Installation of PhreePlot on Linux and Mac systems

1. Requirements

Various binaries are distributed for non-Windows operating systems, particularly Linux and Mac. The OS's supported and their flavours may change from time to time. The notes below provide a guide to their installation. Contacts for queries are given at the end of this document.

PhreePlot will run natively under a variety of non-Windows operating systems but this may require the installation of some external libraries, or an update to existing ones. These supporting libraries include those used by **PhreePlot** itself along with those used by the embedded **PHREEQC** (**phreeqcRM**) library. The actual libraries required depend on your operating system and the compilers that have been used to compile **PhreePlot** and **phreeqcRM**. You may need administrator rights (root permission) to install or update these components. No compilation of **PhreePlot** is required. **Ghostscript** (`gs`) is also required for converting the native **Postscript** output to alternative file formats.

For the `gfortran` version of **PhreePlot**, the following libraries are required:

- `gfortran (part of the gcc distribution)`
- `libgfortran5 (runtime library)`

Other libraries used are: `libstdc++`, `libc`, `libm`, `libgomp`, `linux-vdso`, `libgcc`, `libpthread`, `libquadmath` and `libdl`.

If you have an older version of Linux installed, you may have to update your libraries, especially `gfortran` (if it is 9.3.0 or above, this should be sufficient). Instructions for how to update older systems can be found at https://fortran-lang.org/learn/os_setup/install_gfortran and some instructions are also included below.

The various releases of **PhreePlot** are named according to their build characteristics, e.g.:

`pp version: 1`

`OS: Linux | Darwin`

`compiler: gfortran`

`compiler version: 11.2`

`OS flavour: Ubuntu`

`Chip: x86_64 | arm64`

`PHREEQC: build number`

giving the compressed archive a name such as

```
pp_1-Linux_gfortran_10_Ubuntu_x86_64_15968.tar.bz2
```

All of the shell scripts included in the distribution are for the bash shell. In other shell environments, these should either be modified accordingly or be run explicitly with the bash shell, e.g.:

```
/bin/bash phreeplot.sh
```

2. Getting ready for installation

2.2. LINUX

The source of the libraries required varies with the flavour of Linux being used.

2.2.1 Ubuntu

You need `gcc` and **Ghostscript** (`gs`) installed to run to full capability.

Check in your terminal (or console) if these are installed with: `which gcc`

and

```
which gs
```

If a full path is not returned, then they are not installed. To install, enter the following as needed:

```
sudo apt install gcc
```

```
sudo apt-get install gfortran
```

```
sudo apt-get install ghostscript
```

Once installed, check the version

```
gfortran -v
```

If it is 9.3.0 or above, then this should be sufficient. If not, you may need to update your system:

```
sudo add-apt-repository ppa:ubuntu-toolchain-r/test sudo apt update
```

sudo apt dist-upgrade

```
sudo apt-get install gfortran-10
```

```
sudo update-alternatives --install /usr/bin/gfortran gfortran
/usr/bin/gfortran-10 100
```

These instructions also apply to WSL (Windows Sub Linux) and other Debian-based flavours.

2.2.2 CentOS

```
sudo dnf groupinstall "Development Tools" or
```

```
sudo yum install gcc-gfortran
```

2.2.3 Suse

2.3 MAC OS X

The current release for Mac OS is compiled for the arm64 architecture of the M1 chip.

3. Installation and Setup

Copy the appropriate pp*.bz2 archive to your preferred directory.

Unzip using, e.g. for Ubuntu

```
tar -xvf pp_1-Linux_gfortran_10_Ubuntu_x86_64_15968.tar.bz2
```

When unzipped, it will create a directory 'phreeplot' in your current directory containing the shell script phreeplot.sh and below this, the following sub-directories:

/bin	contains the pp binary
/demo	contains a number of demo examples
/doc	contains the documentation
/lib	contains libPhreeqcRM.a
/system	contains various files used by **PhreePlot**

PhreePlot makes use of two environment variables, PHREEPLOT and PHREEPLOT_PATH to specify the location of files. If the export command is available, these can be set with:

export PHREEPLOT=*/location of the installation, specifically of the system directory/*. export PHREEPLOT_PATH=*/location of the pp binary file/*.

PHREEPLOT_PATH can be added to your PATH, as in the script below, making the **PhreePlot** executable, pp, accessible from any location:

```
export=$PHREEPLOT_PATH:$PATH
```

phreeplot.sh declares these variables and should be executed as

```
source ./phreeplot.sh
```

before executing PhreePlot. Alternatively, a single line could be added to your .bashrc file such as:

```
source /directory_where_phreeplot_is/phreeplot/phreeplot.sh
```

so that the file will be executed each time a terminal is opened.

Note that phreeplot.sh prepends the executable path to the beginning of the existing PATH without deleting any other possible occurrences of the path.

The libraries, and their versions, required to run a given distribution can be found using

```
ldd pp
```

or its equivalent.

If the export command is not available (as with non-bash shells) , use:

```
LD_LIBRARY_PATH “/directory/you/choose"
```

Finally, an internet search with any error messages can often be useful.

4. Testing and running

If you have **sourced** the `phreeplot.sh` script, enter

```
pp -v
```

If the installation was successful, and if it was installed in say the `/home/` directory, you should see something like (versions and dates may differ):

```
Usage:   pp input_file_name [other command line parameters...]


PhreePlot version:                    1 (Linux-gfortran-9.3.0-x64) 09:45:29 14 Oct 2022
PHREEPLOT environment variable:       /home/phreeplot
PHREEPLOT_PATH environment variable:  /home/phreeplot/bin
Phreeqc version:                      3.7.3-15968
Ghostscript version and source:       GPL Ghostscript 9.50 (2019-10-15)(installed)
System directory:                     /home/phreeplot/system/ (root set by PHREEPLOT
environment variable)
```

Scripts can be made to run one or more instances of **PhreePlot** in the normal way.

A test script, `test1.sh`, can be found in the `/demo` directory. This runs the `demo/test/test.ppi` file which produces a predominance diagram for Fe and, if **Ghost-script** is installed, graphical output files in other formats.

```
source ./demo/test.sh
```

A larger range of examples can be found in the demo directory.

```
cd demo
source ./demo.sh
```

5. Contacts

PhreePlot general enquiries: David Kinniburgh, david@phreeplot.org

Linux/Mac installation enquiries: Marino Vetuschi Zuccolini, mailto:marino.zucco-lini@unige.it