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Lawrence Radiation Laboratory
UNIVERSITY OF CALIFORNIA
LIVERMORE

REAL TIME ACQUISITION AND DISPLAY OF MASS SPECTRA

P. D. Siemens

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REAL TIME ACQUISITION AND DISPLAY OF MASS SPECTRA*

P. D. Siemens

Lawrence Radiation Laboratory, University of California
Livermore, California 94550

ABSTRACT

A program package has been developed to perform real time data acquisition and display from a mass spectrometer. In this particular case the data acquisition routine performs multisumming-scaling, but with minor changes the package could do signal averaging or pulse height analysis.

Through a keyboard monitor, the operator has complete control of the experiment with a variety of commands available to him. Among these are commands which provide for: control of the data acquisition, real time log or linear displays, data output on paper tape, teletype, DEC tape or Calcomp, and data reduction (peak stripping and the calculation of isotope ratios).

In our Laboratory, we are just completing the tune-up procedure on a new mass spectrometer. This spectrometer will be used to determine isotopic ratios of trace amounts of heavy elements. A small computer was chosen to be the data acquisition device for several reasons, some of which will be explained in this paper.

By way of introduction, this spectrometer is a three-stage instrument with two magnetic sections and one electrostatic section. Ions, produced by a hot filament, are sorted by their mass/charge ratio in the magnetic sections, while the electrostatic section functions as an energy selector. The magnetic field is swept with a triangular wave over a range of a few hundred gauss, with the center field ranging from essentially zero to 12 kilogauss.

Each half of the sweep is divided into 128 time slots or channels (each time slot is generally about 2 msec long, corresponding to a sweep rate of approximately two sweeps per sec). During each channel time, the number of ions striking the detector are counted. If, during one sweep, the number of ions counted for each channel time are stored in sequential core locations, the resulting array is a spectrum whose peaks represent the abundances of the various isotopes present in the sample. The signal-to-noise ratio of this spectrum is poor, however, so a signal enhancement technique is used in which repetitive sweeps of the spectrum are summed together (commonly called multi-summing-scaling).

A block diagram of the computer system and spectrometer interface is shown in Figure 1. The triangular reference sweep for the magnet sweep control is generated by a 12-bit up-down counter and digital-to-analog converter. The counter is driven from a free running clock that is not under computer control, but the possibility does exist, and is practical, to give the computer control of the sweep generation. A strobe pulse generated every 32 clock pulses is used to load the contents

of the scaler register into the buffer register and to cause a program interrupt notifying the processor that data are available. The scaler register is constructed from 100-MHz emitter coupled integrated circuits, but at the present time, the double pulse resolution of the system is limited by the pulse width from the electron multiplier. In addition to these functions, a sync interrupt is generated once per sweep to insure that the spectrometer and the data acquisition program never get out of sync.

As the software for this mass spectrometer system was formulated, several requirements became clear. First was the need for a good, efficient data acquisition routine. Secondly, the operators of the machine required a very good real-time display capability in order that they might be continually aware of how well the spectrometer was functioning. Finally, it became apparent that all control should be exercised through a keyboard monitor. Experience has shown that there are fewer problems if the operator of a laboratory computer system never touches the front panel switches of the computer.

Since the users of this system range in computer experience from fairly complete knowledge to none at all, a simple method of operation is mandatory. Conflicting with simplicity is the requirement for a very flexible software system. This flexibility was gained by giving the user control of as many functions as possible. For instance, 99 times out of 100, a spectrum is allowed to accumulate until a channel reaches 100,000 counts, at which time the accumulation is automatically halted. However, to prevent operator frustration in that 1 case out of 100, this maximum count limit can be easily changed by operator command.

Once the program has been loaded and started, no direct interaction with the computer front panel is called for. All functions of the program are controlled through a keyboard monitor. However, channeling all control information through the teletype imposes a few problems in programming. First of all, even the best typists make mistakes, so the code must have the capability of allowing

*Work performed under the auspices of the U. S. Atomic Energy Commission.

error correcting from the keyboard. Perhaps more important than this is that the code have error checking capability, and gracefully reject commands that are in error. Secondly, the code should allow the user to change his mind. Any operation, once started, should be capable of being stopped when the user desires. For instance, if the user started a type out of the accumulated data (a process that takes approximately five minutes) and on the basis of the first few channels concludes that the spectrum is not good, there is no reason why the program should force him to wait while the rest of a useless spectrum is typed. In short, one of the important aspects in writing a program that the user will gladly use is to provide him with complete control over every feature of the experiment. The highly touted flexibility of a digital computer is lost unless the software also supplies this flexibility.

The primary task of the software, of course, was the acquisition of the mass spectra data from the spectrometer. A flow chart of the acquisition routine is shown in Figure 2. As can be seen from the flow chart, there are two entry points to the acquisition routine; the sync pulse entry is used once per sweep to synchronize the beginning or ending of the accumulated data mode, and the data flag entry point is used 255 times per sweep. The data are stored in two arrays, the real time data in RT (single precision) and the accumulated data in CHAN (double precision). The data are continuously deposited in the real time array, which stores the current data from the spectrometer. Only one half sweep of data is stored (128 data points) and this is being continuously overwritten by incoming data. A display of this array allows the operator to continuously monitor the performance of the spectrometer, and is the primary display used during a tune-up procedure.

When the STATE flag is in the ACCUMULATE DATA mode, the data are added to the CHAN array, building the desired mass spectrum. Note that when the user commands a start or stop in the data taking, STATE is set to a 1 or 2 respectively. The acquisition routine then synchronizes the start or stop of data acquisition with the beginning or ending of the sweep.

For reasons which are unimportant for the purposes of this paper, the data acquired during the up and down half-sweeps are treated as two separate spectra. If the data are stored sequentially in-core as they come from the spectrometer, the display of the data would show the down-sweep spectrum as the mirror image of the up-sweep spectrum. Normally, however, one would desire to see the low mass data on the left of the display. This was accomplished by having the acquisition routine store the data from the beginning of the data array up for the up-sweep and from the end of the data array down for the down-sweep.

One final problem with the acquisition process should be mentioned. The data from the spectrometer appear at an absolute synchronous rate, placing quite a restriction on the length of time spent in any interrupt service routine.

The display, of course, is one of the major reasons for using a computer in this application. What makes the computer-driven display better than the previous display used? First of all, the computer display is entirely flicker-free, while the previous analog displays were driven at the same

rate as the magnetic sweep—1 to 2 sweeps per second. Secondly, scaling of the linear display is under keyboard control. The full scale value of the linear display can be varied from a value of 2^2 to 2^3 in powers of two. Third, a flicker-free logarithmic display with or without decade lines is available. The data compression afforded by this type of display has proved to be invaluable, but the price paid for the logarithmic display is very minimal, as the routine occupies less than 20 locations and approximates a logarithm in 35 μ sec.¹ Finally, the computer-driven display is capable of expanding a selected number of channels so the user can examine them in more detail. With this expand mode, the user can set a marker at any desired channel, and then expand plus or minus N channels on either side of the marker. In addition, there are two commands to move the marker at approximately one channel per second to either the right or the left and stop when desired.

The display routine, diagrammed in Figure 3, is essentially the main program, as other routines are entered only to service interrupts. The display loop is coded for maximum speed, because in striving for a flicker-free refresh rate of 256 channels every 30 msec, one must remember that every cycle in the loop accounts for more than 1% of the refresh time. For a flicker-free display of 256 channels, then, the loop to display one data point must consist of less than 100 machine cycles. One of the techniques used to achieve this speed is in the area of decision branches. As can be seen from Figure 3, there are three decisions to be made within the main display loop. These decisions could be made by putting the appropriate flag in the accumulator and then executing a skip instruction, but this procedure requires a minimum of three machine cycles. However, the decision can be done in single cycle by depositing the appropriate JMP instruction (this is essentially address modification) in the decision location. This technique alone saves more than 2 msec in the display of 256 channels of data.

Basically, this program is input-output oriented. It can be viewed as a collection of asynchronous program segments that can make conflicting input-output service requests. To resolve these conflicts, a basic input-output processor was written to schedule the response of the requests in an orderly manner.

A request for I/O service is made by transmitting to the Service Request Routine a Service Request Block (see Figures 4 and 5). The Service Request Block consists of three words: a data word to convey needed information to the requested routine, a device number specifying the I/O device, and the starting address of the desired service routine. The Service Request Routine stores this block of data in the Service Request Storage Queue, and then transfers control to the Service Start Routine. This routine sequentially examines Request Blocks in the Storage Queue, and by checking the appropriate Device Busy Flag (a software flag) determines if the requested device is already engaged. If it is busy, the service start routine examines the next entry in the queue. If it is not busy, the appropriate Device Busy Flag is set, and the data word is transmitted to an I/O service initialization subroutine designated by the starting address in the request block. When this requested service has been completed, the End

¹P. D. Siemens, "A Fast Approximation Method for Finding Logarithms," UCRL-71344, 1968. Also to be published in DECUSCOPE, Vol. 7, No. 5.

Service Routine is entered, which clears the Device Busy Flag and then transfers control to the Service Start Routine. In this way, maximum throughput to the I/O devices is achieved.

There are several other I/O operations that have not been mentioned yet. For instance, a spectrum can be punched or read from paper tape, and written or read from DECTape. Also, a spectrum can be printed on a printer (now an ASR 33 teletype, but soon a 100 character/sec printer). Here again, an effort was made to present the data in a very understandable format. To achieve this, the data and channel number were listed in a four-column format with leading zeroes suppressed.

It should be noted that the display and I/O routines are fairly general, and whether the function

that is performed is multi-summing scaling, signal averaging, or pulse height analysis depends on the data acquisition routine.

While much useful data can be obtained with these routines, the software development is not yet complete. Yet to be integrated into this package are the on-line calculational routines to furnish the user with the isotopic ratios immediately after a spectrum has been accumulated.

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Siemens - Fig. 1

SERVICE REQUEST BLOCK

DATA WORD
DEVICE NUMBER
STARTING ADDRESS

Siemens - Fig. 4

Siemens - Fig. 5

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