Software for diffraction data analysis at POLDI available to external users

1. List of programs

The following programs are accessible outside of PSI:

'**dfit**' – data analysis
'**afit**' – data analysis
'showlog' – history of measurements
'**showint**' – counts vs. selected parameters
'**extract_data**' – data extraction

To access these programs, use any available SSH client and make a secure connection (with **X11** forwarding enabled) to '**sinquser-sl6.psi.ch**' (host), and login with the username and password provided by beamline scientist.
After you are logged in, you will be asked to enter your last name. If it is your first time, a personal directory will be created for you, where you will be redirected during your next sessions. You will be able to access all the programs from your folder.

2. Brief description of POLDI programs

2.1 '**dfit**'

This is a general POLDI fitting routine provides the independent fitting of all diffraction peaks. As practice shows, for the majority of polycrystalline materials, the most exact determination of diffraction peaks' positions is reached when peaks are fitted individually (***option*** '**i**') with the following ***global parameters***: **1** (constant background), **2** (linear background) and **5** (linewidth dependence on cosΘ).
Additionally, a folder where data treatment is performed requires a file '**cs.dat**' containing the crystal structure of constitutive phases of examined material, together with '**year.txt**' file defining appropriate instruments parameters for the corresponding year.

2.2 '**afit**'

This fitting routine uses Pawley refinement, by means of that diffraction peaks are fitted simultaneously assuming a certain crystal structure with fixed parameters. Currently this option works only for cubic structures.

2.3 '**showlog**'

Program that gives an overview of the measured data and relevant parameters of the beamline.

2.4 '**showint**'

Program plots the counts-per-monitor values as the function of motor position. It is often used with the purpose to find / align objects relative to neutron beam.

2.5 '**extract_data**'

Program which extracts parameters from fitted '*FitRes.dat' data files, after one has been used either 'afit' or 'dfit' fitting software.

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