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TITLE

NMRCAT-29: A SIMPLIFIED SIGNAL AVERAGER PROGRAM

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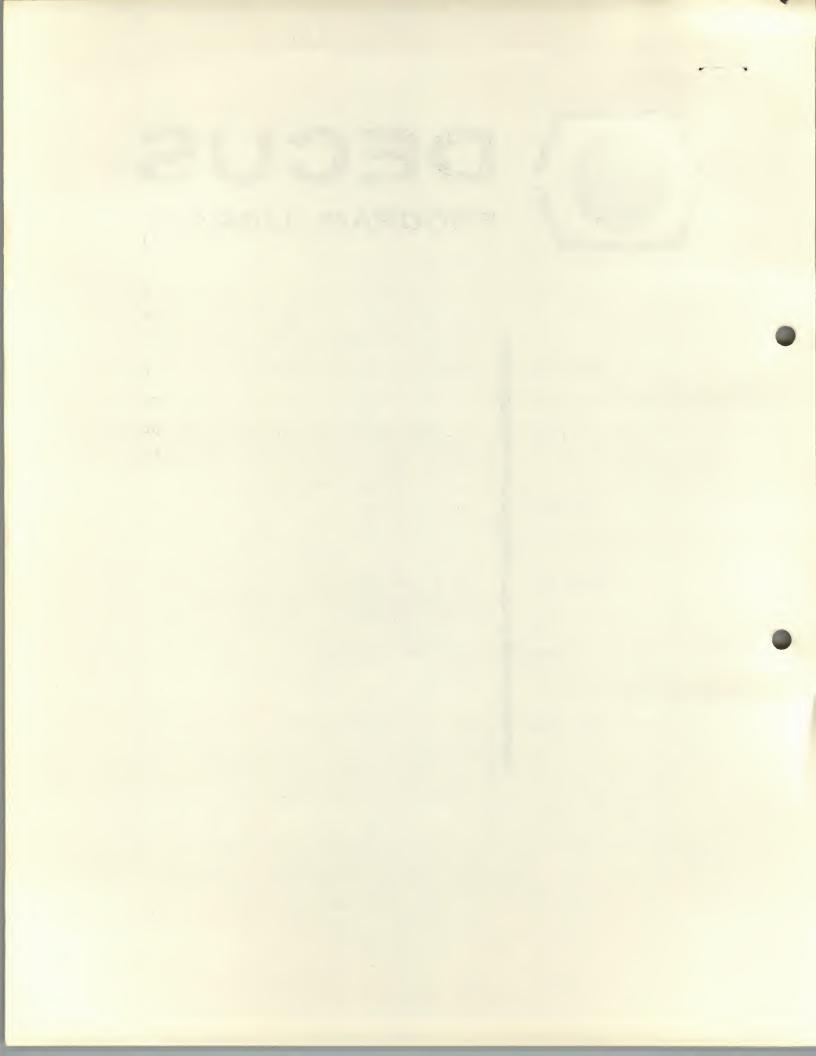
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SOURCE LANGUAGE

PAL III



PROGRAM NMRCAT-29

By James W. Cooper

Programmed at the State University of New York at Buffalo, 1969

The program NMRCAT-29 is a time-averaging program for the PDP-8/I computer specifically designed for use with the HA-60 nmr spectrometer equipped with a digital frequency synthesizer. It generates a linear sawtooth sweep voltage which is used to drive the frequency synthesizer. The synthesizer then sweeps through a pre-set range at a rate controlled by the computer. The program also contains display, printout, plot, integration and calibration routines for examining the accumulated average.

I. USE OF THE AVERAGING PROGRAM NMRCAT-29

- 1. Load the binary tape of the Averaging Program as follows.
- a. Turn on the power to the computer and teletype; the teletype should be switched to LINE.
- b. Place the binary tape in the tape reader while the reader is set to FREE.
 - c. Turn the reader to START.
- d. Set the Switch Register to 7777. This is the position with all 12 switches having their tops pointing out.
- e. Depress LOAD ADD. All the lights in the Program Counter should come on.
- f. Depress START. The tape should begin reading in. If it does not, the Binary Loader program is not resident and must be reloaded. Refer to DEC instructions on reloading the Binary Loader.
- g. When the tape finishes reading in, in about 4 minutes, it should stop at the last set of holes. When it stops the computer should halt with all 12 lights in the accumulator out. (The link may be either on or off). If the accumulator is not equal to 0, it indicates a tape-reading error. To rectify this, reload the tape, starting at instruction d. If this error persists, reload the Binary Loader program.
- 2. Start up the program as follows.
 - a. Set the switch register to 0200 (000 010 000 000).
 - b. Depress LOAD ADD and then START. The teletype should type:

 PROGRAM NMRCAT-29 BY J. W. COOPER
 NUMBER OF SWEEPS =
- c. Type any integer value between 1 and 4095 for the number of sweeps.

If you make a mistake, type enough extra integers to indicate a number greater than 4095 and then type RETURN. When this happens, the computer will type a ?, followed by a carriage return and line feed (abbreviated (CR/LF)) and accept a new value.

When a correct value has been entered, type RETURN. The computer will respond with a CR/LF.

d. If the value of the sweep number is acceptable, the teletype will follow the CR/LF with

NUMBER OF SAMPLES PER POINT (<9) =

This parameter refers to the number of times each point is sampled during a single sweep. To this question, respond with any number between 1 and 8. The purpose of this parameter is to increase the statistical significance of each sweep, by examining each point several times. Follow your typed value with RETURN.

Powers of 2 for this parameter give the most accurate sweep times. Thus, 1, 2, 4, or 8 are preferable to 3, 5, 6 or 7 if the exact sweep time is critical.

e. After responding with a CR/LF, the computer will type:

SWEEP TIME IN SECONDS =

Answer with any value less than 4096. Correct any error as above by typing enough integers to indicate a value larger than 4095. Then type RETURN.

f. The teletype will then type a CR/LF followed by BALANCE

This parameter enables the computer to subtract any DC bias from the input signal. Set the spectrometer so that the output is essentially "zero" baseline and then type RETURN. The computer then digitizes and stores any variation from a zero volt baseline (up to one volt).

g. The teletype will then type a CR/LF followed by REPEAT?

If "Y" is typed, the computer sweeps indefinitely, typing "END" after every N sweeps. If any other character is typed, the sweeping is not repeated.

h. The teletype will next type a CR/LF followed by

TYPE RETURN TO BEGIN AVERAGING

If RETURN is typed, the memory is erased and averaging is begun.

If LINE FEED is typed, the memory is not erased, and additional signals are added to whatever data has already been accumulated.

This feature enables one to change the sweep parameters without disturbing the accumulated data, using the R command.

i. Typing RETURN causes a CR/LF from the teletype, and causes a dot to be displayed at the left hand edge of the scope, representing the rate and position of the sweep. This linear scope sweep is the actual voltage which also causes the synthesizer to sweep the specified decade. If the averaging is to take place over a long period, turn down the scope intensity to avoid burning a dot on the scope, and turn off the teletype.

II. ON-LINE AVERAGING

- 1. During the actual averaging, no other operations can be performed by the computer, but, at the end of any sweep, the computer can be stopped and the operations given below performed. Typing any character on the teletype will cause the sweeping to be interrupted at the end of the current sweep. When the averaging is complete, the teletype will type END, (CR/LF). If the response to REPEAT? was "Y", the computer will continue sweeping.
- 2. Once the averaging has stopped, either at the end of the desired number of sweeps, or whenever the keyboard has interrupted the sweeping, the computer switches to the Display Mode. In the Display Mode, the accumulated average is displayed on the scope, and any of the following commands are applicable:
 - C Contract the display by a factor of 2 each time C is struck
 - X Expand the display by a factor of 2 each time X is struck
 - U Shift the display up by 10% each time U is struck
 - D Shift the display down by 10% each time D is struck
 - S Return the display to its original state

- Go continue averaging without erasing the memory. If the specified number of sweeps has not been completed, sweeping continues until they are complete. If all specified have been completed (i.e., if END has been typed) an additional N sweeps are performed.
- E Erase the memory and the display buffer
- R Restart the program at the beginning
- N Type out the number of the sweep just completed. Thus, to find out how many sweeps have been completed, interrupt the averaging by typing some character while it is sweeping, and at the end of the sweep, type N.
- Type out the contents of the buffer. Since the printer and punch are mechanically linked, the computer halts so that the punch can be turned on. Press CONTINUE after doing this.
 - Leader and trailer tape for the punched output can be generated off line, by pressing the HERE IS key while the teletype is switched to LOCAL.
- K Calibrate. Typing K while in the Display Mode causes a point to be displayed on the scope whose X and Y coordinates are controlled by the knobs O and I of the AX-08. The X and Y outputs of the AX-08 should be connected to the X and Y inputs of the recorder. The X output should also be connected to the synthesizer as before. It is important that neither the spectrometer nor the synthesizer have any settings changed before calibration.

Turn on the recorder and observe that the recorder pen, as well as the scope display, is now controlled by the AX-08 knobs. Adjust the display so that the dot is in an extreme corner of the scope. Then adjust the COARSE TIMING CONTROL until the pen also hovers over a corner of the previously plotted grid. This will be about 4 click stops from the fastest clock setting (or 4 stops from the CCW extreme). Then position the pen over the line of interest and read the frequency from the counter under the scope. Exit from this routine is caused by typing any character on the teletype. The computer then re-enters the display mode.

I Integrate

Typing I switches the computer to the Integrate-Display Mode, which contains two cursors: vertical lines on the display. Integration is accomplished between cursor $\underline{0}$, controlled by AX-08 knob $\underline{0}$ and cursor $\underline{1}$, controlled by AX-08 knob $\underline{1}$. Cursor $\underline{0}$ must be on the left and cursor $\underline{1}$ on the right.

When the cursors are adjusted, type <u>I</u> again, which will cause the teletype to either type out the sum under that portion of the curve, or a vertical arrow. The computer then returns to the Display Mode. If a vertical arrow is typed, an overflow has occurred, and the display must be contracted and integration repeated. After the integral has been typed out, contract the display and re-integrate. If the new integral is not half the old one, continue contracting until it is.

P Plot Routine

Typing \underline{P} causes the computer to enter the Plot-Adjust mode. In this mode, there are four legal commands:

RETURN - This command is executed the first time automatically when the computer enters the Plot-Adjust mode. The teletype types out

LOWER LEFT

and the scope input voltages are set to (-10, -10) volts. Cables should now be connected to a chart recorder from the X and Y axis scope inputs and an adjustment made so that the two voltages actually put the pen in the lower left corner of the chart paper.

LINE FEED - The teletype types

UPPER RIGHT

and the voltages (0,0) are sent to the scope and recorder.

Striking P a second time causes the computer to actually begin the plot. The plotting rate is controlled by the TIMING CONTROL knobs on the AX-08. The COARSE knob has 10 click stop positions and the FINE knob is a ten-turn potentiometer. Keep trying the plot until an appropriate rate is found. Then put the pen in the DOWN position and draw the hard copy. When the plot and border are complete, the computer will halt. (The timing may be speeded up

during the grid plot). Turn off the recorder before pressing CONTINUE. This will prevent the pen from rushing to the center when the computer re-enters the Display Mode.

K Calibrate - This routine can be entered from the Plot-Adjust Mode. It is also the fastest mode of exit from the Plot-Adjust mode, enabling one to return to the Display Mode without actually plotting a spectrum.

Calibration can also be accomplished using the lower left and upper right display voltages from the plot routine. Lower Left represents the upfield extreme of the sweep on the frequency counter and Upper Right represents the downfield frequency limit. Any intermediate position is obtained using the \underline{K} routine as described above.

SUMMARY OF THE USE OF NMRCAT-29

- 1. Load averager tape with Binary Loader: set Switch Register to 7777, press LOAD ADD and START.
- 2. Start Program by setting the SR to 0200, and pressing LOAD ADD and START.
- 3. SWEEPS and TIME are integers less than 4096, SAMPLES PER POINT is an integer less than 9.
- 4. Type RETURN to begin averaging. LINE FEED begins averaging without erasing the memory. Striking any key during averaging will cause an interrupt to occur and the computer to shift to Display Mode.
- 5. In Display Mode, the following commands are operative.
 - C Contract
 - X Expand
 - U Up
 - D Down
 - S Stop return display to unmodified position
 - G Go continue averaging
 - E Erase memory and buffer
 - R Restart program from beginning
 - N Type number of last sweep
 - K Calibrate
 - T Type-punch the contents of the display buffer (press CONTINUE)
 - P Plot the contents of the display buffer

RETURN - Lower Left

LINE FEED - Upper Right

K - Calibrate

P - Plot (press CONTINUE when plot is finished)

I Integrate between cursors.

(The Starting Address of the display routine is 1325).

I. SETTING UP THE SPECTROMETER AND COMPUTER

- 1. Remove the Manual Oscillator Tuning Network circuit card from the model V3507 Slow Sweep Unit. This card is marked, and is the second from the left as you view the back of the unit.
- 2. Connect the Output BNC connector on the front of the Frequency Synthesizer to the MAN OSC OUT connector on the back of the V3507.
- 3. Open the back of the PDP-8/I console rack. The X and Y inputs to the Tektronix 602 Oscilloscope are fitted with T-connectors. To one terminal of the T-connector on the X-axis input, connect a cable, and run it to the banana plug connector attached to the pin connector outlet at the rear of the frequency synthesizer.
- 4. Connect the external recorder jack on the V4391 Mode Selector Panel to analog input 0 of the AX-08 peripheral section of the PDP-8/I. (The input channel used can be changed, if desired from channel 0, to channels 1, 2, or 3 by altering the contents of location 72 from 0 to 1, 2, or 3.)

II. SETTING UP THE NMR SPECTROMETER AND SYNTHESIZER

- 1. Set up the HA-60 to run a normal spectrum in the Field Sweep mode.
- 2. Depress one of the buttons marked SWEEP FREQUENCY RANGE (i.e., 50, 100, 250, 500 or 100 hz) on the V4354 unit. It doesn't matter which button as they don't actually control any function in use. It is only necessary that one be depressed so that a circuit is completed.
 - 3. Set the recorder EXTERNAL/INTERNAL switch to EXTERNAL.
- 4. Set the SIGNAL MONITOR switch to SWEEP FREQ and examine the frequency counter. The number displayed is the frequency of the lock signal. It may be changed by moving the recorder.
 - 5. The frequency synthesizer controls should be set as follows:

POWER - on
DECADE SELECTOR - desired sweep range (i.e., 1, 10, 100 or 1000 hz)
ATTENUATOR - full ccw

Control Selector Panel:

SEARCH DIGIT INTERPOLATOR - REMOTE

SWEEP TIME - Inoperative for this application

SWEEP WIDTH - Inoperative for this application

SYNTHESIZER MODE - LOCAL

6. The sweep range for this application is set by the DECADE SELECTOR to correspond to that desired (i.e., 1, 10, 100 or 1000 hz). These values can be interpolated between by adding a potentiometer to the circuit. The upper limit of the sweep range is the frequency

dialed on the decades of the synthesizer. The lower limit is the frequency dialed minus the sweep range selected.

For example, if the synthesizer were set at 0 0 0 2 7 5 0 . 0 and the DECADE SELECTOR control switch were set at 100 hz, the sweep would go from ca. 2750 hz to 2650 hz. Accordingly, the synthesizer decades should be set so that the signal to be observed lies in the middle of the sweep range.

For example, if the signal to be averaged lies 200 hz below the lock signal, and if the lock signal is at, say, 2510 hz, and if the desired sweep range is 100 hz., then the decades of the synthesizer would be set at 2510 + 200 + 100/2 = 2760 hz. If the averaged signal is 200 hz upfield, the synthesizer would be set to 2510 - 200 + 100/2 = 2360 hz.

- 7. Now set the SIGNAL MONITOR switch to MAN OSC FREQ. The frequency counter should read the same frequency as that of the synthesizer. Be sure that the MANUAL OSCILLATOR power is on. This channel is the one through which the frequency is swept, at an rf power determined by the MANUAL OSCILLATOR RF FIELD MG control. The method for inspecting the actual range of the frequencies swept is described in the next section under the Plot Routine.
- 8. When all of the above adjustments are complete, proceed to the averaging program instructions.