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TOF-VIS, Software for Interactive Exploration of Time-of-Flight Data

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ABSTRACT

TOF-VIS is a fast, highly interactive program for examining time-of-flight neutron scattering data. All spectra from an experiment are displayed simultaneously as an image. The data can be displayed in terms of time-of-flight, energy, wave-vector, or lattice spacing. TOF-VIS has been used for examining data from IPNS and ISIS, and has been useful for diagnosing problems with instruments and detectors as well as for making a quick evaluation of the quality of the data. Hard copy output to a variety of devices using routines built on PGPLOT is now available. TOF-VIS is portable to VMS and UNIX, and is currently implemented primarily using object-based methods in C, MOTIF and X-Windows.

Keywords: Data Visualization, Instrumentation, Neutron Scattering

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I. OVERVIEW

TOF-VIS is a fast, highly interactive program for viewing time-of-flight neutron scattering data. It provides a quick overview of the data from many different detectors for both spectrometers and diffractometers. It could also be used to display changes in the spectrum of a sample as temperature, pressure, time, etc. are varied. It displays three simultaneous views of a collection of spectra in the form of an image plus graphs of two perpendicular cuts across the image (Fig. 1).

The TOF-VIS main or "image" view shows the set of spectra as an image in which rows of the image correspond to spectra from different detectors ordered by detector number or by detector angle with intensity represented by the color or shade of gray. The columns of the image correspond to uniform steps in time, energy, wave-vector, lattice spacing, or "Q". The user can drag the mouse pointer across the image to select rows and columns of the image to be displayed as graphs in the other views. The values of the time, energy, wave-vector, lattice spacing and "Q" values corresponding to points in the image are computed and displayed as the cursor is moved over the image. When the mouse is dragged across the two graph views, digital displays of the corresponding graph variables are displayed in other regions of the window.

The spectrum selected by the cursor can be graphed as a function of time channels, as time channels transformed to the physical units (t , E , λ , d or Q), or as data that has been re-sampled ("rebinned") into equal-sized intervals of physical units. This graph appears at the bottom of the TOF-VIS window. The graph on the left of the TOF-VIS window is a plot of a vertical cut across all spectra for the selected column. This graph displays counts in the "x" direction and either "ID", angle or "Q" in the "y" direction.

To get a closer look at fine details in the data, a "zoom" region can be selected by dragging the cursor to the starting point of the region to be magnified, then holding the middle mouse button

while dragging the cursor to the opposite corner of the region. This can be done in any of the three data views. Each of the three views of the data can be printed to a Postscript printer or to a file. There is a print preview option to check the plot before printing.

Based on user's comments, these capabilities of TOF-VIS have proven useful for several instruments at IPNS and ISIS. Specifically, it is very easy to see dead or noisy detectors and identify modules with faulty electronic components. When sorted by angle, the image makes it easy to see certain instrument specific anomalies and provides a quick look at $S(Q, \omega)$. Also, for spectrometer data, the vertical cut can be used to see the variation of elastic intensity with Q .

II. SOFTWARE STRUCTURE

TOF-VIS uses the X-Window System and MOTIF, and is written in C except for a few FORTRAN routines used only to interface with PGPLOT for hardcopy output. The TOF-VIS program itself is split into three levels: an interface layer, a translation layer, and an application layer. The interface layer constructs the various motif widgets, sets up callback routines that respond to user input, etc. The translation layer consists largely of callback routines that are called in response to user input. The callback routines call on the application layer to carry out the requested action and then display the results in widgets created in the interface layer. The application layer is independent of MOTIF and provides the basic functionality of the application by producing graphs and images as arrays of values, independent of how those are ultimately displayed.

The heart of the application layer is the concept of a spectrum "object". Each spectrum is an instance of a spectrum object. The spectrum object contains the time-of-flight spectrum data values as well as the flight path length, scattering angle and other physically significant quantities. The spectrum object includes methods to access the data and produce an array of values obtained by rebinning the data in an arbitrary collection of time, energy, wave-vector, etc. bins.

The main image display is obtained by first sorting the spectrum objects based on ID or scattering angle. Then the spectrum objects produce the data rebinned in the currently selected units and bin sizes. The rebinned data from each spectrum object is then displayed as one row of the image.

TOF-VIS was originally intended to provide just a quick interactive look at a collection of spectra. Consequently, hard copy output was not supported and this proved to be a significant disadvantage. The latest version of TOF-VIS now has hard copy output based on the freely available plotting package, PGPLOT. Any of the three views of the data may be printed to a postscript file or directly to a postscript capable printer. For UNIX, available printers are obtained from the printcap file, while in OpenVMS the list of available print queues is obtained from system service calls. When a view is printed, appropriately labeled axes, color scales and legends are added.

III. Future Development

TOF-VIS has provided a useful "quick look" at a large collection of spectra. It would be beneficial to combine the visualization capabilities of TOF-VIS with data reduction operations so that this work could be carried out in a user-friendly environment with a good graphical display of the data at each stage of the reduction.

IV. Where to get the software

TOF-VIS may be obtained via FTP from dmikk.msccs.uwstout.edu (144.13.1.16). PGPLOT is available via FTP from astro.caltech.edu (131.215.240.1).

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LIST OF FIGURE CAPTIONS:

Fig. 1, TOF-VIS main window, chopper spectrometer data