AIM

Association for Information and Image Management

1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202

Centimeter

Inches

MANUFACTURED TO AIM STANDARDS
BY APPLIED IMAGE, INC.

1 of 1

Program WALKMAN: A Code Designed to Perform
Electron Single Collision Elastic Scattering
Monte Carlo Calculations

by
Dermott E. Cullen
University of California
Lawrence Livermore National Laboratory
P.O. Box 808
L-294
Livermore, CA 94550

August 1994

MASTER

Program WALKMAN: A Code Designed to Perform
Electron Single Collision Elastic Scattering
Monte Carlo Calculations

by
Dermott E. Cullen
University of California
Lawrence Livermore National Laboratory
P.O. Box 808
L-294
Livermore, CA 94550

August 1994

Introduction

The computer code WALKMAN performs electron single collision elastic scattering Monte Carlo calculations in spherical or planar geometry. It is intended as a research tool to obtain results that can be compared to the results of condensed history calculations.

Code Documentation

This code is designed to be self documenting, in the sense that the latest documentation is included as comment lines at the beginning of the code. Printed documentation, such as this document, is periodically published and consists mostly of a copy of the comment lines from the code. The user should be aware that the comment lines within the code are continually updated to reflect the most recent status of the code and these comments should always be considered to be the most recent documentation for the code and may supersede published documentation, such as this document. Therefore, the user is advised to always read the documentation within the actual code.

The remainder of this report consists of example results and a listing of the documentation which appears at the beginning of the code.

Example Results

The first figure defines the variation of eta vs. element (Z) and electron energy E, for representative values of Z between 1 and 100, and over the energy range 1 keV to 1 GeV.

The next four figures present results for a calculation using $\eta = 1.0 \times 10^{-5}$ in spherical geometry for spheres 1 to 1000 mean free paths thick. The first of these figures presents results as a function of the cosine between the initial electron direction and the point at which they leak from a sphere, as measured relative to the center of the sphere; this defines the lateral displacement (i.e., if there were no lateral displacement we would expect all electrons to emerge from the sphere only along the initial direction). The next figure presents results as a function of the cosine between initial electron and the direction the electron leaks from the sphere, as measured relative to the point the electron leaks from the sphere; these are the results normally defined by condensed history calculations = the angular distribution after transporting at distance t, relative to the point t. The next two figures present results as a function of

the cosine relative to the origin. In the first of these two $\langle 1-\cos \rangle$ relative to the surface vs. $1-\cos$ relative to the center is presented. From the results we can see that even in the most forward direction (little lateral displacement) $\langle 1-\cos \rangle$ is increasing as the electrons transport through thicker and thicker spheres. Relative to $\langle 1-\cos \rangle$ for the single collision angular distribution, after transporting through N mean free paths the $\langle 1-\cos \rangle$ of the emerging angular distribution has increased by roughly a factor of N . The next figure presents results for the distance to leakage (in mean free paths) versus spherical radius. We can see that for forward scattering (small $1-\cos$) on average the electrons have N collisions when they transport through N mean free paths of material; no big surprise there. For progressively larger $(1-\cos)$ the number of collisions increases and for backscatter through 180 degrees the number of collisions roughly double. We can also see that for progressively thicker spheres as the angular distribution approaches isotropic the distance to leakage is more than the mean free path thickness of the spheres (see, 1000 MFP results).

The next two figures present integrals of the angular distribution; the first integrated from $(1-\cos) = 0$ to 2, and the second integrated from $(1-\cos) = 2$ to 2. These are intended to allow us to see the behavior at both ends of the integral.

Results using planar geometry are very similar, particularly for very forward scattering. The one except is the distance to collision. The following figure presents the distance to leakage in planar geometry for planes 1 to 10 mean free paths thick. For distance to leakage in spherical or planar geometry obviously the difference is that in planar geometry as the $\cos$ approaches 90 degrees ($1-\cos = 1$) the distance to leakage approaches infinity, whereas in spherical geometry it always has a finite value; compare the plots of distance to collision for spheres and planes.

Electron Elastic Scattering $A/[(1-\cos(\vartheta))+\eta]^2$
 η vs. Element (Z) and Energy (MeV)

Leakage ($\eta = 10^{-5}$)
Relative to Z Axis

Distance to Leakage ($\eta = -5$)
Mean Free Paths

```

C      PROGRAM WALKMAN
C=====
C
C      BY DERMOTT E. CULLEN
C      UNIVERSITY OF CALIFORNIA
C      LAWRENCE LIVERMORE NATIONAL LABORATORY
C      L=294
C      P.O. BOX 808
C      LIVERMORE, CA 94550
C
C      TELE: 510-423-7379
C      E. MAIL: CULLEN1@LLNL.GOV
C
C      VERSION 90-1 (SEPT. 1990)
C              92-1 (JULY 1992)      *GENERAL CLEAN UP AND IMPROVED
C                                      SPEED
C              94-1 (AUG. 1994)      *IMPROVED SCORNG BINS
C                                      *THICKNESS DEPENDENT SCORING
C                                      BINS TO SPEED CONVERGENCE
C
C      PURPOSE
C=====
C      SINGLE COLLISION ELECTRON SCATTERING IN SPHERICAL OR PLANAR
C      GEOMETRY, TO OBTAIN RESULTS THAT CAN BE COMPARED TO CONDENSED
C      HISTORY RESULTS. NO ATTEMPT IS MADE TO PREPARE GENERAL RESULTS
C      FOR LATER USE IN TRANSPORT CALCULATIONS.
C
C      OVERVIEW OF METHODS
C=====
C      MONTE CARLO IS USED TO TRANSPORT ELECTRONS.
C
C      ONLY ELASTIC SCATTERING IS CONSIDERED.
C
C      ELECTRONS ARE TRANSPORTED IN SPHERICAL OR PLANAR GEOMETRY.
C
C      ELECTRONS ARE TRACKED IN 3-D GEOMETRY, IN X, Y, Z WITH
C      DIRECTION COSINES ALPHA, BETA, GAMMA, STARTING FROM THE
C      CENTER OF A NUMBER OF CONCENTRIC SPHERES OR AT THE SURFACE
C      OF A NUMBER OF Z PLANES, INITIALLY DIRECTED ALONG THE POSITIVE
C      Z AXIS - INITIALLY,
C      X = Y = Z = 0
C      ALPHA = BETA = 0
C      GAMMA = 1
C
C      DISTANCE IS MEASURED IN UNITS OF MEAN FREE PATHS, E.G.,
C      A SPHERE 5 UNITS IN RADIUS IS 5 MEAN FREE PATHS IN RADIUS.
C
C      SINGLE COLLISION SCATTERING IS BASED ON SCREENED COULOMB,
C
C       $P(\mu) * D(\mu) = A * D(\mu) / [(1-\mu) + \text{ETA}]^2$ 
C      MU      = COSINE OF THE SCATTERING ANGLE
C      ETA     = SCREENING PARAMETER
C      A       =  $\text{ETA} * (\text{ETA} + 2) / 2$  = A NORMALIZATION FACTOR
C
C      THE ONLY IMPLIED DEPENDENCE ON ENERGY AND ELEMENT IS
C      THROUGH THE PARAMETER ETA. BY FOCUSING ON ETA WE CAN
C      AVOID HAVING TO PERFORM CALCULATIONS FOR MANY DIFFERENT
C      ELEMENTS AT MANY DIFFERENT ENERGIES, AND INSTEAD WE
C      NEED ONLY BE CONCERNED WITH A RANGE OF ETA.
C
C      THIS DISTRIBUTION IS ANALYTICALLY INVERTED FOR SAMPLING,
C      (AS DESCRIBED IN DETAIL BELOW), RESULTING IN A FAST, ONE
C      LINE DEFINITION OF THE SAMPLED SCATTERING COSINE.
C
C      THEY ARE SCORED - ONLY - THE FIRST TIME THEY CROSS EACH
C      SPHERICAL OR PLANAR SURFACE, FROM INSIDE TO OUTSIDE. EACH
C      HISTORY IS FOLLOWED UNTIL THE ELECTRON LEAKS FROM THE OUTER

```

```

C MOST SPHERE OR THICKEST PLANE OR ARE REFLECTED FROM THE
C PLANE AT Z = 0.
C
C IN ORDER TO SIMULATE CONDENSED HISTORY RESULTS, ENERGY LOSS
C IS NOT INCLUDED DURING TRANSPORT - PRESUMABLY THIS CAN BE
C FOLDED INTO THE RESULTS LATER, ONCE A PATH LENGTH FOR
C TRANSPORT HAS BEEN SAMPLED.
C
C WITH THIS MODEL THE RESULTS ARE A FUNCTION OF,
C 1) ETA - THE SCREEN FACTOR IN  $A/[(1-\cos)+\eta]^2$ 
C 2) RADIUS OR PLANE THICKNESS
C 3) THE COSINE OF THE ANGLE BETWEEN THE RADIUS VECTOR AND
C POINT OF LEAKAGE FROM THE SPHERE =  $Z/R = -1$  TO  $+1$ 
C (THE DISTANCE ALONG THE Z AXIS/RADIUS)
C 4) THE COSINE OF THE ANGLE RELATIVE TO THE Z AXIS AT
C POINT OF LEAKAGE = GAMMA (THE DIRECTION COSINE
C RELATIVE TO THE Z AXIS)
C 5) AN AZIMUTHAL ANGLE ABOUT GAMMA
C
C SINCE THERE IS NO ENERGY LOSS, ETA IS A CONSTANT = AN
C INPUT PARAMETER. SINCE ELECTRONS CANNOT DISAPPEAR THE
C NUMBER OF ELECTRONS CROSSING EACH SPHERE WILL BE THE
C SAME FOR ALL SPHERES.
C
C DEFINITION OF ETA
C =====
C ETA DEPENDS OF ELEMENT (Z) AND ENERGY (E). THE BELOW DEFINITION
C IS FOR ENERGY IN UNITS OF MEV.
C
C  $F(\cos)*D(\cos) = A*D(\cos)/[(1 - \cos) + \eta]^2$ 
C
C WARNING - THE ABOVE EQUATION IS SOMETIMES WRITTEN
C  $F(\cos)*D(\cos) = A*D(\cos)/[(1 - \cos) + 2*\eta]^2$ 
C USING 2*ETA, INSTEAD OF ETA - BE SURE THAT YOU
C INTERPRET ETA AS DEFINED HERE.
C
C  $\eta = C1*[C2 + C3]$ 
C
C  $C1 = C4*(Z^{2/3})/[4*(\tau*(\tau+2))]$ 
C  $C2 = 1.13$ 
C  $C3 = \frac{3.76*[\alpha*Z*(\tau+1)]^2}{\tau*(\tau+2)} * \left[\frac{\tau}{\tau+1}\right]^{1/2}$ 
C  $C4 = 2*(\alpha/0.885)^2$ 
C  $\tau = E/0.511$ 
C  $\alpha = 1/137$  (THE FINE STRUCTURE CONSTANT)
C
C I/O FILES
C =====
C


| UNIT | FILENAME    | DESCRIPTION                                                           |
|------|-------------|-----------------------------------------------------------------------|
| 3    | REPORT      | OUTPUT REPORT                                                         |
| 5    | WALKMAN.INP | INPUT PARAMETERS                                                      |
| 12   | PLOTTAB.CUR | PLOTTAB FORMATTED DIFFERENTIAL RESULTS                                |
| 11   | PLOTTAB.I1  | PLOTTAB FORMATTED INTEGRAL RESULTS<br>[INTEGRAL FOR (1-COS) = 2 TO 0] |
| 15   | PLOTTAB.I2  | PLOTTAB FORMATTED INTEGRAL RESULTS<br>[INTEGRAL FOR (1-COS) = 0 TO 2] |
| 14   | WALKMAN.BIN | RESTART FILE                                                          |


C
C INPUT PARAMETERS
C =====


| LINE | COLUMNS | FORMAT | DESCRIPTION                 |
|------|---------|--------|-----------------------------|
| 1    | 1-10    | I10    | GEOMETRY<br>= 1 - SPHERICAL |


```

```

C                                     = 2 - PLANAR
C      1      11-20      I10      NUMBER OF BATCHES
C      1      21-20      I10      NUMBER OF ELECTRONS PER BATCH
C      1      31-40      I10      NUMBER OF SURFACES (SPHERES/PLANES)
C      1      41-50      D10.3     ETA
C      1      51-60      I10      Z OF ELEMENWNT
C      1      61-70      D10.3     ENERGY OF ELECTRONS (MEV)
C      2-N      1-10      D10.3     SURFACE (SPHERE RADIUS/PLANE Z)
C
C  LIMITATIONS
C  =====
C  YOU MAY INPUT EITHER ETA DIRECTLY, OR THE Z OF AN ELEMENT
C  AND THE ENERGY OF THE ELECTRONS (MEV) AND THE PROGRAM WILL
C  DEFINE ETA. IF BOTH THE Z OF THE ELEMENT AND THE ENERGY ARE
C  POSITIVE THEY WILL BE USED TO DEFINE ETA (IN THIS CASE THE
C  INPUT ETA VALUE IS IGNORED). OTHERWISE THE INPUT VALUE OF
C  ETA WILL BE USED.
C
C  ALL OF THE INPUT PARAMETERS MUST BE POSITIVE. THE NUMBER OF
C  SPHERES OR PLANES MUST BE 1 TO 17. THE RADII OR PLANE Z LOCATION
C  MUST BE IN ASCENDING ORDER.
C
C  A NEGATIVE NUMBER OF BATCHES INDICATES RESTART - SEE DETAILS
C  BELOW (THIS IS THE ONLY EXCEPTION TO THE RULE THAT ALL INPUT
C  PARAMETERS MUST BE POSITIVE).
C
C  IF ANY OF THESE CONDITIONS ARE NOT MET THE PROGRAM WILL
C  TERMINATE.
C
C  EXAMPLE INPUT
C  =====
C      1      2      3      4      5      6      7
C 123456789012345678901234567890123456789012345678901234567890
C  -----
C      1      1000      1000000      3 1.000D-05
C 1.000D+00
C 3.000D+00
C 1.000D+01
C
C  THE ABOVE INPUT PARAMETERS WILL RUN IN SPHERICAL GEOMETRY,
C  1000 BATCHES OF 1 MILLION HISTORIES EACH (A TOTAL OF 1 BILLION
C  HISTORIES) USING ETA=1.0D-05 AND 3 SPHERES BETWEEN 1 AND 10
C  MEAN FREE PATHS THICK.
C
C  IF YOU COMPLETE THIS RUN, OR TERMINATE PREMATURELY (AS DESCRIBED
C  BELOW) YOU CAN RESTART AND CONTINUE RUNNING MORE HISTORIES FROM
C  THE POINT THE PROGRAM TERMINATED BY USING THE ABOVE INPUT, BUT
C  WITH A NEGATIVE BATCH COUNT TO INDICATE RESTART, AS SHOWN BELOW,
C
C      1      2      3      4      5      6      7
C 123456789012345678901234567890123456789012345678901234567890
C  -----
C      1      -1000      1000000      3 1.000D-05
C 1.000D+00
C 3.000D+00
C 1.000D+01
C
C  BOTH OF THE ABOVE EXPLICITLY SPECIFY ETA ON INPUT. TO RUN
C  1 MEV ELECTRONS THROUGH HYDROGEN (Z=1) AND HAVE THE PROGRAM
C  DEFINE ETA INPUT THE FOLLOWING,
C
C      1      2      3      4      5      6      7
C 123456789012345678901234567890123456789012345678901234567890
C  -----
C      1      1000      1000000      3      1 1.000D+00
C 1.000D+00

```



```

C 3.000D+00
C 1.000D+01
C
C IF YOU FOLLOW THE BELOW RECOMMENDATIONS YOU CAN USE THE FOLLOWING
C STANDARD INPUT LINES.
C
C      1      2      3      4      5      6      7
C 123456789012345678901234567890123456789012345678901234567890
C -----
C      1      1000  1000000      1 1.000D-05
C 1.000D+00
C 3.000D+00
C 1.000D+01
C 3.000D+01
C 1.000D+02
C 3.000D+03
C 1.000D+05
C
C START WITH ONLY 1 SURFACE (AS INDICATED ON THE FIRST INPUT LINE)
C ONLY THE FIRST SURFACE WILL BE READ (ALL FOLLOWING SURFACES ARE
C IGNORED). RUN UNTIL YOU HAVE STATISTICAL CONVERGENCE (USE
C PLOTTAB). NEXT RUN USING 3 SURFACES AND 100,000 HISTORIES PER
C BATCH - AGAIN RUN UNTIL CONVERGENCE. NEXT RUN 5 SURFACES, WITH
C 10,000 HISTORIES PER BATCH. FINALLY RUN 7 SURFACES, WITH 1,000
C HISTORIES PER BATCH. THIS APPROACH WILL GET YOU CONVERGED
C RESULTS OVER THE ENTIRE RANGE OF THICKNESSES FAR FASTER THAN
C BY TRYING TO RUN ALL THICKNESSES AT ONCE FROM THE BEGINNING
C (FOR AN EXPLANATION, SEE THE DISCUSSION OF RUNNING TIME BELOW).
C
C RECOMMENDATIONS
C =====
C SPHERICAL OR PLANAR GEOMETRY
C =====
C FOR SMALL VALUES OF ETA THE RESULTS FOR FORWARD SCATTERING MUST
C BE ALMOST IDENTICAL IN EITHER GEOMETRY - IF THE ELECTRONS DO NOT
C MOVE MUCH OFF OF THEIR INITIAL DIRECTION OF TRAVEL THEY CANNOT
C BE SENSITIVE TO GEOMETRY.
C
C SPHERICAL GEOMETRY CAN BE USED TO SIMULATE CONDENSED HISTORY.
C PLANAR GEOMETRY CAN BE USED FOR COMPARISON TO EXPERIMENTAL
C MEASUREMENTS IN PLANAR GEOMETRY - THIS IS PARTICULARLY
C COLNVENIENT FOR BACKSCATTERING MEASUREMENTS.
C
C COMPARISON OF THE LATERAL DISPLACEMENT RESULTS ALLOWS YOU TO
C JUDGE THE VALIDITY OF AFTER ADVANCING SOME DISTANCE Z, 1)
C LATERALLY DISPLACE 90 FROM PATH IN Z DIRECTION (USE PLANE
C GEOMETRY DISPLACEMENT), OR 2) LATERALLY DISPLACE TO CONSERVE
C THE TOTAL CROW FLY DISTANCE (USE SPHERICAL DISPLACEMENT).
C
C VALUES OF ETA
C =====
C THE INTERESTING RANGE OF ETA IS ABOUT 1.0D-2 TO 1.0D-5. FOR
C SMALL VALUES OF ETA THE SINGLE COLLISION ANGULAR DISTRIBUTION
C WILL VARY FROM ABOUT 1/ETA IN THE FORWARD DIRECTION TO ABOUT
C ETA IN THE BACKWARD DIRECTION, E.G., FOR ETA = 1.0D-05, FROM
C 1.0D+5 TO 1.0D-5 = 10 ORDERS OF MAGNITUDE -- WHICH IS VERY
C DIFFICULT TO STATISTICALLY SAMPLE - SO DO NOT USE VALUES OF
C ETA WHICH ARE MUCH SMALLER THAN THIS - YOU WOULD HAVE TO RUN
C AN ENORMOUS NUMBER OF HISTORIES TO OBTAIN GOOD STATISTICAL
C RESULTS OVER THE ENTIRE ANGULAR RANGE.
C
C LARGER VALUES OF ETA CORRESPOND TO ANGULAR DISTRIBUTIONS THAT
C ARE NOT VERY ANISOTROPIC, AND AS SUCH DIFFICULT TO SIMULATE
C USING CONDENSED HISTORY. FOR ETA > 1, THE SINGLE COLLISION
C ANGULAR DISTRIBUTION IS ALMOST ISOTROPIC, AND AFTER A FEW
C COLLISIONS THE ANGULAR DISTRIBUTION OF ELECTRONS WULL ALSO

```

BE ALMOST ISOTROPIC - THE ELECTRONS ARE SIMPLY DIFFUSING IN ALL DIRECTIONS WITHIN THE GEOMETRY, AND IT CAN TAKE MANY COLLISIONS FOR THEM TO FIND THEIR WAY OUT.

IF YOU WISH TO INPUT THE Z OF AN ELEMENT AND AN ENERGY YOU SHOULD FIRST CHECK TO INSURE THAT THE DEFINED VALUE OF ETA IS IN A REASONABLE RANGE. THE EASIEST WAY TO DO THIS IS TO INPUT Z AND ENERGY - THE OUTPUT REPORT WILL DEFINE THE DEFINED ETA - IF IT IS REASONABLE LET THE PROGRAM RUN - IF NOT, STOP THE PROGRAM AND SELECT ANOTHER Z AND E FOR INPUT.

RADIUS OR PLANE THICKNESS

THE INTERESTING, AND REASONABLE, RANGE OF RADIUS OR THICKNESS IS ABOUT 1 TO 1000 MEAN FREE PATHS - WHICH CORRESPONDS TO CONDENSED HISTORY, CONDENSING 1 TO 1000 EVENTS PER SPATIAL STEP. IF YOU USE THICKER MEDIA RUNNING TIME WILL RAPIDLY INCREASE. YOU CAN OBTAIN FAIRLY SMOOTHLY VARYING RESULTS USING ONLY 3 RADII PER DECADE, E.G., ON INPUT SPECIFY 3 RADII AT 1, 3 AND 10 MFP.

RANGES OF RADII OR PLANE THICKNESSES

DEFINING,

EVENT = 1 ELASTIC COLLISION

HISTORY = ALL EVENTS UNTIL THE ELECTRON LEAKS FROM THE OUTER MOST RADII OR THICKEST PLANE

FOR THIN SPHERES (1 TO 10 MFP THICK) THE ANGULAR DISTRIBUTION WILL BE VERY SIMILAR TO THE SINGLE COLLISION DISTRIBUTION (SEE DETAILS BELOW). FOR THICKER SPHERES THE ANGULAR DISTRIBUTION WILL BECOME PROGRESSIVELY SMOOTHER, WITH LESS VARIATION FROM FORWARD TO BACKSCATTER.

THIN SPHERES (1 TO 10 MFP THICK) REQUIRE MANY HISTORIES TO ACCURATELY STATISTICALLY SAMPLE THE LARGE ANGLE SCATTERING, BUT EACH HISTORY DOES NOT INVOLVE MANY EVENTS.

THICK SPHERES DO NOT REQUIRE AS MANY HISTORIES, SINCE THEIR ANGULAR DISTRIBUTIONS WILL BE SMOOTHER, BUT EACH HISTORY WILL REQUIRE MANY EVENTS, E.G., TO TRANSPORT THROUGH A 1000 MFP SPHERE WILL ON AVERAGE REQUIRE ABOUT 1000 EVENTS.

IF YOU TRY TO RUN AN ENTIRE RANGE OF MEDIA FROM 1 TO 1000 MFP THICKNESS IN A SINGLE RUN, IT CAN TAKE AN ENORMOUS AMOUNT OF TIME TO OBTAIN STATISTICALLY GOOD RESULTS FOR THE ENTIRE ANGLE AND RADII RANGE.

A BETTER APPROACH IS TO RUN THE RANGES 1 TO 10, 10 TO 100, AND 100 TO 1000 SEPARATELY. THE RESULTS CAN BE COMBINED IN THE OUTPUT BY STARTING FROM A FEW THIN MEDIA AND PROGRESSIVELY USING THICKER AND THICKER MEDIA - AND THE RESTART OPTION. FOR EACH RUN THE RESTART FILE WILL CONTAIN THE RESULTS FROM ALL PREVIOUSLY RUN CASES, I.E., THE THINNER MEDIA, AND AS YOU ADD MORE AND MORE SURFACES THESE WILL BE COMBINED WITH THOSE ALREADY CALCULATED, AND OUTPUT WILL INCLUDE ALL OF THE RESULTS FOR ALL SURFACES.

WITH THIS APPROACH YOU CAN QUICKLY RUN MANY HISTORIES THROUGH THE THINNER SPHERES, IN ORDER TO OBTAIN GOOD STATISTICAL RESULTS OVER THE ENTIRE ANGULAR RANGE. YOU CAN THEN RUN FEWER HISTORIES THROUGH THE THICKER SPHERES (EACH HISTORY NOW REQUIRING MORE EVENTS, THAN FOR THE THINNER SPHERES) AND AGAIN OBTAIN GOOD STATISTICAL RESULTS.

ROUGHLY SPEAKING IN ORDER TO OBTAIN GOOD STATISTICAL RESULTS OVER THE ENTIRE ANGULAR RANGE, FOR ANY THICKNESS YOU NEED ABOUT 10,000/ETA EVENTS, $\text{ETA}=1.0\text{E}-2$, ABOUT 1 MILLION, $\text{ETA}=1.0\text{E}-5$, ABOUT 1 BILLION EVENTS. FOR VERY THIN MEDIA THERE WILL BE FEW EVENTS PER HISTORY, SO YOU HAVE TO RUN THIS MANY HISTORIES. FOR VERY THICK MEDIA THERE WILL BE MANY EVENTS PER HISTORY, SO YOU CAN RUN FEWER HISTORIES AND STILL GET GOOD STATISTICAL RESULTS, E.G., FOR $\text{ETA}=1.0\text{E}-5$, 1 MFP, RUN 1 BILLION HISTORIES, 1000 MFP, RUN 1 MILLION HISTORIES (ABOUT 1 BILLION EVENTS).

IN THE LIMIT AS THE NUMBER OF MEAN FREE PATHS TIMES ETA EXCEEDS UNITY, THE ELECTRONS WILL BE DIFFUSING IN ALL DIRECTIONS, WITH LITTLE IF ANY CORRELATION TO THEIR INITIAL DIRECTION. IN THIS CASE THE NUMBER OF EVENTS TO LEAK WILL INCREASE RAPIDLY, E.G., FOR $\text{ETA}=1.0\text{E}-02$, 1000 MFP, INSTEAD OF AVERAGING 1000 EVENTS TO LEAKAGE, THE RESULTS WILL SHOW MORE LIKE 20-30,000 EVENTS TO LEAKAGE. THEREFORE IN THIS LIMIT THE RUNNING TIME WILL INCREASE RAPIDLY WITH MEDIA THICKNESS.

BATCH SIZE

AT THE END OF EACH BATCH THE PROGRAM WRITES PLOTTAB FORMATTED RESULTS AND A RESTART FILE, WHICH ADDS OVERHEAD TO EACH BATCH. IN ORDER TO AVOID EXCESSIVE OVERHEAD, DO NOT RUN VERY SMALL HISTORIES PER BATCH. AT A RULE RUN ABOUT 1 MILLION EVENTS PER BATCH - REMEMBER THAT FOR A SPHERE N MFP THICK IT WILL TAKE ABOUT N COLLISIONS (EVENTS) TO LEAK FROM THE SPHERE. SO THAT FOR A MAXIMUM RADIUS MFP THICK YOU CAN FOLLOW THESE GUIDELINES,

- 1 MFP = 1 MILLION HISTORIES PER BATCH
- 10 MFP = 100,000 HISTORIES PER BATCH
- 100 MFP = 10,000 HISTORIES PER BATCH
- 1000 MFP = 1 THOUSAND HISTORIES PER BATCH

EACH OF THESE EXAMPLES WILL RUN A BATCH OF ELECTRONS IN ROUGHLY THE SAME TIME, SINCE ALL REQUIRE ROUGHLY THE SAME NUMBER OF EVENTS.

RUNNING TIME

FOR 2 SPHERES OF RADIUS 1 AND 3 MEAN FREE PATHS EACH BATCH OF 1 MILLION HISTORIES TAKES ABOUT 1 MINUTES ON AN IBM-PC (ABOUT 2 MILLION EVENT IN 60 SECONDS - ABOUT 40,000 PER SECOND).

FOR 5 SPHERES OF RADIUS 1 TO 100 MEAN FREE PATHS EACH BATCH OF 20,000 HISTORIES WILL TAKES ABOUT 15-20 SECONDS ON A SPARC-10 WORKSTATION (ABOUT 2 MILLION EVENTS IN 15-20 SECONDS - ABOUT 120,000 PER SECOND).

TERMINATING EXECUTION

THE PROGRAM WILL WRITE A RESTART FILE AT THE END OF EACH BATCH.

THIS PROGRAM WILL TERMINATE EXECUTION,

- 1) AFTER ALL BATCHES HAVE BEEN RUN, OR,
- 2) AT THE END OF A BATCH, IF ANY KEYBOARD KEY IS PRESSED DURING EXECUTION (ONLY ON IBM-PC)
- 3) IF YOU SOMEHOW KILL IT

REGARDLESS OF HOW THE CODE TERMINATES YOU WILL BE ABLE TO RESTART, UNLESS YOU ARE UNLUCKY ENOUGH TO TERMINATE EXACTLY AT THE END OF A BATCH WHEN THE CODE IS WRITING THE RESTART FILE.

IN ORDER TO AVOID THIS PROBLEM, THE SAFEST TIME TO TERMINATE THE CODE IS IMMEDIATELY AFTER IT HAS PRINTED STATISTICS FOR A BATCH - THIS IMMEDIATELY FOLLOWS WRITING AND CLOSING THE

C RESTART FILE.
 C
 C RESTART FILE
 C=====

C YOU CAN CONTINUE FROM THE POINT THE PROGRAM STOPPED BY USING
 C THE RESTART OPTION. RESTART IS INDICATED ON INPUT BY A NEGATIVE
 C BATCH COUNT.
 C
 C WITH THIS OPTION YOU CAN RUN FOR A PERIOD OF TIME AND THEN LOOK
 C AT THE RESULTS USING PLOTTAB. IF THE RESULTS INDICATE THAT YOU
 C NEED TO RUN MORE HISTORIES, THIS OPTION WILL ALLOW YOU TO
 C CONTINUE FROM THE POINT THAT THE PROGRAM STOPPED. YOU CAN ALSO
 C LET THE PROGRAM RUN TO COMPLETION, EXAMINE RESULTS AND DECIDE
 C WHETHER OR NOT YOU NEED TO RUN MORE HISTORIES.
 C
 C WHEN RUNNING USING THE RESTART OPTION, THE NUMBER OF BATCHES
 C THAT YOU INPUT WILL BE INTERPRETED TO MEAN RUN THIS MANY MORE
 C BATCHES, E.G., IF INPUT INDICATES 1000 BATCHES AND THE RESTART
 C FILE INDICATES 100 BATCHES HAVE ALREADY BEEN RUN, THIS PROGRAM
 C WILL RUN ANOTHER 100 BATCHES (BATCHES 101 TO 1100).
 C
 C WARNING - THE PROGRAM DOES NOT CHECK TO BE SURE THAT YOU ARE
 C CONTINUING EXACTLY THE SAME PROBLEM - IT MERELY
 C COMBINES THE STATISTICS PREVIOUSLY CALCULATED WITH
 C THOSE CALCULATED DURING THE CURRENT RUN.
 C
 C IT IS THE USERS RESPONSIBILITY TO INSURE THAT THE
 C RUNNING CONDITIONS FOR THE CURRENT RUN ARE EXACTLY
 C THE SAME AS THE PREVIOUS RUN, IN ORDER TO INSURE
 C THAT THE STATISTICS FROM THE PREVIOUS RUN, AS READ
 C DURING RESTART, EXACTLY CORRESPOND TO THE CURRENT
 C RUNNING CONDITIONS.
 C
 C THE ONLY EXCEPTION TO THIS RULE IS THAT YOU MAY ADD
 C SURFACES TO SUCCESSIVE RUNS, AS DESCRIBED ABOVE.
 C
 C OUTPUT RESULTS
 C=====

C RESULTS FOR EACH SURFACE ARE OUTPUT AS A FUNCTION OF Z/R (LATERAL
 C DISPLACEMENT) AND GAMMA (COSINE FROM THE INITIAL DIRECTION OF
 C TRAVEL).
 C
 C Z/R AND GAMMA VARY BETWEEN -1 AND +1. SINCE ELASTIC SCATTERING
 C CAN BE SO FORWARD PEAKED (CLOSE TO GAMMA=1), RESULTS ARE OUTPUT
 C VS. 1-Z/R AND 1-GAMMA, IN LOG SPACED BINS BASED ON THE SIZE OF
 C ETA.
 C
 C THIS PROGRAM WILL OUTPUT 6 DIFFERENT RESULTS FOR EACH
 C SPHERE,
 C 1) LEAKAGE RELATIVE TO Z/R (DISTANCE ALONG Z AXIS/RADIUS)
 C 2) LEAKAGE RELATIVE TO GAMMA (DIRECTION COSINE RELATIVE TO Z)
 C 3) <1-GAMMA> RELATIVE TO Z/R
 C 4) DISTANCE TO LEAKAGE RELATIVE TO Z/R
 C 5) THE INTEGRAL OF THE ANGULAR DISTRIBUTIONS 1) AND 2)
 C 6) 1 MINUS THE INTEGRAL OF THE ANGULAR DISTRIBUTIONS 1) AND 2)
 C
 C FOR REFERENCE PURPOSES THE OUTPUT RESULTS FOR THE ANGULAR
 C DISTRIBUTIONS 1) AND 2), AND INTEGRALS 5) AND 6) WILL ALSO
 C INCLUDE ANALYTICAL RESULTS BASED ON THE SINGLE COLLISION
 C ANGULAR DISTRIBUTION. THESE RESULTS ARE IDENTIFIED AS
 C 0.00 MFP FOR THE THICKNESS.
 C
 C RESULTS WILL NOT INCLUDE UNCOLLIDED ELECTRONS. OUTPUT
 C RESULTS WILL BE NORMALIZED TO PER ELECTRON CROSSING
 C EACH SURFACE.
 C

C AT THE END OF EACH BATCH THE RESULTS WILL BE NORMALIZED AND OUTPUT
C IN THE PROGRAM PLOTTAB FORMAT - SO THAT THEY CAN BE IMMEDIATELY
C PRESENTED IN GRAPHICAL FORM. IF YOU WISH TO MONITOR THE RESULTS
C OF THIS CODE WHILE IT IS RUNNING, CONTACT THE AUTHOR FOR A COPY
C OF THE PROGRAM PLOTTAB.

C
C CHECKING FOR CONVERGENCE

C=====

C YOU CAN USE PROGRAM PLOTTAB TO CHECK THE RESULTS FOR CONVERGENCE.
C SINCE THE RESULTS CAN VARY OVER MANY ORDER OF MAGNITUDE THEY
C CAN APPEAR TO BE QUITE SMOOTH AND CONVERGED, WHEREAS IN FACT
C THERE MAY STILL BE SIGNIFICANT FLUCTUATIONS. TO INSURE THAT
C THE RESULTS HAVE INDEED CONVERGED, USE THE PLOTTAB RATIO AND
C SCALING OPTIONS, E.G., THE RATIOS SHOULD BE SMOOTHLY VARYING
C VIEWED USING EITHER LINEAR OR LOG SCALING IN X AND Y.

C
C THE ANALYTICAL SINGLE COLLISION RESULTS INCLUDED WITH THE
C ANGULAR DISTRIBUTION AND INTEGRALS ARE PARTICULARLY USEFUL
C IN CHECKING FOR CONVERGENCE. THE RATIO OF ALL OTHER RESULTS
C TO THESE RESULTS SHOULD BE SMOOTHLY VARYING OVER THE ENTIRE
C ANGULAR RANGE.

C
C SCORING

C=====

C WHEN AN ELECTRON CROSSES A SPHERE THE FIRST TIME THE FOLLOWING
C PARAMETERS ARE SCORED,
C 1) 1 ELECTRON IN A Z/R BIN
C 2) Z/R IN A Z/R BIN
C 3) GAMMA IN A Z/R BIN
C 4) DISTANCE TO LEAKAGE IN A Z/R BIN
C
C 5) 1 ELECTRON IN A GAMMA BIN
C 6) GAMMA IN A GAMMA BIN

C
C CORRELATED RESULTS - VS. BOTH Z/R AND GAMMA, ARE NOT CURRENTLY
C SCORED.

C
C LEAKAGE RELATIVE TO Z/R OR GAMMA

C=====

C FOR OUTPUT EACH DISTRIBUTION IS NORMALIZED TO UNITY WHEN SUMMED
C OVER ALL BINS, I.E., SUM EITHER 1) OR 5), ABOVE. IN ORDER TO
C OUTPUT NORMALIZED DENSITY IN EACH BIN, THE COUNTS IN EACH BIN
C [1) OR 5) ABOVE] IS DIVIDED BY THE SUM OF ALL COUNTS AND THE
C WIDTH OF EACH BIN (A Z/R OR GAMMA RANGE), TO DEFINE AN AVERAGE
C MAGNITUDE OF EACH BIN (Y VALUE ON A PLOT). THE CENTER OF EACH
C BIN IS DEFINED AS THE AVERAGE Z/R OR GAMMA OF EACH BIN, BASED
C ON 2) OR 6) ABOVE, TO DEFINE AN AVERAGE CENTER OF A BIN (X
C VALUE ON A PLOT). ONE (X,Y) POINT IS OUTPUT FOR EACH BIN.

C
C <1-GAMMA> AND DISTANCE TO LEAKAGE RELATIVE TO Z/R

C=====

C THESE QUANTITIES ARE DEFINED AS THE AVERAGE VALUE OF 3) OR
C 4), ABOVE, TO DEFINE AN AVERAGE MAGNITUDE (Y VALUE FOR A
C PLOT). THE CENTER OF EACH BIN IS DEFINED AS DESCRIBED IN
C THE PRECEDING SECTION, I.E., AVERAGE 2), TO DEFINE AN
C AVERAGE CENTER OF EACH BIN (X VALUE FOR A PLOT). ONE (X,Y)
C POINT IS OUTPUT FOR EACH BIN.

C
C INTERPRETATION OF RESULTS

C=====

C LEAKAGE RELATIVE TO Z/R DEFINES THE LATERAL DISPLACEMENT OF
C THE ELECTRONS FROM THEIR INITIAL DIRECTION OF TRAVEL. IF
C THERE IS NO LATERAL DISPLACEMENT ALL OF THE ELECTRONS
C WOULD EMERGE EXACTLY ON THE Z AXIS WITH SOME ANGULAR
C DISTRIBUTION - WHICH NATURALLY DOES NOT HAPPEN. FROM
C THESE RESULTS YOU CAN ESTIMATE JUST HOW FAR THE ELECTRONS

ARE ACTUALLY Laterally Displaced.

Leakage relative to gamma defines the angular distribution of all electrons relative to their initial direction of travel, regardless of where they emerge from a sphere. In principle this should be what condensed history methods calculate.

$\langle 1 - \gamma \rangle$ relative to z/r can be used to see the average change in direction as electrons transport through thicker and thicker spheres. The effect is particularly obvious close to the initial direction of travel, e.g., for thicker and thicker spheres $\langle 1 - \gamma \rangle$ will increase even in the most forward direction relative to z/r .

Distance to leakage relative to z/r can be used to see that generally for small angle scattering an electron that transports through a sphere N mean free paths thick will on average have N collisions (no big surprise here). However, for larger angle scattering an electron will on average have more than N collisions (sometimes considerably more). Comparing distance to leakage for spheres and planes can be informative.

CORRELATED RESULTS

As yet this code does not calculate correlated results, that is for each z/r bin, the angular distribution relative to the z axis (γ) or the radius vector. These results would define the angular distribution for each lateral displacement.

In order to achieve the purpose for which this code is designed (see above) these correlated results are not required - I'll leave this task for some bright young student out there.

APPROXIMATE ATTENUATION ALONG THE INITIAL DIRECTION

Along the initial direction of travel the electrons will be attenuated by $\exp(-z)$ (z in mean free paths) as they collide. However after each collision about $\langle \cos \rangle$ of those colliding will still be traveling in the same direction. In this case the distribution of electrons that have undergone N collisions will be,

$$\exp(-z) * [\langle \cos \rangle^z]^{**N/N!}$$

Summing over all collisions and recognizing that,

$$\exp(\langle \cos \rangle^z) = \text{SUM}(0 \text{ TO INFINITY}) [\langle \cos \rangle^z]^{**N/N!}$$

The approximate attenuation will be,

$$\exp(-z) * \exp[\langle \cos \rangle^z] = \exp[\langle 1 - \cos \rangle^z]$$

That is to say, attenuation according to the transport cross section - rather than the total elastic scattering cross section. For typical values of $\langle 1 - \cos \rangle \sim 1.0E-5$ to $\sim 1.0E-2$, this would represent a tremendous savings in running time if we could use the transport cross section, instead of the total elastic scattering cross section, e.g., for $\langle 1 - \cos \rangle \sim 1.0E-5$, 100,000 mean free paths based on the elastic total, would be only 1 mean free path based on the transport cross section. However, care has to be used in interpreting the above results and accurately applying the transport approximation.

A COMMON MISTAKE IS TO ASSUME THAT THIS MEANS TRANSPORT CALCULATIONS CAN BE PERFORMED USING THE TRANSPORT RATHER THAN TOTAL ELASTIC SCATTERING CROSS SECTION, AND IN ORDER TO COMPENSATE THE ANGULAR SCATTERING CAN BE SAMPLED FROM AN ISOTROPIC DISTRIBUTION.

WRONG!!!

THE PROPER WAY TO INTERPRET THE ABOVE, IS THAT AFTER TRANSPORTING THROUGH SEVERAL TRANSPORT MEAN FREE PATHS THE ANGULAR DISTRIBUTION WILL BE ALMOST ISOTROPIC, AND FROM THIS POINT ON THE TRANSPORT CROSS SECTION CAN BE USED AND THE ANGULAR DISTRIBUTION CAN BE SAMPLED USING ISOTROPIC SCATTERING (FOR AN ISOTROPIC ANGULAR DISTRIBUTION OF ELECTRONS ALL OF THE HIGHER SCATTERING MOMENTS CANCEL OUT, AND ONLY THE ISOTROPIC COMPONENT REMAINS).

HOWEVER, IN TRANSPORTING BETWEEN THE SOURCE OF ELECTRONS AND SEVERAL TRANSPORT MEAN FREE PATHS, THE ABOVE RESULTS TELL US NOTHING ABOUT THE ANGULAR DISTRIBUTION OF THE ELECTRONS. IN THIS RANGE THE TOTAL ELASTIC SCATTERING CROSS SECTION AND THE DETAILED SCATTERING ANGULAR DISTRIBUTION MUST BE USED FOR SAMPLING.

IF WE ASSUME THAT $\langle 1 - \cos \theta \rangle \sim \eta$, THIS MEANS FOR $\eta = 1.0E-5$, YOU MUST TRANSPORT THROUGH AT LEAST $1.0E+5$ MEAN FREE PATHS BEFORE YOU REACH THE POINT WHERE THE TRANSPORT APPROXIMATION BECOMES VALID. SINCE AT LEAST 100,000 MEAN FREE PATHS MUST BE TRANSPORTED THROUGH BEFORE REACHING THIS LIMIT, IN THIS CASE THE RESULTS ARE NOT THAT INTERESTING. FOR LARGER η , SUCH AS $\eta = 1.0E-2$, AFTER ABOUT ONLY 100 COLLISIONS THE TRANSPORT LIMIT WILL BE REACHED, AND IN THIS CASE THE TRANSPORT APPROXIMATION CAN BE USED TO EXTEND RESULTS TO THICKER MEDIA.

ULTIMATELY TO SEE THAT THE TRANSPORT APPROXIMATION DOES NOT WORK FOR BEAMS OF ELECTRONS FOR MEAN FREE PATHS THAT ARE NOT LARGE COMPARED TO THE TRANSPORT MEAN FREE PATH WE NEED MERELY LOOK AT THE RESULTS CALCULATED BY THIS CODE. FOR $\eta = 1.0E-5$, THE TRANSPORT MEAN FREE PATH IS ROUGHLY $1.0E-5$. IF ELECTRONS ARE BEING ATTENUATED ACCORDING TO THE TRANSPORT MEAN FREE PATH WE WOULD EXPECT AT LEAST THE VERY FORWARD PART OF THE ANGULAR DISTRIBUTION (THOSE STILL TRAVELLING ALONG THE INITIAL DIRECTION) AFTER TRANSPORTING THROUGH 10 TO 100 TOTAL MEAN FREE PATH (ABOUT $1.0E-4$ TO $1.0E-3$ TRANSPORT MEAN FREE PATHS), WE WOULD EXPECT ALMOST NO ATTENUATION OF THE FORWARD ANGULAR DISTRIBUTION (ABOUT $\exp(-1.0E-4)$ TO $\exp(-1.0E-3)$). IN REALITY WE SEE ATTENUATION WHICH IS MORE LIKE A LINEAR FUNCTION OF THE NUMBER OF TOTAL MEAN FREE PATHS - FOR 10 MFP, A FACTOR OF 10, FOR 100 MFP, A FACTOR OF 100 - NOTHING LIKE THAT PREDICTED BY THE TRANSPORT APPROXIMATION.

DETAILS OF METHODS

=====

USING EEDL DIRECTLY

=====

IF WE WERE TO USE AN APPROACH SIMILAR TO WHAT WE DO FOR NEUTRONS MERELY CONVERT THE ANGULAR DISTRIBUTIONS TO EQUALLY PROBABLE BINS TO SAMPLE THESE DISTRIBUTIONS. THE PROBLEM WITH THIS APPROACH FOR ELECTRONS IS THAT ENERGETIC ELECTRONS SCATTER THROUGH SUCH SMALL ANGLES THAT ALL OF THE BINS WILL BE VERY CLOSE TO $\mu = 1$, EXCEPT

THE LAST BIN WHICH COVERS THE REMAINING RANGE OF MU ALL THE WAY TO MU = -1, E.G., FOR ENERGETIC ELECTRONS USING A REASONABLE NUMBER OF ANGULAR BINS THE LAST MU INTERVAL CAN BE ALMOST THE ENTIRE MU RANGE FROM MU = (1.0 - 1.0E-04) TO MU = -1.

IF WE LOOK AT OUR BINNED ANGULAR DISTRIBUTIONS AND DERIVE THE AVERAGE SCATTERING ANGLE, OR $\langle 1-\mu \rangle$, WE WILL FIND THAT BECAUSE THE LAST BIN WHICH EXTENDS OVER ALMOST THE ENTIRE RANGE OF MU, THIS WILL CAUSE ELECTRONS TO SCATTER THROUGH TOO LARGE AN ANGLE, AND IT IS NOT BE A VERY GOOD APPROXIMATION TO THE ANGULAR DISTRIBUTION

YOU DON'T HAVE TO RUN AN EXPENSIVE MONTE CARLO CALCULATIONS TO VERIFY THIS POINT - IT IS OBVIOUS THAT IF THE ANGULAR DISTRIBUTION THAT IS SAMPLED CAUSES ELECTRONS UNDERGOING A SINGLE COLLISION TO ROTATE THROUGH TOO LARGE AN ANGLE, THEN THE RESULT OF MONTE CARLO CALCULATIONS BETTER SHOW THIS EFFECT - OR ELSE YOU HAVE MADE A MISTAKE SOMEPLACE.

IF YOU STILL THINK THAT IT IS PRACTICAL TO USE EQUALLY PROBABLE BINS TO ACCURATELY REPRESENT THE ANGULAR DISTRIBUTION OF ELASTICALLY SCATTERED ELECTRONS, HOW MANY BINS ARE NEEDED? THE PROBABILITY OF SCATTERING TO THE RANGE MU = 0 TO -1 (BACK SCATTER) IS ABOUT ETA. THEREFORE FOR ETA = 1.0E-5, IF WE WANTED EQUALLY PROBABLE BINS WITH A MINIMUM OF ONLY 1 BIN COVERING THE ENTIRE MU = 0 TO -1 RANGE, WE WOULD REQUIRE 100,000 EQUALLY PROBABLE BINS - WHICH DOESN'T SOUND VERY PRACTICAL. AGAIN, IN THIS CASE WITH 100,000 BINS WE WOULD STILL HAVE ONLY 1 BIN REPRESENTING THE ENTIRE MU = 0 TO -1 RANGE = 1/2 OF THE ENTIRE COSINE RANGE.

FIRST LEVEL OF APPROXIMATION

THE DETAILED ANGULAR DISTRIBUTION IS NECESSARY TO START FROM IN ORDER TO DEFINE THE ACTUAL ELASTIC SCATTERING CROSS SECTION (THIS WAS DONE IN DERIVING THE DATA IN EEDL).

ONCE THIS IS DONE THE IMPORTANT DETAILS OF THE ANGULAR DISTRIBUTION CAN BE REPRODUCED USING A RELATIVELY SIMPLE MODEL FOR THE ANGULAR DISTRIBUTION.

THE ELASTIC SCATTERING ANGULAR DISTRIBUTIONS IN EEDL ARE DEFINED AS,

$$P(\mu) \cdot D(\mu) = A \cdot R \cdot D(\mu) / [(1-\mu) + \eta]^2 = A \cdot R / (X + \eta)^2$$

WHERE,

MU = COSINE OF SCATTERING ANGLE
X = 1 - COS
R = RELATIVISTIC CORRECTION
A = A NORMALIZATION FACTOR
ETA = SCREENING FACTOR

THIS IS EXACTLY THE EQUATION USED TO DERIVE ALL OF THE DATA IN EEDL - THE ANGULAR DISTRIBUTIONS FOR EACH ELEMENT AND OVER AN ENERGY RANGE WERE CALCULATED, AND INTEGRATED TO DEFINE THE CROSS SECTION, AND THEN NORMALIZED (TO UNITY WHEN INTEGRATED OVER MU) AND OUTPUT INTO THE EEDL DATA BASE.

THE RELATIVISTIC CORRECTION FACTOR (R) IS IMPORTANT TO CONSIDER WHEN CALCULATING THE CROSS SECTION, BUT IT PLAYS A LESS IMPORTANT ROLE IN THE NORMALIZED ANGULAR DISTRIBUTION.

RELATIVE TO THE VARIATION OF $1/(X+\eta)^2$, R IS A SLOWLY VARYING FUNCTION, SO THAT WE CAN INTEGRATE THIS DISTRIBUTION OVER MU, OR X INTERVALS, X_K TO X_{K+1} ,

$$P = A \langle R \rangle [1/(X_K + \eta) - 1/(X_{K+1} + \eta)]$$


```

C      = A<RK> [ (XK+1-XK) / { (XK+ETA) * (XK+1+ETA) } ]
C <RK> = AN AVERAGE VALUE OF R OVER THE INTERVAL XK TO XK+1
C
C NORMALIZATION IS DEFINED BY SUMMING OVER INTERVALS,
C
C 1      = A * SUM(OVER K) <RK> [ (XK+1-XK) / { (XK+ETA) * (XK+1+ETA) } ]
C
C A      = 1 / SUM(OVER K) <RK> [ (XK+1-XK) / { (XK+ETA) * (XK+1+ETA) } ]
C
C FOR SAMPLING WITHIN EACH X INTERVAL, XK IS FIXED, P IS A RANDOM
C NUMBER IN THE RANGE PK TO PK+1 AND WE SOLVE FOR X,
C
C P      = A<RK> [ (X-XK) / { (XK+ETA) * (X+ETA) } ]
C P * { (XK+ETA) * (X+ETA) } = A<RK> (X-XK)
C P * (XK+ETA) * ETA + A<RK> * XK = X * [ A<RK> - P * (XK+ETA) ]
C
C X = [ P * (XK+ETA) * ETA + A<RK> * XK ] / [ A<RK> - P * (XK+ETA) ]
C
C REGARDLESS OF HOW THE ANGULAR DISTRIBUTION IS BINNED THIS IS
C HOW ONE SHOULD INTERPOLATE WITHIN EACH X INTERVAL,
C
C THIS MODEL IS NOT CURRENTLY USED BY THIS CODE, BUT IT COULD
C BE EASILY ADDED, MERELY BY MODIFYING THE SINGLE COLLISION
C ROUTINE (WHAM) TO INCLUDE THE RELATIVISTIC CORRECTION.
C
C NEXT LEVEL OF APPROXIMATION
C =====
C IF WE IGNORE THE RELATIVISTIC CORRECTION, I.E., ASSUME
C R = <RK> = 1, WE CAN INTEGRATE THE ENTIRE DISTRIBUTION,
C
C A      = 1 / SUM(OVER K) <RK> [ (XK+1-XK) / { (XK+ETA) * (XK+1+ETA) } ]
C      = 1 / [ (2-0) / { (0+ETA) * (2+ETA) } ]
C      = ETA * (2+ETA) / 2
C
C SUBSTITUTING FOR A, THE NORMALIZED DISTRIBUTION IS,
C
C P(X) * D(X) = ETA * (2+ETA) * D(X) / (2 * (X+ETA) ** 2)
C
C INTEGRATING FROM X = 0 TO X
C
C P(X) = ETA * (2+ETA) * (1/ETA - 1/(X+ETA)) / 2
C      = ETA * (2+ETA) * (X+ETA - ETA) / (2 * (ETA * (X+ETA)))
C      = ETA * (2+ETA) * X / (2 * (ETA * (X+ETA)))
C      = (2+ETA) * X / (2 * (X+ETA))
C
C SOLVING FOR X,
C
C P(X) * 2 * (X+ETA) = (2+ETA) * X
C 2 * P(X) * ETA = (2+ETA - 2 * P(X)) * X
C
C X = 2 * P(X) * ETA / (2+ETA - 2 * P(X))
C    = 2 * P(X) * ETA / (ETA + 2 * (1 - P(X)))
C
C WHERE P(X) IS A RANDOM VARIABLE BETWEEN 0 AND 1
C
C OR IN TERMS OF MU = 1 - X
C
C MU = 1 - 2 * P * ETA / (2+ETA-2 * P)
C     = (2+ETA-2 * P - 2 * P * ETA) / (2+ETA-2 * P)
C     = (2+ETA-2 * P * (1-ETA)) / (2+ETA-2 * P)
C     = (ETA * (1-2 * P) + 2 * (1-P)) / (ETA+2 * (1-P))
C
C P = 0 CORRESPONDS TO MU = 1 AND P = 1 CORRESPONDS TO MU = -1
C
C SINCE P IS A RANDOM VARIABLE IT IS JUST AS VALID TO USE
C Q = 1 - P - NOTE, Q IS AGAIN MERELY A RANDOM VARIABLE

```

```

C   BETWEEN 0 AND 1.
C
C   MU = (ETA*(2*Q-1)+2*Q)/(ETA+2*Q)
C
C   THIS ALGORITHM MAY BE USED FOR SAMPLING THE SCATTERING COSINE, MU,
C   WHERE Q IS A RANDOM NUMBER BETWEEN 0 AND 1 - A SIMPLE AND FAST
C   1 LINE DEFINITION TO USE TO SAMPLE THE ANGULAR DISTRIBUTION.
C
C   THIS IS THE MODEL CURRENTLY USED BY THIS CODE.
C
C   INTEGRAL OF THE ANGULAR DISTRIBUTION
C   =====
C   P(X) = (2+ETA)*X/(2*(X+ETA))
C
C   X      = R*ETA
C   P(X)   = R*(2+ETA)/(2*(R+1))
C   FOR ETA << 1
C   P(X)   = R/(R+1)
C   P(X)   = 1/2 , R = 1, (1/2 THE INTEGRAL IS FROM X = 0 TO ETA)
C           = 1/10 , R ~ 1/10
C           = 1/100, R ~ 1/100
C
C   FROM THIS WE CAN SEE THAT 1% OF THE INTEGRAL IS BETWEEN
C   X = 0 AND ETA/100, E.G., FOR ETA=1.0E-05, X = 0 TO 1.0E-7,
C   AND 50% IS BETWEEN X = 0 TO ETA. SO THAT FOR SMALL ETA
C   MOST OF THE INTEGRAL WILL CORRESPOND TO VERY SMALL ANGLE
C   SCATTERING.
C
C   1-P(X) = ETA*(2-X)/(2*(X+ETA))
C   THE PROBABILITY OF SCATTERING THROUGH 90 DEGREES, X =1
C   1-P(1) = ETA/(2*(1+ETA))
C   FOR ETA << 1
C   1-P(1) = ETA/2 = 5.0E-06, FOR ETA =10E-5
C
C   X      = 2 - R*ETA
C   1-P(X) = R*ETA**2/(2*(2-R*ETA+ETA))
C   FOR ETA << 1
C   1-P(X) = R*ETA**2/4
C
C   FROM THIS WE CAN SEE THAT THE PROBABILITY OF SCATTERING NEAR
C   180 DEGREES IS VERY SMALL, E.G., FOR R=1, ETA=1.0E-5,
C   1-P(X) ~ 1.0E-10
C
C   MOMENTS OF THE ANGULAR DISTRIBUTION
C   =====
C   <X> DEFINES THE AVERAGE SCATTERING ANGLE, AND THE COMBINATION
C   OF <X> AND <X**2> DEFINE THE VARIANCE OF THE DISTRIBUTION.
C
C   <X>      = ETA*[(2+ETA)/2*LOG[(2+ETA)/ETA] - 1]
C   <X**2>    = ETA*[(2+ETA) - 2*<X> + ETA]
C
C   <X**2> - <X>**2 = ETA*[(2+ETA) - 2*<X> + ETA] -
C                   {ETA*[(2+ETA)/2*LOG[(2+ETA)/ETA] - 1]**2}
C
C                   = ETA*{[(2+ETA) - 2*<X> + ETA] -
C                   ETA*{[(2+ETA)/2*LOG[(2+ETA)/ETA] - 1]**2}}
C
C   TO DEFINE ALL MOMENTS IT IS EASIER TO DEFINE <(X+ETA)**N>
C
C   P(X)*D(X) = [ETA*(ETA+2)/2]*D(X)/[X+ETA]**2
C
C   <(X+ETA)**N> = ETA*(ETA+2)/2] INTEGRAL [X+ETA]**(N-2)*D(X)
C
C   FOR N > 2
C
C   ETA*(ETA+2)/2] {[2+ETA]**(N-1)-ETA**(N-1)]

```

$$\langle (X+\text{ETA})^{**N} \rangle = \frac{\dots\dots\dots}{(N-1)}$$

NOTE, ALL ARE OF ORDER ETA

FOR ETA << 2,

$$\begin{aligned} \langle X \rangle &\sim \text{ETA} * [\text{LOG}(2/\text{ETA}) - 1] \\ &\sim \text{ETA} * [\text{LOG}(2) - 1] - \text{ETA} * \text{LOG}(\text{ETA}) \\ &\quad (\text{NOTE, FOR } \text{ETA} < 1, -\text{ETA} * \text{LOG}(\text{ETA}) > 0 \text{ AND} \\ &\quad -\text{LOG}(\text{ETA}) >> \text{LOG}(2) - 1, \text{ MAKING THIS THE} \\ &\quad \text{DOMINANT TERM, SO THAT}) \end{aligned}$$

$$\langle X \rangle \sim -\text{ETA} * \text{LOG}(\text{ETA})$$

$$\langle X^{**2} \rangle \sim 2 * \text{ETA}$$

$$\langle X^{**2} \rangle - \langle X \rangle^{**2} \sim 2 * \text{ETA}$$

$$\langle (X+\text{ETA})^{**N} \rangle = \text{ETA} * [2]^{** (N-1)} / (N-1), \quad N > 2$$

ETA	<Degrees>	<X>	<X**2>	<X**2>-<X>**2
1.0000E+00	6.9385E+01	6.4792E-01	2.7042E+00	2.2844E+00
1.0000E-01	3.8710E+01	2.1967E-01	1.7607E-01	1.2781E-01
1.0000E-02	1.6922E+01	4.3298E-02	1.9334E-02	1.7459E-02
1.0000E-03	6.5890E+00	6.6052E-03	1.9888E-03	1.9452E-03
1.0000E-04	2.4180E+00	8.9040E-04	1.9984E-04	1.9905E-04
1.0000E-05	8.5777E-01	1.1206E-04	1.9998E-05	1.9985E-05
1.0000E-06	2.9781E-01	1.3509E-05	2.0000E-06	1.9998E-06
1.0000E-07	1.0189E-01	1.5811E-06	2.0000E-07	2.0000E-07
1.0000E-08	3.4486E-02	1.8114E-07	2.0000E-08	2.0000E-08
1.0000E-09	1.1578E-02	2.0416E-08	2.0000E-09	2.0000E-09
1.0000E-10	3.8622E-03	2.2719E-09	2.0000E-10	2.0000E-10

LEGENDRE MOMENTS

=====

$$\langle P_0 \rangle = 1$$

$$\langle P_1 \rangle = 1 - \langle X \rangle$$

$$\begin{aligned} \langle P_2 \rangle &= 1/2 * [3 \langle \text{COS}^{**2} \rangle - 1] \\ &= 1/2 * [3 \langle (1-X)^{**2} \rangle - 1] \\ &= 1/2 * [3 \langle (1-2*X+X^{**2}) \rangle - 1] \\ &= 1/2 * [3 * \{1-2*\langle X \rangle + \langle X^{**2} \rangle\} - 1] \\ &= 1/2 * [2-6*\langle X \rangle + 3*\langle X^{**2} \rangle] \\ &= [1-3*\langle X \rangle + 3*\langle X^{**2} \rangle / 2] \end{aligned}$$

ALL LEGENDRE POLYNOMIALS ARE DEFINED $P_N(\text{COS}) = 1$, AT $\text{COS} = 1$.
 FOR SMALL ETA THE PRODUCT OF ANY LEGENDRE POLYNOMIAL AND THE
 ANGULAR DISTRIBUTION WILL MAKE A SIGNIFICANT CONTRIBUTION TO
 THE INTEGRAL ONLY OVER A VERY SMALL RANGE OF COS, NEAR $\text{COS} = 1$.
 TO ZEROth ORDER THE INTEGRAL WILL BE THE VALUE OF THE LEGENDRE
 POLYNOMIAL AT $\text{COS} = 1$, WHICH IS 1, TIMES THE INTEGRAL OF THE
 ANGULAR DISTRIBUTION, WHICH IS NORMALIZED TO 1. IN THIS CASE
 ALL OF THE LEGENDRE COEFFICIENTS WILL BE OF ORDER 1. TO NEXT
 ORDER THEY WILL ALL BE 1 - ORDER(ETA).

WHAT DOES CONDENSED HISTORY USE?

=====

STARTING FROM THE SIMPLE DISTRIBUTION, DESCRIBED ABOVE, WITHOUT
 THE RELATIVISTIC CORRECTION,

$$\dot{P}(X) * D(X) = \text{ETA} * (2+\text{ETA}) * D(X) / [2 * (X+\text{ETA})^{**2}]$$

$$\begin{aligned} X = 1 - \text{COS}(\text{THETA}) &= \text{THETA}^{**2}/2! - \text{THETA}^{**3}/3! + \dots\dots\dots \\ &\sim \text{THETA}^{**2}/2! \end{aligned}$$

$$D(X) \sim \text{THETA} * D(\text{THETA})$$

$$P(X) * D(X) \sim \text{ETA} * (2+\text{ETA}) * \text{THETA} * D(\text{THETA}) / [2 * (\text{THETA}^{**2}/2+\text{ETA})^{**2}]$$

```

C      ~ 2*ETA*(2+ETA)*THETA*D(THETA)/[(THETA**2+2*ETA)**2]
C
C OR USING CONDENSED HISTORY VARIABLES
C
C      ~ XIC*XI*D(XI)/[(XI**2 + XIA**2)**2]
C
C X1      = THETA
C XIA**2  = 2*ETA
C XIC     = A NORMALIZATION PARAMETER
C
C THE APPROXIMATION,
C
C X = 1 - COS(THETA) ~ THETA**2/2!
C
C WORKS QUITE WELL OUT TO ABOUT 45 DEGREES. BEYOND THIS POINT
C THETA**2/2! RAPIDLY DIVERGES FROM 1 - COS, AND BY 180 DEGREES
C IS ABOUT 2-1/2 TIMES TOO LARGE, MAKING THE DENOMINATOR A
C FACTOR OF (2-1/2) SQUARED TIMES TOO LARGE. THIS AFFECT IS
C PARTIALLY COMPENSATED FOR BY THETA*D(THETA) IN THE NUMERATOR
C INCREASING FASTER THAN D(COS). WHEN PROPERLY NORMALIZED BY
C INTEGRATING OVER THETA FROM 0 TO 180 DEGREES (0 TO PI RADIAN)
C THE RESULT AGREES WELL WITH THE ORIGINAL DISTRIBUTION OUT TO
C ABOUT 60 DEGREES.
C
C BOTTOMLINE: THE SIMPLE SINGLE SCATTERING MODEL INTRODUCED
C ABOVE MAY SEEM TOO SIMPLISTIC TO PRODUCE REALISTIC RESULTS,
C AND YET WE CAN SEE HERE THAT IT IS ACTUALLY A MORE ACCURATE
C MODEL THAN THAT USED IN CONDENSED HISTORY CALCULATIONS; THE
C FORMER APPLIES OVER THE ENTIRE ANGULAR RANGE, WHEREAS THE
C LATTER IS RESTRICTED TO SMALL ANGLE SCATTERING.
C
C SINCE THE OBJECTIVE OF THIS CODE IS TO PRODUCE RESULTS FOR
C COMPARISON TO CONDENSED HISTORY RESULTS, THE SIMPLE SINGLE
C SCATTER MODEL DESCRIBED ABOVE SHOULD BE ADEQUATE.
C
C IT IS WORTH NOTING THAT IF RATHER THAN USING THE
C APPROXIMATION,
C
C X = 1 - COS(THETA) ~ THETA**2/2!
C
C WE USE THE EXACT RELATIONSHIP,
C
C X = 1 - COS(THETA) = 2*SIN(THETA/2)**2
C
C MATHEMATICALLY WE OBTAIN THE SAME DISTRIBUTION WITH EITHER,
C XI      = THETA, OR,
C XI      = 2*SIN(THETA/2)
C
C BUT WITH THE LATTER DEFINITION THERE IS NO RESTRICTION TO
C SMALL ANGLE SCATTERING.
C
C DEFINING ANGULAR SCORING BINS
C =====
C THE MOST IMPORTANT POINT IS HOW THE ANGULAR RANGE IS BINNED
C =====
C FOR SCORING. WITHOUT A GOOD CHOICE YOU CAN EITHER MAKE THIS
C CODE RUN FOREVER, BEFORE YOU OBTAIN STATISTICALLY RELIABLE
C RESULTS, OR LEARN NOTHING ABOUT THE DETAILS OF THE ENTIRE
C ANGULAR DISTRIBUTION.
C
C FROM THE ABOVE DISCUSSION OF THE INTEGRAL OF THE ANGULAR
C DISTRIBUTION IT CAN BE SEEN THAT IT IS NOT PRACTICAL TO
C USE EQUALLY PROBABLE BINS OVER THE ENTIRE ANGULAR RANGE.
C IF THIS WERE DONE 1/2 OF THE BINS WOULD BE BETWEEN (1-COS)
C = 0 AND ETA. SINCE THE PROBABILITY OF SCATTERING TO (1-COS)
C = 1, IS APPROXIMATELY ETA, FOR ETA=1.0E-5 WOULD REQUIRE

```

A MINIMUM OF $1.0E+5$ EQUALLY PROBABLE BINS TO HAVE JUST ONE BIN BETWEEN $(1-\cos) = 1$ TO 2 - THIS SIMPLY WOULD NOT BE PRACTICAL.

HERE, FOR SPEED AND EFFICIENCY, BINS ARE BASED ON THE LOG OF THE PROBABILITY DISTRIBUTION.

$$P(X) = (2+\eta) * X / (2 * (X+\eta))$$

EVALUATING THE PROBABILITY AT ANY 2 POINTS $X = X_1$ AND X_2 ,

$$P(X_1) = X_1 / (X_1 + \eta)$$

$$P(X_2) = X_2 / (X_2 + \eta)$$

$$\log[P_1/P_2] = \log[(X_1/X_2) * (X_2 + \eta) / (X_1 + \eta)]$$

FOR N EQUALLY PROBABLE LOG CHANGES IN PROBABILITY EACH INTERVAL IS $\log[P_1/P_2]/N$ WIDE. UNLIKE USING LINEAR PROBABILITY, WHERE MOST BINS ARE GROUPED IN A VERY SMALL RANGE OF $(1-\cos)$, HERE WE CAN SPAN AS MANY DECADES OF PROBABILITY AS WE WISH, IN AS MUCH DETAIL AS WE WISH, IN ORDER TO REPRODUCE THE ENTIRE ANGULAR DISTRIBUTION.

3 RANGES ARE USED: 1) $P(X) = 0$ TO $1/2$, 2) $1-P(X) = 1/2$ TO $1-P(1)$ [$X = 1$], 3) $X = 1$ TO 2 . THE FIRST BIN IS FROM $X = 0$ TO $\eta/100 = 1\%$ OF THE INTEGRAL. THE FOLLOWING BINS ARE BASED ON EQUAL INCREMENTS IN $\log[P(X)]$ OR $\log[1-P(X)]$, OUT TO $X = 1$. FROM $X = 1$ TO 2 THE NUMBER OF BINS DEPENDS ON THE INTEGRAL $1-P(1) = \%$ SCATTERING TO THE RANGE $X = 1$ TO 2 , AND BINS ARE UNIFORMLY SPACED IN X OVER THIS RANGE.

DIFFERENT SCORING BINS ARE USED FOR EACH MEDIA THICKNESS. AN EMPIRICAL RESULT (SEE BELOW, WHAT DO RESULTS INDICATE?) IS THAT THE ANGULAR DISTRIBUTION AFTER TRANSPORTING THROUGH N MEAN FREE PATHS LOOKS LIKE THE ORIGINAL SINGLE COLLISION DISTRIBUTION WITH η REPLACED BY $N*\eta$. THIS APPROXIMATE SCALING IS USED TO ESTIMATE $P(X)$ TO DEFINE SCORING BINS FOR EACH THICKNESS, USING THE METHOD DESCRIBED IN THE PREVIOUS PARAGRAPH.

THIS BINNING EFFECTIVELY CHANGES THE SAMPLING RANGE OF THE ANGULAR DISTRIBUTION FROM $1/\eta$ TO η (ORIGINAL) TO $1/\eta$ TO 1 - FOR $\eta = 1.0E-5$, THE VARIATION IS REDUCED FROM 10 TO 5 DECADES, WHICH MAKES IT POSSIBLE TO STATISTICALLY SAMPLE THE LOWER PROBABILITY RANGES IN A REASONABLE AMOUNT OF TIME.

WHAT DO THE RESULTS INDICATE?

=====

FROM THE RESULTS THE DISTRIBUTION OF ELECTRONS RELATIVE TO GAMMA (THE DIRECTION COSINE RELATIVE TO THE INITIAL DIRECTION OF TRAVEL) AFTER TRANSPORTING THROUGH SPHERES IS VERY SIMILAR TO THE SINGLE COLLISION RESULTS,

$$A/[X + \eta]**2$$

WITH A LARGER η AND A DIFFERENT NORMALIZATION NEEDED TO CONSERVE ELECTRONS,

$$B/[X + Q*\eta]**2, Q > 1$$

THIS AGREES WITH THE PREDICTION OF FERMI IN HIS 1942 LECTURE NOTES FROM THE UNIVERSITY OF CHICAGO, WHERE HE ESTIMATED

C THAT IF A SINGLE COLLISION ON AVERAGE SCATTERS THROUGH
 C A SMALL ANGLE <THETA>, THEN AFTER N COLLISIONS THE PARTICLE
 C WILL ON AVERAGE HAVE SCATTERED THROUGH AN ANGLE N<THETA>.
 C
 C SINCE THE AVERAGE SCATTERING ANGLE, OR 1-COS, IS DIRECTLY
 C CORRELATED TO ETA, THIS WOULD PREDICT THAT FOR SMALL ETA
 C (SMALL AVERAGE SCATTERING ANGLE), AFTER N COLLISIONS THE
 C DISTRIBUTION WOULD HAVE AN AVERAGE SCATTERING ANGLE N
 C TIMES AS LARGE AS THE SINGLE COLLISION DISTRIBUTION, WHICH
 C IS CONSISTENT WITH THE SAME DISTRIBUTION AS THE SINGLE
 C COLLISION DISTRIBUTION WITH ETA REPLACED BY N*ETA.
 C
 C THIS APPROXIMATION WORKS QUITE WELL TO REPRODUCE MOST OF
 C THE INTEGRAL OF THE ANGULAR DISTRIBUTION. IN ORDER TO REPRODUCE
 C THE LOW PROBABILITY, LARGE ANGLE SCATTER TAIL OF THE DISTRIBUTION
 C A MORE PRECISE MODELS IS,
 C
 C $B/[X + Q*ETA]**K$, $Q > 1$
 C
 C WHERE K IS A SLOWLY VARYING FUNCTION OF THICKNESS, VARYING
 C FROM 2 FOR SMALL THICKNESSES UP TO ABOUT 2.5, FOR 100 MFP
 C AND ETA=1.0E-5.
 C
 C I THOUGHT EVERYTHING WENT TO A GAUSSIAN?
 C =====
 C THE NUMBER OF COLLISIONS WE ARE LOOKING AT IS NOT ENOUGH TO
 C CHANGE THE INITIAL DISTRIBUTION INTO A GAUSSIAN OVER THE
 C ENTIRE ANGULAR RANGE.
 C
 C IF WE LOOK AT A GAUSSIAN,
 C $B*EXP(-Z**2)$ = $B/EXP(Z**2)$
 C = $B/[1 + Z**2 + Z**4/2 + \dots]$
 C ~ $B/[1 + Z**2/2]**2 + \dots$
 C THE FIRST FEW TERMS ARE SIMILAR TO THE ANGULAR DISTRIBUTION
 C = $B/[ETA + X]**2$
 C WITH THE EXPANSION $X = (1 - COS) \sim THETA**2/2$
 C WITH $Z**2/2$ = $THETA**2/2/ETA$
 C $Z**2$ = $THETA**2/ETA$
 C $B*EXP(-THETA**2/ETA) \sim B*ETA/[ETA + THETA**2/2]**2$
 C
 C FOR SMALL X, OR THETA, THE SHAPE WILL BE SIMILAR TO THE ANGULAR
 C DISTRIBUTION, BUT FOR LARGER X THE GAUSSIAN DECREASES FASTER
 C THAN THE ANGULAR DISTRIBUTION AND IF USED AS AN APPROXIMATION
 C WOULD UNDERESTIMATE LARGE ANGLE SCATTERING.
 C
 C COMPUTER DEPENDENCE
 C =====
 C THE CODE IS DIVIDED INTO TWO PARTS,
 C 1) WALKMAN.FOR - COMPUTER INDEPENDENT
 C 2) UTILITY.FOR - COMPUTER DEPENDENT
 C
 C UTILITY.FOR CONTAINS 4 ROUTINES,
 C 1) INITIALIZE RANDOM NUMBER SEQUENCE
 C 2) RANDOM NUMBER GENERATOR
 C 3) DEFINE ELAPSED TIME
 C 4) DEFINE WHETHER OR NOT KEYBOARD KEY HAS BEEN PRESSED
 C
 C UTILITY.FOR IS AVAILABLE FOR USE ON SUN, SGI OR IBM-PC.
 C PLEASE BE SURE TO REQUEST AND USE THE CORRECT UTILITY.FOR
 C FOR YOUR COMPUTER.
 C
 C SINGLE VS. DOUBLE PRECISION
 C =====
 C ALL OF THE CALCULATIONS IN THIS PROGRAM ARE PERFORMED IN DOUBLE
 C PRECISION. FOR VERY SMALL ANGLE SCATTERING, $1 - COS < 1.0E-6$,
 C IT IS IMPOSSIBLE TO ACCURATELY DISTINGUISH BETWEEN $COS = 1$,

C AND COS = 1 - 1.0E-6 (OR SMALLER), IN SINGLE PRECISION,
C BECAUSE WE ARE RUNNING INTO THE ~ 6 DIGITS OF ACCURACY ON A
C 32 BIT PER WORD COMPUTER IN SINGLE PRECISION.

C A SECOND CONSIDERATION IS THAT IN SINGLE PRECISION IT IS
C IMPOSSIBLE TO SAMPLE SMALL PROBABILITY REGIONS AT THE END
C OF THE ANGULAR DISTRIBUTIONS. FOR EXAMPLE, FOR $\eta=1.0E-5$
C THE PROBABILITY OF SCATTERING TO THE RANGE $X = 1$ TO 2 , IS
C ABOUT $5.0E-6$. IF WE SAMPLE FROM $X = 0$ TOWARD 2 , WITH OUR
C RANDOM NUMBER = 0 CORRESPONDING TO $X = 0$, AND 1 TO $X = 2$,
C TO SCATTER TO THE REGION $X = 1$ TO 2 , REQUIRES RANDOM
C NUMBERS BETWEEN 0.999995 AND 1.0 - MOST RANDOM NUMBER
C GENERATORS WILL NEVER RETURN EXACTLY 0 OR 1, SO IN SINGLE
C PRECISION WE WILL RUN INTO A WALL AT ABOUT 0.999999 -
C THE ~ 6 DIGIT SINGLE PRECISION ACCURACY OF A 32 BIT PER
C WORD COMPUTER - AND NEVER SAMPLE THE END OF THE ANGULAR
C DISTRIBUTION.

C WARNING - PLEASE DO NOT TRY THESE CALCULATIONS IN SINGLE
C PRECISION ON 32 BIT PER WORD COMPUTERS. IF YOU
C DO YOU ARE GOING TO BE IN FOR A BIG SHOCK -
C YOU WON'T SAVE THAT MUCH RUNNING TIME, BUT
C YOUR RESULTS COULD BE AT BEST USELESS AND
C AT WORST COMPLETELY MISLEADING.

C=====

DATE

FILMED

10/12/94

END