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16.2
Java-Based Software for Chopper-Spectrometer Data Reduction

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Abstract

We introduce a software application for analyzing time-of-flight data obtained from a chopper spectrometer. This ChopAnalysis Package (CAP) is written in Java to take advantage of its platform independence and Internet accessibility. CAP is a component within the architecture of the Integrated Spectral Analysis Workbench (ISAW) being developed at Argonne. Multiple large data sets, each containing ~1000 spectra, can be examined for removal of noise and contamination. Appropriate sample, background and calibration runs are combined and normalized. Afterward, data from detector groups are binned and converted into various scattering functions in momentum- and energy-transfer (|Q|,E) space. The resulting datasets can be analyzed further by users with additional methods. By virtue of the object-oriented programming (OOP) methods and graphic user interface (GUI) of ISAW, immediate steps of the evaluation are easily displayed in interactive viewers as images or line plots. Repetitive procedures can be executed through command-line scripts. The results can be saved as formatted tables in text files or pasted into other applications.

1. Introduction

The High-Resolution Medium-Energy Chopper Spectrometer (HRMECS) is the first IPNS instrument to employ a new data acquisition system (DAS) and enhanced detector electronics as a part of the upgrade plan of HRMECS currently under way.[1] The protocol for data storage and retrieval via the runfiles within the new DAS, written in Java, permits an efficient entry into the Integrated Spectral Analysis Workbench (ISAW) via a database.[2] A typical HRMECS runfile consists of, besides the instrumental parameters and attributes of sample environment, about 1000 time-of-flight (TOF) detector spectra, each containing up to 4000 channels. The basic steps for initial data reduction include:

i) examine the detector response over all the spectra and, if necessary, remove bad detector spectra for a series of runfiles including sample, background and calibration runs;

ii) calculate the incident energy of each run and check for consistency so that background counts are properly subtracted from the sample runs and the TOF spectra are normalized according to the sample scattering cross section, detector size and relative efficiency; and
iii) rebin data histograms in counts over TOF channels and detector positions into appropriate scattering functions in density distribution over the momentum- and energy-transfer (|**Q**|, E) space.

This procedure is illustrated in Fig. 1. The ChopAnalysis Package (CAP) is built within ISAW, which provides all the necessary components for user interface, data control, and data modeling within the Model-View-Controller architecture as described elsewhere.[2, 3] Since we expect that this procedure would be repeated for a number of runfile sets that belong to an experiment, ISAW includes a scripting language to control the data processing and the steps are automatically logged. For example, a user may easily recall the script of a procedure, edit a few entries corresponding to a new set of runfiles, and execute a part of or the entire procedure. Export of intermediate DataSets in text or table format is also available.

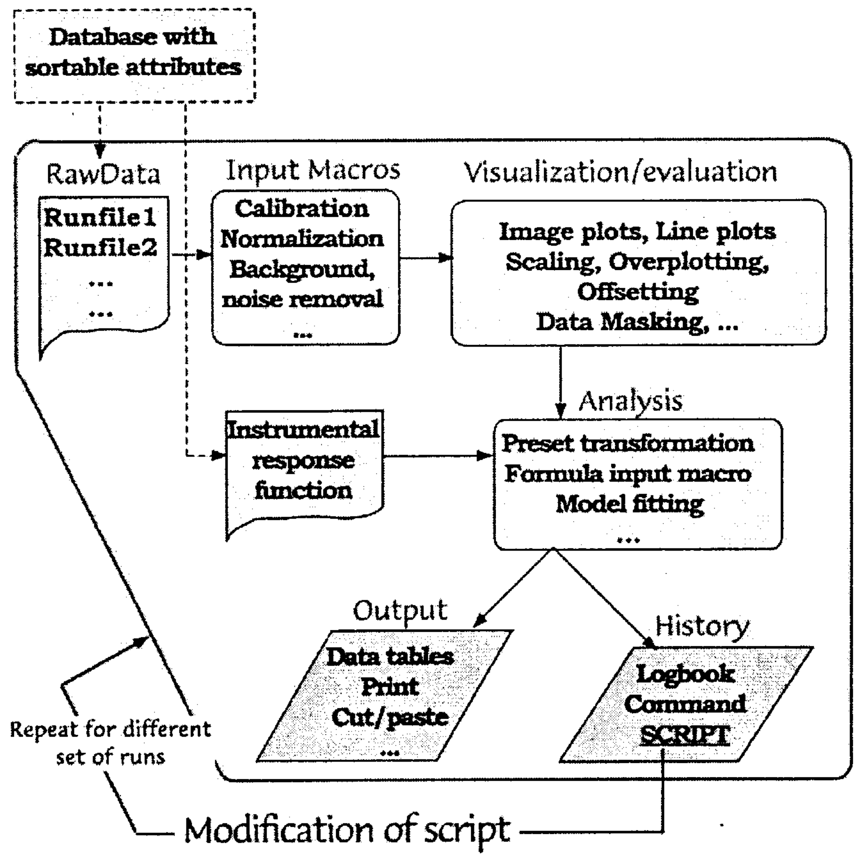

Figure 1. The basic data reduction scheme of the ChopAnalysis Package (CAP).

2. DataSet Evaluation

Fig. 2 displays a typical panel corresponding to detector response in a runfile collected under the pulse-height-spectral mode. The scrollable window on the right is one of many ways to display the detectors' pulse-height spectra (PHS), provided by the IsawGUI.[3] Furthermore, quantitative analysis of the PHS can be done by invoking the proper model/method belonging to the ISAW internal "Peak class", which is designed to handle various characterization and fitting of peak-like spectra. Then the result is shown in the left panel, permitting further examination or eventually the setting of the detector discrimination levels according to an acceptance criterion. At present, the software for evaluation of the PHS and setup of discrimination levels has not been completed, but we would like to emphasize ISAW's powerful features which allow the reuse of existing operators and the easy addition of new operators to perform a variety of spectral analyses.

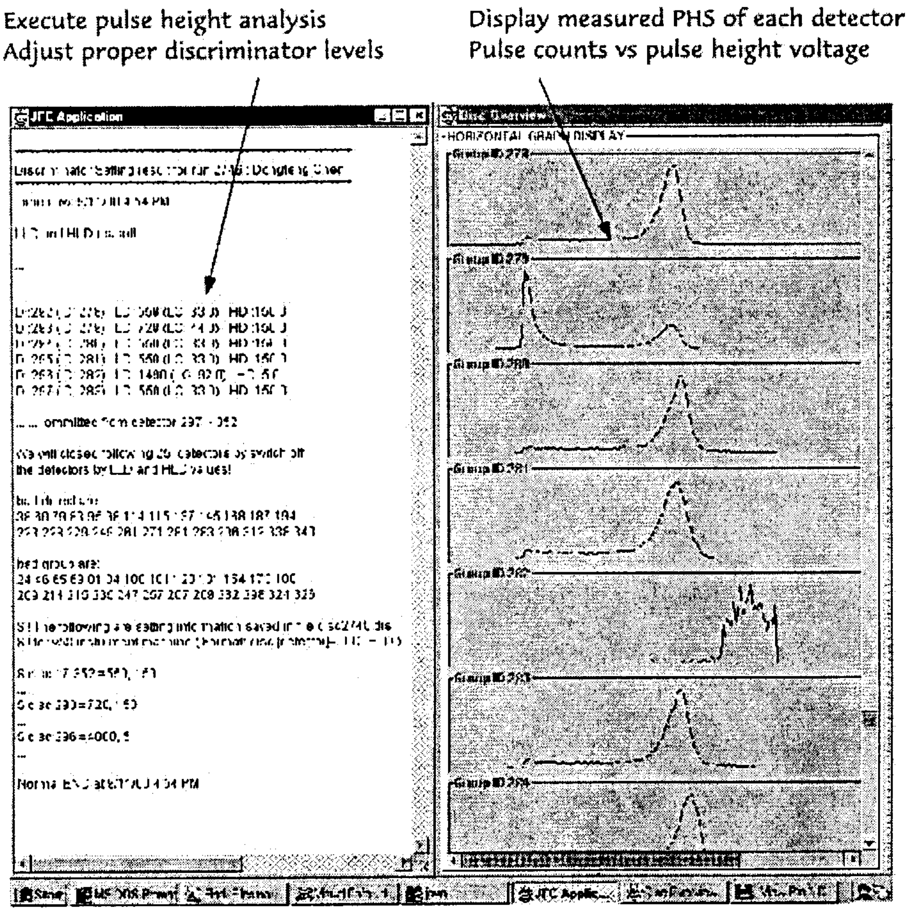

Figure 2. A display of detector pulse-height spectra.

Another important capability of ISAW is the efficient display of all of the detector intensity records (~1000 per runfile) using an image plot with the ability to zoom-in a selected group of TOF profiles. Moreover, it provides a side-by-side comparison of the data before and after applying a filter/operation. For example, a macro of "Remove bad detector data" can be executed within the "Operations" menu, and the result is shown in Fig. 3. If the outcome is desirable, a new DataSet with bad detectors removed is created, and the corresponding script for such an operation is also generated for future treatment of other runfiles.

3. Combining Multiple Runs and Conversion to Various Scattering Functions

Fig. 4 shows the calibration of the incident energy, normalization of background run(s) against sample run(s), and calibration of the intensities according to a vanadium standard run, all done in a menu-driven single step.

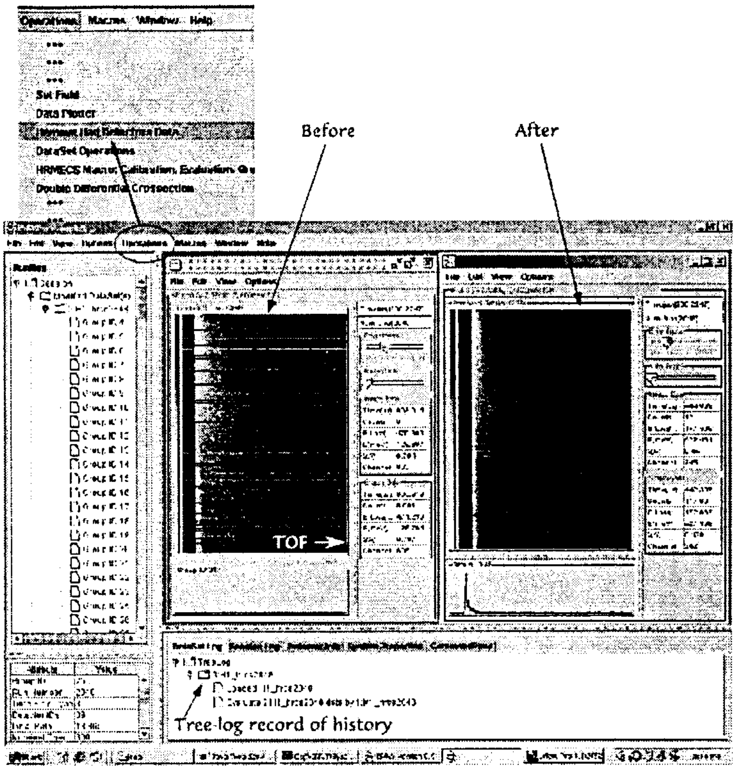

Figure 3. Removal of bad detector data.

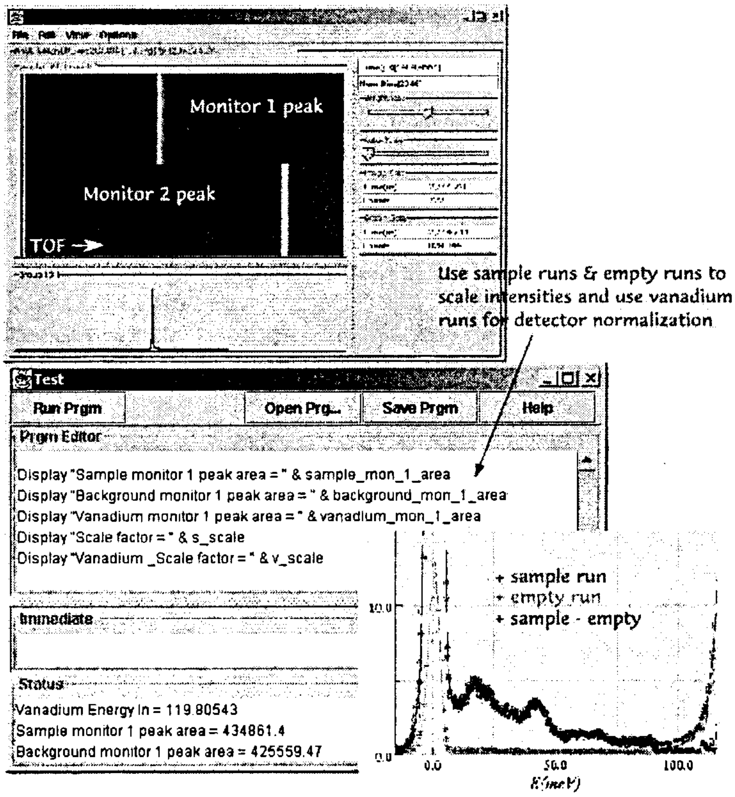

Figure 4. Calibrate incident energy and normalize runs.

The rebinning of data from TOF to (Q,E) space is shown in Fig. 5 and subsequently converting the data to different kinds of scattering functions is shown in Fig. 6.

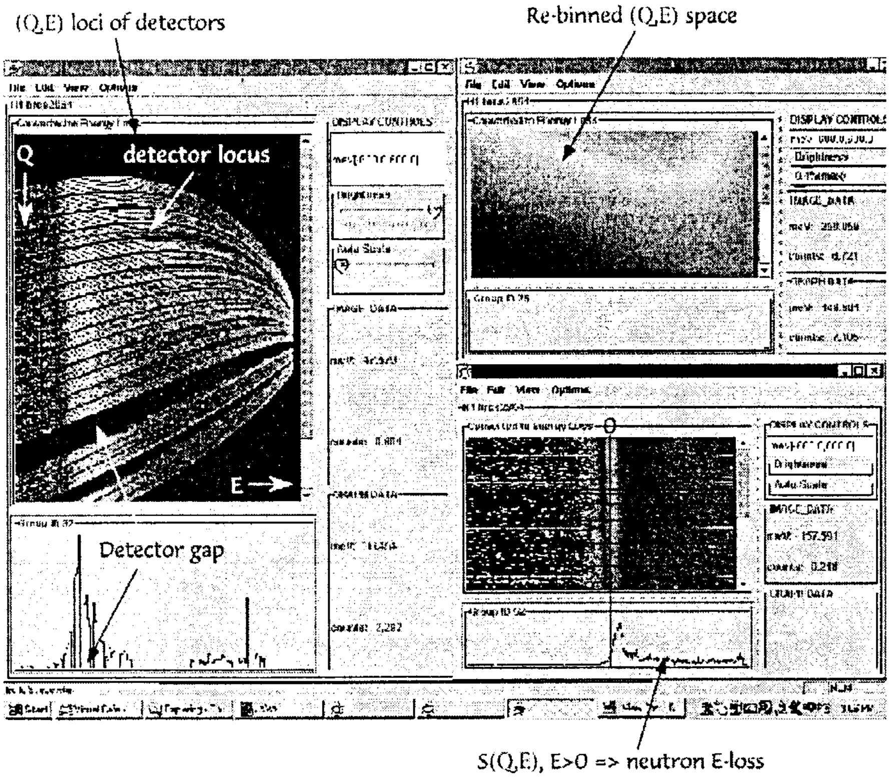

Figure 5. Rebinning data from TOF to (Q,E) space.

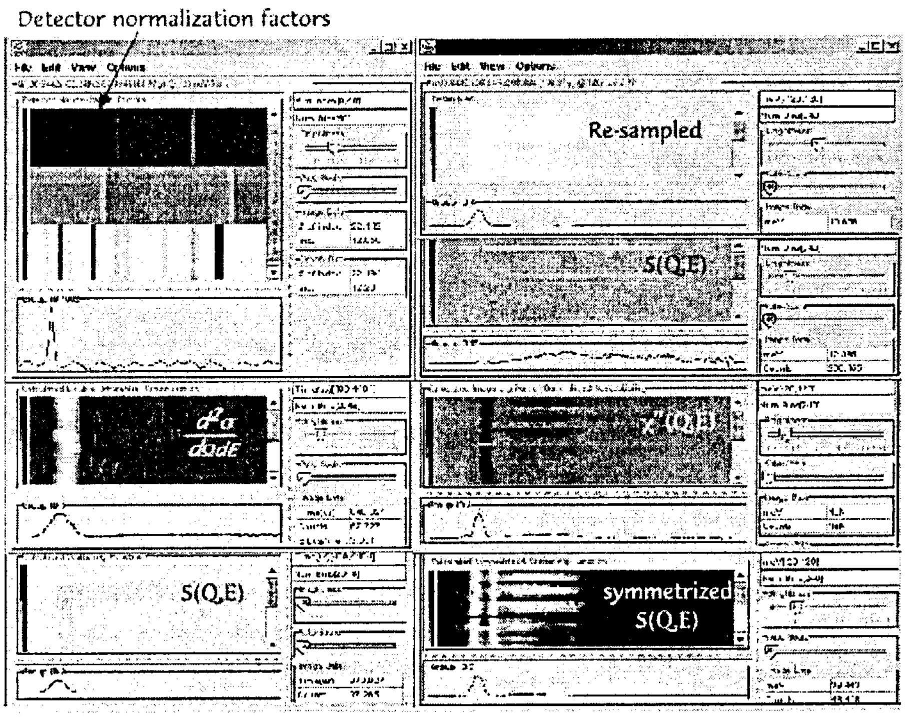

Figure 6. Conversion of data into different scattering functions.

4. Future Plans

We presented a description of the basic tools of the ChopAnalysis Package (CAP) that permit data visualization and reduction of TOF data of a chopper spectrometer to scattering functions within the ISAW software application. Currently this procedure is being tested and refined. Many additional features are planned for future versions, such as run-time monitoring of detector performance, multiple-scattering and multi-phonon corrections, generation of instrumental resolution, and more extensive curve fitting capabilities. CAP is the first software package developed for chopper spectrometers within ISAW. Similar packages will be introduced to other IPNS instruments in parallel to the upgrade of their DAS. Eventually, relevant data sets collected using different instruments could be combined and incorporated in order to produce maximum information benefiting a scientific study. For example, a cut at the elastic region of a scattering function, S(Q, E=0) obtained from a spectrometer would provide a useful comparison with the S(Q) obtained from a total-scattering diffractometer. Also, scattering functions covering different energy ranges with distinct resolutions obtained from direct- and inverse-geometry spectrometers could be combined for an investigation of evolution of excitations over a wide range of (Q,E) space. This is within the design capability of ISAW since the software uses the same data and basic operator classes for all instruments. ISAW can, in principle, be expanded for use by neutron TOF instruments at other facilities because of its platform independence and Internet accessibility. Currently work is under way to extend ISAW's capability of reading data files other than those of IPNS as long as they are written in a standard format such as that defined in NeXus.

Acknowledgement

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3. A. Chatterjee, T. Worlton, J. Hammonds, D. Mikkelson, R. Mikkelson, D. Chen, and C.-K. Loong, in this Proceedings.