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Project report

Overnight measurement script for XAS beamlines at Doris, exercise week in HASYLAB

Introduction

The aim of my project was to modify the ESS script for ONLINE –Tki dedicated for XAS. ONLINE program is used at many experimental stations of HASYLAB. It is SPECTRA running in on-line mode. It controls all beamline components – mirrors, slits, monochromator, sample holders, etc., and performs data acquisition and measurement monitoring. ONLINE runs under Linux (and LynxOS, OpenVMS (Alpha and VAX)). It can communicate with electronic equipment using CAMAC, VME, IEEE-488 or RS232. The default interfaces to ONLINE are the command interpreter and a graphical user interface. In addition there is a network interface which allows remote clients to interact with ONLINE via a tcp socket connection. Finally ONLINE is available as a program library. It can run in simulation mode on any Linux PC.

I was assigned to work at E4 – an X-ray Absorption Spectroscopy beamline. ESS is a script for ONLINE which enables running multiple sample measurements for example to run an overnight measurement. A print screen of the ESS GUI is shown in figure 1. Input parameters are: number of samples to be measured, energy on which the detectors amplification is checked (E-Cal.), name of region file for the measurement (Reg. File), file names for data files of the measured samples, positions of the motor chosen for sample position changing (in fig. 1 MOT16 is chosen), number of repeats for each sample and a comment for the sample.
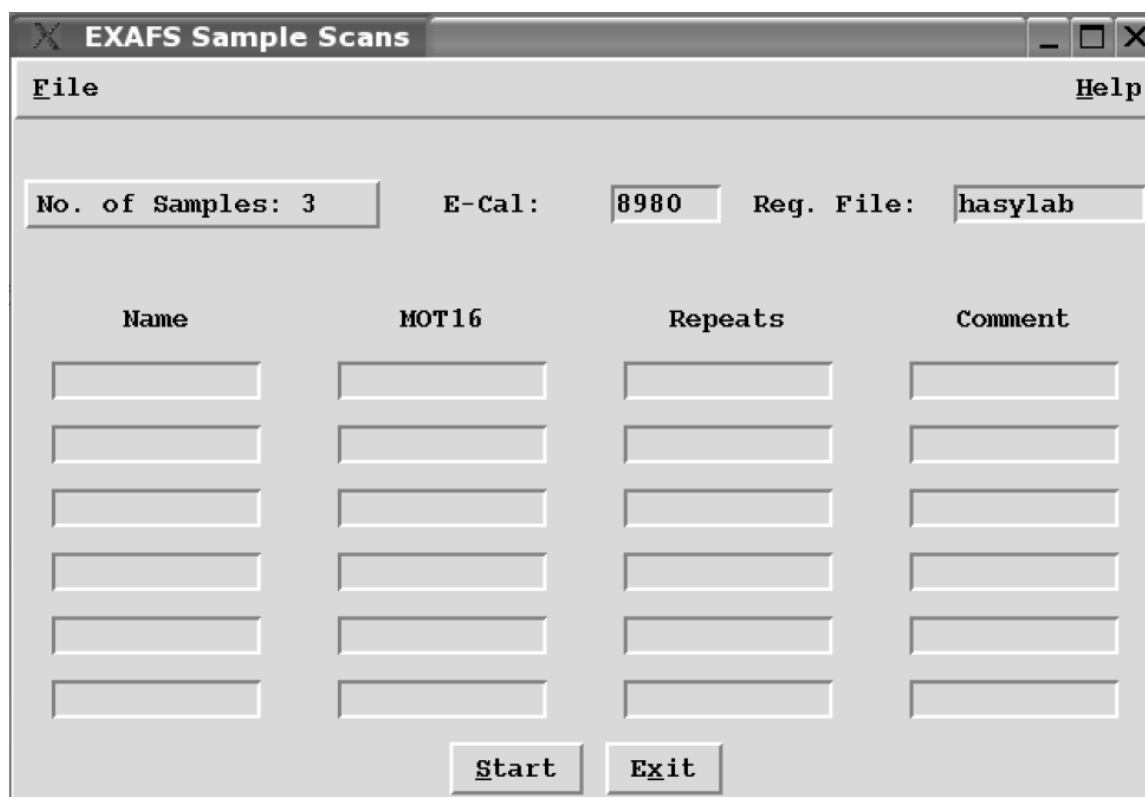
Figure 1: The GUI of ESS script

My assignment

My task was to make the script more "user friendly" by adding more functionality to the GUI window. I had a discussion with beamline scientists using the script. I heard there comments on it and propositions for modifications. One of them was to enable choosing different region file for every sample. This would give a user the possibility to run a series of measurements on different absorption edges. The idea was then rejected, because starting a measurement with different energy requires gas exchange in the ionisation chambers – the experimentalist has to do it by himself.

Another problem was the logarithmic scale of plots drawn live during a measurement run. When the log scale was enabled and there was an injection or some other event which caused a loss of beam, the signal fell down to zero or below, causing a simple mathematical problem with logarithm of zero or a negative number. This made the script stop without measuring the rest of the samples after the injection. The simplest way to fix this problem is to disable the log scale on the live plot. This could be done without any modifications of the ESS script, but required finding the correct button in the correct submenu, what was just another complication for a user not familiar with the software. To simplify it I added a check-button at the bottom of the ESS window, which can turn the log scale on or off.

In February 2007 Adam Webb, a beamline scientist at X1 beamline added some more functionality to the ESS script, adapted for his beamline. He enabled looping the

programmed measurements and also wrote some code to check if the signal amplification is correct. Every XAS beamline uses three ionisation chambers: one for measuring the incoming X-ray intensity, second to measure the intensity after the sample and third to measure the intensity after the reference sample. Signals from these detectors are amplified using Keithley 428 current amplifiers, connected with the beamline computer via IEEE-488 interface. Adam Webb wrote the code checking if the amplification of each detector signal is correct and changing it if it is not. If the amplification was changed, counter offsets have to be measured. This requires beamline specific code, because each XAS beamline (E4, X1, A1, C) uses different ports to communicate with the amplifiers and has different "measure offset" procedures. At A1 and C these procedures are not automatic – the user has to close the beam shutter to measure the counter offsets. At E4 and X1 counter offsets are measured after closing the exit slits by software. Working with the code of ONLINE on all XAS beamlines I found what changes need to be done to adapt the "measure offset" script for A1 and C. Because of user beamtime I was not able to get essential information – what is the exit slit positions sufficient to cut off the beam. Knowing this I could adapt the E4 "measure offset" script to work at A1 and C beamline. Reading Adam Webb's code for checking Keithley's amplifications I found that it would work at E4 without any modifications.

Another simplification I tried to implement in the ESS window was placing a button to change the sample holder motor. It can be done but again – the user has to find this function in a submenu of a different window. To do it in the ESS window would be much simpler. It appeared not to be that easy. This issue must be discussed with Thorsten Kracht. The ESS window after modifications made by Adam Webb and me is shown in figure 2. Added buttons can be seen at the bottom of the window.

Beside the project I also had the opportunity to take part in different XAS experiments running on beamlines E4, A1, X1 and C. I helped in experimental setup, sample preparation and running the experiment.

Figure 2: ESS window after modifications by Adam Webb and me.