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November 13, 1968

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ON-LINE DATA REDUCTION FROM CARY 14, 15, AND 60 SPECTROMETERS*

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ABSTRACT

A 4K PDP 8/S computer with ASR-33 teletype has been installed in this laboratory as the heart of an on-line data-reduction system for the Cary 14, 15, and 60 spectrometers. Data flow is from the spectrometer through a set of Datex mechanical encoders, through an interface designed to our specifications by Berkeley Scientific Laboratories, through the computer, and onto the teletype both as printout and binary punchout. The software system includes a rapid averaging algorithm to eliminate high-frequency noise, a sliding thirteen point least-squares curve fitting, a fully buffered I/O system, and a versatile monitor which virtually eliminates the possibility of unrecoverable operator error.

HARDWARE

A 4K PDP 8/S computer with an ASR-33 teletype has been installed in this laboratory as the heart of an on-line data reduction system for Cary 14, 15, and 60 spectrometers. An interface, designed and built by Berkeley Scientific Laboratories, has been connected to the computer I/O bus so that the computer can sense the status of six input devices. Each of the six devices is assumed to be a set of twelve binary switches. A special set of two switches is connected to device 1 of the interface such that a change in status of either of these switches causes the interface to set the program interrupt flag for the PDP 8/S. Currently a Datex 20-bit shaft encoder, type 22-300-14, which is mechanically linked to the wavelength counter of the spectrometer is connected as devices 1 and 2. The two-switch Gray code of device 1 is connected to a two-bit encoder in the Datex shaft encoder, so that any change in the wavelength encoder status causes the program interrupt flag to be set. A Datex single-turn, 12-bit encoder, type 03-005-1, which is mechanically linked to the pen of the spectrometer, is connected as device 3. The pen and wavelength encoders are part of the standard Cary Digital System, and may be connected interchangeably with that system. Device 4 of the interface is connected to a panel of 12 switches.

SOFTWARE

A library of programs has been written to acquire and process data from Cary spectrometers using the above system. Called "SUPER SPECTRUM," the operating system features fully buffered teletype input/output[1] and a monitor program which permits control to be transferred at will between the various subprograms. Program control is by means of one-letter commands given from the teletype keyboard, and by settings of the computer-console switch register. Provision has been made for future expansion of this operating system. Routines may be added or deleted from the monitor calling program by means of one-word patches. Compatibility with the current program requires that future additions to the system use program interrupt and use "JMP ." rather than "HLT" instructions for delays. Teletype input is achieved by calling the subroutine IN, which returns with the next character in the teletype input buffer in the accumulator. Teletype output is done by calling the OUT subroutine with the character to be printed in the accumulator. The output buffer is emptied and the input buffer is cleared upon entry to the monitor.

Upon entry, the program first calls for the starting and ending wavelengths, the wavelength increment between data points, and the interval over which averaging is to be performed. These and various scaling and identification parameters are entered via the keyboard. Additional control information is entered in the switch register. The keyboard is continually examined, and control is transferred to the monitor whenever the character "←" is typed. From the monitor any of the following routines may be called:

1. Baseline start
2. Spectrum start
3. Data read (from paper tape)
4. Data punch (to paper tape)
5. Backup and retake part of spectrum
6. Clear baseline is zero
7. Echo keyboard
8. Print pen encoder
9. Print wavelength encoder.

The existing program is designed to average the spectrometer pen reading 4096 times or for a specifiable wavelength interval, whichever is less, and store the result internally as a 12-bit integer. The averaging interval is centered about the wavelength to which the averaged value nominally corresponds. The averaging procedure is repeated at specified wavelength intervals within a specified wavelength range. The averaging algorithm used

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is a modified "stable averaging,"[2] where the average M after taking m readings is

$$M_m = M_{m-1} + \frac{f(m) - M_{m-1}}{2^N},$$

where

$$2^{N-1} + 2^{N-2} < m < 2^N + 2^{N-1} + 1,$$

and where f(m) is the value of the mth reading of the signal. Stable averaging is used rather than simple arithmetic averaging, because it can be programmed to execute more rapidly and because it attenuates noise almost as efficiently. The average is computed in double precision using integer arithmetic (24 bits); however, only the most significant 12 bits are kept for later use. Data may be stored as either a spectrum or a baseline, and baselines and spectra may be taken in any order.

Using the output buffering programming, data may be printed on the teletype concurrently with data acquisition, at the experimenter's option. Several output options are available. In addition to printing the wavelength and raw data, a sliding 13-point least-squares average may be applied to the difference of the spectrum and baseline raw data. The resulting smoothed data may be multiplied by a specifiable constant and printed. The difference between the smoothed value and the scaled difference of spectrum and base line raw data may be computed and printed.

The algorithm used in the sliding 13-point least-squares averaging is due to Savitzky and Golay.[3] It is of the form

$$q_0 = \frac{1}{a_7}[a_6 (p_{-6} \pm p_6) + a_5 (p_{-5} \pm p_5) \cdots + a_1 (p_{-1} \pm p_1) + a_0 p_0],$$

where a_0 to a_7 are constants, q_0 is the smoothed value, p_i the raw value, and the signs used in all the inner parentheses are the same. The constants used in the program perform a least-squares fit of 13 points to a third-degree polynomial. By simply changing the constants by means of a patch, the program may be used to calculate the nth derivative using any odd number of points less than or equal to 13, or any odd number of points less than or equal to 13 may be used to fit an nth-order polynomial, where n is an odd integer less than or equal to the number of points used in the fit.

Data may be preserved for later processing by having a paper tape punched containing the control information and the data. If the last data taken before punching is a baseline, the data tape contains the raw baseline data values. If the last data taken is a spectrum, the data tape contains values of (spectrum - baseline) E/OD, where E and OD are constants specified by the operator at the start of each baseline or spectrum.

A routine exists to read the data tapes back into the spectrum baseline data arrays, and another routine permits processing and printing of the data arrays at any time. Programs to print the wavelength and pen position for calibration and test purposes may be called.

Mistakes while acquiring data can be corrected by calling an error-recovery program which enables the operator to retake a portion of the data under carefully defined circumstances.

The program is loaded into the computer memory from a single paper tape punched in Digital Equipment Corporation binary loader format (Digital 8-2-U). It consists of four blocks of code separated by short sections of leader (200 code punches). The first block of code modifies the binary loader to read tape continuously, unless a checksum error is detected. The second block is a copy of Floating-Point Package II (as released by DEC). The third block is the Super Spectrum system, including patches to the Floating-Point package. The final code block restores the binary loader program to its original form, so that the loader halts after reading the final checksum. This means that to the user the tape acts as if it were a single binary tape, and is loaded by following the instructions for the binary loader (Digital 8-2-U).

Great care has been taken to ensure the integrity of the program during execution. To our knowledge once the program is loaded and running, and the console panel is locked, the program can not be destroyed by any operator action except turning the power off while the computer is running. The program has been used for several months without incident by about five operators, most of whom regard the programmed computer as a "black box." The program and data storage occupy all of memory.

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