory a directory called

Downloads/jmol-14.29.54

The exact name will of course depend on the jmol version that you download. Please leave the jmol directory at this place.
Go to the DIFFUSE_INSTALL directory

```
cd $HOME/DIFFUSE_INSTALL
```

run the jmol preparation script

```
./jmol_prepare.sh   jmol-14.29.54
```

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 to your home directory in which the environment variable JMOL_HOME and an abbreviation to start the jmol program are set.

Please check the file $HOME/.profile.local with a suitable editor and remove double lines. Close the terminal and open a new one or run the file .profile.local:

```
source $HOME/.profile.local
```

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 a dummy test structure.

```
discus
read
free
insert Si, 0.0, 0.0, 0.0,  0.1
insert Si, 2.0, 0.0, 0.0,  0.1
insert Si, 0.0, 2.0, 0.0,  0.1
insert Si, 0.0, 0.0, 2.0,  0.1
plot
  program jmol
  outfile   dummy_plot.cif
  select all
  run plot:inter
exit
exit
```

4. Details on preparatory installation procedures

If you desire to learn more about the packages that were installed, a good guide is at :

https://www.moncefbelyamani.com/how-to-install-xcode-homebrew-git-rvm-ruby-on-mac/

Xcode:

XCode in combination with the Command Line Tools adds a lot of developer packages to your MAC. To install manually, start a terminal window. If you do not have a terminal icon, you can find it via Spotlight. Start

Command-Space

type terminal, once it appears select it and press return to start the terminal. Within the terminal type

```
xcode-select  --install
```

A pop up should open, follow the instructions to “Install”.

Command Line Tools:

The Command Line Tools will build a lot of development tools that will come in handy. To install, run the previous command again and follow the instructions that pop up:

```
xcode-select  --install
```

Homebrew:

This is a package manager that lets you install many useful tools:

Type in a single line:

```
ruby -e "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/master/install)"
```

XQuartz

XQuartz brings the “X11” Window system to your MAC. The graphics part of the discus_suite uses this window system to display images and graphs. Once homebrew is installed install the XQuartz package with

```
brew cask install xquartz
```

Compilers, libraries

As the discus_suite will be compiled from the source code, we need of course a compiler, and some libraries which are often not installed by default.

gcc

The gcc GnuCompilerSuite provides the C and fortran compilers needed.

cmake

This is a nice package to handle the compilation of large source code projects.

libpng

The graphics within the suite can write images in the “png” file format.

ghostscript

Allows you to handle PostScript files and convert these to many other formats.

5. 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.