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NUMIT-ONE AMENDMENT #1

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ARMED FORCES RADIOBIOLOGY RESEARCH INSTITUTE
Defense Atomic Support Agency
Bethesda, Maryland

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NUMIT-ONE AMENDMENT #1

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FOREWORD
(Nontechnical summary)

An improvement in NUMIT-ONE (AFRRI Scientific Report SR65-1, October 1965) is described. Simpson's Rule is still used to perform the integration but changes in the coding remove the need for a large array. The number of multiplication operations done during a run has also been vastly reduced resulting in significant savings in machine time.

ABSTRACT

An improvement on NUMIT-ONE, a one-dimensional numerical integration program for the IBM 1620, is reported. Accuracy, input and output formats, source program, flow charts and test problems are discussed.

I. INTRODUCTION

This is an amendment to NUMIT-ONE, a numerical integration program in one-dimension for the IBM 1620 computer, AFRRI Scientific Report SR65-1. Appendix D contains a glossary of terms used in this report.

Further analysis of the problem resulted in the elimination of a large array thereby making the program smaller and the number of multiplication operations fewer. This reduction in size enabled compilation with a larger precision parameter* (thereby increasing accuracy) and the fewer operations decreased the length of running time.

Successive approximations to the integral are now computed with J successively 1, 2, ..., using

$$F_J(a,b) = \frac{\Delta X_J}{3} [f(a) + f(b) + 2 \cdot C_J + 4 \cdot D_J]$$

in which

$$\Delta X_J = \left| \frac{b-a}{2^J} \right|$$

$$C_J = \sum_{m=1}^{2^J-1} f(a + 2m \cdot \Delta X_J), \quad J > 1; \quad C_J = 0 \text{ if } J = 1$$

$$D_J = \sum_{m=1}^{2^J} f(a + [2m-1] \Delta X_J)$$

Thus for the J + 1th iteration:

$$C_{J+1} = D_J + C_J$$

* A precision parameter is the number of arithmetic places to which quantities will be held during computation and may be specified on a control card that precedes the rest of the deck in IBM 1620 FORTRAN II.

and only two summed quantities in the main equation need be multiplied rather than entire arrays.

Input and output formats are slightly changed from the original version.

II. ACCURACY

Reduced truncation error has improved the accuracy. An inherent weakness in Simpson's Rule makes it difficult or impossible to integrate over the intervals of functions where the slope approaches infinity. In the current version it is still difficult but if a large number of iterations are used and the precision parameter is large enough, an accurate answer will be obtained. Test Case 1 (Appendix C) of the current report illustrates this. The slope of this function approaches infinity at the start and end of this interval. By allowing 11 iterations and holding quantities to 10 places, an answer accurate to 5 places was computed.

Breakdown will definitely occur when the integral is close to zero, resulting from an integrand taking on both positive and negative values over the interval of integration. A function such as this should be integrated in parts.

Input for the program has been changed slightly to make this division of the integration interval more amenable and there are no limits on the number of parts used. This situation reveals itself readily by the erratic behavior of DELTA (Δ_J). Test Case 2 (Appendix C) illustrates what happens when integration is attempted over the whole interval of such an integrand and Test Case 3 illustrates the proper method of splitting the integration into parts.

III. INPUT LIMITATIONS

The integrand, $f(x)$, may be any function for which the integral exists; also $(-\infty) < a, b < (+\infty)$, $b \neq a$.

The total number of iterations allowed is $J_{\max}$ (an input parameter) where $2 \leq J_{\max} < 100$. Iteration is stopped whenever either

$$\Delta_J \leq \Delta \quad \text{or} \quad J = J_{\max}$$

While $J_{\max}$ can be any number up to 100, it should not be too high. Each iteration roughly doubles the machine time. Generally, for more than 13 or 14 iterations, machine time is measured in hours.

The integrand, $f(x)$, is provided by a subprogram of the FUNCTION type named FUN(X). FUN must appear on the left of an arithmetic statement whose right is the integrand. The subprogram source deck must be preceded at compilation time by a precision parameter card identical to the precision parameter card, if any was used, of the main source deck.

IV. INPUT AND OUTPUT FORMATS

Input Card Format

The following quantities are specified in the input (floating point numbers are in lower case, fixed point numbers in upper case).

Card 1

Columns 1-80 contain alphanumeric identification. It is reproduced in the output but does not affect the processing.

Card 2

Columns 1-36 Integrand Specification Card. Contains alphanumeric information to identify integrand in output. This does not affect processing.

Card 3

			<u>Format</u>
Columns	1-12	a	E 12.6
Columns	13-24	b	E 12.6
Columns	25-28	Δ	F 4.4
Columns	29-30	$J_{\max}$	I 2

Following card 3 may be any number of cards specifying new values of a, b, Δ , and $J_{\max}$. Input format is the same as card 3. The final card is a trailer card with zeros punched in columns 29-30.

Input Deck Assembly

Input decks are assembled as in the original NUMIT-ONE with the FUN(X) subprogram replacing the POINT subprogram.

Errors in Input

The input error check is the same as before except that in the amended version $J_{\max}$ may have any value up to 99. A check is made to see if $J_{\max} < 2$.

Output

The output has three main stages; the identification is punched as follows:

- (a) Alpha Identification Card
- (b) Program name (NUMIT-ONE)
- (c) $F(X)$ = Columns 1-36 of Integrand Specification Card.

Next, the input a , b , $J_{\max}$, and DELTA 1 are punched followed by the results of the computation with the following data given for each iteration ($J = 2, \dots J_{\text{act}}$):

- (a) Iteration number
- (b) Value of integral
- (c) DELTA

The final value for $\text{DELTA} \leq \text{DELTA } 1$ or $J_{\text{act}} = J_{\max}$ is noted by the term (PASS N) in the last line of the output, where $N = 1, 2, \dots 99$ is the pass number.

If more cards specifying new values of a , b , $J_{\max}$ and DELTA 1 are input, the above cycle will be repeated until all input cards have been processed. The final part of the output is furnished when the trailer card is read. The number of passes (N) is punched, followed by the total value of the integral for all passes. The last card punched, showing satisfactory completion of the program, is "END" and the program stops.

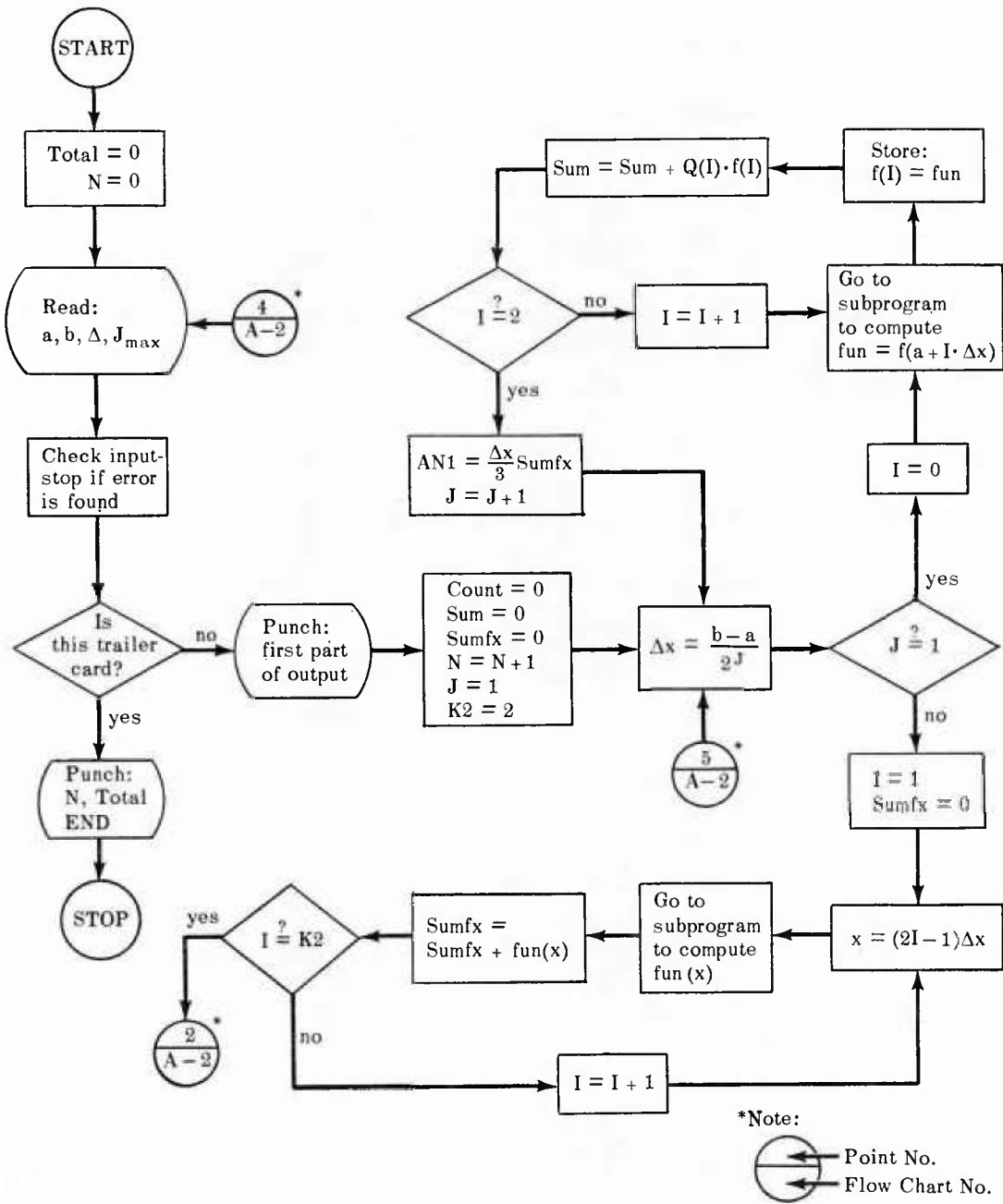
A set of output listings for sample problems is given in Appendix C.

V. OPERATION

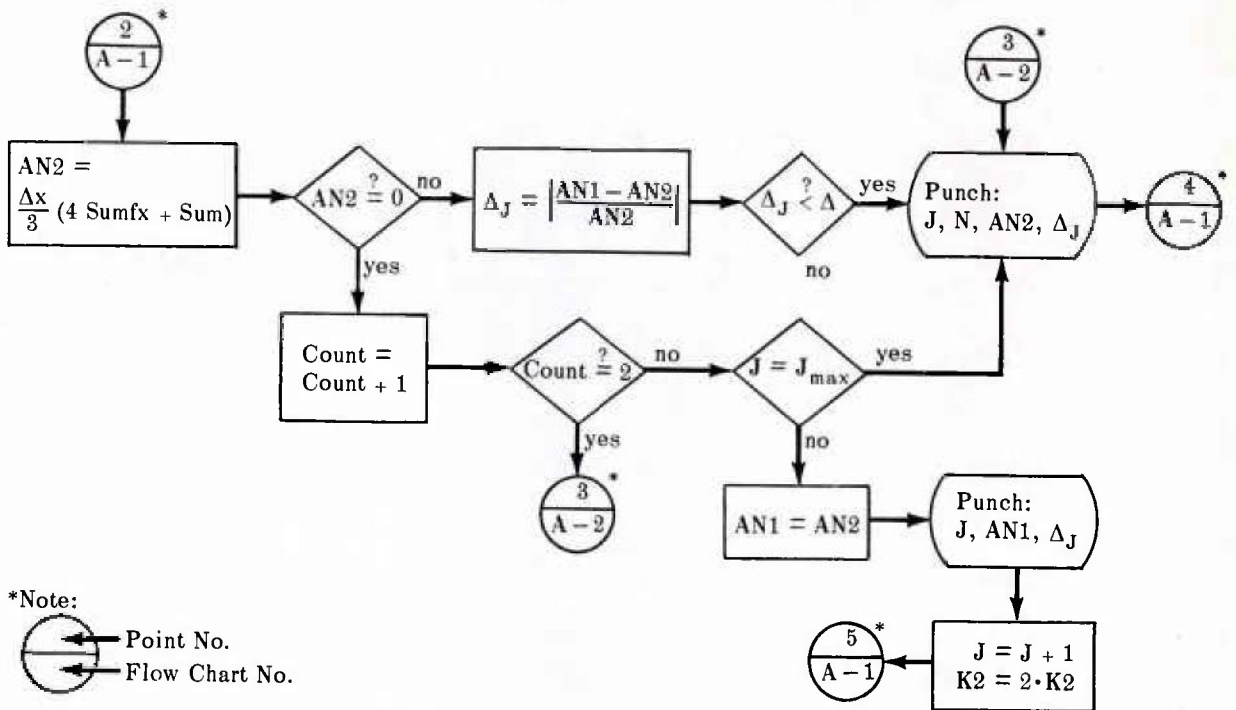
Operation is the same as before except a trailer card is now used to stop the computation. No switches are used.

APPENDIX A

Flow Charts



Flow Chart A-1



Flow Chart A-2

APPENDIX B

Source Program

In the program, the following symbols are used which are unexplained in the mathematical description:

N = counter to keep track of number of passes

DELTA 1 = Δ = input convergence criterion

AN1 = F_{J-1} = previous approximation

AN2 = F_J = current approximation

SUMFX = $\sum_{m=1}^{2^{J-1}} f(a + [2m-1] \Delta x)$

SUM = $f(a) + f(b) + \sum_{m=1}^{\frac{2^J}{2}-1} 2 \cdot f(a+2m \cdot \Delta x)$

COUNT = counter used to count successive times $F_J = 0$

*1010

```

C      NUMERIC INTEGRATION USING SIMPSON- ROCKWELL- 2-16-66  AFRII-NNMC
      DIMENSION F(3),P(3),Q(3),U(9)
      P(1)=1.
      P(2)=4.
      P(3)=1.
      Q(1)=1.
      Q(2)=2.
      Q(3)=1.
      N=0
      TOTAL=0.
C
C      READ INPUT AND ALPHA IDENTIFICATION CARD
      READ102
      PUNCH102
      PUNCH103
      READ 114,(U(I),I=1,9)
      PUNCH115,(U(I),I=1,9)
      1 READ101,A,R,DELTA1,JMAX
C
C      TEST INPUT FOR VALIDITY, IF OKAY PUNCH NEXT PART OF OUTPUT
      IF(JMAX-2)26,26,27
      26 IF(N)25,25,29
      25 PUNCH106
      STOP
      27 IF(R-A)22,28,22
      28 PUNCH104
      STOP
      22 IF(DELTA1)23,24,23
      24 PUNCH105
      STOP
      23 PUNCH109,R,JMAX
      PUNCH110,A,DELTA1
C
C      INITIALIZATION FOR START
      CUNIT=0.
      SUM=0.
      SUMFX=0.
      N=N+1
      J=1
      K2=2
      21 DELX=(R-A)/(2.**J)
      IF(J-1)4,2,4
      2 DO 3 I=1,3
      AI=I-1
      X= A+ AI*DELX
      F(I)=FUN(X)
      SUM = SUM+Q(I)*F(I)
      3 SUMFX=SUMFX+P(I)*F(I)
C      FIRST APPROXIMATION OF INTEGRAL
      AN1=DELX*SUMFX/3.
      J=J+1

```

```

      GO TO 21
C     CALCULATES FUNCTION MIDWAY BETWEEN CURRENT PRINTS
4     SUMFX=0.
      DO 5 I=1,K2
      AT = 2*I-1
      X= A+AT*DFLX
5     SUMFX = SUMFX+FUN(X)
C     NEXT APPROXIMATION
      AN2=DFLX*(4.*SUMFX+SUM )/3.
      IF (AN2)6,12,6
6     DELTA=ARCF((AN1-AN2)/AN2*100.)
      IF (DELTA-DELTA1)17,17,18
18    IF (J-JMAX)19,17,17
19    AN1=AN2
      SUM =SUM +2.*SUMFX
      PUNCH112,J,AN1,DELTA
C     INITIALIZATION FOR NEXT ITERATION LOOP
      J=J+1
      K2=2*K2
C     BACK TO ITERATION IF VALUE HAS NOT CONVERGED ENOUGH
      GO TO 21
C
C     PUNCH FINAL ANSWER FOR THIS PASS AND RETURN FOR NEXT INPUT CARD
17    PUNCH 113,J,N,AN2,DELTA
      TOTAL =TOTAL+AN2
      GO TO 1
C
C     FOR HANDLING ZERO ANSWERS
12    COUNT=COUNT+1.
      IF (COUNT-2.)18,17,17
C
C     PUNCH THE TOTAL ANSWER AND HALT
29    PUNCH116,N,TOTAL
      STOP
101   FORMAT(2F12.6,F4.4,I2)
102   FORMAT(80H
1      )
103   FORMAT(/15X,48HNUMIT ONE (ONE-DIM. INTEGRATION, SIMPSONS RULE) )
104   FORMAT(15X,17HCHECK INPUT - A=R)
105   FORMAT(15X,22HCHECK INPUT - DELTA1=0)
106   FORMAT(15X,32HCHECK INPUT - JMAX OUTSIDE RANGE)
109   FORMAT(35X,10HINPUT DATA/20X,2HA=F12.6,11X,7HJ(MAX)=,I2)
110   FORMAT(20X,2HA=F,12.6,11X,7HDELTA1=F,10.4//15X,10H ITERATION,11X,
1      18HINTEGRAL,13X,5HDELTA)
112   FORMAT(19X,I2,12X,F12.6,10X,F8.3)
113   FORMAT(19X,I2,5H(PASS,I3,1H),3X,F12.6,10X,F8.3////)
114   FORMAT(9A5)
115   FORMAT(16X,7HF(X) = ,9A5,/)
116   FORMAT(32X,12HNO. PASSES =I3/29X,16HTOTAL INTEGRAL = F12.5/39X,
1      13HEND)
      END

```

APPENDIX C

Test Cases

Running time is still highly variable, but in general the time is now 30 to 50 per-cent faster than in the old version as will be noted in the test cases. Also, accuracy has been increased since quantities are now held to 10 significant figures.

Note the integrands of Cases 3(a) and 3(b) are identical to Case 2 and taken to-gether duplicate Case 2. However, Case 3 produced a more accurate answer in a small fraction of the time for Case 2 because the Case 2 integral took on positive and negative values during the iteration attempting to approximate a zero answer while Case 3 integrated nonzero portions and summed them.

Running time, as in the original report, is still dependent on the formula

$$t = K \cdot 2^{J_{act}}$$

Table I gives the new running times for the test cases.

TABLE I

Test #	Integrand	a	b	J_{act}	t	$\frac{t_{new}}{t_{old}} \times 100$	K (min)
1	$\sqrt{(1-x^2)(2-x)}$	-1	1	11	12'50"	51.5	6.27×10^{-3}
2	$\sin(x)$	0	2π	11	16'50"	64.9	8.22×10^{-3}
3(a)	$\sin(x)$	0	π	5	1'	-	8.22×10^{-3}
3(b)	$\sin(x)$	π	2π	5	1'	-	8.22×10^{-3}

TEST CASE 1

INPUT DATA

SOURCE STATEMENT OF SUBROUTINE

```
*1010
```

```
FUNCTION FUN(X)
FUN = SQRTF((1.-X*X)*(2.-X))
RETURN
END
```

OUTPUT DATA

TEST FUNCTION 1

```
NUMIT ONE %ONE-DIM. INTEGRATION, SIMPSONS RULE
F%X# # SQRT%%1.-X*X#2.-X#
```

INPUT DATA

```
B# .100000E&01      J%MAX#13
A#-.100000F&01      DELTA1# .1000E-02
```

ITERATION	INTEGRAL	DELTA
2	.209138E&01	9.838
3	.216390F&01	3.351
4	.218943F&01	1.166
5	.219843F&01	.409
6	.220161F&01	.144
7	.220273F&01	.050
8	.220312F&01	.017
9	.220326F&01	.006
10	.220331F&01	.002
11%PASS 1#	.220333F&01	0.000

```
NO. PASSES # 1
TOTAL INTEGRAL # 2.20333E-00
END
```

TEST CASE 2

INPUT DATA

SOURCE STATEMENT OF SUBROUTINE

*1010

FUNCTION FUN(X)

FUN = SIN(X)

RETURN

END

OUTPUT DATA

TEST FUNCTION 2

NUMIT ONE %ONE-DIM. INTEGRATION, SIMPSONS RULE

F(X) = SIN(X)

INPUT DATA

B# .628319E+01

J%MAX#11

A# .000000E-99

DELTA1# .1000E-02

ITERATION

INTEGRAL

DELTA

3

-.628319E-09

100.000

4

-.523599E-09

20.000

5

.641408E-09

181.632

6

-.615229E-09

204.255

7

-.187841E-08

67.247

8

-.144971E-08

29.571

9

.397608E-09

464.609

10

-.443300E-08

108.969

11%PASS 1#

-.274807E-08

61.312

NO. PASSES # 1

TOTAL INTEGRAL #-2.74807E-09

END

TEST CASES 3(a) and 3(b)

OUTPUT DATA

TEST FUNCTIONS 3(a) and 3(b)

NUMIT ONE %ONE-DIM. INTEGRATION, SIMPSONS RULE
 F%X# SIN%X#

INPUT DATA

B# .314159E&01	J%MAX#11
A# .000000E-99	DELTA1# .1000E-02

ITERATION	INTEGRAL	DELTA
2	.200455E&01	4.481
3	.200026E&01	.214
4	.200001E&01	.012
5%PASS 1#	.200000E&01	0.000

INPUT DATA

B# .628319E&01	J%MAX#11
A# .314159E&01	DELTA1# .1000E-02

ITERATION	INTEGRAL	DELTA
2	-.200455E&01	4.481
3	-.200026E&01	.214
4	-.200001E&01	.012
5%PASS 2#	-.200000E&01	0.000

NO. PASSES # 2
 TOTAL INTEGRAL # 0.00000E-99
 END

APPENDIX D

Glossary

$F_J(a,b)$	-- the approximation of the integral for the Jth iteration over the interval (a,b)
ΔX_J	-- the mesh interval for the Jth iteration
$f(x)$	-- the integrand
C_J	-- the sum of the values of the integrand over the interval (a,b) whose coefficients are 2
D_J	-- the sum of the values of the integrand over the interval (a,b) whose coefficients are 4
J	-- used to denote iteration number
Δ_J	-- convergence number calculated for the Jth iteration
Δ	-- input convergence criterion number
a	-- beginning point of the integration interval
b	-- end point of the integration interval
m	-- used as an index in summation
$J_{\max}$	-- maximum number of iterations permitted
J_{act}	-- actual number of iterations
K	-- constant used in estimating running time

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