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**PROGRAM WEIGHT: A FORTRAN IV PROGRAM FOR EVALUATION OF WEIGHTING
FUNCTIONS USED IN SMALL-ANGLE X-RAY SCATTERING**

Mary G. Buchanan
Robert W. Hendricks

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Mary G. Buchanan and Robert W. Hendricks

SEPTEMBER 1967

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PROGRAM WEIGHT: A FORTRAN IV PROGRAM FOR EVALUATION OF WEIGHTING
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Mary G. Buchanan¹ and Robert W. Hendricks

ABSTRACT

A FORTRAN IV program is presented which evaluates the weighting functions needed to correct observed small-angle x-ray scattering data for the smearing effects of the collimation system. Moments of the weighting functions about both the origin and the mean may also be computed.

INTRODUCTION

In a previous paper, Hendricks and Schmidt² have derived a general equation for evaluating the slit-width and slit-length weighting functions which are necessary for correcting small-angle x-ray scattering data for the smearing effects of the collimation system. Their result, for slit widths, is

$$W_w(u) = L_o L_w [A_w(L_o + L)]^{-1} \int_{x_a(u)}^{x_b(u)} dx e_w(x) \int_{z_a(x,u)}^{z_b(x,u)} dz f_w(z) . \quad (1)$$

The limits of integration are given by

$$\begin{aligned} z_b(x,u) &= \text{Min}(z_{2i-1}; z_{2j-1}) \\ z_a(x,u) &= \text{Max}(z_{2i}; z_{2j}) \end{aligned} \quad (2a)$$

¹Formerly at Computing Technology Center, Oak Ridge Gaseous Diffusion Plant, now at Data Processing Center, E. I. DuPont de Nemours, Spruance Fibers Division, Richmond, Virginia.

²R. W. Hendricks and P. W. Schmidt, "Calculation of Weighting Functions for Collimation Corrections in Small-Angle X-Ray Scattering," Acta Physica Austriaca (in press).

in which

$$z_i = \frac{(L_0 - d_i)(Lu - x) + (-1)^{i+1}(L + L_0)h_i}{L + d_i} \quad (2b)$$

$$z_j = L_0 u - \frac{(L_0 + d_j)x + (-1)^j(L + L_0)h_j}{L - d_j},$$

and

$$x_b(u) = \text{Min}(x_{2i,2i'-1}; x_{2i,2j-1}; w_c) \quad (3)$$

$$x_a(u) = \text{Max}(x_{2i-1,2i'}; x_{2i-1,2j}; -w_c)$$

with

$$x_{ii'} = \frac{L(d_i - d_{i'})u + (-1)^i h_i(L + d_{i'}) + (-1)^{i'+1} h_{i'}(L + d_i)}{d_i - d_{i'}}$$

$$x_{ij} = \frac{(L - d_j)d_i u + (-1)^i h_i(L - d_j) + (-1)^{j+1} h_j(L + d_i)}{d_i + d_j}.$$

The weighting function is nonzero only in the range

$$u_{aaa} \leq u \leq u_{bbb} \quad (4)$$

where

$$u_{bbb} = \text{Min}[u_{2i-1,2i'}(w_c); u_{2i-1,2j}(w_c)] \quad (5)$$

$$u_{aaa} = \text{Max}[u_{2i,2i'-1}(-w_c); u_{2i,2j-1}(-w_c)]$$

$$u_{ii'} = \frac{x}{L} + \frac{(-1)^{i+1} h_i(L + d_{i'}) + (-1)^{i'} h_{i'}(L + d_i)}{L(d_i - d_{i'})}$$

and

$$u_{ij} = \frac{x(d_i + d_j) + (-1)^{i+1} h_i(L - d_j) + (-1)^j h_j(L + d_i)}{d_i(L - d_j)}.$$

In this derivation, the variables have the following meanings: L is the distance from the sample plane to the detector plane, L_0 is the distance from the sample plane to the tube plane, d_i is the distance from the sample plane to the i^{th} collimation edge between the sample plane and the tube plane, h_i is the distance from the i^{th} collimation edge to the camera axis, and d_j and h_j are similarly defined for edges between the sample plane and the detector plane (not including the slit at the detector). The width of the detector slit is $2w_c$, $e_w(x)$ describes the sensitivity of the detector in a direction parallel to the slit width, $f_w(z)$ describes the intensity of the focal spot in the direction of the slit-width, and A_w is a normalization constant which ensures that the area under the weighting function is unity. The weighting function for slit-lengths has the same form and can be evaluated from Eqs. (1) through (5) by making the appropriate changes in notation.

In the original derivation, the subscripts i and j took on all values in the ranges $1 \leq i \leq m$ and $1 \leq j \leq n$, respectively, subject to the condition $i' \leq i$. Here m is the number of pairs of edges between the sample plane and the tube plane, while n is the number of pairs of edges between the sample plane and the detector plane. In that derivation it is not necessary that each member of a pair of edges be equidistance from the sample plane. This leads to the possibility that the denominator in the equations for $x_{ii'}$ and $u_{ii'}$ could be zero for some values of i and i' in their allowable range. For hand calculations, division by zero produces an infinity which is easily handled. However, for computer evaluation, such division must be avoided. Careful examination of the original derivation reveals that if the edges occur in pairs in which each member of the pair is equidistant from the sample plane³ the restriction on i and i' becomes $i' < i$. It is easily verified that under these conditions, the denominators in $x_{ii'}$ and $u_{ii'}$ can never be zero.

³This condition in no way implies that the computation applies only to camera geometries which have real edges which occur in pairs equidistant from the sample. If, as in the Kratky camera, a real edge exists only on one side of the reference line, a dummy edge which is a large distance from the reference line is inserted on the other side of the reference line at the same distance from the sample plane. Such a dummy edge in no way alters the physical situation, but it does meet the mathematical requirements of the equations, and simplifies the computational procedure.

The slit-width collimation correction procedures outlined by Kratky, Porod, and Skala,⁴ and Sauder,⁵ require only knowledge of the k^{th} moment of the weighting function about either the origin or the mean. These moments are readily computed from the relationships

$$M_k = \int_{u_{aaa}}^{u_{bbb}} u^k W_w(u) du$$

and

(6)

$$M_k(\bar{u}) = \int_{u_{aaa}}^{u_{bbb}} (u - \bar{u})^k W_w(u) du .$$

The practical evaluation of Eqs. (1) and (6) is tedious except for geometries having a high degree of symmetry. However, they are ideally suited to computer evaluation. This report describes a FORTRAN IV program which may be used to calculate the weighting function and its moments for small-angle x-ray cameras having a variety of geometries. The reader is referred to the original derivation for a complete discussion of the approximations which limits the validity of the application of Eq. (1) and hence the usefulness of this program. A punched deck for the program may be obtained from R. W. Hendricks.

PROGRAM DESCRIPTION

The object of the program, for which a listing is given in Appendix A, is to evaluate the double integral described by Eq. (1). The integrations are performed by using Simpson's rule for evenly spaced intervals. However, the major portion of the program deals with the calculation of the limits of the integration from Eqs. (2) and (3). Appendix B is a flow chart which explains the operation of the program. The program variables are defined in Appendix C.

⁴O. Kratky, G. Porod, and Z. Skala, Acta Phys. Austriaca 13, 96 (1960).

⁵W. C. Sauder, J. Appl. Phys. 37, 1495 (1966).

Before starting the main portion of the program, a short data format check is performed in loops 1 and 2 to ensure that the input data corresponds to pairs of edges, each member of which is equidistant from the sample plane. If this criterion is not met, an error message is presented in the output, and the computations are terminated.

Using Eqs. (4) and (5), the limits of integration u_{aaa} and u_{bbb} are computed by evaluating the appropriate values of $u_{ii}, (\pm w_c)$ and $u_{ij}, (\pm w_c)$ in loops 3 and 4 or loops 5 and 6, respectively, and comparing the results in SUBMIN and SUBMAX. Then the u increment is calculated as $(u_{bbb} - u_{aaa}) / (NU - 1)$. The initial value of u is set equal to the lower limit, and each successive u up to the upper limit is calculated by adding the u increment to the preceding u value.

In essence, the remainder of the program consists of a series of nested loops. The outside loop (loop 7) calculates the u value. For each value of u , a pair of x limits is calculated in two pairs of inner loops. Loops 8 and 9 find $x_{ii}, (u_\ell)$ while loops 10 and 11 find $x_{ij}, (u_\ell)$. Values of $x_a(u_\ell)$ and $x_b(u_\ell)$ are found in SUBMAX and SUBMIN and the x values are incremented between these limits in the same manner as for u . In order to provide the same degree of accuracy in all of the integrations, the number of x increments (and z increments, to be described below) is the same as the number of u increments (NU). In turn, for each value of u and x a pair of z limits is calculated in loops 13 and 14. The value of z is incremented as before in loop 12, and the function $f_w(z)$ is integrated between these limits. If $f_w(z)$ is not a constant, the appropriate value is found from tabulated input data. It is readily seen that if a value of $f_w(z)$ is to be found for each value of z used in the program, $(NU)^3$ interpolations must be made, while $(NU)^2$ interpolations would be made to find the necessary values of $e_w(x)$. Since NU is of the order of 10^2 , this leads to an unreasonable number of interpolations and excessive machine time. In order to reduce this problem, an alternative procedure has been followed. Immediately upon reading in the $f_w(z)$ data,

a four point Lagrangian interpolation procedure^{6,7} generates a table consisting of $10*(NU - 1)$ equispaced values of $f_w(z)$ and z . Then a table called ZINT(I) is generated which contains a Simpson's Rule integration of $f_w(z)$ from $I = 1$ to $I = I$. With reference to Fig. 1, we find the integral

$$ZANS(MM) = \int_{z_a(x,u)}^{z_b(x,u)} f_w(z) dz \quad (7)$$

may be approximated by

$$ZANS(MM) = ZINT(INTT - 1) - ZINT(INTB) + AREAB + AREAT. \quad (8)$$

The areas AREAB and AREAT are found assuming $f_w(z)$ may be approximated by a straight line from $FWZ(I)$ to $FWZ(I + 1)$.

⁶F. B. Hildebrande, Introduction to Numerical Analysis, p. 60, McGraw-Hill, New York, 1956.

⁷W. E. Milne, Numerical Calculus, , Princeton University Press, Princeton, New Jersey, 1949.

Fig. 1. Schematic Drawing Showing Method for Performing the z-Integrations.

After the integrations have been performed, the corresponding x integral is evaluated. Here, it is not practical to attempt to reduce the number of interpolations in the $e_w(x)$ table in the same manner as for $f_w(z)$. Hence, for each value of $ZANS(MM)$, a value of $EWX(MM)$ is interpolated, and their product $XINT(MM) = EWX(MM)*ZANS(MM)$ becomes the integrand. The values from the x integrations are the unnormalized values of $W_w(u)$. An integration of these values in loop 15 gives the normalization constant. The final values of $W_w(u)$ are obtained by dividing the unnormalized values by this constant. The computation of the various moments is a straightforward integration of the weighting function multiplied by the appropriate factor as indicated by Eq. (6).

DETAILED OPERATING INSTRUCTIONS

The program requires up to 45 input constants and, if $e_w(x)$ and $f_w(z)$ are not constant, two input tables. Each input variable is defined in Appendix D and its format is described in Table D.1. Although the appendix is self-explanatory, a few general remarks are in order.

Experience has shown that for greatest accuracy in the integration, the number of points for which the integration is performed (NU) should exceed 100. Comparison of computed results in which $NU = 101$ with an analytic evaluation of Eq. (1) for a very simple geometry shows that integration errors are less than 0.001%.

The program computation time is critically dependent on (i) the value of NU , and (ii) whether $e_w(x)$ and $f_w(z)$ are constant or are interpolated. It is readily seen that, including the computations necessary for normalization, the running time is roughly proportional to $(NU)^3$. Hence, increasing NU by a factor of 2, increases the running time eightfold. Typical running times on an IBM 360/50 computer for programs having $NU = 101$ are approximately 4 min if $e_w(x)$ and $f_w(z)$ are constant, 17 min if $e_w(x)$ is constant but $f_w(z)$ is read in in tabulated form, and 22 min if both $e_w(x)$ and $f_w(z)$ are read in.

The printed output consists of the input data, including the values of z , $f_w(z)$, x , and $e_w(x)$ if they were given: the normalization factor; the u values and corresponding $W_w(u)$ values; and the moments of the function, if they were calculated. Punched output, if requested, contains only u and $W_w(u)$ values. Two examples are listed in Appendix E.

ACKNOWLEDGMENTS

The authors wish to express their gratitude to J. F. Jamison and R. W. Henderson of the Computing Technology Center, Oak Ridge Gaseous Diffusion Plant for their help in preparing this program.

APPENDIX A

A FORTRAN IV LISTING FOR THE IBM SYSTEM/360 MODEL 50 COMPUTER

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C C C C C C C C

FWZ(LA)#YLAG(SIMPZ(LA),ZVAL,ZWZ,IND,3,NUMZ,IEO)	285
135 CONTINUE	290
CALL SIMP(SIMPZ,FWZ,ZINT,ITONU)	295
C	300
C.....SET UP EWX ARRAY	305
C	310
140 IF(IEX)145,175,145	315
145 READ(5,8015)(XVAL(I),XWX(I),I#1,NUMX)	320
XINCR#(XVAL(NUMX)-XVAL(I))/TWONU	325
SIMPX(I)#XVAL(I)	330
DO 150 LB#2,ITONU	335
150 SIMPX(LB)#SIMPX(LB-1)+XINCR	340
DO 170 LB#1,ITONU	345
DO 160 LP#1,NUMX	350
IF(SIMPX(LB)-XVAL(LP))165,155,160	355
155 EWX(LB)#XWX(LP)	360
GO TO 170	365
160 CONTINUE	370
165 ILP#LP	375
EWX(LB)#YLAG(SIMPX(LB),XVAL,XWX,ILP,3,NUMX,IEC)	380
170 CONTINUE	385
175 ID#I	390
TEMPWC(I)#-WC(I)	395
C****	400
C LOOP ONE	405
C****	410
WRITE(6,8020)	415
8020 FORMAT(1H1,3X,8HSD ARRAY///)	420
LIN#5	425
IFLAG#0	430
DO 190 I#1,M	435
NDX#2*I	440
MDX#NDX-I	445
C	450
C... CHECK TO SEE THAT THE SD ARRAY CONTAINS PAIRS OF EDGES EQUIDISTANT	455
C... FROM THE SAMPLE PLANE TO THE I-TH EDGE, I#1,2,...2*M	460
C	465
IF(SD(NDX).EQ.SD(NDX-1))GO TO 180	470
IFLAG#1	475
WRITE(6,8025)MDX,SD(MDX),NDX,SD(NDX)	480
8025 FORMAT(1H ,3HSD(,I3,3H)# ,F10.5,10H*****ERROR/	485
13HSD(,I3,3H)# ,F10.5,10H*****ERROR)	490
GO TO 185	495
180 WRITE(6,8030)MDX,SD(MDX),NDX,SD(NDX)	500
8030 FORMAT(1H ,3HSD(,I3,3H)# ,F10.5/1H ,3HSD(,I3,3H)# ,F10.5)	505
185 LIN#LIN+2	510
IF(LIN.LE.40)GO TO 190	515
LIN#5	520
WRITE(6,8020)	525
190 CONTINUE	530
C****	535
C END LOOP ONE	540
C****	545
C****	550
C BEGIN LOOP TWO	555
C****	560
WRITE(6,8035)	565

```

8035 FORMAT(1H1,3X,8HTD ARRAY///)
LIN#5
DO 205 I#1,N
NDX#2*I
MDX#NDX-I
C
C... CHECK TO SEE THAT THE TD ARRAY CONTAINS PAIRS OF EDGES EQUIDISTANT
C... THE SAMPLE PLANE TO THE J-TH EDGE, J#1,2,...,2*N
C
      IF(TD(NDX).EQ.TD(MDX))GO TO 155
      IFLAG#1
      WRITE(6,8040)MDX,TD(MDX),NDX,TD(NDX)
8040 FORMAT(1H ,3HTD(,I3,3H)# ,F10.5,10H*****ERROR/1H ,
      13HTD(,I3,3H)# ,F10.5,10H*****ERROR)
      GO TO 200
      195 WRITE(6,8045)MDX,TD(MDX),NDX,TD(NDX)
8045 FORMAT(1H ,3HTD(,I3,3H)# ,F10.5/1H ,3HTD(,I3,3H)# ,F10.5)
      200 LIN#LIN+2
      IF(LIN.LE.40)GO TO 205
      LIN#5
      WRITE(6,8035)
      205 CONTINUE
C****
C      END LOOP TWO
C****
C
C***** WERE ERRORS DISCOVERED IN THE SD AND/OR TD ARRAYS.
C***** IF YES PROCESS THE NEXT CASE.
      IF(IFLAG.EQ.1) GO TO 100
C
C... CALCULATE U(I,IPRIME) AND U(I,J)
C
      NUMIO#0
      NUMIE#0
      DO 220 I#1,M
      DO 220 IP#1,M
      IF(I.LE.IP) GO TO 220
      210 NUMIE#NUMIE+1
      LLI#2*I-1
      LLP#2*IP-1
      UEE(NUMIE)#WC(1)/EL+(POWER(LLI)*(EL+SD(2*IP-1))*H(2*I)+POWER(LLP)
      I* (EL+SD(2*I))*H(2*IP-1))/(EL*(SD(2*I)-SD(2*IP-1)))
      215 NUMIO#NUMIO+1
      LLI#2*I
      LLP#2*IP
      UOO(NUMIO)#WC(1)/EL+(POWER(LLI)*(EL+SD(2*IP))*H(2*I-1)+POWER(LLP)*
      I (EL+SD(2*I-1))*H(2*IP))/(EL*(SD(2*I-1)-SD(2*IP)))
      220 CONTINUE
      NUMA#0
      NUMB#0
      DO 245 I#1,M2
      DO 245 J#1,N2
      LLI#I+1
      IF(MOD(I,2)) 225,230,225
      225 IF(MOD(J,2)) 245,235,245
      230 IF(MOD(J,2)) 240,245,240
      235 NUMB#NUMB+1

```

```

      U(I,J)#WC(I)*(SD(I)+TD(J))/(SD(I)*(EL-TD(J)))+POWER(LLI)*H(I)/SD(I) 855
      I)+POWER(J)*(EL+SD(I))*G(J)/(SD(I)*(EL-TD(J))) 860
      UIO(NUMB)#U(I,J) 865
      NUMB#NUMB 870
      GO TO 245 875
240  NUMA#NUMA+I 880
      U(I,J)#-WC(I)*(SD(I)+TD(J))/(SD(I)*(EL-TD(J)))+POWER(LLI)*H(I)/SD(I) 885
      I)+POWER(J)*(EL+SD(I))*G(J)/(SD(I)*(EL-TD(J))) 890
      UIE(NUMA)#U(I,J) 895
      NUMA#NUMA 900
245  CONTINUE 905
C 910
C... CALCULATE UAAA AND UBBB 915
C 920
      CALL SUBMIN(UIO,UON,UBBB,NUMB,NUMIO) 925
      CALL SUBMAX(UIE,UEE,UAAA,NUMA,NUMIE) 930
      UINC#(UBBB-UAAA)/FLOAT(NU-1) 935
C 940
C.....START U LOOP 945
C 950
      DO 450 L#1,NU 955
      IF(L-1) 250,250,255 960
250  UVAL(L)#UAAA 965
      GO TO 260 970
255  UVAL(L)#UVAL(L-1) + UINC 975
260  IO#0 980
      IE#0 985
C 990
C... CALCULATE X(I,IPRIME) 995
C 1000
      IEE#0 1005
      IOO#0 1010
      DO 265 I#1,M 1015
      DO 265 IP#1,M 1020
      IF(I.LE.IP) GO TO 265 1025
      IOO#IOO+I 1030
      LLI#2*I-1 1035
      LLP#2*IP-1 1040
      XXO(IOO)#(EL*(SD(2*I-1)-SD(2*IP))*UVAL(L)+POWER(LLI)*(EL+SD(2*IP)) 1045
      I      *H(2*I-1)+POWER(LLP)*(EL+SD(2*I-1))*H(2*IP))/ 1050
      I      (SD(2*I-1)-SD(2*IP)) 1055
      IFF#IEF+I 1060
      LLI#2*I 1065
      LLP#2*IP 1070
      XXE(IEE)#(EL*(SD(2*I)-SD(2*IP-1))*UVAL(L)+POWER(LLI)*(EL+SD(2*IP-1) 1075
      I      ))*H(2*I)+POWER(LLP)*(EL+SD(2*I))*H(2*IP-1))/ 1080
      I      (SD(2*I)-SD(2*IP-1)) 1085
265  CONTINUE 1090
C 1095
C... CALCULATE X(I,J) 1100
C 1105
      DO 290 I#1,M2 1110
      DO 290 J#1,N2 1115
      LLJ#J+1 1120
      X(I,J)#((EL-TD(J))*SD(I)*UVAL(L)+ POWER(LLJ) *(EL+SD(I))* 1125
      I      G(J)+ POWER(I) *(EL-TD(J))*H(I))/(SD(I)+TD(J)) 1130
      IF(MOD(I,2)) 275,270,275 1135

```

```

270 IF(MOD(J,2)) 280,290,290      1140
275 IF(MOD(J,2)) 290,285,290      1145
280 IF#IF+1                        1150
    XIE(IE)#X(I,J)                1155
    IE#IF                          1160
    GO TO 290                      1165
285 IO#IO+1                        1170
    XIO(IO)#X(I,J)                1175
    IO#IO                          1180
290 CONTINUE                      1185
C                                  1190
C...   CALCULATE XB(U) AND XA(U)   1195
C                                  1200
    CALL SUBMIN(XIF,XXE,XMIN,IE,IEE) 1205
    CALL SUBMAX(XIO,XXO,XMAX,IO,IOO) 1210
    XMIND(I)#XMIN                  1215
    XMAXD(I)#XMAX                  1220
    CALL SUBMIN(XMIND,WC,XBUI,ID,ID) 1225
    CALL SUBMAX(XMAXD,TEMPWC,XAUI,ID,ID) 1230
    XBU(L)#XBUI                    1235
    XAU(L)#XAUI                    1240
    XINC#(XBU(L)-XAUI(L))/FLOAT(NU-1) 1245
C                                  1250
C.....START X LOOP                1255
C                                  1260
    DO 395 MM#1,NU                 1265
    IF(MM-1) 300,295,300           1270
295 XRAY(MM)#XAU(L)                 1275
    GO TO 305                       1280
300 XRAY(MM)#XRAY(MM-1)+XINC        1285
305 IO#0                            1290
    IE#0                            1295
    JO#0                            1300
    JE#0                            1305
C                                  1310
C...   CALCULATE Z(I)              1315
C                                  1320
    DO 320 I#1,M2                  1325
    LLI#I+1                         1330
    ZI(I)#((ELO-SD(I))*(EL*UVAL(L)-XRAY(MM))+POWER(LLI)*(EL+ELO)*H(I)) 1335
    I/(EL+SD(I))                   1340
    IF(MOD(I,2)) 310,315,310       1345
310 IO#IO+1                         1350
    ZIO(IO)#ZI(I)                  1355
    IO#IO                          1360
    GO TO 320                      1365
315 IF#IF+1                         1370
    ZIE(IE)#ZI(I)                  1375
    IE#IF                          1380
320 CONTINUE                      1385
C                                  1390
C...   CALCULATE Z(J)              1395
C                                  1400
    DO 335 J#1,N2                  1405
    LLJ#J+1                         1410
    ZJ(J)#(ELO*(EL-TD(J))*UVAL(L)-(ELO+TD(J))*XRAY(MM)+POWER(LLJ) * 1415
    I(EL+ELO)*G(J))/(EL-TD(J))     1420

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      IF(MOD(J,2)) 325,330,325
325 JO#JO+1
      ZJO(JO)#ZJ(J)
      JO#JO
      GO TO 335
330 JF#JF+1
      ZJF(JE)#ZJ(J)
      JE#JF
335 CONTINUE
C
CALCULATE ZB(X,U) AND ZA(X,U)
C
      CALL SUBMIN(ZIO,ZJO,ZBU,I,JO)
      CALL SUBMAX(ZIF,ZJF,ZAU,IE,JE)
      ZBU(MM)#ZBU
      ZAU(MM)#ZAU
C
C.....DO Z INTEGRATION
C
      IF(IFZ)340,390,340
340 AREAB#0.
      AREAT#0.
      ZINTB#0.
      ZINTT#0.
      IF(ZAU(MM)-SIMPZ(I))345,345,350
345 IF(ZBU(MM)-SIMPZ(ITONU))370,385,385
350 DO 360 INTB#2,ITONU
      IF(ZAU(MM)-SIMPZ(INTB))355,365,360
355 FWZINB#FWZ(INTB-1)+(ZAU(MM)-SIMPZ(INTB-1))*(FWZ(INTB)-FWZ(INTB-1))
      I/ZINCR
      AREAB#0.5*(SIMPZ(INTB)-ZAU(MM))*(FWZ(INTB)+FWZINB)
      GO TO 365
360 CONTINUE
365 IINTB#INTB
      DO 375 INTT#IINTB,ITONU
      IF(ZBU(MM)-SIMPZ(INTT))370,380,375
370 FWZINT#FWZ(INTT-1)+(ZBU(MM)-SIMPZ(INTT-1))*(FWZ(INTT)-FWZ(INTT-1))
      I/ZINCR
      AREAT#0.5*(ZBU(MM)-SIMPZ(INTT-1))*(FWZ(INTT-1)+FWZINT)
      GO TO 380
375 CONTINUE
380 ZANS(MM)#ZINT(INTT-1)-ZINT(INTB)+AREAB+AREAT
      GO TO 395
385 ZANS(MM)#ZINT(ITONU)
      GO TO 395
390 ZANS(MM)#ZBU(MM)-ZAU(MM)
395 CONTINUE
C
C.....END X LOOP
C
C
C.....DO X INTEGRATION
C
      IF(IFX)400,425,400
400 DO 420 MM#1,NU
      IF(XRAY(MM)-SIMPX(I))405,410,410
405 XINT(MM)#0.

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      GO TO 420
410 IF(XRAY(MM)-SIMPX(1TONU))415,415,405
415 XINT(MM)#ZANS(MM)*YLAG(XRAY(MM),SIMPX,EWX,0,2,1TONU,1EO)
420 CONTINUE
      GO TO 435
425 DO 430 I#1,NU
430 XINT(I)#ZANS(I)
C
C.....WRITE INTERMEDIATE COMPUTATIONS
C
435 IF(KOUT)440,445,440
440 WRITE(6,8050)UVAL(L),XAU(L),XBU(L),(ZAU(ML),ZBU(ML),ZANS(ML),XINT(
      IML),ML#1,NU)
8050 FORMAT(1H1,3H1U#,F9.5,5X,4HXAU#,E14.6,5X,4HXBU#,E14.6/3X,2(3HZAU,
      11X,3HZBU,11X,4HZANS,10X,4HXINT,10X)/(1X,8E14.6))
C
C... CALCULATE UNNORMALIZED WW(U)
C
445 CALL SIMP(XRAY,XINT,XANS,NU)
      WWUP(L)#XANS(NU)*EL*ELO/(EL+ELO)
C
450 CONTINUE
C
C.....END U LOOP
C
C... CALCULATE AW (NORMALIZATION FACTOR)
C
      CALL SIMP(UVAL,WWUP,AANS,NU)
C
C...CALCULATE NORMALIZED WW(U)
C
      DO 455 L#1,NU
      WWU(L)#WWUP(L)/AANS(NU)
455 CONTINUE
C
C CALCULATE THE MOMENTS ABOUT THE ORIGIN
C
C
C... DO WE WANT TO CALCULATE MOMENTS ABOUT THE ORIGIN.
C
      IF(KK) 490,490,460
460 DO 485 MAP#1,KK
      DO 465 LAP#1,NU
465 USTORE(LAP)#(UVAL(LAP)**MAP)*WWU(LAP)
      CALL SIMP(UVAL,USTORE,AMOMNT,NU)
      IF(MAP-2) 470,475,480
470 FIRSTM#AMOMNT(NU)
      GO TO 485
475 SECNDM#AMOMNT(NU)
      GO TO 485
480 THIRDM#AMOMNT(NU)
485 CONTINUE
C
C... DO WE WANT TO CALCULATE MOMENTS ABOUT THE MEAN.
C
490 IF(JJ) 525,525,495
C

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C	CALCULATE THE MOMENTS ABOUT THE MEAN	1995
C		2000
	495 DO 520 MAP#1,JJ	2005
	DO 500 LAP#1,NU	2010
	500 UDIF(LAP) #((UVAL(LAP)-FIRSTM)**MAP)*WWU(LAP)	2015
	CALL SIMP(UVAL,UDIF,AMOMNT,NU)	2020
	IF(MAP-2) 505,510,515	2025
	505 FRSTMM#AMOMNT(NU)	2030
	GO TO 520	2035
	510 SCNDMM#AMOMNT(NU)	2040
	GO TO 520	2045
	515 THRDMM#AMOMNT(NU)	2050
	520 CONTINUE	2055
	525 CONTINUE	2060
	WRITE(6,8055)M,N,NU,KK,JJ,IQUT,IF7,IFX,NUMZ,NUMX,KOUT,EL,ELO,WC	2065
8055	FORMAT(1H1,4X,2HM#,11,3X,2IIN#,11,3X,3HNU#,13,3X,3HKK#,11,3X,3HJJ#,	2070
	111,3X,5HIOUT#,11,3X,4HIFZ#,11/	2075
	21X,4HIFEX#,11,3X,5HNUMZ#,15,3X,5HNUMX#,15,3X,5HKOUT#,11,3X,3HEL#,F8	2080
	3.4,3X,4HELO#,F8.4,3X,3HWC#,F8.4)	2085
	WRITE(6,8060)	2090
8060	FORMAT(1H0,2X,12H SUBSCRIPT I,10X,12H SUBSCRIPT J)	2095
	WRITE(6,8065)(SD(I),TD(I),I#1,8),(H(I),G(I),I#1,8)	2100
8065	FORMAT(1H0, 2(6H D(1)#,F7.3,10X)/2(6H D(2)#,F7.3,10X)/2(6H D(3)#	2105
	1,F7.3,10X)/2(6H D(4)#,F7.3,10X)/ 2(6H D(5)#,F7.3,10X)/2(6H D(6)#,F	2110
	27.3,10X)/2(6H D(7)#,F7.3,10X)/2(6H D(8)#,F7.3,10X)/2(6H H(1)#,F7.3	2115
	3,10X)/2(6H H(2)#,F7.3,10X)/2(6H H(3)#,F7.3,10X)/2(6H H(4)#,F7.3,10	2120
	4X)/2(6H H(5)#,F7.3,10X)/2(6H H(6)#,F7.3,10X)/2(6H H(7)#,F7.3,10X)/	2125
	52(6H H(8)#,F7.3,10X))	2130
	WRITE(6,8070)AANS(NU)	2135
8070	FORMAT(1H0,24HNORMALIZATION FACTOR AW#,E13.5)	2140
	IF(IFX)530,535,540	2145
	530 CALL WOUT1(NUMX,XVAL,XWX)	2150
	535 IF(IFZ)540,545,540	2155
	540 CALL WOUT2(NUMZ,ZVAL,ZWZ)	2160
	545 IF(IQUT) 550,555,550	2165
	550 WRITE(7,8075)(UVAL(I),WWU(I),I#1,NU)	2170
8075	FORMAT(6F13.5,2X)	2175
	555 WRITE(6,8080)	2180
8080	FORMAT(1H1,4X,2H U,7X,6H WW(U),37X,2H U,7X,6H WW(U)/)	2185
	NNU#NU/2	2190
	WRITE(6,8090)(UVAL(I),WWU(I),UVAL(I+NU),WWU(I+NU),I#1,NU)	2195
	IF(MOD(NU,2))560,565,560	2200
560	WRITE(6,8085) UVAL(NU),WWU(NU)	2205
8085	FORMAT(1H ,52X,F11.6,E13.5)	2210
	565 IF(KK)570,100,570	2215
8090	FORMAT(1H ,F11.6,E13.5,28X,F11.6,E13.5)	2220
	IF(KK) 570,100,570	2225
570	WRITE(6,8095)FIRSTM,SCNDM,THRDM	2230
8095	FORMAT(1H0,40HMOMENTS OF THE FUNCTION ABOUT THE ORIGIN//IX,5HIST	2235
	I#,E15.5,10X,5H2ND #,E15.5,10X,5H3RD #,E15.5)	2240
	IF(JJ) 575,100,575	2245
575	WRITE(6,8100)FRSTMM,SCNDMM,THRDMM	2250
8100	FORMAT(1H0,38HMOMENTS OF THE FUNCTION ABOUT THE MEAN//IX,5HIST #,	2255
	IF15.5,10X,5H2ND #,E15.5,10X,5H3RD #,E15.5)	2260
	GO TO 100	2265
	END	2270

SUBROUTINE SUBMIN(A,B,C,M,N)	
DIMENSION A(1),B(1)	5
AMIN#A(1)	10
BMIN#B(1)	15
DO 105 I#1,M	20
IF(AMIN-A(I)) 105,100,100	25
100 AMIN#A(I)	30
105 CONTINUE	35
DO 115 J#1,N	40
IF(BMIN-B(J)) 115,110,110	45
110 BMIN#B(J)	50
115 CONTINUE	55
IF(AMIN-BMIN) 120,120,125	60
120 C#AMIN	65
GO TO 130	70
125 C#BMIN	75
130 RETURN	80
END	85

SUBROUTINE SIMP(XX,FX,AX,NX)	
C PROGRAM AUTHOR ANON.,CENTRAL DATA PROCESSING,1/1/65.	5
DIMENSION XX(2),FX(2),AX(2)	10
DELX#XX(2)-XX(1)	15
AX(1)#0.0	20
DO 105 IX#2,NX,2	25
IF(NX-IX) 100,110,100	30
100 AX(IX)#DELX*(5.0*FX(IX-1)+8.0*FX(IX)-FX(IX+1))/12.0+AX(IX-1)	35
105 AX(IX+1)#DELX*(FX(IX-1)+4.0*FX(IX)+FX(IX+1))/3.0+AX(IX-1)	40
GO TO 115	45
110 AX(NX)#DELX*(-FX(NX-2)+8.0*FX(NX-1)+5.0*FX(NX))/12.0+AX(NX-1)	50
115 RETURN	55
END	60

SUBROUTINE SUBMAX(A,B,C,M,N)	
DIMENSION A(1),B(1)	5
AMAX#A(1)	10
BMAX#B(1)	15
DO 105 I#1,M	20
IF(AMAX-A(I)) 100,105,105	25
100 AMAX#A(I)	30
105 CONTINUE	35
DO 115 J#1,N	40
IF(BMAX-B(J)) 110,115,115	45
110 BMAX#B(J)	50
115 CONTINUE	55
IF(AMAX-BMAX) 120,125,125	60
120 C#BMAX	65
GO TO 130	70
125 C#AMAX	75
130 RETURN	80
END	85

FUNCTION YLAG(XI,X,Y,INDI,NI,IMAX,IFX)	5
C PROG.AUTHORS A.A.BROOKS AND F.C.LONG,CENTRAL DATA PROCESSING,1/1/65.	10
C LAGRANGIAN INTERPOLATION	15
C XI IS INTERPOLATED ENTRY INTO X-ARRAY	20
C N IS THE ORDER OF LAGRANGIAN INTERPOLATION	25
C Y IS ARRAY FROM WHICH YLAG IS OBTAINED BY INTERPOLATION	30
C IND IS THE MIN-I FOR X(I).GT.XI	35
C IF IND#0,X-ARRAY WILL BE SEARCHED	40
C IMAX IS MAX INDEX OF X-AND Y-ARRAYS	45
C EXTRAPOLATION CAN OCCUR,IEX#-1 OR +1	50
DIMENSION X(I),Y(I)	55
IND#INDI	60
N#NI	65
IEX#0	70
IF(N-IMAX) 105,105,100	75
100 N#IMAX	80
IEX#N	85
105 IF(IND)110,110,125	90
110 DO 115 J#1,IMAX	95
IF (XI-X(J)) 120,185,115	100
115 CONTINUE	105
IEX#1	110
GO TO 150	115
120 IND#J	120
125 IF (IND#1) 130,140,135	125
130 IEX#-1	130
135 INL#IND-(N+1)/2	135
IF (INL)140,140,145	140
140 INL#1	145
145 INU#INL+N-1	150
IF (INU-IMAX) 155, 155, 150	155
150 INL#IMAX-N+1	160
INU#IMAX	165
155 S#0.	170
P#1.	175
DO 175 J#INL,INU	180
P#P*(XI-X(J))	185
P#1.	190
DO 170 I#INL,INU	195
IF(I-J)165,160,165	200
160 XD#XI	205
GO TO 170	210
165 XD#X(J)	215
170 D#D*(XD-X(I))	220
175 S#S+Y(I,J)/D.	225
YLAG#S*P	230
180 RETURN	235
185 YLAG#Y(J)	240
GO TO 180	245
END	

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SUBROUTINE WOUT1(NUMX,XVAL,XWX)
DIMENSION XVAL(50),XWX(50)
100 I1#NUMX/4
J1#I1
J2#I1*2
J3#I1*3
WRITE(6,8000)(XVAL(ML),XWX(ML),XVAL(ML+J1),XWX(ML+J1),XVAL(ML+J2),
IXWX(ML+J2),XVAL(ML+J3),XWX(ML+J3),ML#1,I1)
8000 FORMAT(1H1,8X,4HXVAL,11X,3HXXWX,12X,4HXVAL,11X,4HXXWX,11X,4HXVAL,
111X,3HXXWX,12X,4HXVAL,11X,3HXXWX,/(4(1X,F14.6,1X,F14.6)))
NN#MOD(NUMX,4)
IF(NN)105,110,105
105 NN#NUMX-NN+1
WRITE(6,8005)(XVAL(J),XWX(J),J#NN,NUMX)
8005 FORMAT(4(1X,F14.6,1X,F14.6))
110 CONTINUE
RETURN
END

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SUBROUTINE WOUT2(NUMZ,ZVAL,ZWZ)
DIMENSION ZVAL(50),ZWZ(50)
100 I1#NUMZ/4
J1#I1
J2#I1*2
J3#I1*3
WRITE(6,8000)(ZVAL(ML),ZWZ(ML),ZVAL(ML+J1),ZWZ(ML+J1),ZVAL(ML+J2),
IZWZ(ML+J2),ZVAL(ML+J3),ZWZ(ML+J3),ML#1,I1)
8000 FORMAT(1H1,8X,4HZVAL,11X,3HZWZ,12X,4HZVAL,11X,3HZWZ,12X,4HZVAL,
111X,3HZWZ,12X,4HZVAL,11X,3HZWZ,/(4(1X,F14.6,1X,F14.6)))
NN#MOD(NUMZ,4)
IF(NN)105,110,105
105 NN#NUMZ-NN+1
WRITE(6,8005)(ZVAL(J),ZWZ(J),J#NN,NUMZ)
8005 FORMAT(4(1X,F14.6,1X,F14.6))
110 CONTINUE
RETURN
END

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APPENDIX B

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APPENDIX C
PROGRAM VARIABLES

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<u>Variable</u>	<u>Description</u>
AANS(202)	Array containing values of the normalization factor. The last element in the array is the most accurate value.
AMOMNT(202)	Array used in calculating moments of the function.
AREAB	Area under $f_w(z)$ between $z_a(u,x)$ and next highest value of SIMPZ.
AREAT	Area under $f_w(z)$ between $z_b(x,u)$ and next lowest value of ZIMPZ.
EWX(1001)	Array containing calculated values of $e_w(x)$.
FIRSTM	First moment about the origin.
FRSTMM	First moment about the mean.
FWZ(1001)	Array containing calculated values of $f_w(z)$.
FWZINB	Interpolated value of $f_w(z)$ corresponding to $z_a(x,u)$.
FWZINT	Interpolated value of $f_w(z)$ corresponding to $z_b(x,u)$.
G(8)	Array containing h_j .
H(8)	Array containing h_i .
IEX	Flag indicating whether or not x and $e_w(x)$ values are given as data.
IFLAG	Computed flag indicating whether the input data corresponds to pairs of edges with each member of the pair equidistant from the sample plane.
IFZ	Flag indicating whether or not z and $f_w(z)$ values are given as data.
IOUT	Flag indicating form of output.
JJ	Flag indicating whether or not moments about the mean are to be calculated.
KK	Flag indicating whether or not moments about the origin are to be calculated.
M	Number of pairs of slits between sample plane and tube plane.
N	Number of pairs of slits between sample plane and detector plane.
NU	Number values of u .
NUMX	Number of pairs of x and $e_w(x)$ values given as data.
NUMZ	Number of pairs of z and $f_w(z)$ values given as data.
SD(8)	Array containing d_i .
SECNDM	Second moment about the origin.

<u>Variable</u>	<u>Description</u>
SCNDMM	Second moment about the mean.
SIMPX(1001)	Array containing x values that corresponds to $e_w(x)$.
SIMPZ(1001)	Array containing z values that corresponds to $f_w(z)$.
TD(8)	Array containing d_j .
TEMPWC	Contains $-w_c$.
U(8,8)	Values of u_{ij} calculated at $x = w_c$ and $x = -w_c$ used in calculation of the u limits u_{aaa} and u_{bbb} .
UEE(8)	$u_{2i,2i'-1}$.
UDIF(202)	Array containing values of $(u_i - u)^k * W_w(u)$ for each value of u.
UIE(8)	$u_{2i;2j-1}$.
UINC	u increment.
UIO(8)	$u_{2i-1,2j}$.
UOO(8)	$u_{2i-1,2i'}$.
USTORE(202)	Array containing values of $u^k * W_w(u)$ for each value of u.
UVAL(202)	u array.
WC	w_c .
WWU(202)	Array containing normalized $W_w(u)$ for all u values.
WWUP(202)	Array containing unnormalized $W_w(u)$ values for all u values.
X(8,8)	x values used in calculating x limits.
XANS(202)	Array containing results of x integration; last element of the array contains most accurate answer.
XAU(202)	$x_a(u)$.
XBU(202)	$x_b(u)$.
XIE(8)	$x_{2i;2j-1}$.
XINC	x increment.
XINT(202)	Array containing the integrand for x integration; $XINT(I) = EWX(I) * ZANS(I)$.
XIO(8)	$x_{2i-1;2j}$.

<u>Variable</u>	<u>Description</u>
XMAXD	Variable containing maximum x.
XMIND	Variable containing minimum x.
XRAY(1001)	Array containing x values for the integration from XAU to XBU.
XVAL(50)	x values given as data.
XWX(50)	$e_w(x)$ values given as data.
XXE(8)	$x_{2i,2i'-1}$.
XXO(8)	$x_{2i-1,2i'}$.
ZANS(202)	Array containing results of z integration; last element contains most accurate answer.
ZAU(202)	$z_a(x,u)$.
ZBU(202)	$z_b(x,u)$.
ZI(8)	z_i : z values calculated using d_i and h_i .
ZIE(8)	z_{2i} .
ZINT(I)	Array containing the integral of FWZ from SIMPZ(1) to SIMPZ(I).
ZINCR	Increment of z integration.
ZIO(8)	z_{2i-1} .
ZJ(8)	z_j : z values calculated using d_j and h_j .
ZJO(8)	z_{2j-1} .
ZVAL(50)	Array containing z values given as data.
ZWZ(50)	Array containing $f_w(z)$ values given as data.

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APPENDIX D
INPUT VARIABLES

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<u>Variable</u>	<u>Description</u>
EL	The distance from the sample plane to the detector plane; equivalent to L .
ELO	The distance from the sample plane to the tube plane; equivalent to L_0 .
G(J)	The distance from the j^{th} slit to the camera axis; equivalent to h_j .
H(I)	The distance from the i^{th} slit to the camera axis; equivalent to h_i .
IEX	Flag indicating whether or not x and $e_w(x)$ supplied as data; for $IEX = 0$, set $e_w(x) = 1$ for all values of x . When $IEX \neq 0$, values of x and $e_w(x)$ will be read in as data.
IFZ	Flag indicating whether or not z and $f_w(z)$ supplied as data; for $IFZ = 0$, set $f_w(z) = 1$ for all values of z . When $IFZ \neq 0$, values of z and $f_w(z)$ will be read in as data.
IOUT	Flag indicating whether or not a punched deck of the final u and $W_w(u)$ values is to be punched.
JJ	Flag indicating whether or not moments about the mean are to be calculated. $JJ = 0$, do not calculate moments; $JJ = 1$, calculate 1st moment; $JJ = 2$, calculate 1st and 2nd moments; $JJ = 3$, calculate 1st, 2nd, and 3rd moments. 3 is the maximum value of JJ .
KK	Flag indicating whether or not moments about origin are to be calculated. If $KK = 0$, JJ must also be 0. $KK = 0$, do not calculate moments; $KK = 1$, calculate 1st moment; $KK = 2$, calculate 1st and 2nd moments; $KK = 3$, calculate 1st, 2nd, and 3rd moments. 3 is the maximum value of KK .
KOUT	Flag indicating whether or not the values of u , $x_a(u)$, $x_b(u)$ versus $z_a(x,u)$ and $z_b(x,u)$ are printed out. This information is helpful in error analysis. $KOUT = 0$, no printout; $KOUT \neq 0$, printout.
M	Number of pairs of slits between sample plane and tube plane; $1 \leq M \leq 4$.
N	Number of pairs of slits between sample plane and detector plane; $1 \leq N \leq 4$.
NU	Number of u values to be calculated; $NU - 1$ is the number of intervals to be used in evaluating the integrals. $NU \leq 200$.
NUMX	Number of pairs of x and $e_w(x)$ supplied as data.
NUMZ	Number of pairs of z and $f_w(z)$ supplied as data.

<u>Variables</u>	<u>Description</u>
SD(I)	Array of distances from sample plane to the i^{th} slit between the sample plane and the tube plane; $1 \leq I \leq 2*M$.
TD(J)	Array of distances from sample plane to the j^{th} slit between sample plane and detector plane; $1 \leq J \leq 2*N$.
X(NUMX)	Array of x values.
XWX(NUMX)	Array of $e_w(x)$ values.
Z(NUMZ)	Array of z values.
ZWZ(NUMZ)	Array of $f_w(z)$ values.

Table D.1. Format of Information Shown on Data Cards

Card Number ^a	Format	Variables
1	11I5	M, N, NU, KK, JJ, IFZ, IEX, IOUT, NUMZ, NUMX, KOUT
2	3F10.4	EL, ELO, WC
3	8F10.3	SD(I), where I = 1,2, ..., 2*M
4	8F10.3	H(I)
5	8F10.3	TD(J), where J = 1,2, ..., 2*N
6	8F10.3	G(J)
7-19	8F10.3	Z(K), ZWZ(K) alternately; K = 1,2, ..., NUMZ
20-31	8F10.3	X(K), XWX(K) alternately; K = 1,2, ..., NUMX

^aCards 7-31 are not necessary if IFZ and IEX are both 0. Provision has been made for 50 values each of X, XWX, Z, and ZWZ. If the user requires fewer than this number, the number of data cards required for the values can be reduced. For example, if NUMZ = 25, there would be 25 Z values and 25 ZWZ values. Therefore, the Z and ZWZ values would only occupy cards 7-13 and the X and XWX values would be started in data card number 14. If Z and ZWZ values are not read in as data, the X and XWX values start in data card number 7. Reading Z, ZWZ, X, and XWX values in as data is optional. The only restriction is that if Z values are fed in, ZWZ values must be furnished; the same applies for X and XWX.

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APPENDIX E

SAMPLE CALCULATIONS

Example 1: Computations for a typical Kratky Camera geometry. Note the use of dummy edges at $H(I)$ for $I = 2$ and $I = 3$, and at $H(J)$ for $J = 1$ and $J = 2$. There were no $e_w(x)$ or $f_w(z)$ input data.

Example 2: Same as example 1 except with $e_w(x)$ and $f_w(z)$ values read in as input data.

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EXAMPLE 1

M#3 N#1 NU#101 KK#3 JJ#3 IOUT#0 IFZ#0
 IEX#0 NUMZ# 0 NUMX# 0 KOUT#1 EL#209.0000 ELO#188.0000 WCN 0.2600

SUBSCRIPT I	SUBSCRIPT J
D%1<# 22.000	D%1<# 18.000
D%2<# 22.000	D%2<# 18.000
D%3<#117.000	D%3<#*****
D%4<#117.000	D%4<#*****
D%5<#138.000	D%5<#*****
D%6<#138.000	D%6<#*****
D%7<#*****	D%7<#*****
D%8<#*****	D%8<#*****
H%1<# 0.0	H%1<#999.999
H%2<#999.999	H%2<#999.999
H%3<#999.999	H%3<#*****
H%4<# 0.0	H%4<#*****
H%5<# 0.120	H%5<#*****
H%6<# 0.0	H%6<#*****
H%7<#*****	H%7<#*****
H%8<#*****	H%8<#*****

NORMALIZATION FACTOR AW# 0.26394E-01

U	WWTUC	U	WWTUC
-0.001196	0.0	0.004457	0.12870E 03
-0.001083	0.52425E 00	0.004570	0.12544E 03
-0.000970	0.20970F 01	0.004683	0.12217E 03
-0.000857	0.47182E 01	0.004796	0.11891E 03
-0.000744	0.83879E 01	0.004909	0.11564E 03
-0.000631	0.13106E 02	0.005022	0.11238E 03
-0.000518	0.18873E 02	0.005135	0.10911E 03
-0.000405	0.25688E 02	0.005248	0.10585E 03
-0.000292	0.33551E 02	0.005361	0.10258E 03
-0.000179	0.42463E 02	0.005474	0.99319E 02
-0.000066	0.52424E 02	0.005587	0.96054E 02
0.000047	0.62960E 02	0.005700	0.92789E 02
0.000160	0.73349E 02	0.005813	0.89524E 02
0.000274	0.83585E 02	0.005926	0.86260E 02
0.000387	0.93666E 02	0.006039	0.82994E 02
0.000500	0.10359E 03	0.006152	0.79730E 02
0.000613	0.11337E 03	0.006265	0.76465E 02
0.000726	0.12298E 03	0.006379	0.73200E 02
0.000839	0.13245E 03	0.006492	0.69935E 02
0.000952	0.14176E 03	0.006605	0.66670E 02
0.001065	0.15091E 03	0.006718	0.63405E 02
0.001178	0.15991E 03	0.006831	0.60140E 02
0.001291	0.16839E 03	0.006944	0.56875E 02
0.001404	0.17569E 03	0.007057	0.53610E 02
0.001517	0.18177E 03	0.007170	0.50345E 02
0.001630	0.18665E 03	0.007283	0.47080E 02
0.001743	0.19034E 03	0.007396	0.43815E 02
0.001856	0.19281E 03	0.007509	0.40550E 02
0.001969	0.19408E 03	0.007622	0.37285E 02
0.002082	0.19416E 03	0.007735	0.34022E 02
0.002195	0.19303E 03	0.007848	0.30859E 02
0.002309	0.19069E 03	0.007961	0.27850E 02
0.002422	0.18747E 03	0.008074	0.24996E 02
0.002535	0.18421E 03	0.008187	0.22296E 02
0.002648	0.18094E 03	0.008300	0.19750E 02
0.002761	0.17768E 03	0.008414	0.17358E 02
0.002874	0.17441E 03	0.008527	0.15121E 02
0.002987	0.17115E 03	0.008640	0.13038E 02
0.003100	0.16788E 03	0.008753	0.11109E 02
0.003213	0.16462E 03	0.008866	0.93349E 01
0.003326	0.16135E 03	0.008979	0.77148E 01
0.003439	0.15807E 03	0.009092	0.62489E 01
0.003552	0.15482E 03	0.009205	0.49374E 01
0.003665	0.15156E 03	0.009318	0.37803E 01
0.003778	0.14829E 03	0.009431	0.27774E 01
0.003891	0.14503E 03	0.009544	0.19286E 01
0.004004	0.14176E 03	0.009657	0.12344E 01
0.004117	0.13850E 03	0.009770	0.69437E 00
0.004230	0.13523E 03	0.009883	0.30863E 00
0.004344	0.13197E 03	0.009996	0.77140E-01
		0.010109	0.0

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EXAMPLE 2

M#3	N#1	NUM101	KK#3	JJ#3	IOU#0	IFZ#1
IE#1	NUM#	26	NLM#	49	KOUT#1	EL#209.0000
						ELO#188.0000
						WC# 0.2500

SUBSCRIPT I	SUBSCRIPT J
D%1<# 22.000	D%1<# 18.000
D%2<# 22.000	D%2<# 18.000
D%3<#117.000	D%3<#*****
D%4<#117.000	D%4<#*****
D%5<#138.000	D%5<#*****
D%6<#138.000	D%6<#*****
D%7<#*****	D%7<#*****
D%8<#*****	D%8<#*****
H%1<# 0.0	H%1<#999.999
H%2<#999.999	H%2<#999.999
H%3<#999.999	H%3<#*****
H%4<# 0.0	H%4<#*****
H%5<# 0.120	H%5<#*****
H%6<# 0.0	H%6<#*****
H%7<#*****	H%7<#*****
H%8<#*****	H%8<#*****

NORMALIZATION FACTOR AW# 0.39193E-02

XVAL	XWX	XVAL	XWX	XVAL	XWX	XVAL	XWX
-0.240000	0.0	-0.120000	0.0	0.0	1.000000	0.120000	0.0
-0.230000	0.0	-0.110000	0.0	0.010000	0.990000	0.130000	0.0
-0.220000	0.0	-0.100000	0.0	0.020000	0.960000	0.140000	0.0
-0.210000	0.0	-0.090000	0.150000	0.030000	0.910000	0.150000	0.0
-0.200000	0.0	-0.080000	0.360000	0.040000	0.840000	0.160000	0.0
-0.190000	0.0	-0.070000	0.510000	0.050000	0.750000	0.170000	0.0
-0.180000	0.0	-0.060000	0.640000	0.060000	0.640000	0.180000	0.0
-0.170000	0.0	-0.050000	0.750000	0.070000	0.560000	0.190000	0.0
-0.160000	0.0	-0.040000	0.840000	0.080000	0.360000	0.200000	0.0
-0.150000	0.0	-0.030000	0.910000	0.090000	0.190000	0.210000	0.0
-0.140000	0.0	-0.020000	0.960000	0.100000	0.0	0.220000	0.0
-0.130000	0.0	-0.010000	0.990000	0.110000	0.0	0.230000	0.0
0.240000	0.0						

ZVAL	ZWZ	ZVAL	ZWZ	ZVAL	ZWZ	ZVAL	ZWZ
0.0	1.000000	0.120000	0.700000	0.240000	0.400000	0.360000	0.650000
0.020000	0.095000	0.140000	0.650000	0.260000	0.300000	0.380000	0.700000
0.040000	0.090000	0.160000	0.600000	0.280000	0.450000	0.400000	0.750000
0.060000	0.850000	0.180000	0.550000	0.300000	0.500000	0.420000	0.800000
0.080000	0.800000	0.200000	0.500000	0.320000	0.550000	0.440000	0.850000
0.100000	0.750000	0.220000	0.450000	0.340000	0.600000	0.460000	0.900000
0.480000	0.950000	0.500000	1.000000				

U	WWXUK	U	WWXUK
-0.001196	0.0	0.004457	0.99113E 02
-0.001083	0.0	0.004570	0.95599E 02
-0.000970	0.0	0.004683	0.92412E 02
-0.000857	0.0	0.004796	0.89558E 02
-0.000744	0.0	0.004909	0.87034E 02
-0.000631	0.0	0.005022	0.84834E 02
-0.000518	0.0	0.005135	0.82936E 02
-0.000405	0.96722E-01	0.005248	0.81309E 02
-0.000292	0.10983E 01	0.005361	0.79912E 02
-0.000179	0.26700E 01	0.005474	0.78693E 02
-0.000066	0.44681E 01	0.005587	0.77595E 02
0.000047	0.83282E 01	0.005700	0.76553E 02
0.000160	0.17069E 02	0.005813	0.75506E 02
0.000274	0.32384E 02	0.005926	0.74403E 02
0.000387	0.54886E 02	0.006039	0.73206E 02
0.000500	0.83960E 02	0.006152	0.71889E 02
0.000613	0.11855E 03	0.006265	0.70436E 02
0.000726	0.15701E 03	0.006379	0.68844E 02
0.000839	0.19443E 03	0.006492	0.67116E 02
0.000952	0.22578E 03	0.006605	0.65256E 02
0.001065	0.24909E 03	0.006718	0.63271E 02
0.001178	0.26391E 03	0.006831	0.61160E 02
0.001291	0.27060E 03	0.006944	0.58923E 02
0.001404	0.27037E 03	0.007057	0.56561E 02
0.001517	0.26502E 03	0.007170	0.54073E 02
0.001630	0.25692E 03	0.007283	0.51460E 02
0.001743	0.24836E 03	0.007396	0.48722E 02
0.001856	0.24001E 03	0.007509	0.45857E 02
0.001969	0.23201E 03	0.007622	0.42868E 02
0.002082	0.22433E 03	0.007735	0.39752E 02
0.002195	0.21688E 03	0.007848	0.36512E 02
0.002309	0.20957E 03	0.007961	0.33150E 02
0.002422	0.20238E 03	0.008074	0.29655E 02
0.002535	0.19532E 03	0.008187	0.26040E 02
0.002648	0.18838E 03	0.008300	0.22297E 02
0.002761	0.18157E 03	0.008414	0.18429E 02
0.002874	0.17489E 03	0.008527	0.14457E 02
0.002987	0.16833E 03	0.008640	0.10637E 02
0.003100	0.16189E 03	0.008753	0.72342E 01
0.003213	0.15559E 03	0.008866	0.44370E 01
0.003326	0.14943E 03	0.008979	0.23447E 01
0.003439	0.14342E 03	0.009092	0.97317E 00
0.003552	0.13757E 03	0.009205	0.24815E 00
0.003665	0.13191E 03	0.009318	0.11975E-01
0.003778	0.12646E 03	0.009431	-0.12315E-04
0.003891	0.12124E 03	0.009544	0.0
0.004004	0.11626E 03	0.009657	0.0
0.004117	0.11154E 03	0.009770	0.0
0.004230	0.10710E 03	0.009883	0.0
0.004344	0.10295E 03	0.009996	0.0
		0.010109	0.0

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