

1. Installation

1.0 Preparation

DISCUS requires several libraries and general build tools to have been installed on your MAC. The installation script should install these, yet I've seen MAC variants where this does not seem to work. It might be best to install xquartz and homebrew prior to the discuss installation. Open a **terminal**. Click on the magnifying glass and enter **terminal**. Once you have opened the terminal please type:

```
conda deactivate                # Only needed if you have Anaconda active!
export CONDA_SHLVL=0
cd $HOME
xcode-select --install          #(there are two '-' in front of install)
```

Once xquartz is installed, it seems best to restart the computer.
Then, visit: <https://brew.sh/> and install Homebrew according to the current installation guide.

During the DISCUS installation, please keep Anaconda turned off, afterwards you can activate Anaconda again with:

```
export CONDA_SHLVL=1
conda activate
```

1.1 One touch installation

Please make sure that you remove all old versions of the installation script, both from the Downloads folder and your \$HOME folder.
Download the latest installation script **bbb_install_script_mac.sh** from the DiffuseCode download site at: <https://github.com/tproffen/DiffuseCode/releases/>.

Run this script, if necessary adjust the source path... To run the script, open a **terminal**. Click on the magnifying glass and enter **terminal**. You might have to check in **System Preferences** under the **Security & Privacy** for the setting regarding **Full Disk Access**. Please make sure that the check box to the left of the **terminal** entry is checked. Once you have opened the terminal please type:

```
cp ${HOME}/Downloads/bbb_install_script_mac.sh  ${HOME}
cd ${HOME}
chmod u+x $HOME/bbb_install_script_mac.sh
$HOME/bbb_install_script_mac.sh
```

The script will ask for the type of installation (globally for all users into /usr/local/bin or locally into \$HOME/bin). If the script needs to install packages you will be asked for your (SUDO) password. If you do not have sudo rights, please ask your local administrator for help with the first installation. On a MAC I recommend to install the DISCUS SUITE locally.

If you have an active ANACONDA environment, there is a good chance that the CONDA

environment messes up the compilation of Fortran during the linker stage. It seems best to turn off CONDA prior to the installation:

```
conda deactivate  
export CONDA_SHLVL=0
```

Once the installation is finished, CONDA can be activated again:

```
export CONDA_SHLVL=1  
conda activate
```

The script will create a local installation directory \$HOME/DIFFUSE_INSTALL. For future work with the DISCUS_SUITE I suggest to use a different directory for your macros and data.

At a first time installation of discuss, (really just the first time installation of xquartz) you will have to restart your Mac at this point.

Once the installation is finished, open a new terminal/konsole and type

```
discus_suite
```

Enjoy!

Future updates can be run via the script [bbb_install_script_mac.sh](#) or simply by the discuss_suite command '**update**'.

0.1 Occasional glitches

Occasionally, an operating system update might mess up the links to dynamically linked libraries. In this case the pre-compiled version is likely not working for you any longer. To force a fresh compilation, change to your home directory and run the install script with optional parameters:

```
$HOME/Downloads/bbb_install_script.sh code=git install=local
```

The full scope of the optional parameters is:

<code>code=pre</code>	! Use a precompiled DISCUS version
<code>code=git</code>	! Use the current source code released at GitHub
<code>code=archive.tar.gz</code>	! Use the archive called “archive.tar.gz”, often something like ! DIFFUSE_CODE_v.6.03.00.tar.gz
<code>install=fetch</code>	! Get the latest installer from GitHub
<code>install=local</code>	! Use the current installer
<code>install=archive.tar.gz</code>	! Use the archive called “archive.tar.gz”, often something like ! DIFFUSE_INSTALL_local.tar.gz
<code>prepare=libraries</code>	! Install and update libraries
<code>prepare=none</code>	! Skip the check for new libraries

I have experienced issues on MacOS upon a change of the major operation version. This is likely to mess up `xcode`, `brew` and possibly `xquartz`. As first remedy, try to run the script “`prepare_macos.sh`” that is located within `DIFFUSE_INSTALL`:

```
cd $HOME
source ./DIFFUSE_INSTALL/prepare_macos.sh
```

Now try the DISCUS installation again. If it still does not work, you might have to uninstall “`brew`”, “`xquartz`” and “`xcode`” and then install them again.

A first remedy that seems to work is to force reinstallation of “`xcode`”, and then an upgrade of the `gcc` compiler: Try:

```
cd $HOME
xcode-select --install          #(there are two '-' in front of install)
brew upgrade gcc
```

On some installations of the MacOS operating system the software installer states that is in a “shallow” state. Unfortunately this does not seem to trigger an error message but still several of the required libraries will not have been installed. Commonly, the compilation of our graphics library, respectively `DISCUS_SUITE` itself will trigger an error message related to a missing “*X*” library. If you encounter this error, please step into the installation directory and run the preparatory script `prepare_macos.sh`. Once its finished scroll back to the beginning, and you should see a message that “`brew`” is “shallow” and a command line how to “unshallow” `brew`. Please copy this line into your terminal and execute this line. Thereafter, run the `prepare_macos.sh` script and finally go back to the home directory and run the main installation script.

0.2 Rare (?) glitches

On older versions of the MacOS operating systems (prior to 10.13?) the installation of the Java and JavaRuntimeEnvironment (JRE) seems to fail, with an error message that the archive is too old / has expired. The only effect on discus is that you will not be able to plot a structure directly from the discus plot menu. Instead, write a cif file and use other available software to plot the structure.

The following glitch should have been fixed with version 6.09.02. The Cellar folder is created and used by homebrew. Depending on the MacOS version it is located at `"/usr/local/Cellar"` or at `"/opt/homebrew/Cellar"`. The new installation scripts use brew tools to find this folder.

I have encountered one case, where there was no directory `"/usr/local/Cellar"`. I thought this should have been standard. I am not sure to which folder optional programs and libraries will be installed if this is missing. A careful fix might be to create this folder. Warning, I do not know what effect it might have on other program/applications.

```
sudo mkdir /usr/local/Cellar
```

Try the discus installation again.

1. Detailed 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 DISCUS_INSTALL-v6.08.02.tar.gz contains a shell script

`prepare_macos.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-v6.08.02.tar.gz to your home directory

`cp Downloads/DISCUS_INSTALL-v6.08.02.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 `DISCUS_INSTALL`.

Execute the shell script:

`prepare_macos.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-v6.05.00.tar.gz to your home directory

```
cp Downloads/DISCUS_INSTALL-v.6.05.00.tar.gz $HOME
```

If necessary adjust the source path...

Unpack this archive:

```
cd $HOME
tar -zxf DISCUS_INSTALL-v.6.05.00.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 6.05.00

```
cd $HOME/DIFFUSE_INSTALL
cp Downloads/DiffuseCode-v6.05.00.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
./prepare_macos.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-v6.05.00.tar.gz
```

or alternatively

```
./install_discus_suite.sh DiffuseCode-v6.05.00.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 this 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 built 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 with 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.moncefbellyamani.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 cmake with source code directory as parameter.

cmake should open a graphical interface:

```
cmake ../DiffuseCode-5.29.1/
```

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.