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SOFTWARE DEVELOPMENT ON CHOPPER SPECTROMETERS FOR MLF, J-PARC

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ABSTRACT

We report the current status of software development for inelastic spectrometers such as high-intensity chopper spectrometer, 4SEASONS, and cold neutron disk-chopper spectrometer, AMATERAS, at Materials and Life Science Facility (MLF), J-PARC. This development work consists of several parts, i.e. the control system on spectrometer (data acquisition and devices), support for decisions of experimental conditions, sample environment (direction alignment), data reduction and visualization. At commissioning of spectrometers, using actual neutron beam, we have already utilized our software in the processes of obtaining neutron signals by event recording data, transforming them to histograms and visualizing the results. Especially, using event data, we have successfully demonstrated to visualize two-dimensional maps of dynamical structure factors measured with different incident energies simultaneously obtained by one measurement by multiple incident energy measurement on 4SEASONS.

1. Introductions

In Materials & Life Science Facility (MLF) of J-PARC, several inelastic spectrometers such as 4SEASONS, high-intensity chopper spectrometer, and AMATERAS, cold neutron disk-chopper spectrometer have been constructed and have started their operation. At the same time, the development of software to control instrument devices and to analyze data for users is also our urgent task for operating these instruments. The development for chopper instruments consists of several parts, i.e. the instrument control(data acquisition and devices), support for decisions of experimental conditions, data reduction and visualization.

In this development works, we considered to utilize some features of computing environments peculiar to MLF. One feature is that software developments should be based on two software frameworks, i.e. MLF software frameworks [1] and Manyo Library [2], which had been developed simultaneously with ours. MLF software framework gives software scalability and flexibility for the various measurements and the enormous data. These are achieved by distributing processes through the network with XML (eXtensible Markup Language) message over HTTP (Hyper Text Transport Protocol). Manyo Library is the framework for the analysis software development and provides general-purpose functions as common modules in manipulating data. By using these frameworks, the unifying of user experiences and the sharing of development resources for software are achieved with high level. Another feature is the event data recording methods. MLF decided to employ this method instead of the traditional histogram recording method. In the event recording method, the time and position information of "WHEN" and "WHERE" one neutron is detected at a detector are recorded in the raw data as an event. On making histogram for analysis, users can freely and flexibly decide or remake the binning of both time and position from event data after measurement.

We have already produced a series of software with these features and have started to use them in actual measurements. Some developments, especially in data reduction part, have been progressed under the collaboration between J-PARC and HANARO in Korea. The results of this collaboration will also be utilized on a chopper spectrometer for HANARO, which is under construction. In this paper, we describe the current status of our works.

2. Software development and status

Currently, a seriese of software for the instrument control, the informative visualization, the data reduction, the data visualizations and the commands sequence

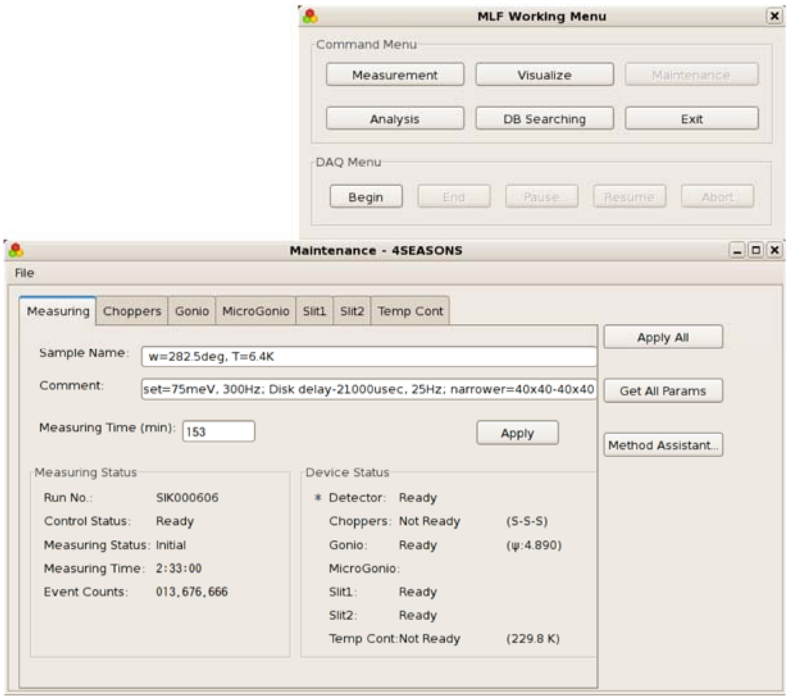

Fig.1 Screen shots of GUI for controlling devices. Upper is main menu and control DAQ system. Lower is to show all status and to control devices.

control is produced. Each module in software has both the command-based interface on Python and the graphical user interface (GUI) constructed by wxPython [3]. These are developed and executed on Linux.

2.1. Instrument control

An inelastic spectrometer consists of many devices to be controlled by users on measurements. For example, 4SEASONS has a DAQ system, 3 choppers, 2 beam narrowers, sample temprature control and goniomator for a direction of sample. Figure 1 shows the screen shot of GUI for the device control software working on 4SEASONS. This software has several GUI tabs for an interface to set parameters of each device. The first tab shows current status of all managed devices as shown in Fig.1. If all devices conditions are "Ready", users can start DAQ system. Device conditions are updated every second. All parameters of devices are stored in a XML file on the hard disk for logging and reusing conditions.

2.2. Informative visualization

This software, shown in Fig. 2, is a utility to help users in their making decision on the experimental conditions such as chopper frequencies, choice of incident energies, choices of slit packages of Fermi-choppers or slit width of disk-choppers and so on. Before users measurements, they can consider experimental parameters by referring visual information in the space for momentum transfer (**Q**) and energy transfer ($\hbar\omega$). Reachable space is determined by certain crystal orientation and instrumental conditions given. This software can display **Q**-$\hbar\omega$ space, expected flux at sample position and **Q** and $\hbar\omega$ resolution at the specific point. At ISIS, there are already many handy utilities for determining such measurement conditions, i.e. CHOP and TOBYPLOT [4]. However, these utilities were completely run independently from the others, which caused users to feel uneasy in using the programmes more effectively. One of the aims of our new software is to combine decision-making and optimization utility and hardware control

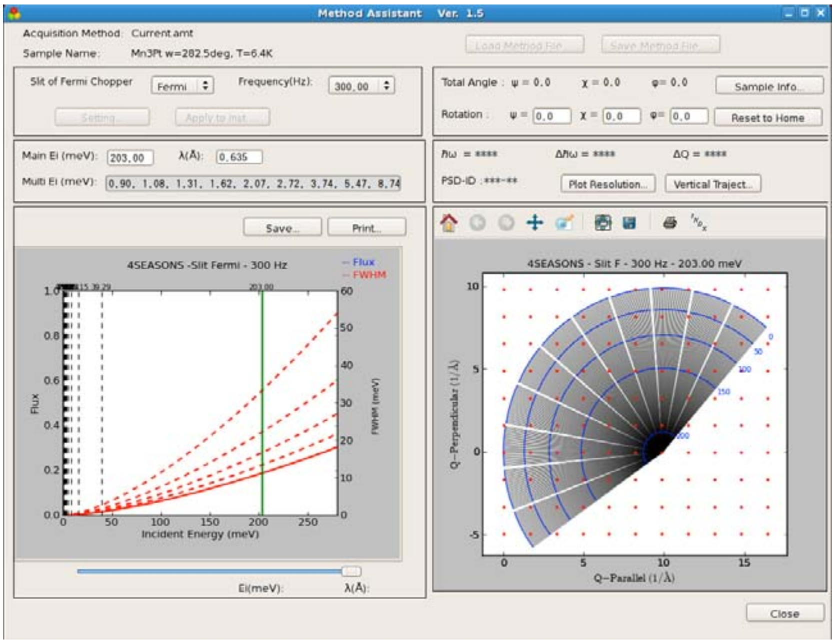

Fig.2 Screen shots of the informative visualization software

software tightly in order to make it easy to setup the experimental conditions determined by pre-experiment decision.

2.3. Data reduction

The structure of basic data reduction software is shown in Fig. 3. When all neutron events are stored as series of events with their own unique time tags, they will be called into the first step of the data reduction software, "Event to Histogram". Here, it will be converted to histograms, which will be further checked to discriminate data from bad detectors by so-called masking process. Then time-of-flight (TOF) of the data is converted to the energy transfer by using detector information embedded in a histogram data. After the conversion, the data of individual segments of detectors will be constructed by using information described in a mapping file. For example, circular averaging (averaging on same |**Q**| value) can be done at this part. After that, background treatments (subtraction of empty can data and constant background correction), normalization by monitor counts, Vanadium correction and correction of detector efficiency will be carried out. Then S(**Q**, $\hbar\omega$) or S(ϕ, $\hbar\omega$) is obtained that will be used in other analysis programmes developed by ourselves or at other institutes.

We developed each process in data reduction as an indivitual module in Python or C++ on the Manyo Library framework. Therefore, users can access each module from Python interface. Data histograms are sotred in data container of Manyo library, called ElementContainer, which has a role to deliver data between modules. This container can also store header information for meta-data, such as detector position, angle, masking and so on. Therefore, ElementContainer also has a role of parameter file.

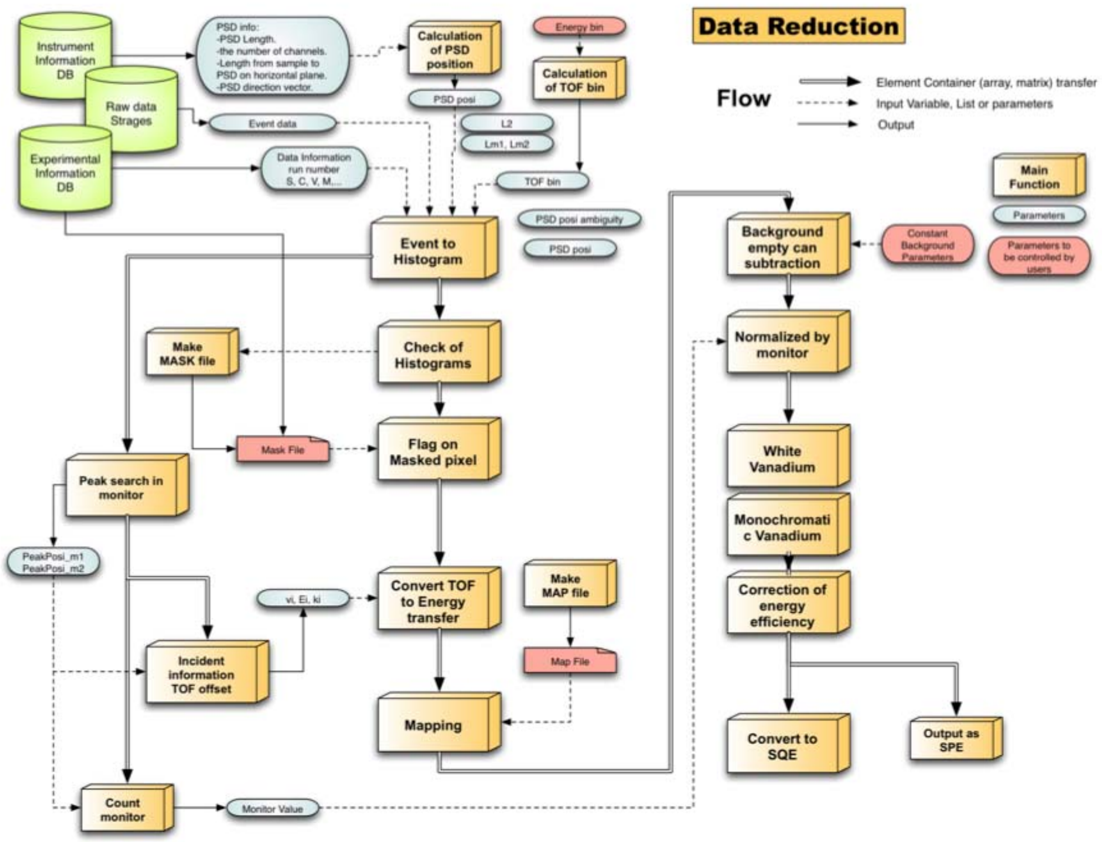

Fig.3 The structure for basic data reduction software

Currently we have not yet completed our works for some modules, such as the vanadium correction, detector efficiency correction and so on. In near future, we equip lack modules and unify several common modules into one module to be useful for users.

2.4. Visualization

Visualization software helps users to treat and visualize any data at data reduction steps, such as the simple TOF data and the S($\mathbf{Q},\hbar\omega$) data measured in inelastic neutron scattering instruments, which have the five dimensions (three axes for Qx, Qy, Qz, one axis for $\hbar\omega$ and the intensity). Functions of visualization softwaer are mainly consisted of several parts, PSD map visualization, 1D-plotter (X and Y axes), 2D-plotter (X, Y axes and the intensity) and the data slicing software from a higher dimensional space to a lower dimensional one for single crystal sample. These plotters can be controlled by command line on Python or by commands in the other software.

The slicing software (Fig. 4(1)) can import several data containers (ElementContainer) of S($\mathbf{Q},\hbar\omega$) from all detectors, which are produced by data reduction software. Some parameters are read from header information of ElementContainer. By inputting sample lattice parameters and parameters for projection, users can slice and plot the data. At the present status, this software can only slice and plot the data. Any functions for advanced analysis, fitting and convolution of resolution are not prepared yet and will be parts of future project. In the main panel, users can handle up to 5 individual data in 5 dimensional spaces of S($\mathbf{Q}$, $\hbar\omega$) data. Users can choose imported data by clicking tabs on

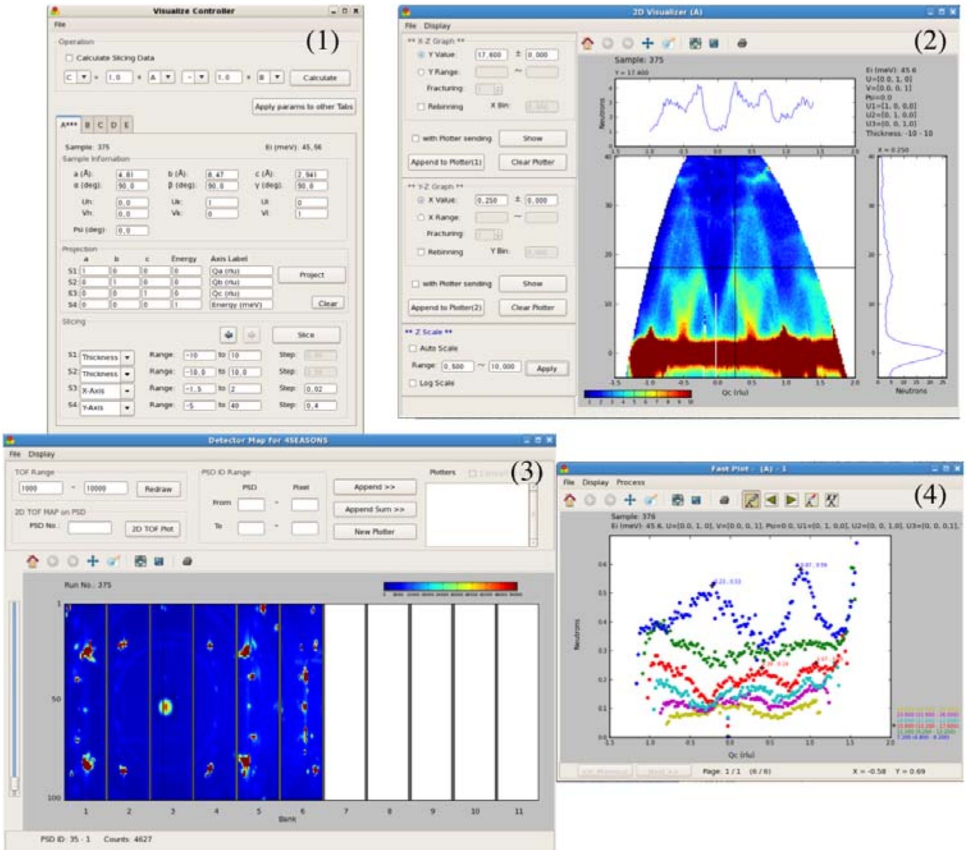

Fig.4 Screen shots of visualization software.
(1) slicing modules for single crysta data
(2) 2D plotter
(3) PSD map visualization
(4) 1D plotter

GUI. In addition, it is possible to calculate arithmetic operation between 2 data containers and to put the result into another tab. Slicing and plotting functions are included in this panel also. For given parameters, projecting and slicing are carried out to send the results to the outer 2D-Plotter for display on the screen.

2D-Plotter (Fig. 4(2)) can plot not only the sliced data of single crystal sample but also the powder/grassy sample. Using the 2D-plotter, users can cut the 2D data by mouse on GUI and the resulting data is then sent to the outer 1D-plotter (Fig.4 (4)) for display on screen. 1D-Plotter is usually used just to plot several histograms. As same as other ordinary plotters, this plotter has several basic functions such as changing types of lines and markers, scaling plot region and so on. Also this plotter can read and write text data file to import/export any histogram data. More advanced functions for data analysis will be implemented in future.

2.4. Command sequence control

This software helps users to make procedures for executing analysis commands (Fig. 5). Users can select necessary command from the Command List placed on left column of the window, which the instrument scientist prepared beforehand, and entry to the Sequence List in the middle. A set of arguments for selected command in the Sequence List shows in a frame on the bottom. The contents in the arguments frame change dynamically by the motion of selecting command. By pushing the Start button, this software executes commands in the Sequence List step by step. If any error happenes on executing command or the process is interrupted by Stop button, the process stops but all parameters and returned values from each command are kept. Resume button can be used to restart the process. The icons in the head of a line of command list are the status of each command, which indicates feasible, error and executing status. Users can send data to visualization software from this directly. In addition, the command sequence can be saved as a file of python script, which can be directly executed on console. Currently, commands executalble on this software are limited to the use for analysis. We have a plan to extend

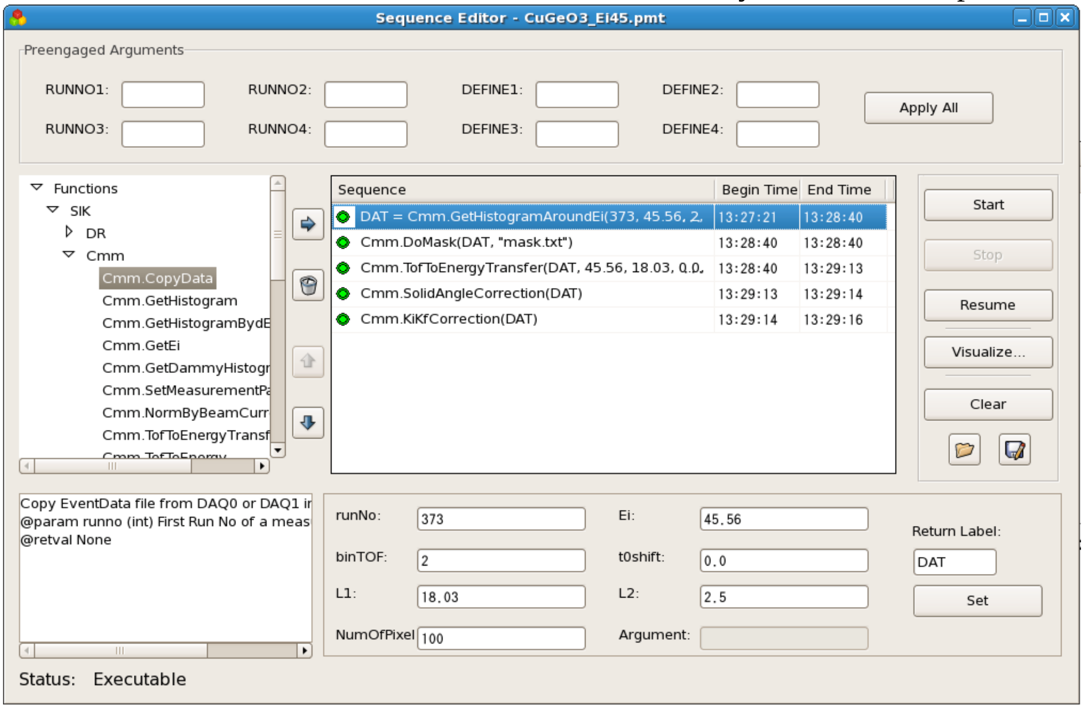

Fig.5 Screen shot of the command sequence control software

the use of this software to control instrument and devices.

3. Demonstration

On commissioning of 4SEASONS in MLF in 2009, using actual neutron beam, we have started to utilize our software in the processes of obtaining neutron signals as event-by-event data, transforming them to histograms and visualizing the results. Especially, using event data, we have successfully demonstrated to visualize two-dimensional maps of dynamical structure factors measured with different incident energies simultaneously obtained by one measurement by multiple incident energy measurement on 4SEASONS [5].

The data used for the demonstration is separated in 20 event files with a total size of 2.4 GB for 19200 segments to detect neutrons. In data reduction process, we only use only the event data to histogram, converting TOF to energy, correction of solid angle and ki/kf correction. It takes less than 2 minutes to execute data reduction for an incident energy using a PC with one CPU of quad-core with memory of 8 GB. The reduction data are sent to visualization software, which takes 1 or 2 seconds. Once imported, visualization processes for projection, slicing and plotting are sufficiently fast (1 or 2 seconds) enough for users to use. Fig. 6 shows an example plot.

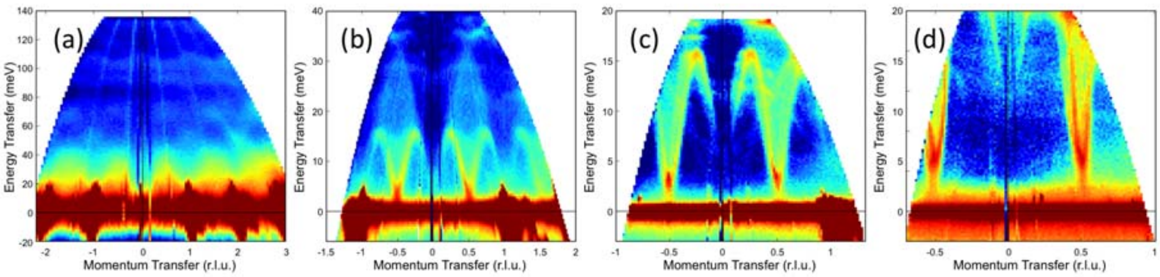

Fig.6 The example plots for software demonstration.
Sample : CuGeO3, (a) Ei = 150.7 meV, (b) 45.4 meV, (c) 21.5 meV, (d) 12.6 meV

4. Summary

A series of software for chopper spectrometers in MLF has been developed, which is including results of software developments, i.e. MLF software framework, Manyo Library project and the collaboration between J-PARC and HANARO. As results, we have successfully demonstrated to analyze event data and visualize then using our own software. However, some problems have been left. One is that we still have many bugs and much lack of functions required by users. We need to continue to develop and improve software with instrument scientists and users. The other is the way to offer the environment to treat and analyze data for outside users of J-PARC. This is hard task because this is deeply connected to MLF computing environment and we need further discussions in view of the policy for computing in MLF/J-PARC.

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