TUTORIAL ROOTPROF

Help on-line

The RootProf help on-line site is www.ba.ic.cnr.it/softwareic/rootprof. You can also type RootProf on google and open the first link, which points to users.ba.cnr.it/ic/crisrc25/RootProf/RootProf_help.html

Download

You should go to the url www.ba.ic.cnr.it/softwareic/rootprof and click download (link on the right). You will need to create an account or sign in. Then you will receive the file *RootProfProgramFiles.zip* (~ 2 Mb), containing the RootProf files and demos. You can also download the file *Tutorials.zip,* containing the tutorials.

Install

Unzip the file *RootProfProgramFiles.zip*. Among other files, it contains:

RootProfGui.C --> the Graphical User Interface or RootProf, which can be used to generate the command file and run the program.

RootProf_v15.C --> the program file

README.txt --> a file containing relevant information

a subdirectory ./DemoFiles containing:

fileInput* --> demo command files

output* --> demo output files

remaining files are demo data input files.

RootProf can be run on your computer upon installation of the package ROOT. Please download the latest version of ROOT from root.cern.ch/releases. For each release, you will find binary distributions. Choose the one compatible with your OS. If you have Windows 10, you should first install the Windows Subsystem for Linux (WSL) supplied by Microsoft (installation steps can be found in www.computerhope.com/issues/ch001879.htm), and then choose the ROOT binary compatible with the linux distribution set in your WSL. After unpacking/installing the binary, and before using ROOT you should use a special script distributed with ROOT:

source <pathname>/root/bin/thisroot.sh (there are versions for [t]csh and fish, too.)

where <pathname> is the location where you unpacked the ROOT distribution. Typically add these lines to your .profile or .login files.

PLEASE INSTALL ROOT BEFORE THE ROOTPROF TUTORIAL SESSION

RUN

Run ROOT by typing root or clicking on the ROOT icon.

A root prompt will appear on your terminal in case of Linux, or on a new terminal in case of windows:

```
root>
```

Go to the directory containing the RootProf files. You can change directory from the ROOT prompt by using the command

```
root> gSystem->cd("workdir")
```

where workdir is the full path of the directory containing the RootProf files

You can check the actual directory by using the command

```
root> gSystem->pwd()
```

As an alternative, if you have the ROOT directory in your path, you can launch ROOT from the directory containing the RootProf files.

Write the command

```
root> .x RootProfGui.C
```

and the RootProf GUI will appear. From it you can generate the command file and run RootProf from the command file generated by the GUI or from any other command file you have in your directory. The output will appear on the ROOT terminal window, while plots will appear in graphic windows on your terminal.

To launch RootProf without GUI, write the command

```
root> .x RootProf_v15.C("fileInput")
```

To redirect the output text into the file outputFile, type:

```
root> .> outputFile

.x RootProf_v15.C("fileInput")

.>
```

In the case of Linux, RootProf can be run directly from the terminal, by typing:

```
root  'RootProf_v15.C("fileInput")'
```

EXERCISE 1

Perform First Sight analysis on X-ray powder diffraction profiles, executing RootProf_v15.C with the command file *fileInputFirstSight*

You should type the command:

```
root> .x RootProf_v15.C("fileInputFirstSight")
```

Explanation of the graphic and text output can be found in the file *TutorialQualitative.pdf* (chapters 1 and 2).). It is available on the help online, session TUTORIALS, link “Qualitative analysis”.

EXERCISE 2

Perform First Sight analysis on X-ray powder diffraction profiles by using the RootProf GUI and the command file *fileInputFirstSight*

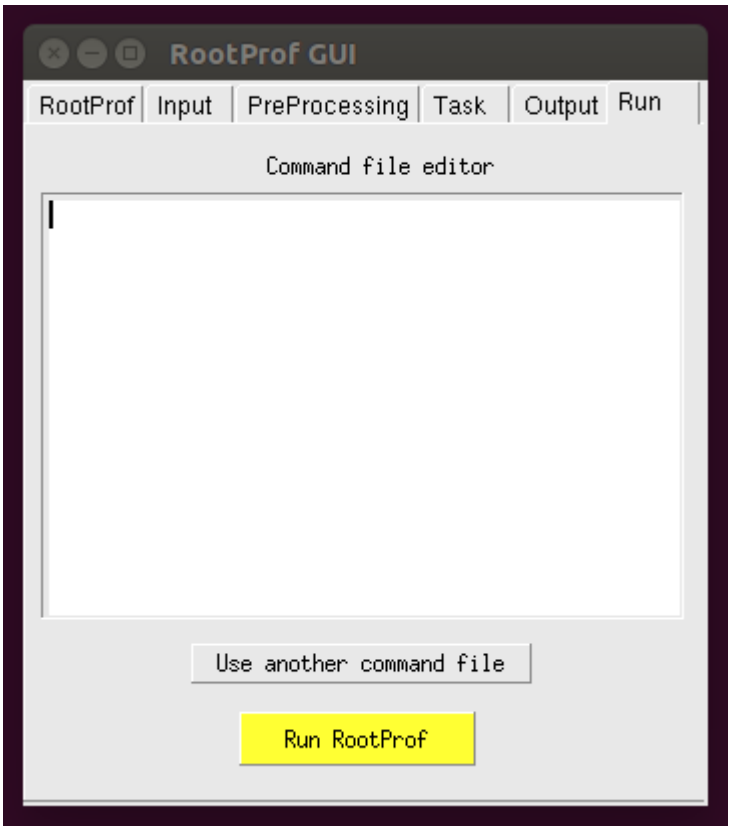
You should type the command:

```
root> .x RootProfGui.C
```

and use the GUI to run RootProf with the already existing command file *fileInputFirstSight*.

Please refer to the help online: session USER GUIDE, link “The Graphical User Interface”.

TIP: use the GUI page *Run*



EXERCISE 3

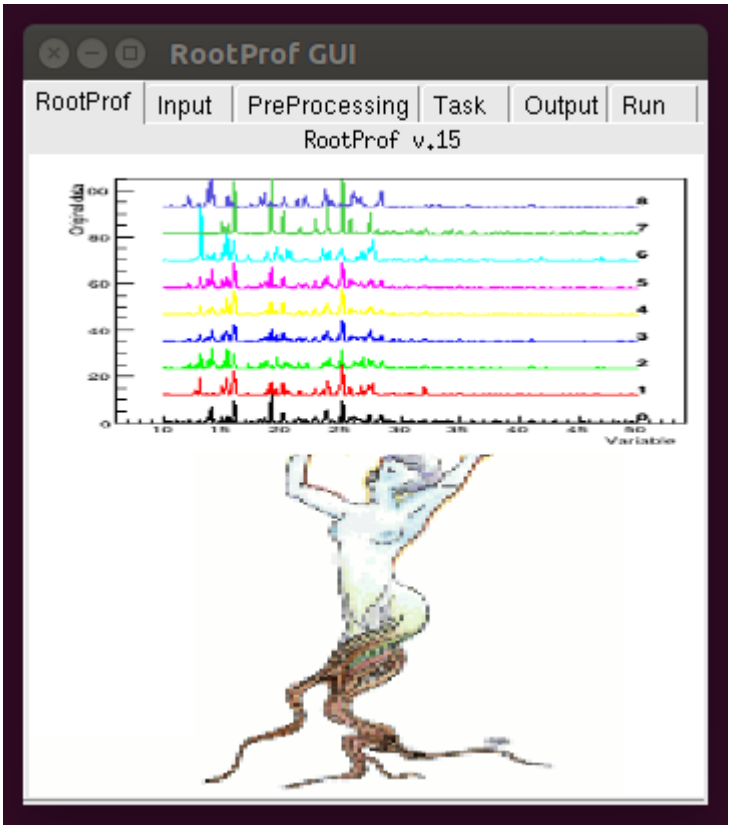
Perform First Sight analysis on X-ray powder diffraction profiles by using the RootProf GUI

You should type the command:

```
root> .x RootProfGui.C
```

and use the GUI to generate a command file to perform First Sight analysis.

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “General Commands”.



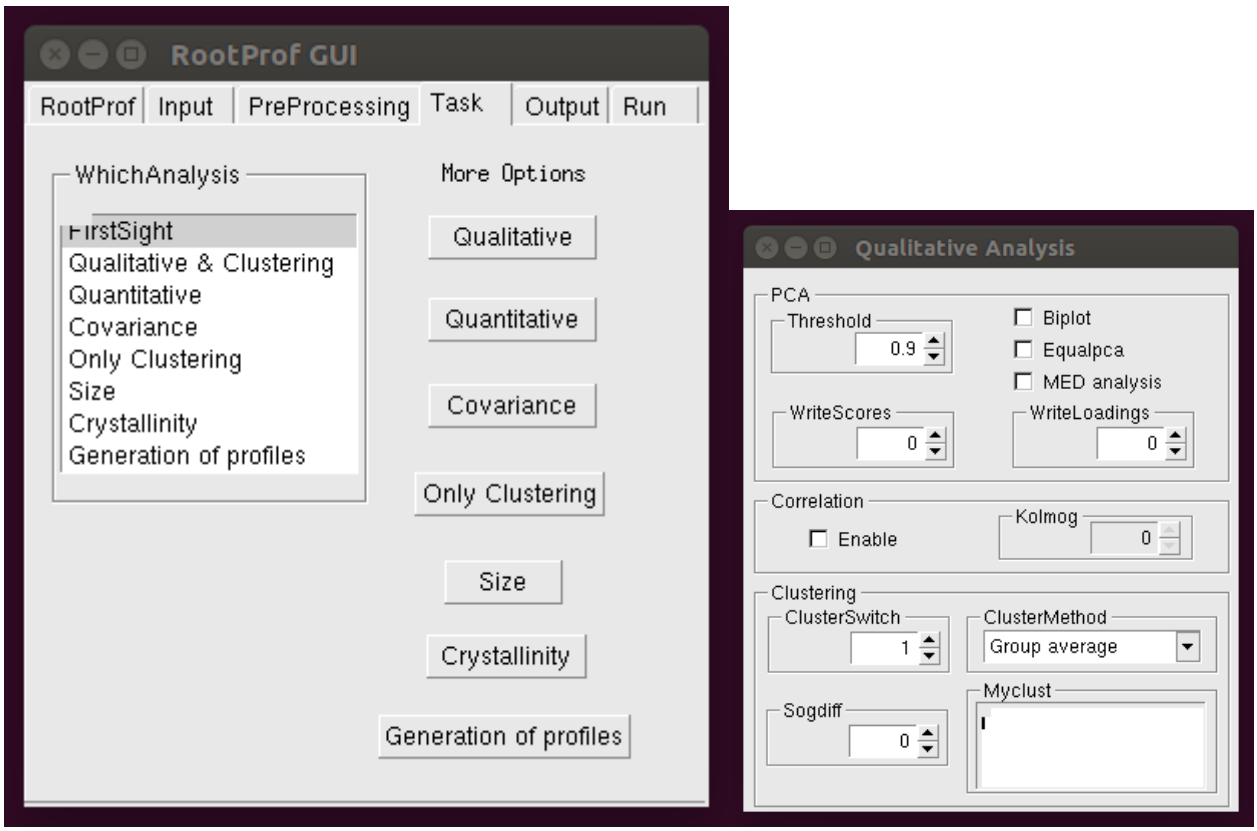
EXERCISE 4

Perform Qualitative analysis on X-ray powder diffraction profiles by using the command file *fileInputQualitative* and/or the RootProf GUI.

TIP: use the GUI page *Task* with More Options: *Qualitative.*

Explanation of the graphic and text output can be found in the file *TutorialQualitative.pdf* (chapter 3). It is available on the help online, session TUTORIALS, link “Qualitative analysis”.

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “Qualitative Analysis”.



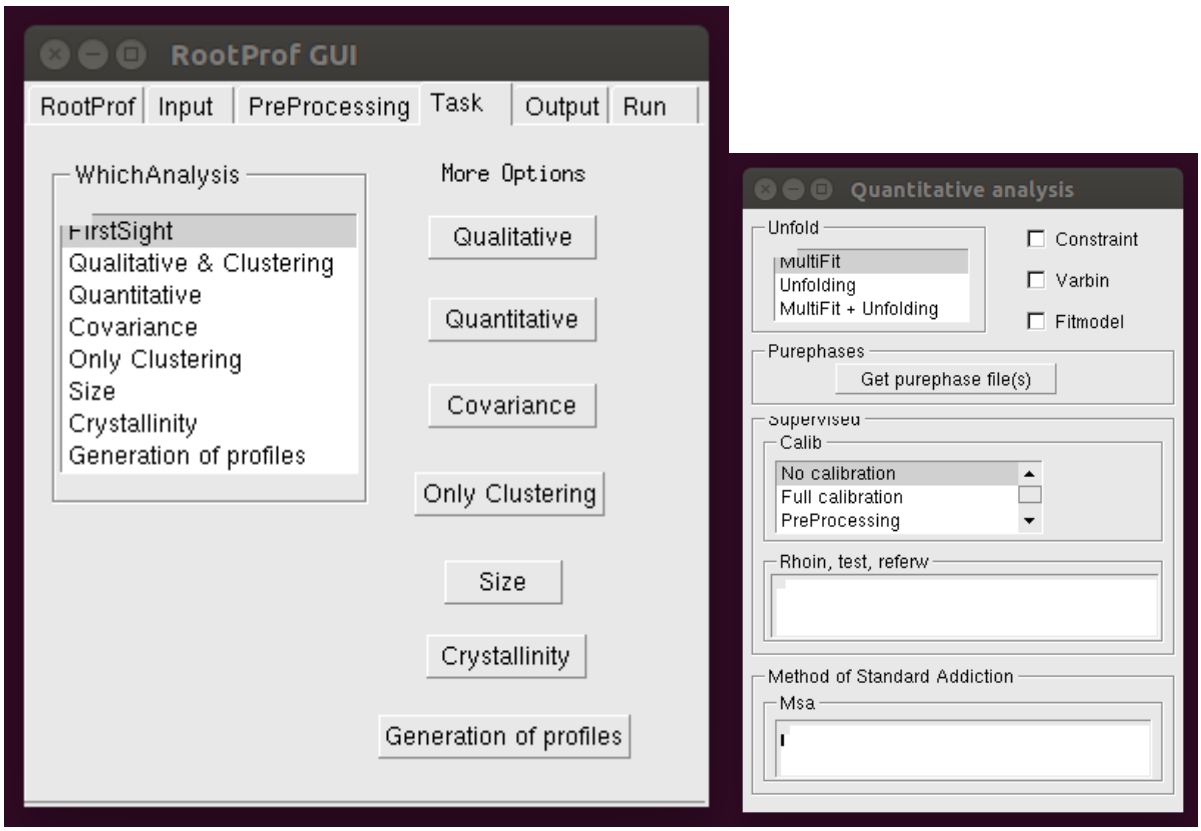
EXERCISE 5

Perform Quantitative analysis on X-ray powder diffraction profiles by using the command file *fileInputQuantitative* and/or the RootProf GUI.

TIP: use the GUI pages *Task* with More Options: *Quantitative.*

Explanation of the graphic and text output can be found in the file *TutorialQuantitative.pdf* (chapters 1 and 2). It is available on the help online, session TUTORIALS, link “Unsupervised quantitative analysis”.

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “Quantitative Analysis”.



EXERCISE 6

Perform Quantitative analysis on X-ray powder diffraction profiles by using the Unfolding procedure.

You can use the command file *fileInputQuantitativeUnfolding* and/or the RootProf GUI.

Explanation of the graphic and text output can be found in the file *TutorialQuantitative.pdf* (chapter 4). It is available on the help online, session TUTORIALS, link “Unsupervised quantitative analysis”.

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “Quantitative Analysis” (command *unfold*).

TIP: use the GUI pages *Task* with More Options: *Quantitative* (*Unfod* option: *Unfolding*)

EXERCISE 7

Perform Supervised Quantitative analysis on X-ray powder diffraction profiles by using the command file *fileInputCalibrationLSQ* and/or the RootProf GUI.

Explanation of the graphic and text output can be found in the file *TutorialCalibration.pdf* (chapters 1 and 3). It is available on the help online, session TUTORIALS, link “Supervised quantitative analysis”.

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “Quantitative Analysis”.

TIP: use the GUI pages *Task* with More Options: *Quantitative* (*Calib* option: *Pure fase rescaling*)

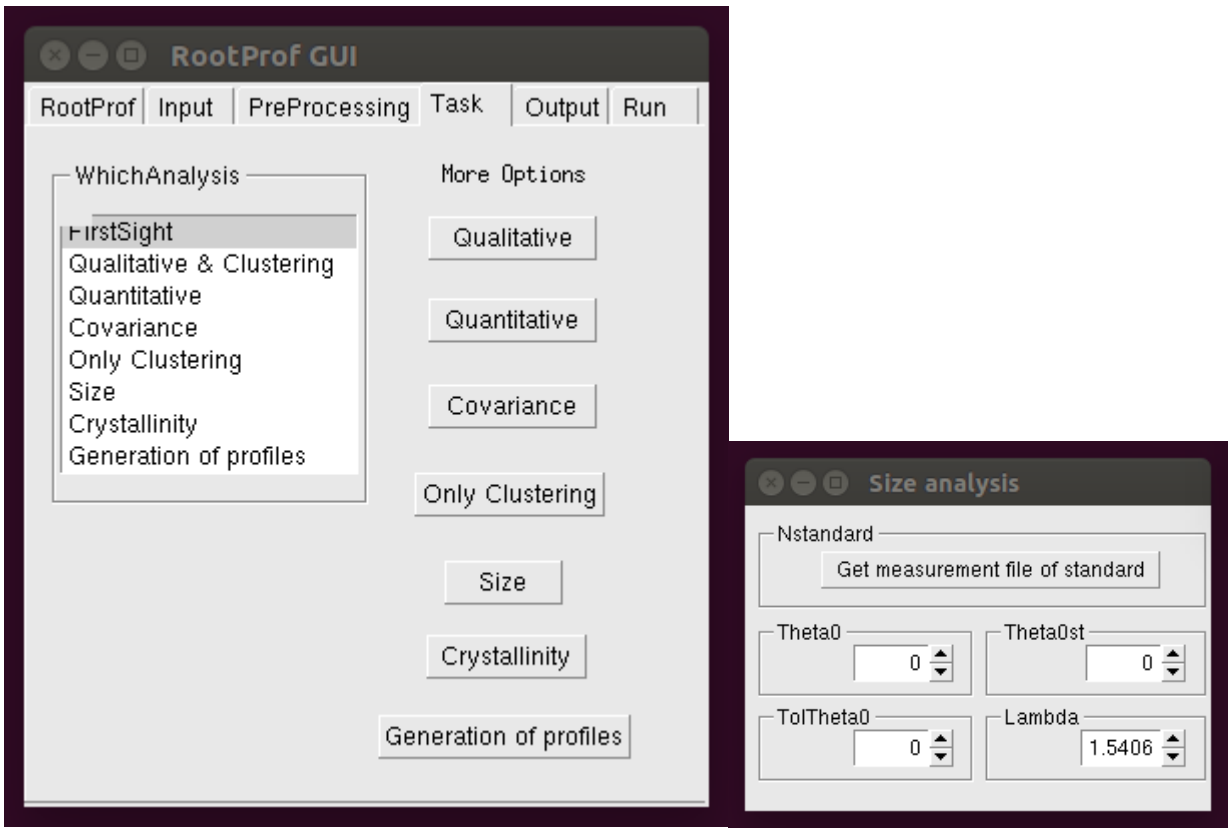
EXERCISE 8

Perform Size analysis on X-ray powder diffraction profiles by using the command file *fileInputSize* and/or the RootProf GUI.

TIP: use the GUI pages *Task* with More Options: *Size.*

Explanation of the graphic and text output can be found in the file *TutorialSize.pdf*. It is available on the help online, session TUTORIALS, link “Size analysis”.

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “Size Analysis”.

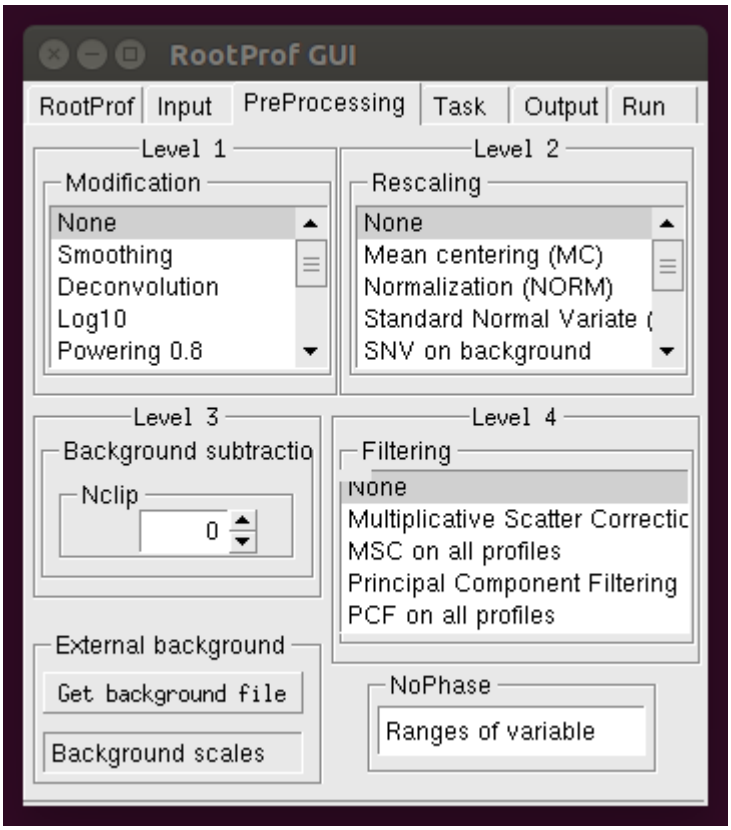


EXERCISE 9

Perform First Sight, Qualitative and Quantitative analysis on FT-IR spectra by using the command files *fileInputIRFirstSIght, fileInputIRQualitative fileInputIRQuantitative* and/or the RootProf GUI.

Explanation of the graphic and text output can be found in the file *TutorialIR.pdf* (chapters 1, 2, 3, 4). It is available on the help online, session TUTORIALS, link “Analysis of FT-IR spectra”.

TIP: Play with the Preprocessing step by using the GUI page *Preprocessing* to improve Qualitative and Quantitative analyses.



EXERCISE 10

Perform MSA analysis on X-ray powder diffraction profiles by using the command file *fileInputMSA* and/or the RootProf GUI.

TIP: use the GUI pages *Task* with More Options: *Quantitative.*

Please refer to the help online: session USER GUIDE, links “The Graphical User Interface” and “Quantitative Analysis” (command *msa*).