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TITLE	8-POINT QUADRATIC SMOOTH WITH FPP-12
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8-POINT QUADRATIC SMOOTH WITH FPP-12

DECUS Program Library Write-up

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DESCRIPTION

The FPP-12 performs floating point calculations 100 times faster than the software version. However, the new processor was apparently designed to operate on data stored as floating point numbers.

A FPP/PDP-12 program has been developed for smoothing an array of $4095_{(10)}$ data points, stored as single 12 bit words, using an 8-point quadratic fit.

The program is more versatile than the original Four-Point Smoothing Program (DECUS NO. 12-72) because the operator may choose a filter factor by force fitting the middle 2 data points, the middle 4 data points, or the middle 6 data points of the 8 points used to calculate the best quadratic. The latter choice offers the greatest smoothing. The net effect for gas chromatography data taken 3 points/sec shows a net peak height reduction of only the least significant bit.

The SETX, LDX, XTA and ATX instructions are combined to examine 8 successive 1-12 bit data words anywhere in 32 k core, float, fit to quadratic, smooth the desired center points, fix, and restore them back into their original 1-12 bit word location, advancing by one data point through the array.

The program invokes the standard least-squares fit technique whereby the A, B, and C coefficients of the least-squares quadratic are obtained by simultaneous solution of the equation set:

$$\begin{aligned}\bar{y} &= A + B\bar{x} + C\bar{x}^2 \\ \overline{xy} &= A\bar{x} + B\bar{x}^2 + C\bar{x}^3 \\ \overline{x^2y} &= A\bar{x}^2 + B\bar{x}^3 + C\bar{x}^4\end{aligned}$$

where \bar{y} , \bar{x} , \bar{x}^2 , \overline{xy} , etc. designate average values of the respective quantities associated with the 8-point data array. Rather than require the FPP-12 to perform all operations associated with simultaneous solution of the three equations, the determinantal expansion was performed by hand in the interest of conserving processor time. Relative x-coordinate values of one thru eight are assigned the eight data points involved in each quadratic fit-smooth operation. This allows assignment of numerical values to \bar{x} , \bar{x}^2 , \bar{x}^3 , and \bar{x}^4 so that the solutions to A, B, and C can be expressed in terms of three remaining unknowns, \bar{y} , \overline{xy} , and $\overline{x^2y}$. One obtains:

$$A = 15.5714 \bar{y} - 7.28571 \overline{xy} + 0.714826 \overline{x^2 y}$$

$$B = -7.28571 \bar{y} + 4.04762 \overline{xy} - 0.428571 \overline{x^2 y}$$

$$C = 0.714286 \bar{y} - 0.428571 \overline{xy} + 0.0476190 \overline{x^2 y}$$

Consequently, the FPP-12 is simply assigned the task of calculating \bar{y} , \overline{xy} , and $\overline{x^2 y}$ for a data set and applying the foregoing equations to obtain A, B, and C, and smoothing the data by assigning values on the quadratic to 2, 4, or 6 central data points in the 8-point array.

In addition to saving two-thirds the core necessary to store the data as floating point numbers, the program was written in single-word addressing which reduces the core necessary to reside the program by one-half from that used for double-word addressing.

Time comparisons of the FPP-12 system shows the run time of 20 seconds to smooth 4095₍₁₀₎ points using a 8-point smooth while the DEC software floating point package took 4 minutes, 15 seconds using a 4-point quadratic fit. In addition, the FPP-12 is operating in parallel to the PDP-12 CPU, so one can actually see the smoothing occurring.

USAGE

The program FPSMOOTH, submitted on LINCtape is actually two programs combined. The program is loaded by DIAL with starting address of 4021 (L). The first section, CONTAPE, is a Qanda display routine written in LINC mode to flash three scope displays and load data from tape Unit 1 into the second 4 k memory bank. The first display states:

To Continue
Type "C"

The Sense switch 0 must not be set to advance to the second display which asks:

Total Time _____
Total No. Points _____

Respond using octal numbers up to 7777. Entry examples for this frame are as follows:

2260 Carriage Return (1200(10) seconds)
7640 Line Feed (4000(10) points)

The third display asks for the starting tape block of unit 1 where data begins and the number of blocks:

Tape Blk _____
No. Blks _____

eg. $\frac{100}{20}$ Carriage Return
Line Feed

Upon typing the linefeed, the data is loaded from tape and CPU jumps to 0200(L) to begin section two of the combined program.

NOTE: DIAL-MS has been modified on tape submitted. With SNS 0 set, the system disk storage device is NOT initialized; it works just like Dial-1. This was necessary on our system having only 1 DF-32, to allow loading of FOCAL-12 and the FPPASM assembler. (Courtesy of Dale Lewellyn, DEC, Chicago, Illinois)

Section two, called FIT8DECS, is written in 8 mode and assembled by FPPASM, the FPP-12 assembler. The starting address is 0200(L). The first subroutine sets up the display for a total of 7777(8) points, initializes the FPP-12 APT, displays data, and checks teletype for "C".

Upon typing C2, C4, or C6, the data is displayed while the FPP-12 is smoothing, force fitting the middle 2, 4, or 6 data points of the 8 point array depending on the user response.

When the FPP-12 has completed the smoothing, the CPU regains control continuing the CRT display. The data may be re-smoothed.

The program will not be completed until the GLC data is printed out in worksheet format, listing retention time, peak heights, peak areas, etc., but the program does demonstrate the use of the FPP-12 on a mini-computer to smooth data stored as 1-12 bit word, operating in parallel with CPU.

NOTE: Only four locations need modification to allow the program to force-fit the center 2, 4, or 6 data points to the quadratic. They are tabulated as follows:

	2	4	6
Location Lok1(1154)	7776	7774	7772
Location Lok2(1156)	0003	0002	0001
Location Lok3(1160)	0002	0001	0000
Location Lok4(1205)	7774	7773	7772

The use of equipment described in this paper does not constitute an endorsement by the Food and Drug Adm.

REFERENCES

- 1). PDP-12 Systems Reference Manual, DEC., Maynard, Massachusetts 01754 (DEC-12-SRZA-D) 1970.
- 2). FPP-12 User's Manual, DEC., Maynard, Massachusetts 01754 (DEC-12-GQZA-D) 1971.
- 3). FPP-12 Assembler, DEC., Maynard, Massachusetts 01754 (DEC-12-AQZA-D) 1971.
- 4). ADTAPE/ADCON Manual, DEC., Maynard, Massachusetts 01754 (DEC-12UW2A-D) 1970.

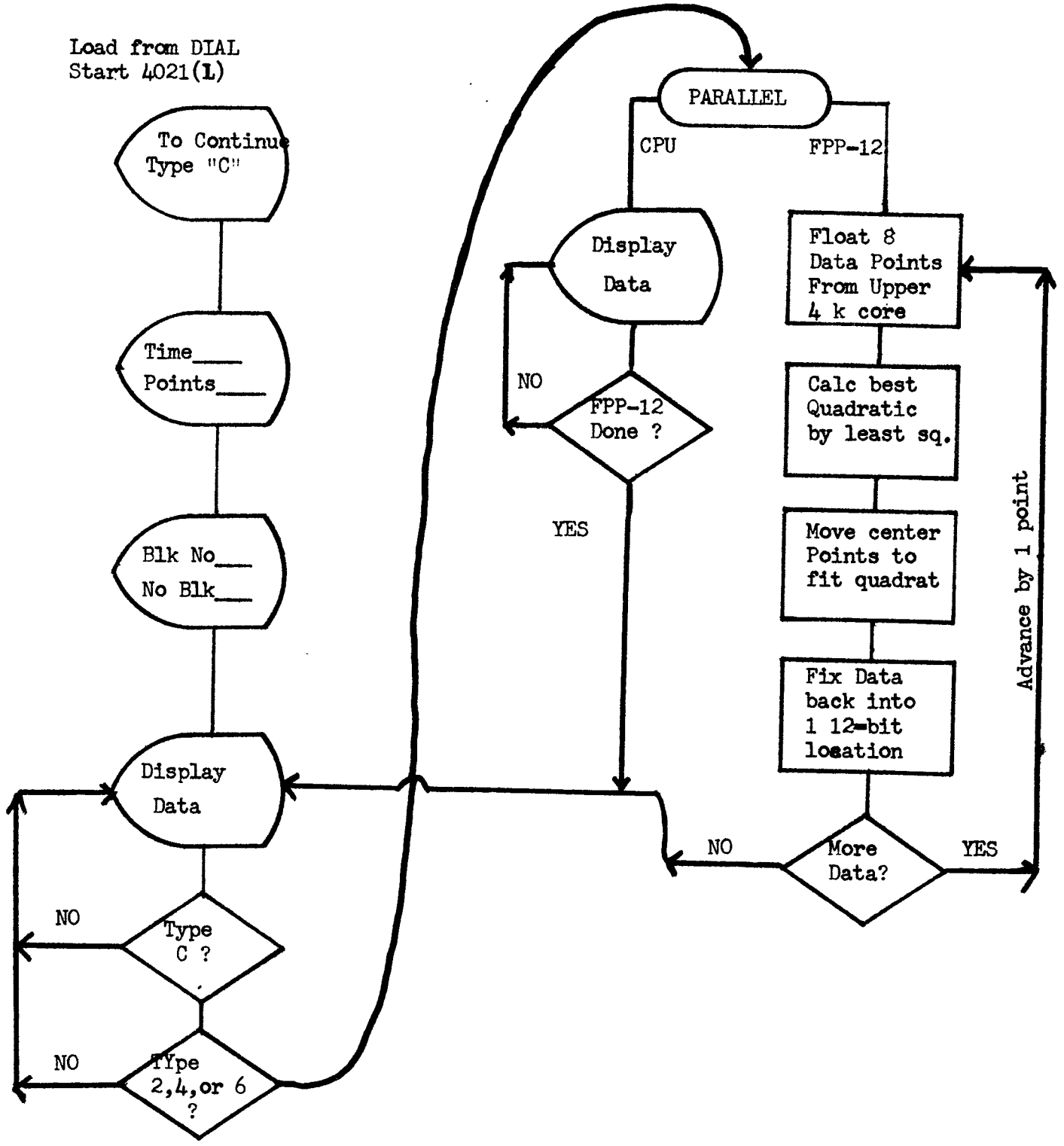
5). Qanda Manual, DEC (DEC-12-FISA-D) 1970.

6). See below

NOTE: The use of equipment described in this paper does not constitute an endorsement by the Food and Drug Administration.

6). Alber, L. L., Overton, M. W. & Smith, D. E. "Four-Point Smooth Using FPP-12", DECUSCOPE, 1972.

8-Point Quadratic Smooth With FPP-12 Flow Diagram



LINCTAPE INDEX

FPSMOOTH

NAME	SOURCE		BINARY	
	BN	BLKS	BN	BLKS
PIP			247	21
PATCH			47Ø	4
FPPTST	246	1		
FOCAL-12			215	25
MARK12			656	7
CONTAPE	516	13	531	5
FPSMOOTH	245	1	2Ø2	13
DIALMSNØ	244	1		
FPPASM			474	22
FITRDECS	162	10	172	1Ø
DATA			100	20