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Real-time Reduction of Nuclear Physics Data*

Abstract: Small scientific computers have been widely used in research laboratories for on-line data acquisition to improve the efficiency of data collection and to perform sophisticated data manipulation before storage. An equally productive use of such computers is for the subsequent reduction of these data in real time, permitting interaction between investigator and computer and providing immediate interpretation of masses of data. This report describes the philosophy and techniques developed for the SCANS (Stanford Computers for the Analysis of Nuclear Structure) system for the reduction in real time of multichannel pulse-height spectra, which comprise the bulk of data in Nuclear Physics. The programming language for users is FORTRAN, to provide flexibility and ease in introducing and modifying sophisticated concepts such as nonlinear least-squares fitting. Software interface to specific real-time hardware devices such as oscilloscope display and light pen is accomplished via library subroutines which perform a variety of general purpose services. Several different applications of this approach to various types of data spectra are discussed to illustrate the degree of mutual interaction achieved between investigator and computer and the resultant optimization of reduction techniques to suit particular types of data.

Introduction

Improved data acquisition techniques in experimental nuclear physics have intensified the need for more sophisticated methods of reduction of those data to meaningful parameters characteristic of the experiments. Design considerations for computer-oriented data acquisition systems must include not only the control of measuring devices and monitoring of data flow, but also the equally important task of handling the data thus accumulated.

The purpose of this report is to describe the philosophy and methods of data reduction in real time developed for a typical system and to present workable techniques for implementing the computation. The configuration outlined is that of the SCANS (Stanford Computers for the Analysis of Nuclear Structure) system.

SCANS System

The SCANS System[1] was developed for investigation of nuclear structure with reaction energies in the range of 1 to 60 MeV. Its primary task is the processing of data in the form of single- or multi-parameter arrays, where the address of each word represents a particular magnitude of pulse height from a detector and the contents of the word represent the number of such events detected. Each location in memory corresponds to a particular channel (or bin) of the output of an analog to digital converter (ADC), and the array is considered as a multichannel pulse-height spectrum, as illustrated in the Figures, indicating the number of counts per channel detected as a function of pulse height (channel number).

The on-line data acquisition and final data analysis procedures utilized by the SCANS System will not be described here. What is of primary interest is the solution to the intermediate problem of reducing masses of raw data and extracting characteristic information in real time with the utmost flexibility and control afforded the investigator. There are three major criteria which influenced the development of the system.

(1). The system must operate in real time, reducing arrays of data with on the order of a thousand words in a matter of minutes, and have immediate response to any request for computation.

(2). Communication between system and operator must be as flexible and powerful as possible, so that the investigator may be kept fully informed of trends in relevant parameters of his data, and may in response control the reduction techniques to utilize those most appropriate for his data.

(3). The programming language must be a high-level language such as FORTRAN, to provide the user with flexibility and ease in introducing and modifying highly sophisticated concepts of data handling.

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The optimum compromise between the demands of these criteria resulted in a FORTRAN-compatible system for a small scientific computer (a PDP-7 or PDP-9 with 8K of memory), in which the capabilities of immediate response and varied modes of communication inherent in such small computers are combined with the sophistication of computation generally utilized only in larger and more remote systems.

Subroutine interface

The standard FORTRAN instruction set makes no provision for real-time control and display because of the complex and singular requirements of individual installations. Specialized library subroutines have, therefore, been developed to access specific real-time hardware devices such as oscilloscope display and light pen for a variety of frequently encountered circumstances.

The standard library of interface subroutines for the SCANS system is listed in Table 1. Oscilloscope displays are generated by the —SCOPE series of routines. PTSCOPE and FPTSCOPE display single-parameter multi-channel pulse-height spectra, with the number of channels, first channel number, positioning, scale factors, and data array specified as arguments. The number of counts per channel is displayed versus channel number. XYSCOPE and FXYSCOPE display data in a similar manner, where the channel numbers are not necessarily contiguous.

PT3DSCOPE displays a two-dimensional array in three dimensions, with the polar and azimuthal angles from which the oscilloscope display is "viewed" variable in 1-degree steps by switches on the console. The three coordinates of the array are arbitrary, but might represent, for example, X = energy of detected particles, Y = incident energy for several accumulated spectra, and Z = events counted per channel.

Because of memory size limitations, all of these routines display data arrays directly, without storing scaled or normalized display arrays. The scale factors are therefore calculated on the fly, point by point, each time the array is displayed. During display the central processor time is devoted exclusively to computing the display, but this does not represent any serious disadvantage in real time. The purpose of a display is to interrogate as well as inform the operator and the program usually cannot proceed without further instructions, based on the operator's judgment.

The routines PTPEN and FPTPEN are used to interrogate the light pen for use with PTSCOPE and FPTSCOPE, and the routines XYPEN and FXYPEN are used similarly with XYSCOPE and FXYSCOPE. In each case a small cross is displayed on the oscilloscope screen each time the routine is called. If the light pen detects any of the dots of the cross, the cross is repositioned at the centroid of the detected points, and this position is returned (normalized to appropriate display routine scale factors) to the calling program. The routines are thus able to indicate the last position specified as well as modify that position. The calculation of a centroid permits the use of a coarse opening on the light pen for ease in viewing the scope face.

Similarly, the routines PTPLOT and FPTPLOT and the routines XYPLOT and FXYPLOT are compatible with the corresponding display routines, creating a hard copy on an X–Y plotter of the view on the oscilloscope screen. The routine CALIBRATE is used to calibrate the plotter for the desired set of scale factors.

The control routines LISTEN and ISENSE are used for branching within programs. LISTEN interrogates the teletypewriter, returning an argument of a number if a numeric character is hit, —1 if a non-numeric character is hit, or 0 if no character is hit. Its main purpose is to provide a cutoff time for a display loop and some instruction from the operator as to which task to perform next. ISENSE reads a set of sense switches, including a 16-position switch which provides a scale factor for displays. These switches are part of an IDIOT (Indicating Digitizer for Input/Output Transformation) box.

The input/output routines are special purpose routines for reading and punching paper tape in formats compatible with hard-wired analyzers. The DUMP routines transfer arrays of data directly from the memories of these analyzers. The utility programs are used for general-purpose translations of information from one medium to another.

Typical application

These subroutines and function subprograms provide a complete link between FORTRAN and the real-time input/output devices. The investigator who wants to

Table 1 FORTRAN compatible subroutines for real-time data analysis.

Purpose	*Fixed Arguments*	*Floating Arguments*
Display	PTSCOPE	FPTSCOPE
	XYSCOPE	FXYSCOPE
		PT3DSCOPE
Light Pen	PTPEN	FPTPEN
	XYPEN	FXYPEN
Plotting	CALIBRATE	
	PTPLOT	FPTPLOT
	XYPLOT	FXYPLOT
Control	LISTEN	
	ISENSE	
Input/Output	INPUT ND 180	INFLT ND 180
	INPUT VICTOREEN	INFLT VICTOREEN
	DUMP ND 180	FDUMP ND 180
		OUTFLT
Utility	CREASE (Card Reader for Ease in ASCII Source Editing)	
	ACTION (Analyzer-Computer Transfer of *I/O* for Nuclear data)	

Program 1

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C       GRASP 3/16/68
C       GAUSSIAN REDUCTION AND ANALYSIS OF SPECTRUM PEAKS
C       ALBERT ANDERSON, STANFORD UNIVERSITY
        DIMENSION IDATA(513), LTPEN(10, 6)
        WRITE(2, 1)
    1   FORMAT (12H GRASP 3/68)
  100   WRITE(2, 101)
  101   FORMAT (4H I/0)
  102   MAXY = ISENSE(-0)
        CALL PTSCOPE (NUMBER, 1, 0., 1., .1, MAXY, IDATA)
        CALL PTPEN (NUMBER, 1, LTPENX, MAXY, LTPENY)
        CALL LISTEN(L)
        IF (L), 200, 102, 103
  103   GO TO (110, 120, 130, 140, 150, 160, 170, 180, 190), L
  120   CALL INPUTN (NUMBER, IDATA)
        GO TO 102
  170   WRITE (2, 171) IDATA(LTPENX), LTPENX
  171   FORMAT (/17, 15H CTS AT CHANNEL 15)
  190   CALL DUMPND (NUMBER, INITIAL, IDATA)
        GO TO 102
  200   WRITE (2, 201)
  201   FORMAT (/5H PEAK)
  202   MAXY = ISENSE(-0)
        CALL PTSCOPE (NUMBER 1, 0., 1., .1, MAXY, IDATA)
        LTPENX = LTPEN(N, LT)
        CALL PTPEN (NUMBER, 1, LTPENX, MAXY, LTPENY)
        CALL LISTEN(L)
        IF(L) 300, 202, 203
  203   GO TO (210, 220, 230, 240, 250, 260, 270, 280, 290), L
```

incorporate data display or branch control into his program can do so merely by calling the appropriate routine. The statements listed in Program 1, which were abstracted from a typical data reduction program GRASP,[2] indicate how these routines are used.

The program is composed of three sections, each section providing a display and branching structure, of which only the control sections for the first two are indicated. The first section provides for reading, writing, and editing the data. The second section utilizes the light pen to identify a peak to be fit. The fitting process and parameter extraction for any particular peak are performed in the third section.

The first display loop is located in statements 102–103. An array IDATA with NUMBER channels is displayed with its baseline 10% above the base of the scope display, along with a light pen cross positioned at LTPENX and LTPENY. The vertical scale factor MAXY is taken from the 16-position switch by ISENSE(−0). The display is repeated until a key on the teletypewriter is struck, causing a branch either to the second loop at statement 200 or to one of ten branches within the first loop.

If the number 2 is struck on the teletypewriter, for example, the program reads paper tape from a Nuclear Data 180 analyzer into the array IDATA. Striking the number 9 similarly fills the array from the analyzer directly through an electronic dump. Striking the number 7 produces a printed record of the horizontal location of the light pen. The second loop starting at statement 200 indicates how various stored values of an array LTPEN can be altered with the light pen.

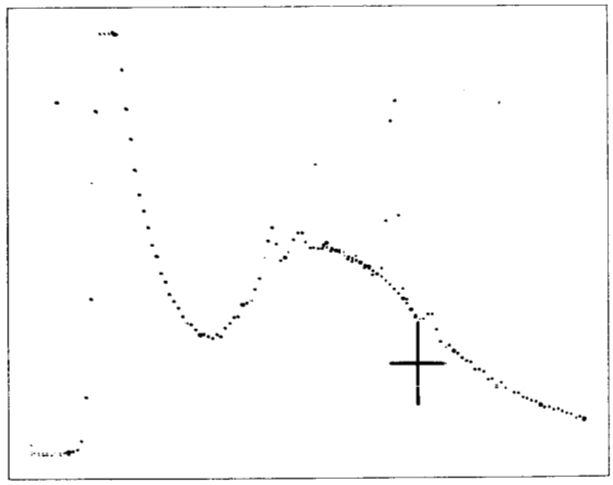
Data reduction

The parameters of prime interest in the multichannel pulse-height spectra accumulated as data in nuclear reaction experiments are the area (number of events detected), position (generally a measure of the corresponding particle energy), and width of each peak in the spectrum, after correction for background contribution.

For the simplest type of spectrum analysis[3] the background spectrum can be fit on either side of a peak with the method of least squares and be subtracted from the data. The sum of counts in the difference spectrum yields the area, and the centroid locates the position. A typical spectrum is illustrated in Fig. 1, with the fitted background interpolated beneath the peak. The light pen cross is used to indicate to the analysis program the region of background to be included in the fitting procedure.

For more complex situations, where the areas of the peaks span a wide range or where the peaks are not well separated, more consistent results can be obtained by fitting the peaks as well, either with analytic functions or with reference shapes. Several general-purpose fitting programs exist for locating and fitting peaks of various types in such spectra automatically, but in most cases the requisite flexibility and accuracy are attained at considerable expense of memory, and the programs are suitable only for fairly large computers.

Figure 1 Multichannel pulse-height spectrum including interpolated fit to background underneath prominent peak. Light pen cross is used to indicate fitting region to the program.



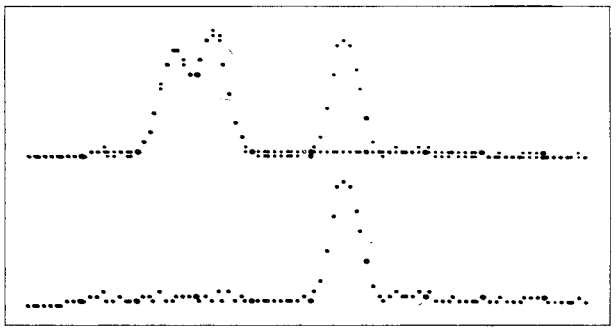


Figure 2 Deuteron energy spectrum from $^{40}A(p, d)$ reaction showing fit to two peaks simultaneously with Gaussian peaks plus polynomial background. Upper curve superimposes fit on data; lower curve shows difference between data and fit to peaks.

We have found it invaluable in adapting fitting programs to small computers to provide several modes of communication between the computer and the investigator to permit the strongest possible interaction between them. The requisite flexibility and accuracy are thus attained by intercession of the investigator at appropriate points in the fitting procedure.

There are three major benefits which accrue from this interaction. (1) In the initial stages of data reduction for a specific type of data, the investigator is able to introduce fairly arbitrary procedures and criteria into a general fitting program. (2) The progress of the fitting procedure for typical spectra may be monitored and analyzed in detail to optimize the techniques for the particular data to be reduced: the criteria developed may then be incorporated into automating the fitting, with confidence in the results. (3) Even when the procedures are automated to the extent that very little is demanded of the investigator, he may obtain additional insight into the nature of his data by occasionally analyzing the data reduction process in detail.

Nonlinear least-squares fitting

The primary tool for reduction of nuclear reaction data with the SCANS system is the consistent fitting of data with nonlinear functions by the method of least squares.[4] There are three major classifications for programs using this technique: (1) determination of peak parameters (area, position, width) by fitting with analytic functions; (2) determination of peak parameters by interpolating between reference shapes; and (3) fitting of data with arbitrary analytic functions with large numbers of parameters.

Typical of the first classification is the program GRASP (Gaussian Reduction and Analysis of Spectrum Peaks).[2] This program fits data in the form of multichannel pulse-height spectra with a function comprising a series polynomial (up to 5th order) plus one or two Gaussian peaks simultaneously.

A typical fit is illustrated in Fig. 2, which shows three peaks from an energy spectrum of deuterons emitted from the $^{40}A(p, d)$ reaction for a proton bombarding energy of 18 MeV. The upper curve shows the data with a fit to the double peak plus background superimposed. The lower curve shows the difference spectrum between the data and the fit to the double peak (background is not subtracted).

In operation, the investigator identifies background regions on either side of the peak, and identifies the region for fitting the peak, with the light pen and teletypewriter. The peaks and background are fit over different regions of the spectrum (although in each case the fit is to the sum of the functions) because the peaks are not perfectly Gaussian, and contributions to χ^2 in the tails of the peaks are not valid.

The fitting procedure is straightforward except that the investigator can specify externally with sense switches any of the parameters and/or hold them fixed throughout the fitting. The difference spectrum is particularly useful in discovering anomalies in the fit, which indicate discrepancies between the data and the parameterized description. By varying one or more parameters externally, the investigator can study the relationship between fluctuations in the data and uncertainties in the parameter.

Nonanalytic function

Typical of the second classification of data reduction is the program GRASS (Gamma Ray Analysis by Spectrum Stripping).[5] This program fits gamma ray energy distributions in the form of multichannel pulse-height spectra with a function comprising a measured background plus up to five peaks interpolated from reference line shapes for monoenergetic gamma ray sources. The positions of the peaks are fit iteratively and the areas are fit simultaneously. Provision is included for increasing the widths of peaks by folding in a rectangular shape, whose width is optimized.

A typical fit is illustrated in Fig. 3, which shows two peaks from an energy spectrum of gamma rays emitted from the $^{7}Li(p, \gamma)$ reaction for a proton bombarding energy of 10.0 MeV. The upper curve shows the data with a fit superimposed. (The low-energy tail on the left is extrapolated with a straight line to zero energy.) Note the asymmetry of the peaks, which precludes the use of an analytic function to describe the peaks. The fits are interpolated (or extrapolated) from two reference line shapes corresponding to two different gamma ray energies.

This program is more highly automated than GRASP; once the investigator has specified to the program the procedure for determining starting values for the least-squares fitting, and the regions over which to fit, the program can reduce spectra automatically, retrieving data

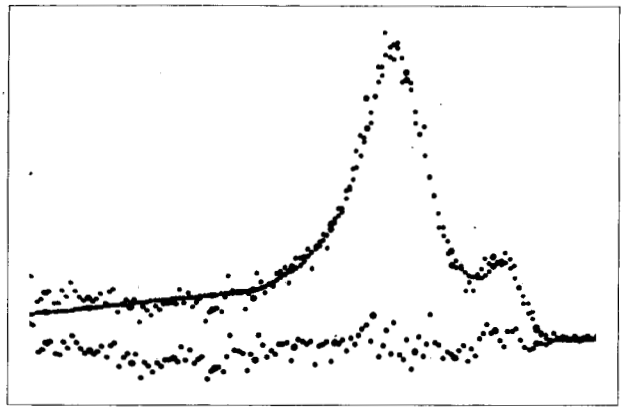


Figure 3 Gamma ray energy spectrum from ^{7}Li(p, γ) reaction showing fit to two peaks simultaneously interpolated from reference shapes. Upper curve superimposes fit on data; lower curve shows difference spectrum.

from magnetic tape (or electronic dump from an analyzer) and typing or punching the extracted parameters for subsequent analysis.

Interaction between the computer and investigator plays a major part, however, in establishing the optimum conditions for fitting the particular data. Not only is it important to choose the fitting regions carefully, a task which is considerably simplified by coordinating light pen and oscilloscope display, but it is also necessary, when fitting such data with a large number of parameters, to determine initial values for the parameters with accuracy, if not precision. The χ^2 hypersurface may have a number of local minima, only one of which corresponds to the desired estimates of the parameters. The starting values of the parameters must be specified close enough to the final values that the search along the χ^2 hypersurface will not veer away from that minimum.

Searching the χ^2 hypersurface

Typical of the third classification above is the subroutine SESAME (Spectrum Evaluation by a Search Analysis with Maximum Efficiency).[6] This program fits multichannel pulse-height spectra with arbitrary functions containing a considerable number of parameters. The search utilizes a second-order Taylor's expansion of χ^2 to determine an analytic solution for the minimum of the χ^2 hypersurface. Partial derivatives of χ^2 are estimated by sampling the value of χ^2 in the neighborhood of the starting point.

The search converges rapidly if the starting point is close to the desired minimum of the χ^2 hypersurface, but may converge slowly if the starting point is not close. In particular, if the curvature of the hypersurface is negative, strict application of the method would force convergence to a relative maximum rather than a minimum.

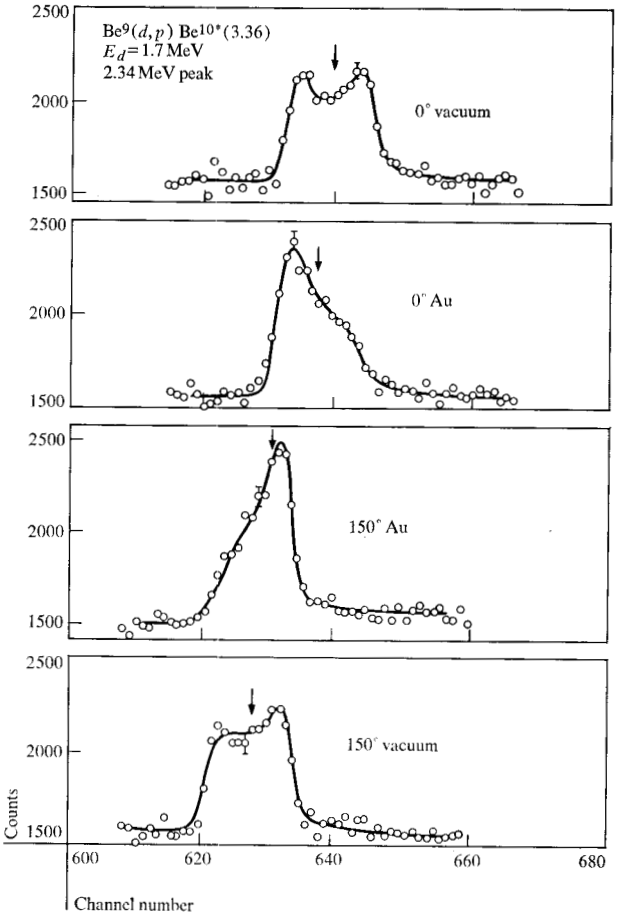


Figure 4 Gamma ray spectra from the ^{9}Be(d, p) reaction for recoil nucleus decaying in vacuum, and stopping in gold. Fit includes parameters for angular distribution of recoil nucleus and Doppler shift of gamma ray energy.

For this reason, communication between computer and investigator is invaluable. By monitoring the progress of the search on the oscilloscope, the investigator is able to adjust (via the teletypewriter) the values of parameters which are not being optimized properly. At the same time he may omit (via sense switches) from some stages of the search those parameters which are already fairly well optimized. Thus the investigator can insure the accuracy and improve the speed of the search by analyzing its progress.

A typical fit is illustrated in Fig. 4, which shows line shapes of the gamma-ray spectra from the 3.37 MeV level of ^{10}Be produced in the ^{9}Be(d, p) reaction at a deuteron bombarding energy of 1.7 MeV. The different shapes of the peaks result from the Doppler effect. Information pertaining to the lifetime of the recoil nucleus can be obtained by studying the change in shape when the nucleus is free to recoil in vacuum and when it is stopped in an absorber such as gold.

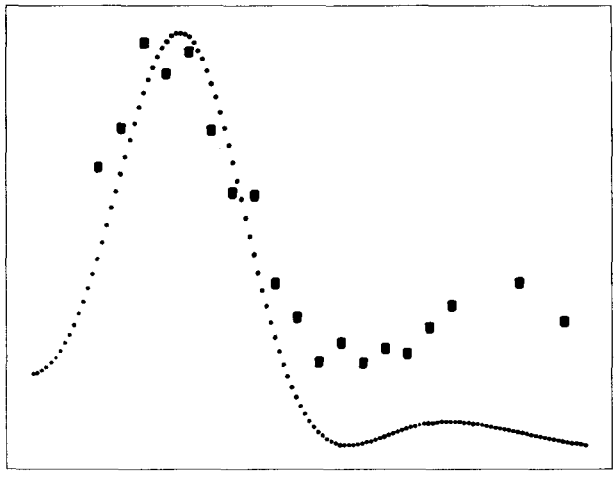


Figure 5 Angular distribution for deuterons emitted from the $^{27}Al(p, d)$ reaction. The smooth curve is a plane wave Born approximation calculation, with parameters adjusted to fit the data points. Note that the position but not the magnitude of the second maximum is predicted correctly.

In spite of the large number of parameters (up to ten), excellent fits to the data can be obtained rather quickly if the investigator is aware of the condition of the χ^2 hypersurface.

Communication

The common denominator in the three data reduction programs described above is interactive communication between computer and investigator. The power of the computer is utilized to perform fairly sophisticated non-linear least-squares fitting, but where appropriate the scientific training and intuition of the investigator is utilized to guide and control the data reduction.

Four different modes of communication are used for this purpose: (1) The teletypewriter permits the use of numbers and phrases in conventional input/output as well as providing a method for branching to different parts of programs. (2) Sense switches permit the inclusion or rejection of various parameters, provide easily variable scale factors for display, and facilitate automation via pre-selected branching paths. (3) The oscilloscope display is invaluable in monitoring the comparison between data and parameterized description, and in studying the validity of various fitting procedures in terms of that comparison. (4) The light pen permits rapid digital identification of prominant features of data and serves as a powerful tool for specifying graphic information to the computer program.

The most important aspect of this intercommunication is that the investigator is able to consider his data not merely in terms of parameters describing the fit, but also in terms of graphic presentations of the data, both in original and in reduced form.

Analysis

Typical of the application of such communication to the analysis of reduced data is the program DIRECS (DIrect REaction Cross Sections).[2] This program calculates angular distributions for particles emitted from stripping reactions (using a plane wave Born approximation) and displays the calculation superimposed on a measured angular distribution.

A typical fit is illustrated in Fig. 5, which shows the cross section as a function of angle for deuterons emitted from the $^{27}Al(p, d)$ reaction. The positions of the peaks are a characteristic feature of the stripping reaction, depending primarily on the value of the transferred angular momentum quantum number l and the radius of interaction R. A better fit to the main peak (and a subsequently smaller value of χ^2) can be obtained with a different set of values for l and R but the second peak is not predicted at all with this choice. Applying his knowledge of the shortcomings of the theory (the positions of the peaks are predicted well, but not the relative heights), the investigator chooses the correct combination of l and R.

Once the comparison between theory and experiment is well explored, the estimation of parameters could, of course, be automated. But until that happy state comes about, graphic communication between investigator and computer can greatly facilitate that exploration.

Conclusions

Small scientific computers which are routinely used for data acquisition are thus eminently suited for data reduction on a fairly sophisticated scale. Not only are they able to perform such reduction, but their use in real time significantly increases the confidence possible in the extracted parameters. The use of graphic display with light pen to provide interactive communication with the investigator permits a detailed understanding of the mechanism of the fitting process in relation to the data and provides a means for modifying the procedure to adapt to prevailing conditions. The use of FORTRAN as the operating environment greatly facilitates this flexibility.

The prime consideration in a research laboratory is to evaluate experiments performed under conditions which are variable and often unprecedented. General procedures can become obsolete by the time they are fully automated. The important advantage which real-time interaction offers is the possibility of customizing sophisticated procedures of data reduction to particular kinds of data by combining the intuition of the investigator with the power of the computer.

The slowness of small scientific computers relative to large batch-processing systems is offset by the fact that they can be economically dedicated to operate in real time. Comparisons of the total time for data reduction in the two types of systems must include the effort spent in

preparing and organizing data for reduction. In a real-time environment these tasks are performed synchronous with computation, and are greatly facilitated by real-time displays and immediate response to questions stimulated by the prevailing circumstances.

Another important consideration is that reduction of data in real time, in synchronization with the experiment, provides immediate interpretation of the results of the experiment and prompt response by the investigator to discrepancies or unexpected trends. Until true time-sharing becomes more of a reality, this need can only be filled by computers small and inexpensive enough to be dedicated to the inefficient use that real time operation requires. In addition there is the undeniable asset of being able to control the computer's operating system within the user's environment: the system is much more easily available when it is wholly owned and operated by its prime users.

Acknowledgments

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