

## PkFit & Filing v3

for

### Mac OS X

Last update : 19 Sept 2007 (+ 19 Sept 07)

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**Filing:** A tool to handle data files of three-axis spectrometers (TAS)

**PkFit:** A tool to fit data from neutron three-axis spectrometers (TAS)

Ref:

A. Bouvet, A. Filhol (1997) Technical report ILL97BO03T, Institut Laue-Langevin, France.

<<http://www.ill.fr/tas/pkfit/readme.html>>

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## I- VERSION 3

### I.1- Main features

The version 3 of PkFit & Filing for Mac OS X is based on the X11 graphic library PGplot which is available for most platforms. PGplot is used both for plotting the data and also for the design of a human interface with buttons, menus, edit fields, etc. Since PGplot was never designed for that the resulting interface is not very comfortable. Furthermore, the main concern for the Mac OS X version are bugs in their rarely used keyboard input routines. This is true for the PGplot libraries available from the net, e.g. :

<<http://www.astro.caltech.edu/~tjp/pgplot/>> v5.2

<<http://www.ill.fr/Computing/pgplotSS.html>>

Therefore we used our own modified version of PGplot.

Main features of the current version of PkFit and Filing

- 1- It is X11 based. An xterm is required to run these applications and thus do not expect a nice Apple like interface !
- 2- It makes use of an improved version of PGplot and supports Aquaterm.
- 3- It supports the most recent (April 07) ILL data file formats for TAS instruments.
- 4- It supports the most recent (April 07) file formats for polarised neutrons on TAS instruments, including CRYOPAD files.
- 5- Both applications are provided as:
  - a line command application: to be launched from an X11 terminal
  - a bundled application: to be launched by double-clicking the icon (see the launcher description § II-1).

### I.2- FAQs

- Which Mac OS version are supported ?  
10.3.9 or higher

- What about Macintel computers ?

The current PkFit and Filing are compiled for PPC computers but are fully functional on Macintel computers owing to Rosetta. Universal binary versions are foreseen.

- What are the differences with the Mac OS classic version

The calculation routines are the same but the PGplot based interface of the Mac OS X version cannot pretend to compete with the interface based on Apple's APIs

- Why X11 for the Mac OS X version ?

The Mac OS classic version used the graphic library TSIgraphics which is dead for long (source code not available). The interface was pure Fortran with direct calls to Apple's APIs. This is only possible with the Absfort Fortran compiler and the effort to switch from Mac OS classic to Mac OS X was huge. It was thus easier and faster to port the Unix version to Mac OS X without bothering too much with the quality of the interface.

- What is the future of PkFit & Filing

A much better interface is being prepared based on Winteracter <[www.winteracter.com](http://www.winteracter.com)>, an advanced and multiplatform graphical library.

## II- INSTALLATION NOTES

### II.1- X11 terminal

PkFit and Filing v3 cannot run without an X11 terminal.

Apple provides X11.app which can be installed using "Optional Installs.mpkg" from the DVD "Mac OS X Install DVD".

To see the icon of this installer, scroll down the window contents.

Remember that you can past command to that X11 terminal using "option click" only. The usual "command-V" is inactive.

Also exist some third parti X11 terminal.

### II.2- Installing PGplot + Aquaterm.app

Both are required even if you prefer the classical X11 terminal to the Aqua look and feel.

#### II.2.1- Installing Aquaterm.app

- via SourceForge : <<http://aquaterm.sourceforge.net>>

version 1.0.1 (universal binary)

This is the easiest solution since the installer is provided in the form of a .dmg file

- via FinkCommander <-- do not use !

This installs an older version and not at the right place, i.e. :

/sw/Library/Frameworks/AquaTerm.framework/Versions/A/AquaTerm

while PkFit wants:

/Library/Frameworks/AquaTerm.framework/Versions/A/AquaTerm

#### II.2.2- Installing PGplot

##### ATTENTION

PGplot (from SourceForge or other) is normally installed in: /sw/lib/pgplot

PkFit uses a modified version instead which is installed in: /usr/local/lib

The minimal installation is as follows :

#### Mac OS 10.4 (Tiger) PPC or Macintel

Warning: you must have administrator privileges.

Install PGplot from the files in the folder "PkFit\_MacOS10.4\_PPC":

Create the following directory

```
sudo mkdir -p /usr/local/lib
```

In the commands below, replace "??yourAccount??" by the appropriate characters ###

```
cd /Users/??yourAccount?~/PkFit_MacOS10.4_PPC/pgplot-olilog/

sudo mv libgplot.dylib /usr/local/lib
sudo mv pgxwin_server /usr/local/lib
sudo mv grfont.dat /usr/local/lib
sudo mv rgb.txt /usr/local/lib

sudo mv libg2c.dylib /usr/local/lib
sudo mv libg2c.0.dylib /usr/local/lib
sudo mv libg2c.0.0.0.dylib /usr/local/lib

sudo mv libgcc_s.1.dylib /usr/local/lib
sudo mv libgcc_s.1.0.dylib /usr/local/lib
sudo mv libgcc_s.10.4.dylib /usr/local/lib
sudo mv libgcc_s.10.5.dylib /usr/local/lib

cd /usr/local/lib
sudo ln -s libgcc_s.1.0.dylib libgcc_s.dylib
sudo ln -s libgcc_s.1.dylib libgcc_s_ppc64.1.dylib
sudo ln -s libgcc_s.1.dylib libgcc_s_x86_64.1.dylib
```

#### Mac OS X Jaguar (10.3.9) <- gcc & g77 3.4.6

Warning: you must have administrator privileges.

Install PGplot from the files in the folder "PkFit\_MacOS10.3.9\_PPC":

```
### replace the ??? below by the appropriate characters ###
cd /Users/??yourAccount?~/PkFit_MacOS10.3.9_PPC/pgplot-olilog/

sudo mv libgcc.0.dylib /usr/local/lib
sudo mv libg2c.0.0.0.dylib /usr/local/lib
sudo mv libgplot.dylib /usr/local/lib
sudo mv pgxwin_server /usr/local/lib
sudo mv grfont.dat /usr/local/lib
sudo mv rgb.txt /usr/local/lib
cd /usr/local/lib
sudo ln -s libg2c.0.0.0.dylib libg2c.dylib
sudo ln -s libg2c.0.0.0.dylib libg2c.0.dylib
sudo ln -s libgcc_s.1.0.dylib libgcc_s.dylib
```

### II.3- Environment variables

Defining these variables is compulsory only if you prefer to launch PkFit and Filing using line commands in an X11 terminal (see § II.4.1). Bundled applications (i.e. with double-clickable icons) automatically set the variables for you (see § II.4.1 and II.4.3).

Create a .bashrc file or append the following command lines to the existing one.

```
export PGPLOT_DIR=/usr/local/lib
export PGPLOT_FONT=/usr/local/lib/grfont.dat
export PKFITDATA=~/.Documents/ <- or any valid path to a data folder (must end with a slash)
export PGPLOT_DEV=/xserv <- classical xterm
or
export PGPLOT_DEV=/aq <- aquaterm interface (supports printing)

???? is this useful ????
export PATH=/usr/local/lib:$PATH
```

#### Attention:

X11 Xterm sees .bashrc but does not see .bash\_profile  
Terminal.app sees .bash\_profile

You may experience the alternatives yourself: .bash\_login or .profile or even /etc/profile

Remember that, when you log in, Bash reads first /etc/profile then [.bash\_profile or .bash\_login ou .profile] but only one of the last three ! Furthermore .bashrc is not read when you log in.

### II.4- Installing and launching the application

#### II.4.1- Installing

Depending on your system, go to either folder PkFit\_MacOS10.3.9\_PPC or PkFit\_MacOS10.\$\_PPC

Ligne command applications :

folder : "terminal-app"

move the files to a folder referenced in the variable \$PATH

Packaged applications :

Drag and drop the icons of PkFit-Olilog317.app and Filing-Olilog317.app to the folder Applications

## II.4.2- Using command lines

Warning: you must have administrator privileges

- copy the files "pkfit" and "filing" (unix applications) to a folder referenced in the PATH variable  
e.g. /usr/bin (or /usr/local/bin but check with printenv)  
    cd xxxxx <- path to the folder containing the application files  
    sudo mv pkfit /usr/bin  
    sudo mv filing /usr/bin
- define the environment variables in .bash\_profile (see §II.3)
- open an X11 terminal
- optionally set a new data file path (environment variable PKFITDATA (see §II.3))
- type command  
    pkfit

## II.4.3- Using the bundled form of the applications

- double-click the icon of the application  
    PKFITDATA will be defaulted to "~"  
    X11 will be automatically started and the application will launch.
- drag&drop a data folder to the icon of the application  
    PKFITDATA will automatically set to the path of the folder

See section 6 for more details on the launcher.

## III- TECHNICAL NOTES

### III.1- The launcher

It is based on a generic Script Launcher by Martin Fuhrer (mfuhrer@alumni.ucalgary.ca): XDroplet 1.0.1.

<<http://automators.net/news/freshmeat-net-announcements-mac-os-x/xdroplets-1-0-1-default-branch/>>

It combines a Java application (droplet), an AppleScript file (main.scpt) and a shell script (launcher.sh) to launch an X11 terminal, set all necessary environment variables and then launch the application itself.

The contents of the application's bundle is as follows:

```
Application/Contents
  Info.plist    <- (6.1)
  MacOS
    droplet
      pkfit     <- (6.3)
  PkgInfo
  Resources
    droplet.icns
    droplet.rsrc
    InfoPlist.strings <- (6.1)
    launcher.sh      <- (6.5)
    PkFit-appl.icns  <- (6.2)
  Scripts
    main.scpt       <- (6.4)
```

#### III.1.1- Info.plist

Some tags have been modified

```
<key>CFBundleIconFile</key>
<string>PkFit-appl</string>
<key>CFBundleGetInfoString</key>
<string>v3.0 @2007 Institut Laue-Langevin and Olilog</string>
<key>CFBundleVersion</key>
<string>1.0.0</string>
<key>CFBundleShortVersionString</key>
<string>PkFit-Pgplot Application 3.0, PPC, X11</string>
```

#### III.1.2- Bundle icon

The file "PkFit-appl.icns" is the icon of the bundle and is referenced in Info.plist (see 6.1)

#### III.1.3- Application

The folder "MacOS" must contain only two files: droplet and either pkfit or filing

#### III.1.4- AppleScript file main.scpt

This AppleScript has been substantially modified to fit our requirements

- 1- the contents of the folder Contents/MacOS is analysed and any parasitic file (e.g. tmp.tmp, .log, or debug files) is moved out of the bundle
- 2- application not running: if a folder or a file is dropped on the bundle icon, its path is placed in the environment variable PKFITDATA and then the application is launched
- 3- application already running: if a folder or a file is dropped on the bundle icon, its path is written to the preference file of the application (not yet available)

Variable to be set to the name of the application stored in the folder MacOS :

```
property appName : "pkfit"
-- property appName : "filing"
```

#### III.1.5- Shell script launcher.sh

This script has been modified:

- the bundle can now be placed in any folder
- all environment variables are set (see §II.3)
- space characters in file path are no longer a problem

Variable which can be modified:

```
export PGPLOT_DEV='/xserv'      #-- xterm
#export PGPLOT_DEV='/aq'       #-- Aquaterm
```

#### IV- HISTORY OF THE MAC OS X VERSIONS

##### 4 May 2007, known Bugs

If the application is in "~/ " if will crash (segmentation fault) when trying to move the tmp.tmp file from "~/ " to the same location. If PKFITDATA is undefined, the creation of the .LOG file fails and the application crashes.

##### 10 April 2007, PkFit+Filing 3.1.7 (1.1.7)

PkFit +Filing (Mac OS 10.4 et 10.3.9 PPC)

Support of new ILL file formats

- CRYOPAD files with a new PAL coding (old one was "1.x") or with a unique value e.g. 2.
- CRYOPAD files with PAL values equal to e.g. 4. and values 1.,2. or 3. absent
- CRYOPAD files: when selecting a PAL value, all available values are shown (max. 18) and the missing ones are replaced by NO

Example of file contents:

```
DATA_:
PNT  PAL  CNTS  QH  QK  QL  EN  M1  M2  TI  A1  A2  A3  A4  A5  A6  TT  TRT  THI
THF  IPi  IPf  INDi  INdf  INgi  INAi  INgf  INAf
1.  2.  38.  1.1400  0.3800  1.7000  40.000  500.  0.  455.45  -9.00  -18.03  137.36  9.70  -13.76  -27.55  1.9580  2.0020  17.47
27.17  1.002  -1.781  3.500  -3.507  1.300  2.900  2.500  2.900
2.  2.  35.  1.2000  0.4000  1.7000  40.000  500.  0.  458.21  -9.00  -18.03  134.36  12.42  -13.76  -27.55  1.9560  1.9950  21.65
34.07  1.002  -1.779  3.500  -3.506  1.300  2.900  2.500  2.900
3.  2.  42.  1.2600  0.4200  1.7000  40.000  500.  0.  459.66  -9.00  -18.02  132.24  14.76  -13.76  -27.55  1.9570  1.9980  24.75
39.57
```

##### 28 March 2007, PkFit+Filing 3.1.6 (1.1.6)

Versions of PkFit +Filing for both Mac OS 10.3.9 and 10.4 PPC

- files .LOG and tmp.tmp are now created in the folder \$PKFITDATA instead of the current working directory.

Support of new ILL file formats

- CRYOPAD files with/without POLAN lines. If POLAN lines are missing a pre-fetch is performed for the maximum value of PAL.

##### 21 March 2007, PkFit+Filing 3.1.5 (1.1.5)

- version specific for Mac OS 10.3.9 (uses gcc-g77-3.4.6)

- the g77 version from fink does not work (problem with libg2c ?)

Support of new ILL file formats

- search for the variable SCAN:

When line COMND was in the form:

```
sc ipi 0.0 dipi 0.1 np 21 ti 300 fcu 0.5
```

and when the column was

```
"|P|"
```

this column was not found due to a character case problem.

- polarized neutrons: now support variables names Fi and Ff in addition to F1 and F2.

##### 20 March 2007, PkFit+Filing 3.1.4 (1.1.4)

Improvement of the Aquaterm interface:

- more responsive,
- cosmetic bugs corrected
- PGplot modifications for Aquaterm :
  - a buffer is added for moveto, lineto.
  - suppress moveto, lineto to a destination point identical to the origin.
  - default font set to "Monaco"

##### 16 March 2007, PkFit+Filing 3.1.3 (1.1.3)

Compatibility with Mac OS classic data files ended by a <cr> character instead of a <lf>

- when opened, each file is analyzed and <cr> are replaced by <lf> through a temporary file "tmp.tmp"

##### 9 March 2007, PkFit+Filing 3.1.2 (1.1.2)

Workaround to errors in ILL's data formats

- line STEPS of IN22: the parameter is missing !

PkFit thus analyzes the line COMND to fetch its value

A message gives the STEP value which has been retrieved

```
STEPS invalid, line COMND analyzed instead
```

```
STEPS =
```

```
DEN = 0.2500
```

##### 8 March 2007, PkFit 3.1.1 (1.1.1)

Workaround to errors in ILL's data formats

- incorrect syntax of lines STEPS :

```
STEPS: EN = 1.0000
```

```
STEPS: QH = 0.0000, QK = 0.0000, QL = 0.0000
```

instead of

```
STEPS: DEN = 1.0000
```

```
STEPS: DQH = 0.0000, DQK = 0.0000, DQL = 0.0000
```

- Suppression of debugging messages

##### 7 March 2007, PkFit 3.1 (1.1)

Data input bugs:

- buffer aLinePart too small (126 character) set to 255

- the maximum number of columns is increased to 40

Workaround to errors in ILL's data formats

- line FORMT: ',F,' '(F,' ',F)' are replaced by ',F9.0,' '(F9.0,' ',F9.0),'

- line FORMT: format overflows like \*(F,A,I), are corrected on the fly

Default data path

- the environment variable PKFITDATA now sets a default path :  
export PKFITDATA=/monDossier/mesDonnees/

**8 Feb 2007: PkFit 3.0 (1.0)**

PGplot, PkFit and Filing modified to make the interface more usable.

**xterm:** problem solved

- delete key and arrow keys are operational
- unnecessary clicks or <cr> are trapped and are no longer a problem
- on ne peut pas passer d'un champ éditable à l'autre par un clic, il faut d'abord faire un <rc>
- pas de bouton par défaut activable par la touche <rc>. Il faut cliquer.
- boutons inactifs lorsqu'un champ éditable est activé.

**aquaterm**

- same as for xterm...
- but arrow keys does not work (would require a modification of aquaterm itself).
- use keys '<' et '>' instead.

**Oct 2004- first test compilation (L-P Regnault)**

He successfully recompiled the Linux version for Mac OS X

- corrected a bug in the 4D resolution calculation using the Popovici method (bug not present in the Mac OS classic version)
- the original PGplot interface is hardly usable and very touchy
- most ILL file formats posterior to 1997 are not supported
- Mac OS classic data file must be converted to Unix (end of line <lf> instead of <cr>)

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