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AUTHOR	Gerald W. Delaney
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MADCAP IV

A Multiplexed ADC and Analog Plotter Program

Author: G. W. Dulaney
Digital Equipment Corp., Maynard, Mass.

ABSTRACT:

The program was designed as a foundation from which the construction of routines for data acquisition and analysis can be more easily done. By the use of short overlays, it is able to accept many forms of input data including analog output from peripheral equipment such as a mass spectrometer, ESR, NMR, curve follower, etc. This output is converted into digital form using the AXØ8 Lab Peripheral's 9-bit ADC. The mode of input for mass spec, ESR, and NMR requires signal averaging to remove noise. This is accomplished by performing 'boxcar integration,' which consists of averaging a certain number of consecutive samples to generate a data point in a controlled period of time. The lowest S/N increase for 6Ø-cycle noise and one scan is about a factor of ten (128 samples per point at 5Ø points per second), and it can be as high as 4Ø (2Ø48 samples per point) for a slow scan of more than 2.0 seconds per point.

Important, also, is the program's utilization of a general-purpose X-Y analog plotter in parallel with the AXØ8 oscilloscope output as opposed to the more expensive incremental plotter normally employed for computer output plotting.

Output is in the form of printed (and/or punched) information and a scaled plot which can be either a line plot or point plot with optional axes and tic marks drawn in.

The MADCAP IV Basic Package accepts digital data input from paper tape or the keyboard for plotting. Included in the Basic Package are routines to compute the best line between adjacent points for plotting to prevent plotter servo overshoot and a one-page program modifier routine which operates much like ODT-8 in that locations in core can be changed to suit a special purpose. Without the modifier, about $18ØØ_{10}$ locations are available for overlays and data.

Analog input routines are supplied as separate, short binary tapes to be added to the Basic Package. Overlays currently available include a flexible signal averager, a routine to use a photoelectric curve follower, and a specialized routine to accept data from a mass spectrometer to generate ionization efficiency curves. Integration and curve smoothing routines also are available to massage data after acquisition. All data acquisition and reduction routines are re-executable without reloading the binary tape.

The Basic Package has been used as the basis for the LORCAP Package which can input data, compute Lorentzian peak spectra, compute residuals between original and calculated data, integrate either type of data, strip out undesired peaks, remove nonlinear baseline, and smooth data using an eleven-point parabolic function. Results of any of these operations can be displayed on the oscilloscope and/or plotted and are easily executed from the ASR keyboard. LORCAP can be converted by means of a short overlay to handle Gaussian peaks.

The LORCAP Package has been used in the analysis of Mossbauer and NMR data and with the addition of a Gaussian line shape overlay, it can find application in the simulation of IR, visible, and other forms of spectroscopic data.

The author encourages response from users of the program with respect to how well it meets their applications, any new routines they may wish to make available for use with it, their satisfaction (or lack of it, too) with the concepts used, and any changes they wish to propose.

I. REQUIREMENTS:

The system on which the program was written and used was a basic 4K PDP-8/I LAB-8 Computerpack with high-speed reader. Peripherals necessary (See Appendix 2) are the AXØ8 Lab Peripheral, ASR-33, and an oscilloscope. A Hewlett-Packard 2D-2 X-Y analog plotter with remote relay actuated pen lift and Y-axis retransmitting potentiometer and a Hewlett-Packard F3B photoelectric curve follower also were used with good results. A felt-tip pen was found advantageous in making point plots and, in fact, a simple sheet metal holder was fashioned which made use quite satisfactorily of dime-store refill cartridges. A relay driver and relay were added to the AXØ8 and triggered by SØ for pen up-down control on the plotter.

Hardware desired and/or necessary for signal averaging are preamps with a gain of approximately 2Ø for accepting approximately 5Ø mv signals - a FLIP-CHIP type A2ØØ operational amplifier is suitable - and a relay output - FLIP-CHIP type W8ØØ is useful here. The scans are initiated by an external trigger (e.g., +1 to -3 volts) impressed on S1 of the AXØ8. This can be done a variety of ways and is, of course, dependent on the nature of the signal source device. For NMR or ESR instruments unequipped for computer output, a microswitch actuated by the recorder carriage can be used to switch in a simple battery circuit to trigger the computer. The end-of-scan marker from SØ of AXØ8 (-3 to Ø volts for 1 sec., and then back to -3 V) can be divided down and inserted into the Y axis of the instrument's recorder to allow accurate calibration.

These are merely suggestions for thought, and the user can obviously apply his ingenuity to better implement and utilize the signals.

The arithmetic and I/O routines utilize Floating Point Package #2 (DIGITAL 8-5B-S), a relocated version of DECUS No. 8-44 Modified Output Controller, and overlays written by the author to allow use of a high-speed reader punch under control of C(56). The resulting FPP is herein called the Modified Fl. Pt. Pkg. #2 and has been incorporated into both the Basic Package and the LORCAP Package.

II. USAGE:

The FPP accepts all standard input formats; e.g., any of the following are accepted as 1.0: "1", "1.Ø", "1EØ", "1.ØEØ", "Ø.1E1", and "1ØE-1".

In each case, the number is terminated by anything other than a digit, "E", or a period. A space is suggested as a terminator. Leading spaces and spaces following a plus or minus sign are ignored, a RETURN not immediately preceded by a digit is ignored, and plus signs are converted to spaces on output. On input, a RETURN is not echoed with a LINEFEED.

A number can be cancelled on input if RUBOUT is struck before a terminator is entered. An exclamation point is echoed; then the user can enter the correct value.

The subroutine which handles the response to questions will accept only "Y" or "N" as valid input. All other characters generate "?" and are ignored. No terminator is needed.

Insure that the BIN loader is in core - see CONSOLE MANUAL for instructions to load it. For all systems except LORCAP, load the Basic Package (which includes the Modified FPP) into desired reader, turn Teletype on line, LOAD ADDRESS 7777, set bit Ø = Ø to use high-speed reader and press START. The tape has only one checksum. Now load any desired overlays; e.g., the mass spec routine and/or the integrator, etc., by placing them in desired reader and hitting CONTINUE.

The LORCAP Package is a two-part binary tape, the second of which is a set of operating instructions that will be typed out when the program is started. The first section contains all that is needed to operate and the second section is optional.

All data input routines, including LORCAP, use SA=Ø2ØØ. A heading is typed then the user can type in a title of any desired length, terminating it with ALTMODE. The discussion is now separated into parts descriptive of each mode of operation.

A. Digital data input:

Answer "N" to ANALOG INPUT? and give the number of points to be retained for NO. POINTS=. Up to 5ØØ points with X data or up to 1ØØØ without X data can be entered. If X data is to be entered, answer "Y" to HAVE X DATA? The program then requests PTS. TO SKIP=, i.e., the number of points to ignore on read in. This feature allows the user to select any contiguous section or block of points from the data tape. Scaling variables for Y data (and X, if present) are entered next. RANGE should be chosen to be at least as large as the difference between the largest and smallest values within the data block. MIN is the smallest value, or less, in the block. These are used to scale the data to fit within a Ø-5ØØ range for display and can be chosen to maintain exact intensity (and X axis) calibration, if necessary. If no X data is to be entered, X RANGE and MIN are not asked for. Then the user is asked TTY I/O? Load the data tape and prepare the desired reader before answering. "N" will start reading from the high-speed reader. When input is complete, scope display commences. See Section II.G for further instructions.

B. Mass Spec Analog Input:

This mode was designed for measuring relative ion current as a function of accelerating voltage, wherein the accelerating voltage is manually incremented on a pot. A voltage proportional to the ion current is sampled and averaged by injecting an external trigger pulse (+1.5 going to -1.5 volts) into S1 of the AXØ8 to begin each data point. 2Ø48 samples are averaged per point, and the results for each point can be printed out as soon as they are complete. This requires about 1.5 second per point. The currently accumulated data is displayed on the scope while waiting for the next trigger pulse.

To enter this mode, answer "Y" to ANALOG INPUT and enter the desired MULTIPLEX CHANNEL. To print and/or punch the data as it is taken, answer "Y" to OUTPUT? and prepare the punch before answering TTY I/O?; "N" assumes the high-speed punch is to be used. In this mode, the number of points is left unspecified, and the user can enter up to 1ØØØ points or terminate entry when desired. The program will punch leader tape if output was desired and then await the first trigger pulse. If output was not requested, the Teletype bell is rung when each point is complete.

When it is desired to terminate data entry, set BIT 11=1. Trailer is punched if output was requested, then the program types out the number of points taken before scope display commences. See Section II.G.

C. Curve Follower Input:

Note: For plotters other than HP 2D-2 and/or curve followers other than HP F3B, refer to manuals supplied by the manufacturer.

Connect the Y output of the F3B to Y input of recorder, place recorder in LF mode and connect the multipin plug into receptacle on rear of recorder marked RETRANSMITTING SLIDEWIRE. Make signal connection to AXØ8 and insert pickup head in pen holder. See manuals for more detail.

Answer "Y" to ANALOG INPUT?, give desired MULTIPLEX CHANNEL, and select desired PT. INDEX (Table 1). An illegal PT. INDEX results in it being requested again. The program now types an instruction to set up X ZERO and GAIN on recorder to encompass desired region to be sampled. See Section II.G under PLOT for detail on the plotter calibration routine. Axes can be drawn on the original, if desired.

When range is set, turn RC clock COARSE to first or second position from slowest (Ø.5 to 1 sec/cycle) and type "0". Center pickup head over line, increasing follower SENSITIVITY and GAIN just short of oscillation. Type "G" to begin data input. When input is complete, the scope display routines are entered.

Turn recorder to standby and set follower gain sensitivity fully counter-clockwise. Refer to Section II.G for output details.

D. Slow Scan Signal Averaging Input:

In this mode, a remote trigger (+ TO -) impressed on S1 of AXØ8 commences the scan after a specified delay time. Up to about 5ØØ scans can be taken and averaged. After each scan, an outgoing trigger is available from SØ of the AXØ8. It is a -3 to Ø volt pulse lasting about 1 second. A new scan must again be triggered thru S1.

Digital data input via Section II.A is unavailable with the Averager, and Y axis tic marks are not made.

After starting at Ø2ØØ, type a title, hit ALTMODE, and supply desired multiplexor channel, point index, and SEC/SCAN.

If the input for PT. INDEX and SEC/SCAN give a value less than .Ø16 sec/pt, new input is requested, starting from PT. INDEX. Then set the MAX SCANS (<5ØØ), and, finally, the delay time in secs. (<4ØØ) (See Tables 1 and 2.)

Input commences with the first trigger and continues to the end of the scan. While in progress, the scope will follow the ADC's as they are performed with the X axis scaled to the number of points.

The run can be interrupted at the end of the scan in progress by setting BIT Ø of the SR to 1 at which time the number of scans taken is printed and scope display of stored data commences. The size of the display can be changed by typing "D" on the ASR to decrease size or "M" for magnification. Typing "S" to stop display allows the user the option of returning to accept more data (up to MAX. SCANS) or terminate the run as it stands by giving the desired answer to MORE SCANS? After termination, the scope routines are entered. If the integrator and/or one of the smoothers is desired, this can now be loaded with the BIN loader. Restart program at Ø2Ø1 to reenter scope routines. See Section II.G for further details.

Computer memory cycle time is used for the time base; thus, accuracy will vary from one machine to another but reproducibility is quite good.

Accuracy can be improved to about Ø.5% using the following calibration method:

1. Accurately measure the scan time, T, with 5ØØ points (PT.INDEX=3), 18Ø seconds or more for SEC/SCAN (defines ST below), and Ø for DELAY as the input. Since there is a one-second delay loop used for the end of scan marker, carefully watch the PC and MA lights to detect the actual end of the scan. For convenience, C(36Ø5) can be changed from 6331(XRIN) to 76Ø4(LAS) to allow SR bit 1 to trigger the scan.

2. Compute new memory cycle time, MCT:

$$MCT = (1.45\emptyset X1\emptyset^{-6})\ xST/T$$

(1.45Ø microseconds was the value assembled into the Averager.)

3. A short routine is available at startup only by SA Ø4ØØ to allow resetting the MCT to a new value. The routine is destroyed by data. After entry of the calibration value, the routine exits to Ø2ØØ; i.e., the normal starting address.

Table 1:

Number of Points Assigned

According to PT. INDEX

PT. INDEX	Follower	Averager	Min.Sec./Scan
1	125	5Ø	Ø.8
2	25Ø	1ØØ	1.6
3	5ØØ	5ØØ	8.Ø
4		1ØØØ	16.Ø

Table 2:

Number of ADC Samples per Point as

a Function of Time Density for Averager:

Seconds/Point	Samples/Point
.015 > Ø.5	128
Ø.5 > 1.Ø	512
1.Ø > 2.Ø	1Ø24
2.Ø >	2Ø47

E. MODIFIER Routine (Resides in the Basic Package):

The routine is similar to "ODT-8" but is used only for making changes in core locations and uses only one page of core. LA 24ØØ, hit START, and the routine will give a carriage return-linefeed. To open a location, type the octal value then a space. The contents are then typed out followed by a colon. Insert the correction then type "C" to enter the correction. If no correction is desired, hit the SPACE bar or RETURN. To inspect the next location after closing one, type "N" and the location and contents are printed with a colon. To reopen the same; i.e., last, location used, type "S". RUBOUT will terminate any operation and restart the routine.

A jump into any part of core can be made by typing "R" for return, then the location and a SPACE. (Be sure to set any controlling SR bits used in that routine.)

Of the currently available routines for use with MADCAP IV, only a 1ØØØ-point signal averaging run and LORCAP destroy the MODIFIER. It can be reloaded after averager data acquisition, but is never available to LORCAP in its normal configuration.

As may often happen in certain experiments, a data set may contain a few obviously "bad" points. If allowed to remain, they will mar performance of the scaling, smoothing, and other routines. Roughly tagging their positions on the scope, they can be located and reset using the MODIFIER. Unless changed, the data array starts at location $4\emptyset\emptyset_8$.

F. Utility Routines for MADCAP IV:

1. SMOT29 and SMOT11:

Two data smoothing routines are available which can be loaded at start time with all but a 1ØØØ-point signal averaging run (load after the run) or LORCAP (already contains SMOT11). Both are modifications of M. W. King's LESQ29 and LESQ11 (DECUS No. 5/8-69). Only one or the other may be present at a time.

To execute smoothing type FILTER: (or F:) during scope display. Up to 5Ø seconds may be required for 1ØØØ points with SMOT29. When the operation is complete, the scope routines are entered. The data can be smoothed as many times as desired.

2. INTEG:

This is a numerical integration routine using the second order Simpson's Rule. It is executed by typing INTEGRATE: (or I:) during scope display. It requests a value for a PIVOT LINE with a value in a range of Ø-5ØØ. This value will be subtracted from each data point. In essence, the routine computes the running area around the pivot at each point then scales the data down to a range of 5ØØ. The factor used is printed out then the scope routines are entered. It can be executed as often as desired, each time supplying the appropriate PIVOT LINE. Like the smoothers, a 1ØØØ-point signal averaging run will destroy the integrator; but it, too, can be loaded after the run. It requires about 5 seconds for 1ØØØ points. LORCAP contains its own version of INTEG.

G. Program Control During Scope Display:

All routines of MADCAP exit to the scope display routines. During the display, the Teletype keyboard is active and will accept a variety of commands which initiate data treatment, output, and new input. Hence, once the Basic Package is started, it becomes independent of the switch register and is totally keyboard oriented. Certain of the analog data input overlays do, however, require use of the switch register.

The Basic Package allows the following commands. Each begins with a unique letter but allows any number of characters to be entered after that character until receipt of a colon which executes the command, if it is legal, or a RUBOUT which deletes the command. Illegal; i.e., undefined, commands and RUBOUT force a return to the scope display.

SCALE:	Scales the Y data to a range of Ø-5ØØ(10) and prints out the scaling parameters used.
OUTPUT:	Outputs the Y data onto the device to be specified by the user in answer to TTY I/O?. "N" assumes use of the high-speed punch. In either case, prepare the device (turn it on, run leader, etc.) before answering the question since output commences immediately upon receipt of "Y" or "N".
PLOT:	Plots the data using a solid line or as points depending upon the response to LINE PLOT?. "N" assumes a point plot is desired. Upon receipt of "Y" or "N", the plotter calibration routines are entered. In this submode, the keyboard is again used to direct control. The legal characters are X, Y, O, M, and G and are typed without colons, etc., simply as the single character. Before typing M or G, set the RC clock COARSE switch on

PLOT: (cont'd.)

first or second from slowest position. This controls pen speed. During drawing of lines, the COARSE switch can be changed, but do not move it during point plots or when drawing tic marks. The FINE control potentiometer can be changed anytime. Because of the Ø to -1Ø volt display signals, it is convenient to use the following calibration sequence. Type "X" (gives approximately Ø volts) and set the X zero pot of the recorder; type "O" and set the X variable range pot; repeat until satisfactory then calibrate the Y axis similarly.

X = Move pen to maximum X coordinate.

Y = Move pen to maximum Y coordinate.

O = Move pen to X-Y origin.

M = Mark off a frame to inscribe the plot and put quadrant tic marks on the X and Y axes.

G = Exit the calibration routine and commence plotting.

When the plot is complete, a message is printed requesting that the plotter be turned off (or put on standby). Do so immediately, since the scope display is restarted which will drive the pen wild in its effort to follow the scope analog signals. The keyboard is live during plotting, so unless premature termination is desired (shut plotter off then hit SPACE bar and a colon to do so), do not depress any of the keys. A simple way to arrest the scope display after the plot is to hit the SPACE bar as soon as it starts, shut plotter off, then type a colon.

REENTER: Allows reentry of digital data; i.e., it jumps to the routine to allow the user to enter a new set of data points from tape or Teletype. Note: This option is not available to the Averager.

ANALOG: Restarts an analog data input overlay, if present, and if not, the command is equivalent to REENTER.

The integrating and smoothing overlays, if present, can also be initiated. See Section F. If they are not present, the scope display is restarted.

FILTER: Filters or smooths the Y data using SMOT11 or SMOT29 (11- or 29-point parabolic least squares fitting).

INTEGRATE: Integrates the Y data after subtracting the user supplied value for PIVOT LINE, scales the integral to a range of 5ØØ(10), and prints the scale down multiplier.

In all cases, only the first character of a command is decoded; thus, the single letter followed by a colon will suffice. Exercise caution in doing so.

If, for some reason, the user must stop the program, depress the STOP console switch. The scope display can be restarted by SA=Ø2Ø1 or a program restart can be made by SA=Ø2ØØ.

H. LORCAP IV Package:

1. General Description:

As described in the abstract, LORCAP is a set of data processing routines as opposed to data acceptance. It was written to work with Lorentzian spectra as can be obtained from Mössbauer and NMR spectrometry and can be a useful model to simulate IR and UV data. The functional Lorentzian expression relating height, width, and arbitrary X-axis position is as follows:

$$Y_i = \sum_{j}^{N} H_j W_j^2/((X_i - P_j)^2 + W_j^2)$$

where Yi is the sum of intensities at point i over N peaks characterized by their independent H_j's, W_j's, and P_j's. The result for a single peak is an envelope similar to a Gaussian peak but having more extended "tails". The width, defined as the half-width at half-height, corresponds to a Gaussian sigma value, the height and position have identical correspondence, and the area is directly proportional to the height-width product.

LORCAP will handle up to 1ØØØ points total including X data, if needed. Thus, up to 5ØØ but an equal number of points for each type (raw and calculated) or 1ØØØ points of either type, all without X data, may be entered.

If X data is desired, it requires on array equal to the number of points and the spectrum calculator will use it if its presence was so declared in answer to HAVE X DATA?. If the answer was negative, an equally incremented X axis scaled to X RNG and X1 is used.

2. Usage of LORCAP:

The binary tape is in two parts. Load the second only if the operating instructions are desired. This section was included to aid those users who, like the author, usually forget, loan, or otherwise incapacitate the manual or book needed while on the system. The instructions are loaded into the data array and are destroyed when data is entered. Hence, they are typed out only when the program is first started. Similarly, but within the first section, a short dialog subroutine, which loads into the peak parameter array and allows several structural changes to be made, is used only at startup.

LORCAP uses SA Ø2ØØ, types a heading, then asks for the initial data block number. Two data blocks are assumed, Ø for raw data and 1 for calculated or LORCAP data. If raw data is to be entered first, type Ø, or type 1 if a spectrum is to be calculated first.

The program then desires some information which is used to change the structure of LORCAP slightly. The first choice allows the spectrum calculator to compute absorption dips (descending from a baseline) or peaks (growing up from baseline). Supply the desired answer to WANT ABSORPTION 'DIPS'?. The next option allows the assignment of equal widths to all peaks, hence, requiring the width be entered only for the first peak when the parameters are entered. Answer ALL WIDTHS EQUAL? as desired. If "N", a width must be entered for each peak. Both options are fixed until the program is reloaded. If the second part of the binary tape was loaded, a brief set of LORCAP's operating instructions will now be printed out.

After the initial dialogue, CALC'N INPUT? is asked. To enter raw data, answer "N". Raw data entry is identical to that described in Section II.A. If "Y", a set of variables and parameters are to be entered and used to calculate a spectrum. Give the NO. POINTS to be assigned to each array, answer HAVE X DATA? to describe the raw data or give "N" if none is to be entered, and type in the NO. PEAKS to be convoluted (up to 25). The X RNG,X1,INT.MPLR, and BASE are then requested. The X axis used in the calculation can be scaled to any desired units by appropriately setting the range (difference of right from left extreme) and first X value (left extreme) for X RNG and X1. If X data is present, use the same values given for X RANGE and XMIN. The INT.MPLR is an arbitrary multiplier of all heights and the baseline. This allows scaling the Y axis to suit. The product of INT.MPLR and the sum of the largest height and BASE must be less than 5ØØ to prevent scope display overlap. For example, to allow entry of heights scaled to a largest peak of 1ØØ with a base of 1Ø, enter a value of 4.555 (5ØØ/11Ø) for INT.MPLR to get a fully scaled display, assuming no intensity is acquired by overlap of peaks.

Finally, the table of heights, widths, and positions for all peaks is entered. If the user specified all widths to be equal, width is entered for only the first peak, and then HGT followed by POS for all subsequent peaks. When the parameters for a peak are complete, a carriage return-linefeed is issued, and when all input is complete, the message COOL IT. is typed. The program is now computing the spectrum and will require about Ø.Ø6 seconds per point per peak; e.g., five peaks and 1ØØØ points take about five minutes to compute. When complete, a carriage return-line feed is issued and scope display commences.

During scope display, LORCAP uses an expanded version of the Basic Package keyboard command decoder. Each command begins with a unique pair of characters as opposed to one and block Ø and 1 can be alternately displayed by typing "Ø" and "1". Illegal commands generate "?" and are ignored. As in the Basic Package, the command is not tested for validity until a colon is received and a RUBOUT will cancel it and return to the scope display.

The following four commands assume that raw data is in block Ø and calculated data is or will be in block 1. Therefore, the user should be displaying block 1 before entering one of these four commands (even though no real data may be in that array).

COMPUTE: Computes a spectrum from a new set of variables and parameters to be entered. This is logically equivalent to answering "Y" to CALC'N INPUT? on startup.

ALTER: Alters the parameters indexed by their PEAK & PARA #'S where the peak number is indexed in the order of initial entry (it is not a function of the parameters), and the para numbers are as follows, even if the equal widths modification is in effect; i.e., although entered as equal, the widths of all peaks are handled independently and can be reset to any desired value.

N, 1:	height of peak N;
N, 2:	width of peak N;
N, 3:	position of peak N.

Also

Ø, 1:	intensity multiplier;
Ø, 2:	baseline.

Current values for the parameters can be printed out thusly:

N, Ø:	prints parameters for peak N;
Ø, Ø:	prints out all parameters. Exit is made without computing the spectrum in either case.

When desired alterations are complete, type:

Ø,-1:	exit alteration mode and compute a spectrum from the current parameters.

SWAP: Swaps block Ø and block 1 data.

SUBTRACT: Gives point-by-point subtraction of block 1 data from block Ø and adds $25Ø_{10}$ to each resultant point. Double subtraction will restore the original array.

All of the following operations can be performed on whichever array is currently displayed. For brevity, CDA is defined as the currently displayed array. In all cases, including the above four commands, the program will use the latest value supplied for the block number; i.e., if it has been already set to the desired value previously, it need not be reinserted, except in the interest of safety.

STRIP: On entering the first time, a pair of bright spots are placed on the scope. Their positions are controlled by analog input potentiometers through multiplex channels 34-37 of the AXØ8. The top pair control the "left side" point's X and Y coordinates, resp., and the bottom pair similarly govern the "right side" point. Three options will be available: (1) replace the data with the best straight line from one point to the other; e.g., strip out a peak; (2) subtract a sloping baseline from all data points; and (3) subtract the straight line between the points from the data between points; i.e., partial baseline restoration.

For option one, carefully place the two test points to remove the desired section of the data. They will normally be somewhere on the data curve. The X positions need not be precise for option two. Simply place the test points with the proper slope and amplitude, usually lying just under the data curve. The points do not have to be located at the X axis extrema. Data processing using option three often involves performing option two first and then removing the residual non-linear baseline in short segments via option three. Position the points as would be done for option one, but usually, the points should not lie on the data but be somewhat below it. One, in fact, may often lie near the bottom of the screen as in the case of NMR data treatment, for example. After the points are positioned, the STRIP routines must be reentered, this time to select and execute one of the above options. To execute option one, answer "Y" to STRIP PEAK?. If "N", answer "Y" to FULL BASE? for option two and, if again "N", option three, partial baseline subtraction, is performed. All options require very little time and exit to the display.

If, upon entering STRIP the second time, the message BAD X POINTS! is issued, the user has inverted the left-right X axis relationship of the test points. The routine immediately cancels the stripping operations and exits to the display. The user must then reenter STRIP and reset the points before proceeding.

SCALE:	Scales the CDA to a range of Ø-5ØØ and prints the factors used.
SMOOTH:	Smooths the CDA using a slightly modified SMOT11. SMOT29 is not available.
INTEGRATE:	Integrates the CDA after subtracting the value of PIVOT LINE from each point. The assumed Y axis range is 5ØØ, independent of the intensity multiplier used to compute LORCAP data. The integral is scaled to a range of 5ØØ and the scale down multiplier is printed. A modified INTEG is used.
OUTPUT:	Prints and/or punches the CDA data on the device to be specified in answer to TTY I/O?. See Section II.G under OUTPUT.
PLOT:	Enters the plotter calibration routine. See Section II.G under PLOT.
DIGITAL:	Enters the digital data input routine to allow entry of new data points. See Section II.A.
RESTART:	Restarts the program. This is equivalent to SA=Ø2ØØ.

3. Hints on the Use of LORCAP:

   a. A left to right decreasing X axis can be implemented by specifying a negative X RNG and setting X1 to the left side value, as usual. This is useful in handling NMR data.

   b. An overlapped Y axis may result after using STRIP. The normal perspective can be regained by calling SCALE.

   c. After startup, the program configuration giving peaks or dips and allowing input of equal widths can be changed thusly:

      Change C(BSCHNG) to 7Ø41 for dips
      or to 7ØØØ for peaks

      Change C(WIDSWT) to Ø for equal width input
      or to 1 for normal operation

      Restart the program at SA=Ø2Ø1.

   d. When manipulation of the calculated array results in its destruction, type 1, call ALTER, and enter Ø,-1 for peak and parameter numbers to recompute the spectrum. This results from the fact that the parameters used to compute a spectrum are unaffected by all operations except ALTER and COMPUTE.

   e. If user was viewing block Ø instead of 1, these commands result in the listed symptoms:

      SWAP: Will have no effect whatsoever.
      SUBTRACT: A straight line appears in the center of the screen.
      ALTER and COMPUTE: If a spectrum is calculated, it will go into block Ø.

      Although much mention has been made of the relationship of block Ø and 1, they are, in fact, independent of all operations except SWAP and

SUBTRACT. Hence, data tapes can be read, and computed spectra can be placed into either or both arrays. This finds use if it is desired to subtract a standard or calibration data tape from another data tape, assuming the X axes are identical.

f. The choice for PIVOT LINE for the integrator must be fairly accurate, but in the event that it was not, the integral can be "corrected" by using STRIP to remove a wedge then rescaling, if necessary.

g. To use LORCAP immediately after any one of the available MADCAP acquisition routines was executed, it is not necessary to have the data punched out. It will remain untouched in core so long as the LORCAP instruction patch is not loaded.

Load only the first section of LORCAP, use SA=Ø2ØØ, answer "N" to CALC'N INPUT? and supply NO. POINTS and answer HAVE X DATA? Now, press STOP switch on console, LA Ø2Ø1 and hit START. The data will be displayed on the scope and other operations can now proceed as usual.

The author is fully cognizant of the fact that peak stripping, extensive smoothing, etc., can be used to manufacture data of <u>any</u> desired shape and form; thus a note to thesis advisors: Bear a watchful eye on graduate students using the program. And, a note to those graduate students: Think! Will the results be challenged? Mr. John Steichen of Rice University who prompted and aided in many of the ideas used herein is acknowledged for allowing use of these comments.

4. Usage of Gaussian Curve Overlay:

After loading first (and second, if desired) section of LORCAP, load the GASCAP overlay. The functional equation used is changed to

$$Yi = \sum_{j}^{N} Hj * E x P (-(X-Pj)**2/(2*Wj**2))$$

with the parameters as described in Section H.1. The overlay changes the envelop calculator routine and adds the necessary exponentiation routine. Because of the latter, the data arrays are cut from 5ØØ points to 464 points; i.e., the total data array is 928 points, instead of 1ØØØ, allowing 464 points each for raw data and calculated data or 928 points of either type - all without X data. All other operations, starting addresses, etc., remain the same as described in Section H.1.

III. CONSTRUCTION OF ROUTINES FOR USE WITH MADCAP IV:

A. General Structure of MADCAP:

All currently available routines for MADCAP IV operate in real time; i.e., program interrupt is not used. This allows coding of new routines to be done in a straightforward manner without the need to identify and resolve concurrent peripheral I/O. Admittedly simple minded and inefficient this approach is satisfactory since there is little else of a useful nature that could be done simultaneously with the few operations that are performed.

Operating in real time and without recourse to an accurately and reproducibly calibrated clock, the averaging routines use memory cycle time to determine real time intervals. Hence, for a given machine, reproducibility is excellent, but absolute time will vary from one machine to another.

However, if the user desires, analog input routines can be written using program interrupt if he constructs the necessary interrupt handler and flow controller. It must be borne in mind that all I/O thru MADCAP and its overlays normally wait for ready or completion flags.

The program is centered around the AXØ8 LAB PERIPHERAL which can perform an ADC (analog-to-digital conversion) from a prespecified multiplexor channel in about 17 microseconds giving a two's complement, nine-bit signed integer result. Nine-bit DAC (digital-to-analog conversion) is performed for the scope and plotter driving signals. Hence, for both ADC and DAC, the numerical range is 512_{10}. This fact was highly instrumental in the formation of the algorithms for data acquisition, storage, and display.

Data storage after all types of input should consist of single-precision integers in a range of $Ø-5ØØ_{10}$. These are the numbers used for X - Y displays and printout and will be characterized within the program by two parameters, "PTSWT" in location 66 and "NPTS", the number of points, in location 67.

For Y-only data input (limited to 1ØØØ points), PTSWT=1, for digital input wherein the user is supplying X data, PTSWT=Ø and the maximum number of data points is 5ØØ. The X array is scaled and stored as Ø-5ØØ integers following the Y array.

The acquisition and storage of Y data by the analog input overlays differ from each other as follows. The

CURVE FOLLOWER routine makes an ADC for each point to which is added 256_{10}, making all results positive. That value between Ø-512 is then stored as single precision. The MASS SPEC routine will take 2Ø48 ADC samples adding 256 to each and store the intermediate sum as a double-precision integer. After the sum is complete, the result is divided to a Ø-512 integer for storage.

The SIGNAL AVERAGER routine, similarly, takes a number of samples (see Table 2) for each data point during each scan, adding 256 to each sample, and the samples are then summed as a double-precision integer. After sampling is complete for that point, the intermediate sum is divided to a range of Ø-512 and added to the current scan sum for that point using a pseudo-18 bit storage scheme; i.e., the scan sum uses sesqui-precision storage requiring only 50 per cent more registers than there are data points in the scan.

When the input is terminated, the "18-bit" integers are divided by the number of scans taken to give a result between Ø-512 for storage.

Note that for analog input which covered the full range of the converter, the data must be scaled down from

Ø-512 to Ø-5ØØ to prevent wrap-around during scope display and plotting. For axes marking, 12 display units are reserved on each axis to prevent overdrawing the axes onto data.

B. Some Subroutines Available in MADCAP:

The more useful and commonly used suboutines are addressed indirectly through page zero (locations 2Ø-37). A description of each follows:

(AC=accumulator; FAC=floating point AC in locations 44-46)

FLOATR (JMS I FLOTER):

Converts contents of AC to a floating point number in FAC. Previous contents of FAC are lost.

FIXR (JMS I FIXER):

Converts FAC to an integer leaving result in AC and location 45. Values $>$ 2047 or $<$ -2047 are then truncated to those limits.

READER (JMS I READXY):

Accepts numeric input (ignoring all but carriage returns). It can be implemented in or outside the interpreter. In either case, the floating point result is in the FAC. If outside, execute JMS I READXY and if inside, execute READ.

STALL (JMS I HOLD):

Is a variable time delay subroutine using the RC clock of AXØ8. The variable SET, if Ø, runs clock for 32 pulses, and if non-zero for 8 pulses; i.e., four times faster.

ASRRED (JMS I TELRED):

Accepts and prints an 8-bit ASCII character on the Teletype, leaving the character in the AC.

INITIZ (JMS I INIT):

Is called to initialize array pointers and counters for data storage. Three anto-index registers are set:

YIND=YONE (a page zero constant),

XIND=YONE+NPTS (# of points),

ZIND=YONE;

It clears the X display coordinate sum, TXSM; and sets a counter,

CNTR=-NPTS.

ZIND is used for restorage when a value is extracted by YIND and is to be replaced after some modification.

RETLF (JMS I CRTLFD):

Issues a carriage-return and line feed.

ASKER (JMS I QUERY):

Allows input of "Y" or "N" in answer to a question. All other characters generate "?" and ASKER will await proper response. Upon receipt of "Y", it exits leaving AC=0. For "N", AC=1. The calling program can then branch according to the response. ASRRED is used for ASCII I/O.

UPPEN and DNPEN (JMS I PENUP or PENDN):

Use enable register and external register of AXØ8 to, respectively, set SØ and clear it to operate a relay which controls plotter pen attitude. Each subroutine calls STALL before and after the operation.

HEDER1 and HEDER2 (JMS I HEADR1 or HEADR2):

Output stripped ASCII as generated by MACRO-8 Assembler. All headings and titles are handled using these. There is only one special character, the up-arrow (336_8), which is used to generate a carriage return-line feed in the middle of a text string. Each separate message begins with a carriage return-line feed.

HEDER1 takes the content of PC+1 in core as the starting address of the message thus allowing the message to be stored anywhere in core. If multiple and always consecutive headings are to be printed, the first message is printed using JMS I HEADR1 followed by address and consecutive messages thru JMS I HEADR2 without need for message address. For example,

```
.
JMS I HEADR1
HDI
.
.
JMS I HEADR2
.
.
.
HDI, TEXT / THIS IS FIRST.↑/
    TEXT/↑ THEN THIS.↑↑/
```

When assembled by MACRO-8 and executed will produce

```
(CL)
THIS IS FIRST. (CL)
(CL)
(CL)
THEN THIS. (CL)
(CL)
```

("CL"=Carriage return-line feed)

After a call thru HEADR1 to initialize the message address, text can be printed while in interpreter mode by executing HEDIT; e.g.,

```
.
JMS I HEADR1
HDI
.
.
JMS I 7
.
HEDIT
.
FEXT
```

If the messages are not always printed consecutively, each must be output by JMS I HEADR1 followed by address.

ADCONV (JMS I ADCON):

Is a general-purpose subroutine to perform an ADC on the channel specified in the AC on entry. The result is left in the AC.

RESET (JMS I DISMOV):

Resets DAC levels for the scope display to contents of XDIS and YDIS which have been set up elsewhere.

PLTINC (JMS I PLTMOV):

Sets up scope or plotter display depending on C(AC). If C(AC)=-1 use RESET for scope display; if zero, call an incrementer routine to move along the best straight line between current position and XDIS, YDIS; and if +1, use RESET but keep pen up for a while to allow stabilization at new position, then lower the pen.

ASKIO (JMS I IOASK):

Requests if user wants TTY I/O. The answer sets IOSWT to Ø for Y and to +1 for N. IOSWT is checked by both the input and output ASCII routines to choose the device before transferring each character. A value of Ø uses Teletype and +1 uses high-speed reader/punch.

Also available are several operations executable while within the floating point package interpreter:

HEDIT: (See above)

READ: Input a floating point number ignoring non-numeric characters (decimal point optional, E format acceptable). It is logically equivalent to JMS I READXY.

OUTPUT: Print F. P. number under control of C (62). If C(62)=Ø, use exponential format and if non-zero, print integer of that many digits.

NEGATE: Will negate C(FAC).

SQUARE and SQROOT are available, as usual.

FLOT: Is used as a memory reference instruction to float contents of a single-precision operand into the FAC. It supplants FNOR as a MRI and FNOR is reduced to the status of NEGATE, SQUARE, etc., which do not have operands and work only on the current C(FAC).

With the exception of FLOT but including FNOR, these interpretor instructions can only be called to a depth of one. Hence, a new user function to be called thru the interpreter cannot use them but must call those operations thru indirect subroutine calls while outside interpreter mode. These addresses are as follows:

```
HEDIT:   JMS I HEADR2

OUTPUT:  JMS I 6

READ:    JMS I READXY

NEGATE:  JMS (6ØØØ)

SQUARE:  JMS (6163)

SQROOT:  JMS (6656)

FNOR:    JMS (66ØØ)
```

With the exception of ASRRED and KBDNTR routines (in Basic Package), SERVIS (in LORCAP) and MULT (in Signal Averager), all ASCII I/O is handled using routines common to the Modified Fl. Pt. Pkg. #2; specifically, output is implemented with JMS (7344) and input thru READER using JMS (74ØØ). These can be reached thru page zero by JMS I OUT and JMS I READXY or READ as described above. Note: After a SR start sequence, a TLS is not necessary.

C. General Layout for New Routines:

The following logical considerations should be met for the writing of new analog input routines. See enclosed core map for available space.

1. Assemble starting address of routine into location NOTDIG and into ADRTAB+5,

2. Print headings and read in any necessary run parameters,
3. Set NPTS and PTSWT to characterize data; e.g., use subroutine DATYP, and any other needed variables,
4. Initialize array storage (JMS I INIT),
5. Perform data acceptance, perhaps using JMS I ADCON,
6. When complete, reduce data such that all Y values are = or <500, and
7. Execute JMP I REETRN to go to display routines.

   For more detailed, yet simple, examples, the reader should check the listings for the mass spec and line follower routines.

The basic layout of data treatment routines is similar.

1. Set up entry logic, one of two ways.
   a. Put starting address of routine in location SPOVR1 or SPOVR2 and use SR SA=Ø2Ø2 or Ø2Ø3, resp.
   b. or use keyboard command by putting desired first letter code character and starting address in the tables CHRTAB+X and ADRTAB+X, resp., where X is 6, or greater if SMOT 11 or 29 and INTEG are desired (see below).

In either case, the routine is entered by an indirect jump.

2. Initialize arrays, print headings, get input, etc.

3. Perform manipulations.

4. JMP I REETRN is commonly the last instruction.

See listing of SMOT29 or INTEG for more detail on applications. SMOT11 or 29 use the character "F" in location CHRTAB+6 and has its address in ADRTAB+6. INTEG uses the character "I" in CHRTAB+7 with the address in ADRTAB+7. New routines cannot use the characters Z, S, R, P, O, A, F, or I as the first letter and the address must be in a corresponding location in ADRTAB. Z is used as a dummy character to fill out the table. Table size allows up to five routines to be added to the Basic Package in this manner.

APPENDIX 1:

INSTRUCTIONS FOR ASSEMBLING MADCAP IV:

CORE PACKAGE:

This consists of those locations as shown on the accompanying core map. The source tapes do not include any overlays or the floating point package.

The MACRO-8 ASSEMBLER is needed to handle the stripping of the ASCII text. After loading the assembler, the NEW ASSEMBLER SYMBOL TABLE is loaded to include AXØ8 microinstructions and delete un-needed pneumonics. The source tapes are then loaded for PASS I. Only the source tapes are re-entered for PASS II (and III, if desired) -6 hours are needed to print out PASS III for the entire set of MADCAP and overlays onto a Teletype.

Refer to the MACRO-8 PROGRAMMING MANUAL, DEC-Ø8-CMAA-D, for complete instructions in the use of the assembler.

The high-speed assembler uses the high-speed reader for all input and can be modified to use the ASR-33 for all output, including the binary tape, by making these changes:

Change C(6Ø3) to 6Ø46

Change C(6Ø3) to 6Ø41

Change C(3Ø26) to 6Ø44

Change C(3Ø27) to 6Ø41

OVERLAYS:

These are all assembled separately from the CORE PACKAGE by means of the USER SYMBOL TABLE, which defines the symbols used in the CORE PACKAGE such that overlays can be written using the same pnuemonics.

As above, the MACRO-8 ASSEMBLER is loaded as is the NEW ASSEMBLER SYMBOL TABLE. Then the USER SYMBOL TABLE is loaded (It should be considered part of the source program.), followed by the ASCII source tape(s). The pass is terminated with a short tape containing a dollar sign.

The MADCAP IV BASIC PACKAGE can be made by loading the MODIFIED FL. PT. PKG. #2 then the CORE PACKAGE and, using ODT-8 (DEC-Ø8-COCO-D-LOW VERSION), punching them out with a single checksum.

The user can also load the various overlays he desires after the CORE PACKAGE and include them in the final package. The LORCAP PACKAGE can be made in this manner.

APPENDIX 2:

MODIFYING MADCAP FOR USE WITH OTHER ANALOG I/O DEVICES:

In any case, data or display variables must not fall outside the range of + and -1023_{10}. Otherwise, the integer arithmetic ingrained in the entire structure of MADCAP will give strange results.

The most likely modification desired, obviously, is to live without the AX08 Lab Peripheral. This can be done by changing the various routines as described below. One common difficulty will be handling ADC's and DAC's with more than 9 bits. Four registers on page zero govern display size. These are: XLIM, the left extreme; YLIM, the bottom limit; XRNG, which is X axis data range; and YRNG, the Y axis range. For the AX08 they were set to 6, -250, 500, and 500, resp., when assembled. The axes marking routine, MARKER, used quadrant fractions of the ranges and requires the 6-unit buffer at both ends of each axis to draw the enclosing frame. The first page of the Core Package listing describes the assembly variables. The Core Package can be reassembled with the desired values; e.g., double the values to implement 10-bit DAC.

If the DAC is 1Ø bits and the above alterations are made, no change should be necessary to use a 1Ø-bit ADC. The Signal Averager is limited to 25Ø scans, however.

In the display routine, a register, GTX+3, can be loaded with CLL RAR, for example, to implement a system with a 1Ø-bit ADC but 9-bit DAC.

Although effort was made to code MADCAP to allow these modifications, the author cannot guarantee complete success since it was not possible to test them. He is willing, however, to confer with interested parties having difficulty implementing such changes.

Here is a breakdown of possibly necessary changes:

A. Basic Package:

All analog I/O is handled by five subroutines starting from location 43Ø7. These are RESET, DNPEN, UPPEN, STALL, and ADCONV (not used by the Basic Package itself) and are described in Section III. It is fairly simple to overlay the necessary IOT's for all except perhaps those implementing the enable and external registers and the RC Clock of the AXØ8. STALL can be emulated with a nested pair of ISZ loops or if an analog input is available; i.e., a potentiometer delivering + to -1 volt or so into an ADC, it can be used to get variable delay times. The delay period should be in the range of Ø.1 to 2 seconds.

Although quite awkward, UPPEN and DNPEN can be written to wait for a Teletype flag to allow manual lifting and lowering of the pen.

B. LORCAP:

Use is made of all the analog I/O routines and four analog inputs going into consecutive multiplexor channels. The first channel is written in as 34_8 but this can be reset by changing C(PL34) to the desired channel.

C. Curve Follower Input:

It uses only those routines in the Basic Package.

D. Mass Spec Input:

The external register is used to sense a Schmitt trigger. This can be implemented by monitoring an ADC channel for any desired preset level as detected by the software. Change locations LOOP3, LOOP3+1, and PTLOOP + 7 to 11.

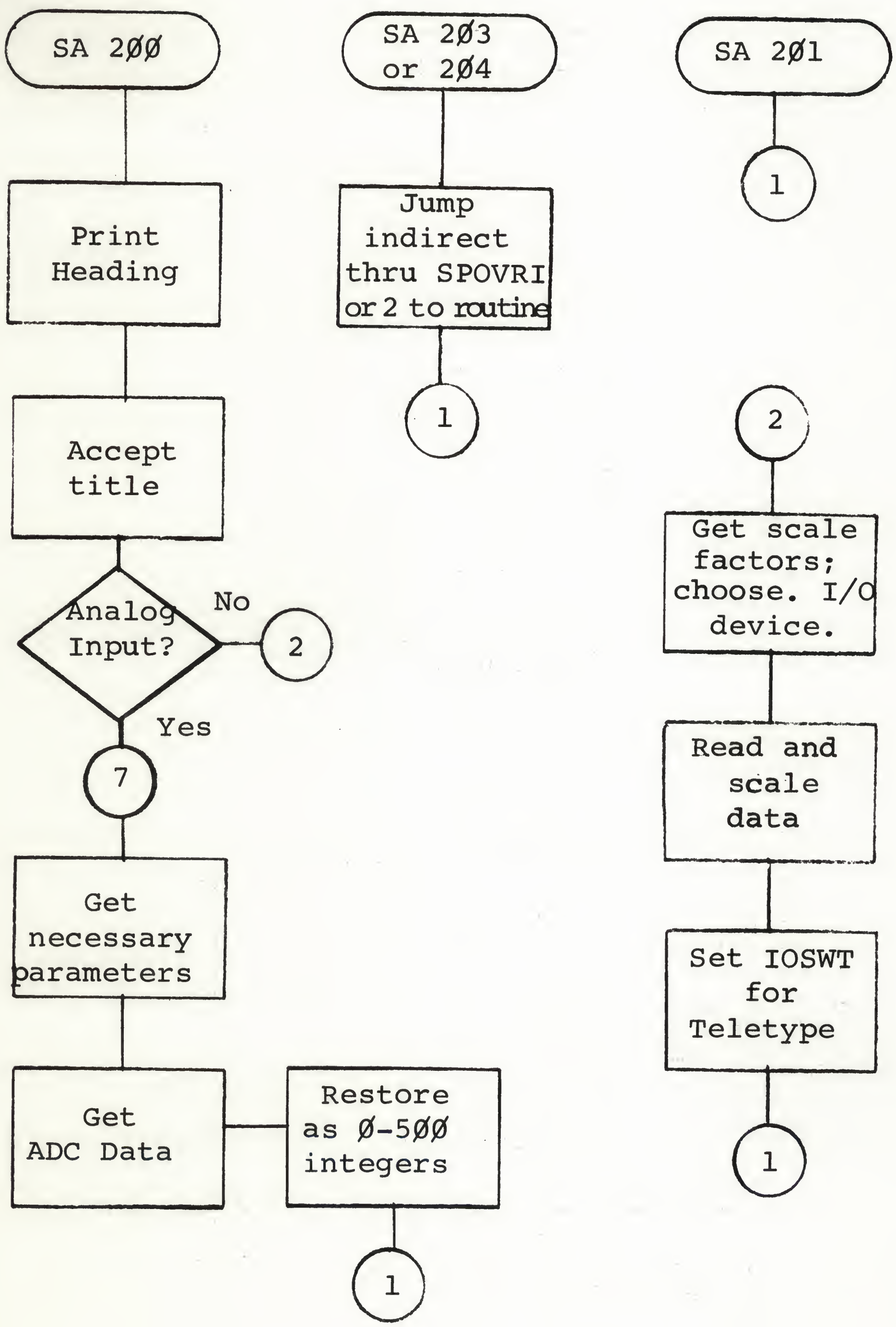
E. Signal Averager:

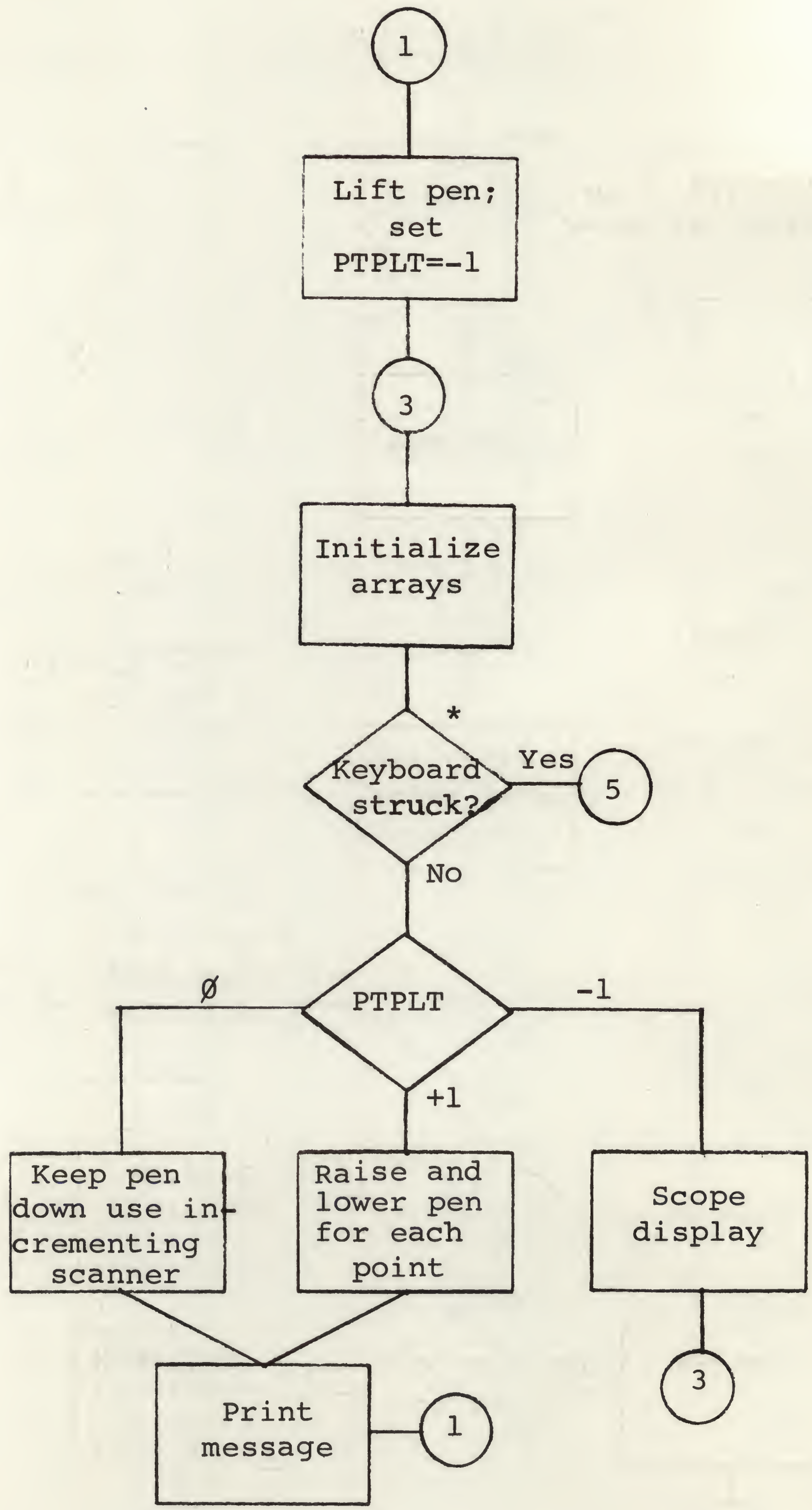
All special analog I/O is performed in subroutine AVGMR. What is needed here is a starting trigger mechanism, another programmed but accurate delay loop, and, if desired, a means for the computer to signal the end of a scan. The changes here are reasonably easy to make with a variety of hardware approaches.

APPENDIX 3:

Functional Flow Chart

for Basic Package:

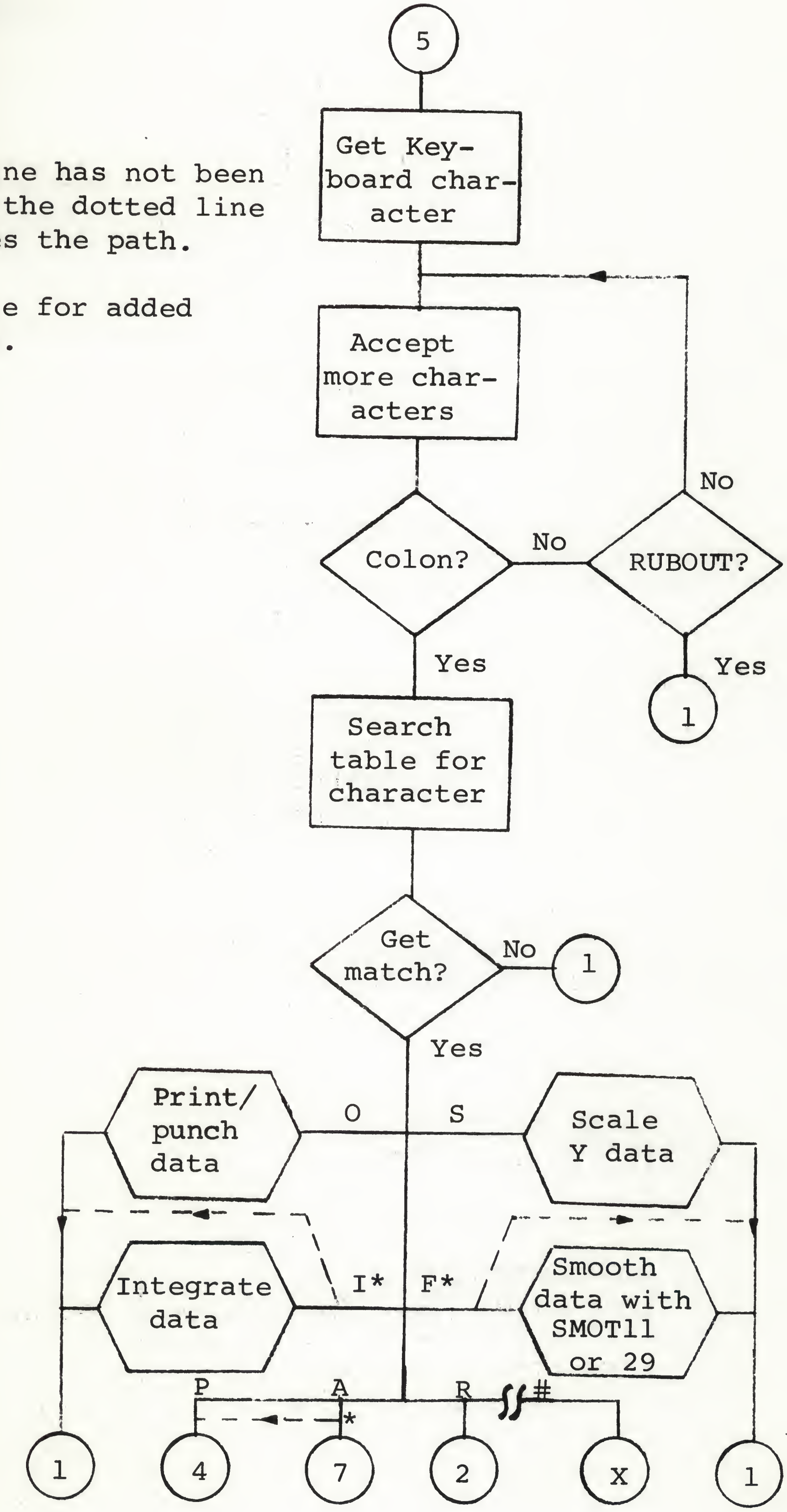


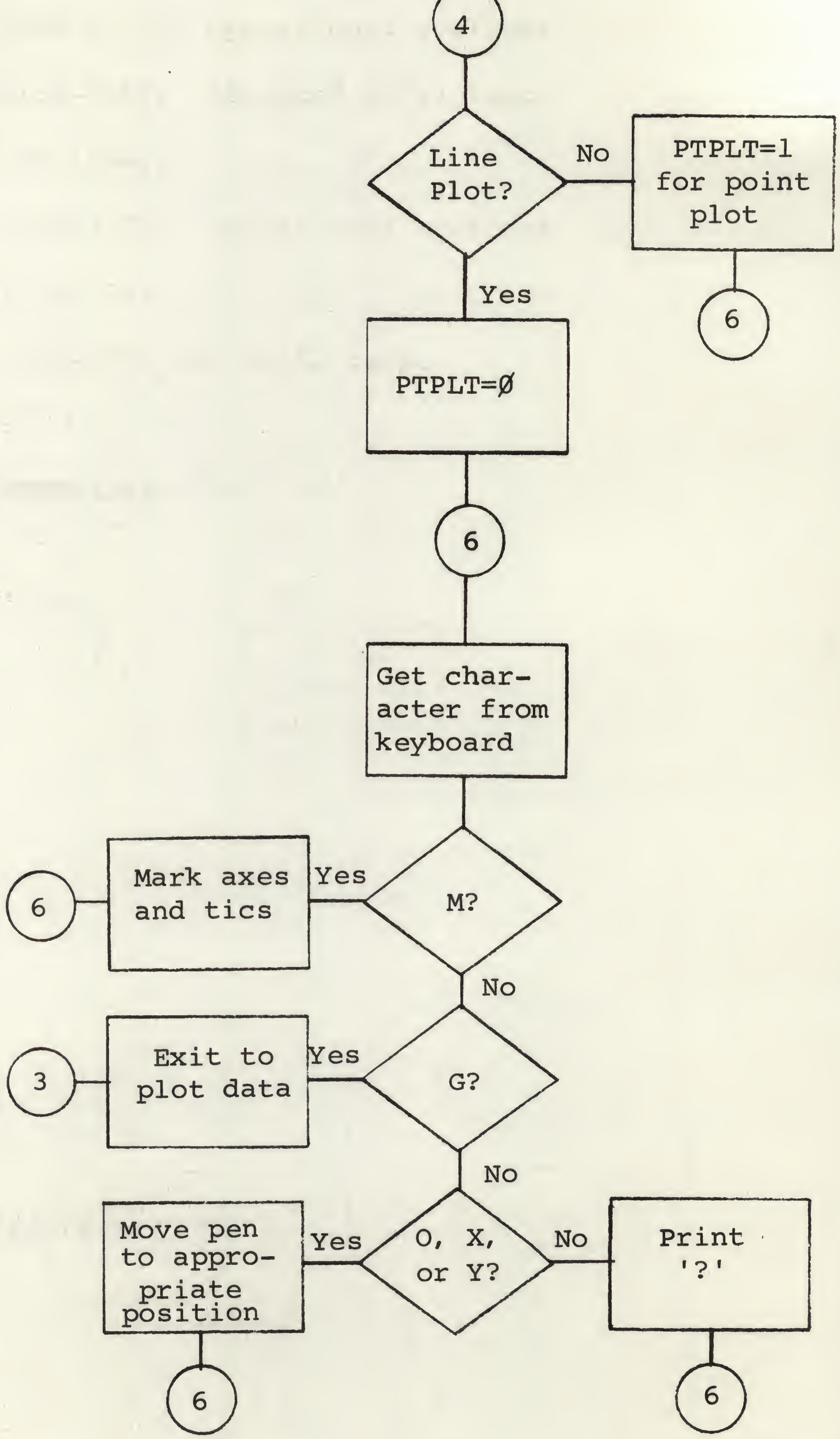


*Keyboard flag is checked before each point.

*If routine has not been loaded, the dotted line indicates the path.

#Available for added routines.




4
Line Plot?
No
PTPLT=1 for point plot
6
Yes
PTPLT=Ø
6
Get character from keyboard
M?
Yes
Mark axes and tics
6
No
G?
Yes
Exit to plot data
3
No
O, X, or Y?
Yes
Move pen to appropriate position
6
No
Print '?'
6

APPENDIX 4:

CORE MAP FOR MADCAP ROUTINES:

(All locations are in octal.)

Basic Package:

2-144 :	FPP registers, subroutine references, etc.
2ØØ-377 :	Main calling routine and display
24ØØ-2577:	MODIFIER routine
4ØØØ-5377:	Operational routines
54ØØ-7577:	Modified FPP

The following assume all registers of the Basic Package:

LORCAP Package:

145-177 :	Subroutine reference, constants, etc.
4ØØ-235Ø:	Reserved for data
235Ø-2462:	Reserved for peak parameters, contains initial dialog routine on startup
2463-3777:	Operational routines

Note that the MODIFIER is lost.

Averager:

145-177 :	Subroutine references, constants, etc.
34ØØ-3777:	Operational routines

Also, the code used by the Basic Package for digital input and Y axis tic marks is overlayed. MODIFIER is destroyed by a 1ØØØ-point run.

Mass Spec:

3600-3777: Operational routines

4160-4167: Stripped ASCII text

Curve Follower:

3600-3777: Operational routines

SMOT11 and 29:

3200-3322 and 3355, resp.

INTEG:

3000-3144

APPENDIX 5:

Samples of Program Output:

(Text in parentheses is added comments; underlined text is user input)

(Basic Package, SMOT11, and INTEG were loaded with BIN Loader. Then used SA=Ø2ØØ.)

MADCAP IV!	
TITLE: EXAMPLE OF USE OF BASIC PACKAGE	(Terminated with ALT MODE)
ANALOG INPUT?N	(Want data tape input)
NO. POINTS= 1ØØ HAVE X DATA?N PTS. TO SKIP = Ø	
RANGE & MIN Y:+ 5ØØ - Ø	(Spaces between + or - sign and number are ignored)
DATA:	
TTY I/O?N	(Use high speed reader) (Scope display began after input)
S:	(Scale the data)
MIN= 46 MAX= 335 MPY= 1.73Ø	
P:	(Plot the data)
CALIBRATE: LINE PLOT?Y	(Connect points with best straight line)
YXO ?	('?' from illegal characters - spaces)
_?_?_?OM	('M' to draw axes and tic marks)
G	('G' begins plot)

APPENDIX 5: continued

TURN PLTR OFF!	(Plot is complete; scope display restarts)
O:	(Output the data)
TTY I/O?N	(Use high speed punch)
R:	(Re-enter data from tape)
NO. POINTS = 1ØØ	
HAVE X DATA?N	
PTS. TO SKIP = Ø	
DATA:	
TTY I/O?N	(Use high speed reader)
F:	(Filter the data)
I:	(Integrate it)
PIVOT LINE (Ø-5ØØ)=1Ø	
MPY=Ø.233296E-Ø1	(Scale down multiplier)
P:	(Plot data)
CALIBRATE:	
LINE PLOT?N	(Make point plot)
G	
TURN PLTR OFF!	

APPENDIX 5: continued

(Loaded LORCAP IV, first section, then used SA=Ø2ØØ)

```
LORCAP IV!

TITLE:  SAMPLE OF LORCAP IV

INITIAL DATA BLOCK NO. = Ø               (Enter data in BLOCK Ø)
WANT ABSORPTION 'DIPS'?N                 (Use 'peak' spectra)
ALL WIDTHS EQUAL?Y

CALC'N INPUT?N                           (Input the data)

NO. POINTS= 1ØØ
HAVE X DATA?N
PTS. TO SKIP = Ø

RANGE & MIN
Y:5ØØ Ø

DATA:

TTY I/O?N                                (Use high speed reader)

SCALE:                                   (Scale the block Ø data)

MIN=   46
MAX=  335
MPY= 1.73Ø
OUTPUT:                                  (Output block Ø data)
TTY I/O?Y                                (Use Teletype)

     2     2     3     5     5     7     7     9    1Ø    12
    14    14    16    17    21    22    24    28    29    33
    36    4Ø    45    48    54    59    64    71    78    87
    95   1Ø6   116   13Ø   144   159   178   197   22Ø   246
   279   31Ø   343   375   41Ø   441   467   488   498   5ØØ
   49Ø   472   446   415   382   349   317   285   256   23Ø
   2Ø2   182   163   147   131   119   1Ø7    97    88    8Ø
    73    66    61    55    5Ø    45    42    38    35    31
    28    26    22    21    19    17    16    14    12    1Ø
     9     9     7     5     5     3     3     2     2     Ø
```

APPENDIX 5: continued

STRIP:	(Put test points on scope)
ST:	(After positioning them, re-enter STRIP)
STRIP PEAK?N	
FULL BASE?Y	(Restored sloping baseline)
SCP?	(Hit a RUBOUT)
SCALE:	(Scale Block Ø data)
MIN= 229	
MAX= 38Ø	
MPY= Ø.821	
ST:	
STRIP:	(Enter STRIP again)
STRIP PEAK?N	
FULL BASE?N	(Remove portion of baseline)
SCALE:	(Scale data)
MIN= Ø	
MAX= 5ØØ	
MPY= 1.ØØØ	
FILTER:?	(Illegal command)
SMOOTH:	(Smooth data)
SM:	(Smooth data again)
ST:	(Enter STRIP)
ST:	
STRIP PEAK?N	
FULL BASE?N	(Remove more baseline)
SMOO:	(Smooth again)

(NOTE: All of the above was performed on BLOCK Ø.)

Ø1CO:	(Typed 1 and entered COMPUTE)
NEW CALCULATION:	
NO. POINTS=1ØØ	(Must be same as Block Ø)
HAVE X DATA?N	
NO. PEAKS=2	

APPENDIX 5: continued

X RNG, X1, INT.MPLR, BASE:	
1Ø 1Ø 5 1Ø	
HGT,H-WIDTH,POS:	
8Ø 1 15	
70 17	(No width needed, '1' is assumed)
COOL IT.	
Ø1Ø1Ø11SC:	(Alternately displayed arrays then SCALED Block 1)
MIN= 65	
MAX= 449	
MPY= 1.3Ø2	
Ø1Ø11SUBTRAAAAAACT:	(Typed 1 then, effectively, SU: for SUBTRACT:)
SU:	(SUBTRACT again to restore array)
ALTER:	(ALTER para's)
PEAK & PARA #'S:Ø 2	(Alter base)
TO:15	
PEAK & PARA #'S:1 1	(Alter height of peak 1)
TO:85	
PEAK & PARA #'S:Ø -1	(Exit ALTER)
COOL IT.	(Computing Spectrum)
AL:	(Enter ALTER again)
PEAK & PARA #'S:Ø Ø	(Get para listing)

```
X RNG, X1, INT.MPLR, BASE:
 Ø.1ØØØØØE+Ø2 Ø.1ØØØØØE+Ø2  Ø.5ØØØØØE+Ø1 Ø.15ØØØØE+02
HGT,H-WIDTH,POS:
 Ø.85ØØØØE+Ø2 Ø.1ØØØØØE=Ø2 Ø.15ØØØØE+Ø2
 Ø.7ØØØØØE+Ø2 Ø.1ØØØØØE+Ø1 Ø.17ØØØØE+Ø2
```

AL:	(Enter again)
PEAK & PARA #'S:1 Ø	(List only first peak Paras)
Ø.85ØØØØE+Ø2 Ø.1ØØØØØE+Ø1 Ø.15ØØØØØE+Ø2	
AL:	(Enter again)
PEAK & PARA #'S:1 2	(Width of peak 1)
TO: 1.5	
PEAK & PARA #'S:1 3	(Position of peak 1)
TO:16	
PEAK & PARA #'S:2 1	(Height of peak 2)

APPENDIX 5: continued

TO:75	
PEAK & PARA #'S:1 4	(PARA 4 is illegal)
PEAK & PARA #'S:- 1	(PEAK-1 is illegal)
PEAK & PARA #'S:25 -1	(PEAK 25 is ignored; PARA -1 for exit)
COOL IT.	
ST:	(Enter STRIP)
ST:	
STRIP PEAK?N	
FULL BASE?Y	(Remove sloping baseline)
Ø1SM?	(Smooth Block 1)
SC:	(Scale it)
MIN= 13	
MAX= 468	
MPY= 1.Ø99	
IN:	(Integrate Block 1)
PIVOT LINE (Ø-5ØØ)=Ø	
MPY= Ø.12578ØE-Ø1	
1Ø1AL:	(Enter ALTER)
PEAK & PARA #'S:Ø -1	(Recompute spectrum)
COOL IT:	
SU:	(Get residuals)
SC:	(Scale them)
MIN= - 42	
MAX= 343	
MPY= 1.299	
IN:	(Integrate residuals)
PIVOT LINE (Ø-5ØØ)=25Ø	
MPY= Ø.49Ø629E-Ø1	
RESTART:	(Restart program)
LORCAP IV!	
TITLE:	(Hit ALTMODE)
CALC'N INPUT?N	
NO. POINTS= 1ØØ	
HAVE X DATA?N	
PTS. TO SKIP = 1Ø	(Skip first 10 points on tape)

APPENDIX 5: continued

1SWAP:	
P:?	(Invalid command)
ØPL:	(Plot Block Ø)
CALIBRATE:	
LINE PLOT?Y	
OXOXOXOXOXOYOYOYOYOYOYOYOM	(Calibrate plotter, draw axes and tics)
G	
TURN PLTR OFF!	
Ø1PL:	(Plot Block 1)
CALIBRATE:	
LINE PLOT?N	
G	
TURN PLTR OFF!	

WELL, THAT IS ALL THERE IS TO IT!!!:?

(This was typed during scope display and '?' means it was an invalid command, obviously.)

APPENDIX 5: continued

(Loaded first section of LORCAP, then Gaussion overlay.
Used SA=Ø2ØØ)

GASCAP IV!

TITLE: SAMPLE OF USE OF GAUSSIAN OVERLAY

CALC'N INPUT?N

NO. POINTS = 1ØØ
HAVE X DATA?N
PTS. TO SKIP = 1Ø! Ø (Wanted Ø, not 1Ø; hit RUBOUT)

RANGE & MIN
Y:5ØØ Ø

DATA:

TTY I/o?N

CO:

NEW CALCULATION:

NO. POINTS = 1ØØ
HAVE X DATA?N
NO. PEAKS = 1
X RNG, XI, INT.MPLR, BASE:
1ØØ Ø 5 Ø
HGT,H-WIDTH,POS:
9Ø 6 5Ø! 55 (Wanted 55, not 5Ø; hit RUBOUT)

COOL IT. (Computing spectrum)
Ø11ØØØDI: (Get new data into Block Ø)

NO. POINTS = 1ØØ
HAVE X DATA?N
PTS. TO SKIP = Ø

APPENDIX 5: continued

RANGE & MIN
Y:500 0

DATA:

TTY I/O?N

(All operations same as LORCAP)

APPENDIX 5: continued

AVERAGER!

TITLE: SAMPLE OF SIGNAL AVERAGER

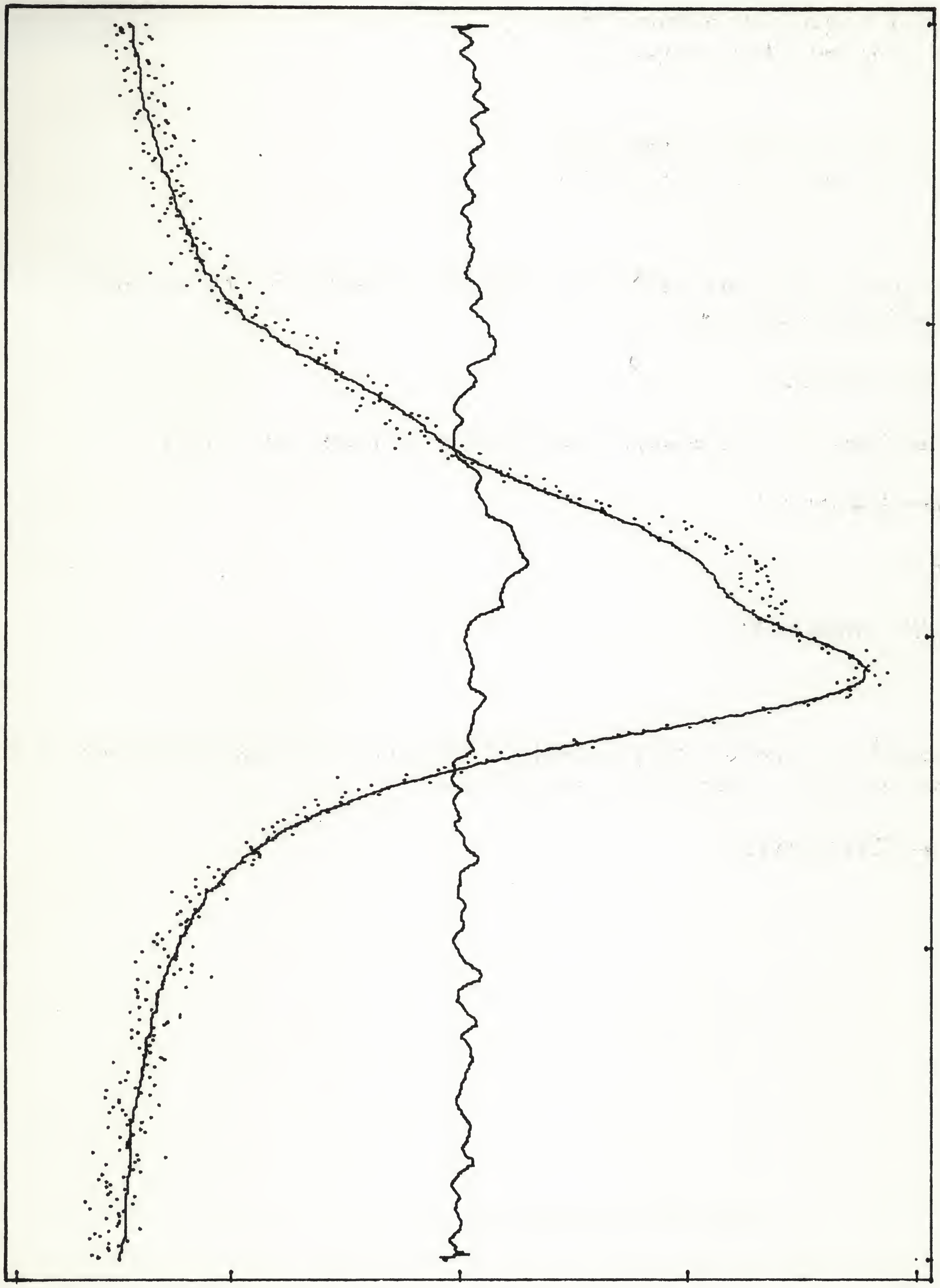
(Loaded Basic Package and Averager overlay; used SA=Ø2ØØ)

MPX CHAN=28	(Must be decimal)
PT. INDEX = 1	(50 points)
SEC/SCAN=.6	(Too little time)
PT. INDEX=1	
SEC/SCAN= 1.0	
MAX SCANS = 3	
DELAY (SEC)= Ø	(Input commenced and three scans were taken)
A:	(Restart analog input)
PT. INDEX =1	
SEC/SCAN=1Ø	
MAX SCANS=2	
DELAY (SEC)=Ø	(Input began on first trigger)
No. SCANS= 1	(Bit Ø of SR was set to interrupt)
DDDMMMMMMDDDS	('D' to decrease size,'M" to magnify, 'S' to stop)
MORE SCANS?Y	(Continued averaging, went to completion and scope display began.)
I:	(No action; INTEG not loaded)
F:	(No action; FILTER not loaded)
DI:	(Ditto: invalid command)
RE:	(Restart, input routine)
PT. INDEX=3	(500 points)
SEC/SCAN=6Ø	
MAX SCANS=1	
DELAY(SEC)=Ø	

Remaining operations as in Basic Package (Reloaded Averager overlay only; used SA=Ø4ØØ to reset machine cycle time.)

MACHINE CYCLE TIME (SEC) = 1.5E-6

(Program continues as if SA=Ø2ØØ)



OVERLAY PLOT OF EIGHT PEAK
LORCAP ON DATA POINTS, WITH
RESIDUALS (SMOOTHED):

DECtape #1 contains copies of the source and binary tapes.

M4BIN.1 is equivalent to tape 1 of 4
M4BIN.2 is equivalent to tape 2 of 4

and

M4SRC.1 is equivalent to tape 1 of 6
M4SRC.2 is equivalent to tape 2 of 6

etc.

To get punch copies from the DECtape using PIP on the PDP-10, the source files can be directly transferred, e.g.,

PTP: ← M4SRC.1

but the binary files must always be tranferred using image mode, e.g.,

PTP:← M4BIN.1/I

and also,

DSK;/X←M4BIN.1/I

etc.

DECtape #2 is an edited, complete PAL-10 listing of all the program segments. A line printer listing is acquired thusly, using PIP:

LPT: ← DTAN:M4LST