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Abstract

Bremstrahlung from secondary electrons and positrons created by pair creation has been treated by a simplified method which neglects electrons/positrons movements inside materials using a discrete ordinate code. Bremsstrahlung from recoil electrons after Compton scattering must also be considered for precise calculations of the photon dose inside materials.

It is required to provide data concerning the double differential bremsstrahlung yields after pair production and Compton scattering for a discrete ordinate code. The EGS4 user code, ucbrempc.mor, was written for this purpose.

In this paper, outlines of ucbrempc.mor and the input data are presented together with the calculated results for lead.

1 Introduction

Movements of electrons/positrons inside materials are generally not considered in most photon transport codes, especially in the case of a discrete ordinate method. Bremsstrahlungs photons after pair production are treated by simplified methods concerning their angular distribution using an isotropic distribution[1] or the direction of a photon before pair creation[2].

Pair-produced particles have production angles relative to the incident photon direction, given by $\theta = m_0c^2/k$, where m_0c^2 is the rest-mass energy of the electron and k the energy of the incident photon. A bremsstralung photon, on the other hand, is emitted at an angle relative to the incident electron direction, given by $\theta = m_0c^2/\check{E}_0$, where $\check{E}_0$ is the total energy of the incident electron. In addition, electrons/positrons suffer many elastic scatterings inside the material and change their directions. Therefore, the angular distributions of bremsstrahlung photons are complicated and strongly depend on the material and the incident photon energy.

Bremsstrahlung photons from a recoil electron after Compton scattering also contribute to the dose inside a material and must be considered.

It is required to provide double differential yields of bremsstrahlung photons after pair production and/or Compton scattering for precise calculations by a discrete ordinate photon transport code.

An elecromagnetic cascade shower Monte Carlo code, EGS4[3], was used for this purpose. The usercode of EGS4, ucbrempc.mor, was written to calculate the required photon yields after pair production and/or Compton scattering.

Outlines of ucbrempc.mor and its input data are given below together with the results for 16 MeV photons in lead.

2 Outline of ucbrempc.mor

2.1 Main Program

2.1.1 Material data file

Material data produced using pegs4 must be included in a material data file named "paircom.xsec" in this user code. If all material data necessary are included in this file, one can assign the material to be calculated as part of the input data mentioned below.

2.1.2 Input data

The following items are necessary to define the input data, and must be included in the input data file, named "paircom.inp".

1. Material name (24 characters)
2. Number of energy bins (less than 100)
3. Upper energy of each bin (in MeV, lowest energy is assumed as 0.0)
4. Number of angular bins (less than 100)
5. Upper angle of each angular bin (in degrees, smallest angle is assumed to be 0.0 degree)
6. Incident photon energy (in MeV)
7. Type of interaction (0:pair creation, 1:Compton scattering)
8. History number

A sample of paircom.inp is as follows:

```
WATER-IAPRIM-PHOTX                                  "Material name"
43                                                  "Number of energy bin"
0.01,0.02,0.03,0.045,0.06,0.08,0.1,0.15,0.2,0.3,
0.4,0.45,0.51,0.512,0.6,0.7,0.8,0.9,1.0,1.125,
1.25,1.375,1.5,1.75,2.0,2.25,2.5,3.0,3.5,4.0,
4.5,5.0,5.5,6.0,6.5,7.0,7.5,8.0,9.0,10.0,
12.0,14.0,16.0
40                                                  "Number of angular bin"
5.4,9.9,14.4,18.9,23.3,27.8,32.2,36.7,41.4,45.5,
50.0,54.4,58.9,63.3,67.8,72.2,76.7,81.1,85.6,90.0,
94.4,98.9,103.3,107.8,112.2,116.7,121.1,125.6,130.0,
134.5,138.9,143.3,147.8,152.2,156.7,161.1,165.6,170.1,
174.6,180.0
16.00                                               "photon energy in MeV"
1                                                   "0:pair, 1:Compt"
400000                                              "History number"
```

2.1.3 Cut-off energy and production angle after pair production and Bremsstrahlung

A bremsstrahlung photon must be discarded immediately after creation to calculate the double differential bremsstrahlung yield. The photon cut-off energy, PCUT is, therefore, set to the upper energy (20 MeV in this example).

In the default EGS4, the production angle of a pair-produced particle or bremsstrahlung photon is set to $\theta = m/k$ or $\theta = m/\check{E}_0$, respectively. The option to sample the production angle precisely is used both for pair production and bremsstrahlung by setting the flags of IPRDST and IBRDST to 1.

2.1.4 Sampling of information of an electron/positron after an interaction

In an ordinary calculation, the user code calls SUBROUTINE SHOWER with information about the type of particle (IQI), total energy (EI), positions (XI, YI, ZI), direction cosines (UI, VI, WI), region of source particle (IRI) and weight of the source particle (WTI).

It is necessary to calculate the energy, and the direction cosines after the interaction must be determined at first in this case. The following statements are put before CALL SHOWER. IPACO is a flag used to indicate the type of interaction defined in the input data: 0 for pair creation and 1 for Compton scattering, respectively.

```
X(1)=XI0; Y(1)=YI0; Z(1)=ZI0; U(1)=UI0; V(1)=VI0; W(1)=WI0;
E(1)=EI0; IR(1)=IRI0; IQ(1)=IQI0; WT(1)=WTI0;
NP=1; MEDIUM=MED(2);

IF(IPACO.EQ.0) ["Pair creation"
CALL PAIRS;

EIB(1)=E(1); EIB(2)=E(2);
UIB(1)=U(1); UIB(2)=U(2); VIB(1)=V(1); VIB(2)=V(2);
WIB(1)=W(1); WIB(2)=W(2); IQIB(1)=IQ(1); IQIB(2)=IQ(2);
NELPO=2;]

ELSE ["Compton"
CALL COMPT;

IF(IQ(1).NE.0) [
EIB(1)=E(1); UIB(1)=U(1);
VIB(1)=V(1); WIB(1)=W(1); IQIB(1)=IQ(1);]
ELSE [
EIB(1)=E(2); UIB(1)=U(2);
VIB(1)=V(2); WIB(1)=W(2); IQIB(1)=IQ(2);]
NELPO=1;
]

DO IPC=1,NELPO [
IF(EIB(IPC).EQ.0.0) [STOP;]

XI=XI0; YI=YI0; ZI=ZI0;
UI=UIB(IPC); VI=VIB(IPC); WI=WIB(IPC);
IRI=IRI0; IQI=IQIB(IPC); WTI=WTI0;
EI=EIB(IPC);
LATCHI=0;ISOP=IQI;
TOTKE=TOTKE+EI+IQI*PRM;
```

2.1.5 AUSGAB

A discarded photon after bremsstrahlung was scored depending on its energy and directional cosine W(NP) for the double differential bremsstrahlung yield. The energy and angular bins are defined in the input data in the main program.

```
IF(IQ(NP).EQ.0) [

DO IE=1,NEBIN[
IF(E(NP).LE.ETAB(IE)) [EXIT;]
]

IEBIN=IE;
IF(IEBIN.GT.NEBIN) [IEBIN=NEBIN;]

DO IANG=1,NABIN [
IF(W(NP).GT.WIANG(IANG)) [EXIT;]
]

IF(IANG.GT.NABIN) [IANG=NABIN;]
PHEIW(IANG,IEBIN)=PHEIW(IANG,IEBIN)+DPWT;

]
```

Full lists of ucbrempc.mor are given in Appendix.

3 Calculated Results for 16 MeV Photons

Figs. 1 and 2 show the double differential photon yields in lead produced by 16 MeV photons after pair production and Compton scattering, respectively. The results are shown as photons/Sr./MeV per pair production or Compton scattering.

In Fig. 1, positron annihilation gammas (0.511 MeV), which do not depend on the angular bin, are clearly shown.

At pair production, 1.022 MeV is used to create an electron and positron pair and, therefore, the maximum energy of the electron or positron is 14.978 MeV in this case. This energy is divided between the electron and positron. On the other hand, the maximum energy of a Compton recoil electron is 15.75 MeV, as calculated by the following equation:

$$E_{max} = h\nu_0 \frac{2h\nu_0/m_0c^2}{1+2h\nu_0/m_0c^2}, \tag{1}$$

where $h\nu_0$ is the incident photon energy before the interaction. The shape at the highest energy part is the reflection of these differences.

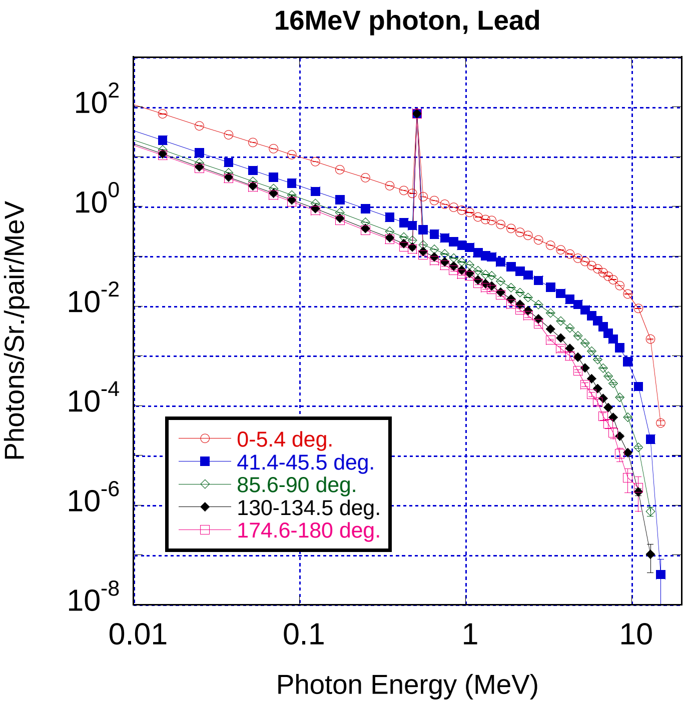

Figure 1: Double differential bremsstrhlung yield per pair production inside lead with 16 MeV photons.

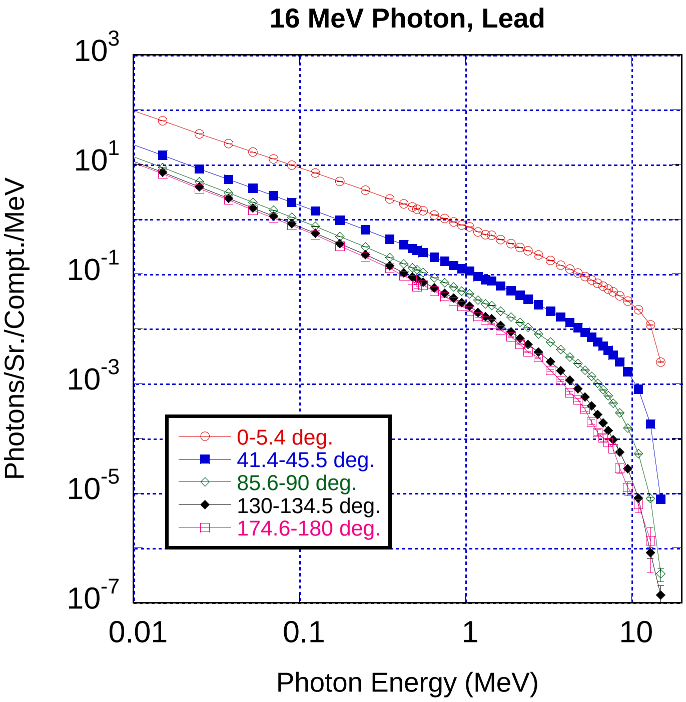

Figure 2: Double differential bremsstrhlung yield per Compton scattering inside lead with 16 MeV photons.

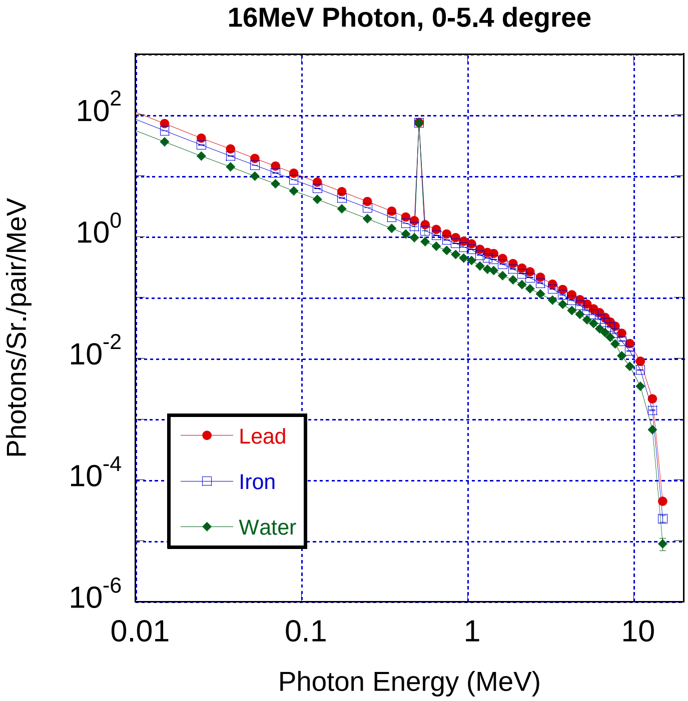

Figure 3: Double differential bremsstrhlung yield between 0 and 5.4 degrees per pair production inside lead, iron and water with 16 MeV photons.

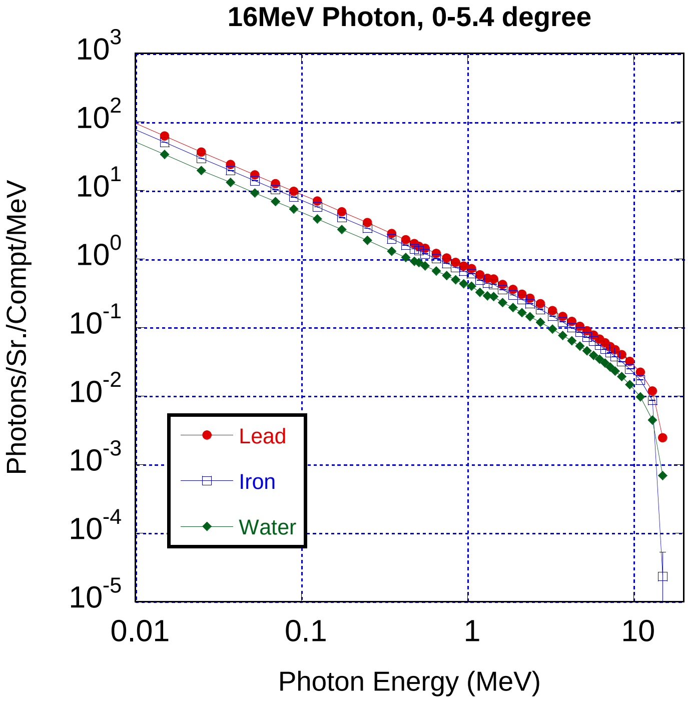

Figure 4: Double differential bremsstrhlung yield between 0 and 5.4 degrees per Compton scattering inside lead, iron and water with 16 MeV photons.

Figs. 3 and 4 show the double differential photon yields between 0 and 5.4 degrees in lead, iron and water produced by 16 MeV photons after pair production and Compton scattering, respectively.

In general, the photon yields, except for the annihilation photons, slightly decrease with a decrease in the atomic number of the material. This tendency is due to the fact that the ration between the collision and radiative stopping power increases with a decrease in the atomic number.

References

[1] Radiation Shielding Information Center Code collection package CCC-336/ASFIT-DS2: Gamma ray transport code for one dimentional finite system, Contributed by the Reactor Research Center, Kaplakkam, India, and ORNL.

[2] K. Takeuchi and S. Tanaka, "PALLAS-1D(VII): A code for discrete integration of transport equation in one-dimentional plane and spherical geometry", *JAERI-M 82-214* (1984).

[3] W. R. Nelson, H. Hirayama and D. W. O. Rogers, "The EGS4 Code System", *SLAC-265*, Stanford Linear Accelerator Center, (1984).

Appendix: Lists of ucbrempc.mor

```
!INDENT M3;
!INDENT F2;
"******************************************************************"
"****************************  High Energy Accelerator Research    *"
"****************************  Organization (KEK)                  *"
"***   U C B E M P C *******                                       *"
"****************************  EGS4 USER CODE -- 13 Feb 2002/0930  *"
"******************************************************************"
"                                                                  "
"  PROGRAMMER:   HIDEO HIRAYAMA                                    "
"                High Energy Accelerator Research Organization(KEK)"
"                1-1 Oho, Tsukuba, Ibaraki, 305-0801                "
"                JAPAN                                             "
"                                                                  "
"******************************************************************"
"                                                                  "
"  PROGRAM:      UCBREMPC                                          "
"                                                                  "
"                EGS4 user code to calculate bremmstrahlung        "
"                production after pair creation or Compton.        "
"                Energy mesh, angular mesh, material and photon    "
"                energy are read from file (paircom.dat).          "
"                                                                  "
"******************************************************************"
"                                                                  "
"                     F E A T U R E S                              "
"                                                                  "
"    - USES ENERGY CONSERVATION PROGRAM CALLED ECNSV1
"
"    - USES 'COUNTER' ROUTINE CALLED NTALLY                        "
"                                                                  "
"******************************************************************"
"                                                                  "
"       THE FOLLOWING 'STEPS' REFER TO THE STEPS OUTLINED          "
"       IN THE EGS3 USER MANUAL (SLAC-210).                        "
"       VARIOUS EGS USER NOTES (EUN'S) HAVE BEEN CREATED           "
"       TO SUPPLEMENT SLAC-210 FOR THE CORRECTIONS, CHANGES
"
"       AND ADDITIONS THAT ARE IN EGS4.                            "
"                                                                  "
"******************************************************************"
"******** STEP 1.  USER-OVER-RIDE-OF-EGS-MACROS ******************"
"******************************************************************"

REPLACE{$CALL-HOWNEAR(#);} WITH
 {$CALL-HOWNEAR-FOR-SLAC-PLANE-GEOMETRY({P1});}

"                ****                                           "
"THIS IS THE MACRO THAT SHOULD RETURN THE CLOSEST PERPENDICULAR
"
"DISTANCE TO ANY SURFACE WHIC FORMS A BOUNDARY FOR THE CURRENT
"
"REGION. IN THIS APPLICATION T IS REPLACED BY THE MACRO FOLLOW- "
"ING WHICH IS SPECIALIZED FOR THE SLAC PLANE GEOMETRY.          "
"IT IS THE USER'S RESPONSIBILITY TO PROVIDE THIS MACRO FOR HIS  "
"OWN GEOMETRY.                                                  "
"++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++   "

; "BUFFER FLUSH"
REPLACE{$CALL-HOWNEAR-FOR-SLAC-PLANE-GEOMETRY(#);} WITH

"       ===================***=========================="
   {;ZL=Z(NP);IRL=IR(NP);
   ZLEFT=ZL-PCOORD(3,IRL-1);ZRIGHT=PCOORD(3,IRL)-ZL;
   {P1}=MIN(ZLEFT,ZRIGHT);}

"THIS ROUTINE IS INTENDED TO BE USED TO CALCULATE THE MINIMUM   "
"PERPENDICLAR TO THE NEAREST BOUNDING SURFACE. THIS VERSION IS  "
"SPECIALLY DESIGNED FOR THE SLAC PLANE GEOMETRY PACKAGE.        "
"A DIFFERENT VERSION IS NEEDED FOR OTHER GEOMETRY PACKAGES.     "
```

```
"GEOMETRICAL INFORMATION"
"SLAC DEFINITION OF /GEOM/ AND RE-DEFINITIONS FOR /PLADTA/      "
"****                                                           "
REPLACE {;COMIN/GEOM/;} WITH {;COMIN/PLADTA/;}

"------------------------------------------------------------------"
" Select random number generator: 0=RAN6 1=RANMAR                  "
"RANMAR is a Lagged-Fibonacci Method pseudo random number generator"
"devised by George Marsaglia and Arif Zaman.                       "
"------------------------------------------------------------------"
REPLACE {$RNGEN} WITH {1}

REPLACE {;COMIN/RANDOM/;} WITH {
 {SETR B=$RNGEN}
 [IF] {COPY B}=0 [
   ;COMMON/RANDOM/IXX;
   ]
 [IF] {COPY B}=1 [
   ;COMMON/RANDOM1/URNDM(97),CRNDM,CDRNDM,CMRNDM,IXX,JXX;
   ]
   }
REPLACE {$RANDOMSET#;} WITH {
 {SETR B=$RNGEN}
 [IF] {COPY B}=0 [
   IXX=IXX*663608941;{P1}=IXX*0.23283064E-09;IF(IXX.LT.0){P1}={P1}+1.0;
   ]
 [IF] {COPY B}=1 [
    {P1}=URNDM(IXX)-URNDM(JXX); IF({P1}.LT.0.) {P1}={P1}+1.;
    URNDM(IXX) = {P1};
    IXX=IXX-1; IF(IXX.EQ.0) IXX=97;
    JXX=JXX-1; IF(JXX.EQ.0) JXX=97;
    CRNDM=CRNDM-CDRNDM; IF(CRNDM.LT.0.) CRNDM=CRNDM+CMRNDM;
    {P1}={P1}-CRNDM; IF({P1}.LT.0.) {P1}={P1}+1.;
   ]
   }
"This should be called somewhere near the beginning of the main routine"
"before any random numbers are asked for";
REPLACE {$RNG-INITIALIZATION;} WITH {;
 {SETR B=$RNGEN}
 [IF] {COPY B}=0 [;]
 [IF] {COPY B}=1 [ IXX=0; JXX=0; CALL RMARIN;
      DO II=1,20005[
      $RANDOMSET XX;
      IF(II.GT.20000) OUTPUT (MOD(INT(XX*16.**JJ),16),JJ=1,7);
      (8X,7I3); ]
    ]
 }

PARAMETER $MXPLNS=2; "NUMBER OF PLANE"
PARAMETER $MXSPHE=1; "Number of shpere"
PARAMETER $NCASES=1000000; "MAXIMUN NUNBER OF CASES"
PARAMETER $NCASES=400000; "MAXIMUN NUNBER OF CASES"
PARAMETER $NBATCH=500;  "Number of batch"
PARAMETER $NEBIN=100;   "Number of energy bin"
PARAMETER $ANGBIN=100;   "Number of angular bin"

"******************************************************************"
"******************* ADDITIONAL (NON-EGS) MACROS ******************"
"******************************************************************"

"                      N O N E                                     "

"******************************************************************"
"************************** DECLARATIONS **************************"
"******************************************************************"

;COMIN/DEBUG,BOUNDS,BREMPR,EDGE,ELECIN,ETALY1,GEOM,PHOTIN,SPH
DTA,
       MEDIA,MISC,NTALY1,RANDOM,STACK,THRESH,UPHIOT,USEFUL,USER/;
COMMON/LINES/NLINES,NWRITE,NCOUNT,ILINES;
COMMON/TOTALS/PHEIW($ANGBIN,$NEBIN),WIANG($ANGBIN),ETAB($NEBIN)
,
              NEBIN,NABIN;
```

```
COMMON/PASSIT/NREG,NPLAN;
DIMENSION PHEIWPB($ANGBIN,$NEBIN,$NBATCH),EIB(2),UIB(2),VIB(2),
WIB(2),IQIB(2),SANG($ANGBIN),ANG($ANGBIN),EBIN($NEBIN);
REAL*8 TOTKE,AVAILE,DEPE;
       "NEEDED FOR ENERGY CONSERVATION TABULATION"

CHARACTER*4 MEDARR(24,1);

"******************************************************************"
"*************** START OF EXECUTABLE CODE *************************"
"******************************************************************"

OPEN(5,FILE='paircom.inp',STATUS='UNKNOWN');
OPEN(6,FILE='mortjob.output',STATUS='UNKNOWN');
OPEN(7,FILE='mortjob.out7',STATUS='UNKNOWN');
OPEN(8,FILE='mortjob.dummy',STATUS='UNKNOWN');
OPEN(12,FILE='paircom.xsec',STATUS='OLD');

"******************************************************************"
"******** STEP 2.  PRE-HATCH-CALL-INITIALIZATION COMES NEXT *******"
"******************************************************************"

NMED=1; "NUMBER OF MEDIA"

READ(5,:FMTMA:) (MEDARR(I,1),I=1,24);
:FMTMA:FORMAT(24A1);

DO J=1,NMED [
DO I=1,24 [MEDIA(I,J)=MEDARR(I,J);]]

NPLAN=$MXPLNS;    "NUMBER OF PLANES"
NREG=NPLAN+1; "NUMBER OF REGIONS (INCLUDING OUTSIDE VACUUM"
"                       REGION)                                       "
"SET MEDIUM INDEX FOR EACH REGION"

/MED(1),MED(NREG)/=0;   "VACUUM REGIONS"

MED(2)=1;    "MEDARR material"
PCUT(2)=20.0;   "Discard photon immediately"

"******************************************************************"
"***************** STEP 3.  HATCH-CALL COMES NEXT *****************"
"******************************************************************"

CALL HATCH;

"OUTPUT VARIOUS QUANTITIES ASSOCIATED WITH THE MEDIA"

OUTPUT;  ('1QUANTITIES ASSOCIATED WITH EACH MEDIA:',//);

DO J=1,NMED [
OUTPUT (MEDIA(I,J),I=1,24);  (/,1X,24A1);
OUTPUT RHO(J),RLC(J);  (5X,' RHO=',G15.7,' G/CM**3     RLC=',
   G15.7,' CM');
OUTPUT AE(J),UE(J);  (5X,' AE=',G15.7,' MEV    UE=',G15.7,' MEV');
OUTPUT AP(J),UP(J);  (5X,' AP=',G15.7,' MEV    UP=',G15.7,' MEV');
]

OUTPUT;(/' INFORMATION OF MEDIUM AND CUT-OFFFOR EACH REGION'//);
DO I=1,NREG [
IF(MED(I).EQ.0) [OUTPUT I,ECUT(I),PCUT(I);
(' MEDIUM(',I3,')=VACUUM',18X,'ECUT=',G10.5,' MEV, PCUT=',G10.5,' MEV');
]
ELSE [OUTPUT I,(MEDIA(II,MED(I)),II=1,24),ECUT(I),PCUT(I);
(' MEDIUM(',I3,')=',24A1,'ECUT=',G10.5,' MEV, PCUT=',G10.5,' MEV');]
]

DO I=1,NREG [IF(IEDGFL(I).NE.0) [CALL EDGSET(NREG); EXIT;]]

"******************************************************************"
"*********** STEP 4.  HOWFAR-INITIALIZATION COMES NEXT ************"
"******************************************************************"
```

```
"DEFINE VARIOUS THICKNESSES/DISTANCES"

TDE=100.0;   "Thickness of sample in cm"

"DEFINITION OF PLANES"

"SET ALL COORDINATES AND NORMALS TO ZERO TO BEGIN WITH"
DO J=1,NPLAN [
  PCOORD(1,J)=0.0;  PCOORD(2,J)=0.0;  PCOORD(3,J)=0.0;
  PNORM(1,J)=0.0;   PNORM(2,J)=0.0;   PNORM(3,J)=1.0;
]

"NOW PUT IN THE EXCEPTIONS"

PCOORD(3,1)=-100.0;
PCOORD(3,2)=TDE;

OUTPUT; ('1PCOORD AND PNORM VALUES FOR EACH J-PLANE (I=1,3):',//);
DO J=1,NPLAN [
OUTPUT J,(PCOORD(I,J),I=1,3),(PNORM(I,J),I=1,3);
(I5,6G15.7);]

"******************************************************************"
"********** STEP 5.  INITIALIZATION FOR AUSGAB COMES NEXT *********"
"******************************************************************"

CALL ECNSV1(0,NREG,TOTKE);"  INITIALIZE ESUM ARRAY FOR ENERGY"
"                            CONSERVATION CALCULATION."
"                            NREG=NUMBER OF REGIONS"
"                            TOTKE=TOTAL KE (DUMMY VARIABLE HERE)"
"                                  (MUST BE REAL*8)"

CALL NTALLY(0,NREG);

NCOUNT=0;  "PARTICLE HISTORY COUNTER"
ILINES=0;  "INITIALIZE LINE-OUTPUT COUNTER"
DEPE=0.D0; "ZERO THE ENERGY DEPOSITION AT SCINTILATOR"
PEFF=0.0;  "Zero of the peak efficiency"

DO IANG=1,40 [
DO J=1,$NEBIN [
PHEIW(IANG,J)=0.0;]]

READ(5,*) NEBIN;
READ(5,*) (ETAB(J),J=1,NEBIN);

READ(5,*) NABIN;
READ(5,*) (ANG(IANG),IANG=1,NABIN);
DO IANG=1,NABIN [
WIANG(IANG)=COS(ANG(IANG)/180.0*PI);
IF(IANG.EQ.1) [SANG(IANG)=2.0*PI*(1.0-WIANG(IANG));]
ELSE [SANG(IANG)=2.0*PI*(WIANG(IANG-1)-WIANG(IANG));]
]

"USAGE: IPRDST=0 => EGS4 DEFAULT ANGLE SELECTION                  "
"       IPRDST=1 => LOWEST ORDER ANGULAR DISTRIBUTION             "
IPRDST=1;

"USAGE: IBRDST=0 => EGS4 DEFAULT ANGLE SELECTION                  "
"       IBRDST=1 => KOCH AND MOTZ (1959) EQ. 2BS ANGLE SELECTION  "
IBRDST=1;

IBRSPL=1; "Set brems splitting flag"
IF(IBRSPL.NE.0) [
  NBRSPL=100;"Splitting number"
  FBRSPL=1.0/FLOAT(NBRSPL);  "Weight after splitting"
  ]

"******************************************************************"
"****** STEP 6.  DETERMINATION OF INCIDENT PARTICLE PROPERTIES ****"
"******************************************************************"

IQI0=0;  "INCIDENT PARTICLE"
```

```
READ(5,*) EI0;
EI0=EI0-IQI*PRM;   "TOTAL ENERGY OF PARTICLE (MEV) "

AVAILE=EI0 + IQI0*PRM;  "AVAILABLE K.E. (MEV) (MUST BE REAL*8)"
EKIN=AVAILE;

ECUTMN=ECUT(2);  EK0=EKIN;   "*PRESTA*"
$PRESTA-INPUTS;  "INPUT THE *PRESTA* VARIABLES"

EISING=EI;  "SINGLE PRECISION ENERGY VARIABLE"

READ(5,*) IPAC0;
"0: after pair creation, 1:after Compton scattering"
XI0=0.0; YI0=0.0; ZI0=0.0;  "STARTING COORDINATES (CM)"
UI0=0.0; VI0=0.0; WI0=1.0;  "INCIDENT DIRECTION COSINES"
IRI0=2;  "ENTRANCE REGION DEFINITION"
WTI0=1.0;  "WEIGHT FACTOR OF UNITY"

IDINC=-1; "AN IDENTIFIER (LIKE IARG) TO MARK INCIDENT PARTICLES"

$RNG-INITIALIZATION;
IXXST=IXX;

NWRITE=10;  "NUMBER OF INCIDENT CASES TO PRINT OUT"


READ(5,*) NCASES;
"MAXIMUM NUMBER OF INCIDENT CASES TO RUN"
NBATCH=$NBATCH;  "NUMBER OF BATCH"
NCASPB=NCASES/NBATCH; "NUMBER OF CASES PER BATCH"
NOFBAT=0;  "NUMBER OF BATCH FINISHED"

NLINES=15; "NUMBER OF LINES TO PRINT OUT"

TOTKE=0.0;

"*******************************************************************"
"******************** STEP 7. SHOWER-CALL---NEXT ******************"
"*******************************************************************"

DO I=1,NCASES ["START OF SHOWER CALL LOOP"

X(1)=XI0; Y(1)=YI0; Z(1)=ZI0; U(1)=UI0; V(1)=VI0; W(1)=WI0;
E(1)=EI0; IR(1)=IRI0; IQ(1)=IQI0; WT(1)=WTI0;
NP=1; MEDIUM=MED(2);

IF(IPAC0.EQ.0) ["Pair creation"
CALL PAIRS;

EIB(1)=E(1); EIB(2)=E(2);
UIB(1)=U(1); UIB(2)=U(2); VIB(1)=V(1); VIB(2)=V(2);
WIB(1)=W(1); WIB(2)=W(2); IQIB(1)=IQ(1); IQIB(2)=IQ(2);
NELP0=2;]

ELSE ["Compton"
CALL COMPT;

IF(IQ(1).NE.0) [
EIB(1)=E(1); UIB(1)=U(1);
VIB(1)=V(1); WIB(1)=W(1); IQIB(1)=IQ(1);]
ELSE [
EIB(1)=E(2); UIB(1)=U(2);
VIB(1)=V(2); WIB(1)=W(2); IQIB(1)=IQ(2);]
NELP0=1;
]

DO IPC=1,NELP0 [

IF(EIB(IPC).EQ.0.0) [STOP;]

XI=XI0; YI=YI0; ZI=ZI0;
UI=UIB(IPC); VI=VIB(IPC); WI=WIB(IPC);
```

```
IRI=IRI0; IQI=IQIB(IPC); WTI=WTI0;
EI=EIB(IPC);
LATCHI=0;ISOP=IQI;
TOTKE=TOTKE+EI+IQI*PRM;

IF(NCOUNT.LE.NWRITE.AND.ILINES.LE.NLINES) [
  OUTPUT EI,XI,YI,ZI,UI,VI,WI,
  IQI,IRI,IDINC;   (7G15.7,3I5);
  ILINES=ILINES+1;]

CALL SHOWER(IQI,EI,XI,YI,ZI,UI,VI,WI,IRI,WTI);

]

IF(MOD(I,NCASPB).EQ.0)[
NOFBAT=NOFBAT+1;
DO IANG=1,NABIN [
DO IE=1,NEBIN [
PHEIWPB(IANG,IE,NOFBAT)=PHEIW(IANG,IE)/NCASPB;
PHEIW(IANG,IE)=0.0;
]]
]

NCOUNT=NCOUNT + 1;
IXXEND=IXX;   "LAST RANDOM NUMBER USED"

"END OF SHOWER CALL LOOP"]

"******************************************************************"
"******************** STEP 8. OUTPUT OF RESULTS *******************"
"******************************************************************"

OUTPUT NCOUNT,IXXST,IXXEND,AVAILE,TOTKE;
('1',I10,' CASES COMPLETED',
     //,' IXXST=',I12,/,' IXXEND=',I12,//,' AVAILABLE K.E.=',
     G15.5,' MEV',/,' TOTKE=',E15.5,' MEV',//);

OUTPUT;(' PRESTA algorithm is used.'/);

IF(IPACO.EQ.0) ["After pair"
OUTPUT EI0;(' Bremss. after pair, Photon energy =',G15.5,'MeV');
WRITE(7,:FMT0:) EI0;
:FMT0:FORMAT(' Photon Energy=',G15.5,'MeV'/
' EUP,  photons/Sr./pair');
]
ELSE ["After Compt"
OUTPUT EI0;(' Bremss. after Compt, Photon energy =',G15.5,'MeV');
WRITE(7,:FMT01:) EI0;
:FMT01:FORMAT(' Photon Energy=',G15.5,'MeV'/
' EUP,  photons/Sr./Compt');
]

OUTPUT ;(/' Doublel differentila bremsstralung ');
DO IANG=1,NABIN [
IF(IANG.EQ.1) [ANG0=0.0; ANG1=ANG(1);]
ELSE [ANG0=ANG(IANG-1); ANG1=ANG(IANG);]
OUTPUT ANG0,ANG1;(' Angle ',F6.1,' -- ',F6.1,' degree');
WRITE(7,:FMT1:) ANG0,ANG1;
:FMT1:FORMAT(' Angle ',F6.1,' -- ',F6.1,' degree');

OUTPUT;
(' Upper energy',10X,' photons/Sr. ');

DO IE=1,NEBIN [
IF(IE.EQ.1) [ELOW=0.0;]
ELSE [ELOW=ETAB(IE-1);]
EUP=ETAB(IE);
DELTAE=EUP-ELOW;

IF(ELOW.GT.EI0) [EXIT;]

/AVENEW,DESCI2/=0.0;
```

```
DO J=1,NOFBAT [
AVENEW=AVENEW+PHEIWPB(IANG,IE,J)/NOFBAT;
DESCI2=DESCI2+PHEIWPB(IANG,IE,J)*PHEIWPB(IANG,IE,J)/NOFBAT;
]
SIGMAW=SQRT((DESCI2-AVENEW*AVENEW)/(NOFBAT-1));
AVENEW=AVENEW/SANG(IANG);
SIGMAW=SIGMAW/SANG(IANG);

OUTPUT EUP,AVENEW,SIGMAW;
(1X,G10.4,'--',G15.5,'+-',G15.5);

WRITE(7,:FMT2:) EUP,AVENEW,SIGMAW;
:FMT2:FORMAT(3E10.3);
]]


"NEXT, CALL THE SUBROUTINE ECNSV1 TO WRITE-OUT THE ENERGY
DEPOSITION"
"TOTALS---TO CHECK ENERGY CONSERVATION FOR ONE THING"

CALL ECNSV1(1,NREG,TOTKE);

CALL NTALLY(1,NREG);

STOP;
END;  "END OF MAIN PROGRAM"

%E
"******************************************************************"
"                KEK, High Energy Accelerator Research Organization"
SUBROUTINE AUSGAB(IARG);
"                                EGS4 SUBPROGRAM - 13 Feb 2002/1730"
"******************************************************************"
;COMIN/DEBUG,EPCONT,ETALY1,MISC,NTALY1,SPHDTA,STACK/;
COMMON/TOTALS/PHEIW($ANGBIN,$NEBIN),WIANG($ANGBIN),ETAB($NEBIN)
,
              NEBIN,NABIN;
COMMON/PASSIT/NREG,NPLAN;
COMMON/LINES/NLINES,NWRITE,NCOUNT,ILINES;
REAL*8 DPWT,DEPE;
IRL=IR(NP);   "SET LOCAL VARIABLE"
DPWT=WT(NP);

"KEEP TRACK OF THE ENERGY DEPOSITION---FOR CONSERVATION
PURPOSES"
ESUM(IQ(NP)+2,IRL,IARG+1)=ESUM(IQ(NP)+2,IRL,IARG+1)+EDEP*DPWT;
NSUM(IQ(NP)+2,IRL,IARG+1)=NSUM(IQ(NP)+2,IRL,IARG+1) + 1;


IF(IQ(NP).EQ.0) [

DO IE=1,NEBIN[
IF(E(NP).LE.ETAB(IE)) [EXIT;]
]

IEBIN=IE;
IF(IEBIN.GT.NEBIN) [IEBIN=NEBIN;]

DO IANG=1,NABIN [
IF(W(NP).GT.WIANG(IANG)) [EXIT;]
]

IF(IANG.GT.NABIN) [IANG=NABIN;]
PHEIW(IANG,IEBIN)=PHEIW(IANG,IEBIN)+DPWT;

]

IF(NCOUNT.LE.NWRITE.AND.ILINES.LE.NLINES) [
OUTPUT E(NP),X(NP),Y(NP),Z(NP),U(NP),V(NP),W(NP),
  IQ(NP),IRL,IARG;   (7G15.7,3I5);
ILINES=ILINES+1;]

RETURN;
```

```
END;  "END OF SUBROUTINE AUSGAB"

%E
"****************************************************************"
"                 KEK, High Energy Accelerator Research Organization"
SUBROUTINE HOWFAR;
"                                 EGS4 SUBPROGRAM - 13 Feb 2002/1730"
"****************************************************************"
;COMIN/DEBUG,EPCONT,GEOM,STACK,THRESH/;
COMMON/PASSIT/NREG,NPLAN;

IRL=IR(NP);  "SET LOCAL VARIABLE"

IF(IRL.LE.1.OR.IRL.EQ.NREG) [IDISC=1; RETURN;]

NPL1=IRL; NPL2=IRL-1;
NRG1=IRL+1;
NRG2=IRL-1;

$PLAN2P(NPL1,NRG1,1,NPL2,NRG2,-1);

RETURN;
END;  "END OF SUBROUTINE HOWFAR"

%E
```

```
"*********************************************************************"
"                                  STANFORD LINEAR ACCELERATOR CENTER"
SUBROUTINE ECNSV1(NTREE,NREG,TOTKE);
"                                  EGS4 SUBPROGRAM -  8 MAY 1983/1730"
"*********************************************************************"
"   SUBROUTINE FOR KEEPING TRACK OF ENERGY CONSERVATION---TO BE
"
"   USED WITH EGS USER CODES.  WHEN NTREE=0, THE PROGRAM IS
"
"   ENTERED IN ORDER TO INITIALIZE THE ESUM ARRAY TO ZERO.           "
"   OTHERWISE, IT IS ENTERED FOR TOTALING AND OUTPUTTING THE
"
"   RESULTS.  THE ESUM ARRAY IS NEEDED IN SUBROUTINE AUSGAB,
"
"   WHERE EDEP (ENERGY DEPOSITION) IS ADDED TO THE ELEMENT OF
"
"   THE ARRAY CORRESPONDING TO THE VALUE OF IQ, IR, AND IARG.        "
"*********************************************************************"
COMIN/DEBUG,ETALY1/;  "INSERT IN ALL SUBPROGRAMS THAT USE ESUM"
REAL*8 ROWSUM(4,$MXREG),COLSUM(4,5),SUMSUM(4),GSUM,TOTKE;

"   CHECK WHETHER NREG IS GE $MXREG.  IF IT IS, STOP AND OUTPUT.    "
IF(NREG.GT.$MXREG) [
MDUMMY=$MXREG;
OUTPUT NREG,MDUMMY;
(///,' ***** NOTE: STOPPED IN SUBROUTINE ECNSV1 BECAUSE NREG= ',
 I5,' IS LARGER THAN $MXREG= ',I5,' *****');
STOP;]

IF(NTREE.EQ.0) [  "INITIALIZE ESUM TO ZERO AND RETURN"
DO I=1,4 [DO J=1,NREG [DO K=1,5 [ESUM(I,J,K)=0.D0;]]]
RETURN;]

"   REACH THIS POINT WHEN FINAL TALLY IS TO BE MADE."

"   FIRST, INITIALIZE SUMS"

GSUM=0.D0;

DO IQ=1,4 [
SUMSUM(IQ)=0.D0;
DO IR=1,NREG [ROWSUM(IQ,IR)=0.D0;]
DO ICODE=1,5 [COLSUM(IQ,ICODE)=0.D0;]
"   END OF IQ-LOOP"]

"   SUM IQ=1,2,3 INTO IQ=4 OF ESUM FOR ALL IR- AND ICODE-VALUES"

DO IR=1,NREG [
DO ICODE=1,5 [
DO IQ=1,3 [
ESUM(4,IR,ICODE)=ESUM(4,IR,ICODE) + ESUM(IQ,IR,ICODE);
]]]

"   NORMALIZE DATA TO TOTKE"

DO IQ=1,4 [
DO IR=1,NREG [
DO ICODE=1,5 [
ESUM(IQ,IR,ICODE)=ESUM(IQ,IR,ICODE)/TOTKE;
]]]

"   SUM-UP COLUMNS AND ROWS"

DO IQ=1,4 [
DO IR=1,NREG [
DO ICODE=1,5 [
ROWSUM(IQ,IR)=ROWSUM(IQ,IR)+ESUM(IQ,IR,ICODE);
]]

DO ICODE=1,5 [
DO IR=1,NREG [
COLSUM(IQ,ICODE)=COLSUM(IQ,ICODE)+ESUM(IQ,IR,ICODE);
]]
"   END OF IQ-LOOP"]

"   NOW GET TOTAL FOR IQ AND GRAND TOTAL"

DO IQ=1,4 [
DO IR=1,NREG [
DO ICODE=1,5 [
SUMSUM(IQ)=SUMSUM(IQ)+ESUM(IQ,IR,ICODE);
IF(IQ.LE.3) [GSUM=GSUM+ESUM(IQ,IR,ICODE);]
]]]


"   NOW WRITE-OUT THE RESULTS OF THE ENERGY DEPOSITION SUMMARY"

DO IQ=1,4 [
IF(IQ.LE.3) [
IQNOW=IQ-2;
OUTPUT IQNOW;
('1ENERGY DEPOSITION SUMMARY FOR PARTICLES WITH IQ=',I2,///,
55X,'IARG',/,19X,'0',15X,'1',13X,'2',14X,'3',14X,'4',16X,'ROW SUM',
/,3X,'REGION',/);
]
ELSE [
OUTPUT;  ('1ENERGY DEPOSITION SUMMARY FOR ALL PARTICLES:',///,
55X,'IARG',/,19X,'0',15X,'1',13X,'2',14X,'3',14X,'4',16X,'ROW SUM',
/,3X,'REGION',/);
]

DO IR=1,NREG [
OUTPUT IR,(ESUM(IQ,IR,ICODE),ICODE=1,5),ROWSUM(IQ,IR);
  (I7,5X,5G15.7,5X,G15.7);
"   END OF IR-LOOP"]

OUTPUT (COLSUM(IQ,ICODE),ICODE=1,5),SUMSUM(IQ);
(/,3X,'COL SUM',2X,5G15.7,5X,G15.7);

"   END OF IQ-LOOP"]

OUTPUT GSUM; (/////,' TOTAL FRACTION=',G15.7,
'     NOTE: THIS NUMBER SHOULD BE VERY CLOSE TO UNITY');


RETURN;
END;  "END OF SUBROUTINE ECNSV1"

%E
"******************************************************************"
"                                STANFORD LINEAR ACCELERATOR CENTER"
SUBROUTINE NTALLY(NTREE,NREG);
"                                EGS4 SUBPROGRAM -  8 MAY 1983/1730"
"******************************************************************"
"   THIS PROGRAM KEEPS 'TALLY' OF THE NUMBER OF TIMES AUSGAB IS    "
"   ENTERED FOR VARIOUS REASONS, ETC.  IT GIVES THE USER A 'ROUGH' "
"   IDEA OF WHETHER CERTAIN EVENTS ARE RARE OR NOT.                "
"   CAUTION *** DO NOT USE THESE NUMBERS IN ANY STATISTICAL SENSE] "
"******************************************************************"
COMIN/DEBUG,NTALY1/;
INTEGER ROWSUM(4,$MXREG),COLSUM(4,5),SUMSUM(4),GSUM;

"   CHECK WHETHER NREG IS GE $MXREG.  IF IT IS, STOP AND OUTPUT."
IF(NREG.GT.$MXREG) [
MDUMMY=$MXREG;
OUTPUT NREG,MDUMMY;
(///,' ***** NOTE: STOPPED IN SUBROUTINE NTALLY BECAUSE NREG= ',
 I5,' IS LARGER THAN $MXREG= ',I5,' *****');
STOP;]

IF(NTREE.EQ.0) [  "INITIALIZE NSUM TO ZERO AND RETURN"
DO I=1,4 [DO J=1,NREG [DO K=1,5 [NSUM(I,J,K)=0;]]]
RETURN;]

"   REACH THIS POINT WHEN FINAL TALLY IS TO BE MADE."
"   FIRST, INITIALIZE SUMS"

GSUM=0;

DO IQ=1,4 [
SUMSUM(IQ)=0;
DO IR=1,NREG [ROWSUM(IQ,IR)=0;]
DO ICODE=1,5 [COLSUM(IQ,ICODE)=0;]
"   END OF IQ-LOOP"]

"   SUM IQ=1,2,3 INTO IQ=4 OF NSUM FOR ALL IR- AND ICODE-VALUES"

DO IR=1,NREG [
DO ICODE=1,5 [
DO IQ=1,3 [
NSUM(4,IR,ICODE)=NSUM(4,IR,ICODE) + NSUM(IQ,IR,ICODE);
]]]

"   SUM-UP COLUMNS AND ROWS"

DO IQ=1,4 [
DO IR=1,NREG [
DO ICODE=1,5 [
ROWSUM(IQ,IR)=ROWSUM(IQ,IR)+NSUM(IQ,IR,ICODE);
]]

DO ICODE=1,5 [
DO IR=1,NREG [
COLSUM(IQ,ICODE)=COLSUM(IQ,ICODE)+NSUM(IQ,IR,ICODE);
]]
"   END OF IQ-LOOP"]

"   NOW GET TOTAL FOR IQ AND GRAND TOTAL"

DO IQ=1,4 [
DO IR=1,NREG [
DO ICODE=1,5 [
SUMSUM(IQ)=SUMSUM(IQ)+NSUM(IQ,IR,ICODE);
IF(IQ.LE.3) [GSUM=GSUM+NSUM(IQ,IR,ICODE);]
]]]


"   NOW WRITE-OUT THE RESULTS"

DO IQ=1,4 [
IF(IQ.LE.3) [
IQNOW=IQ-2;
OUTPUT IQNOW;
(’1SUMMARY OF EVENT COUNT FOR PARTICLES WITH IQ=’,I2,///,
55X,’IARG’,/,19X,’0’,15X,’1’,13X,’2’,14X,’3’,14X,’4’,16X,’ROW SUM’,
/,3X,’REGION’,/);
]
ELSE [
OUTPUT;  (’1SUMMARY OF EVENT COUNT FOR ALL PARTICLES:’,///,
55X,’IARG’,/,19X,’0’,15X,’1’,13X,’2’,14X,’3’,14X,’4’,16X,’ROW SUM’,
/,3X,’REGION’,/);
]

DO IR=1,NREG [
OUTPUT IR,(NSUM(IQ,IR,ICODE),ICODE=1,5),ROWSUM(IQ,IR);
  (I7,5X,5I15,5X,I15);
"   END OF IR-LOOP"]

OUTPUT (COLSUM(IQ,ICODE),ICODE=1,5),SUMSUM(IQ);
(/,3X,’COL SUM’,2X,5I15,5X,I15);

"   END OF IQ-LOOP"]

OUTPUT GSUM; (/////,’ TOTAL NUMBER OF EVENTS=’,I15);


RETURN;
END;  "END OF SUBROUTINE NTALLY"
```

```
%E

%C80
"-----------------------------------------------------------------"
" Start of PRSTAAUX MORTRAN - Auxiliary codes required by PRESTA. "
"--------------------------   Taken from NRCCAUXP MORTRAN.        "
"                            24 August 1989 WRN                   "
"-----------------------------------------------------------------"
"                                                                 "
"*********************************************************************"
"                           *        *                               "
"                           * FIXTMX *                               "
"                           *        *                               "
"                           **********                               "
SUBROUTINE FIXTMX(ESTEP,MEDIUM);
"                                                                    "
"  THIS ROUTINE CHANGES THE STEP SIZE ALGORITHM USED IN EGS SO
THAT   "
"  THE STEP SIZE ARRAYS FOR TMXS CORRESPOND TO AN ARBITRARY,BUT
"
"  FIXED FRACTIONAL ENERGY LOSS ESTEPE.                              "
"  IT IS ONLY NECESSARY FOR LOW ENERGY ELECTRON PROBLEMS SINCE
"
"  TYPICALLY THE 200*TEFF0 RESTRICTION ON TMXS IS MORE STRINGENT
"
"   FOR ELECTRONS WITH ENERGIES ABOVE A FEW MEV
"
"                                                                    "
"  NOTE THAT THE $TMXS-OVER-RIDE MACRO MAY STILL BE IN FORCE IN
EGS.  "
"                                                                    "
"  THE ROUTINE CHANGES THE VALUES ONLY FOR THE MEDIUM 'MEDIUM'
"
"  AND IT SHOULD PROBABLY BE USED FOR ALL MEDIA IN A PROBLEM.
"
;"                                                                   "
"  THE ROUTINE MUST BE CALLED AFTER HATCH HAS BEEN CALLED AND
BEFORE  "
"  THE SIMULATION IS BEGUN.                                          "
"                                                                    "
"  THE ROUTINE IS INDEPENDENT OF WHAT UNITS ARE BEING USED, AS
LONG   "
"  AS THEY ARE CONSISTENT( E.G. CM, RL OR G/CM**2 )                  "
"                                                                    "
"  IF CALLED WITH IOLDTM=0 (PASSSED IN COMIN USER) THE TMXS ARRAYS
ARE"
"  ADJUSTED TO GIVE A FIXED ESTEPE AND ARE SUBJECTED TO THE TMIN
AND  "
"  CONSTRAINTS.                                                      "
"  IF CALLED WITH IOLDTM=1 THE CURRENT EGS ALGORITHM IS USED.
"
"  IF CALLED WITH IOLDTM=0 AND ESTEPE=0 THE CURRENT EGS
ALGORITHM IS  "
"  USED.                                                             "
"  IF CALLED WITH IOLDTM=1 AND ESTEPE=0 THEN ESTEPE=1.0 IS USED.
"
"                                                                    "
"  FOR A DETAILED DISCUSSION OF THE USE OF THIS ROUTINE, SEE
"
"  'Low Energy Electron Transport with EGS' in Nuclear Instr. and    "
"  Methods A227 (1984)535-548.  D.W.O. Rogers                        "
"                                                                    "
"  FOR A DISCUSSION OF THE NEW FEATURES (V03+) OF THIS ROUTINE,
"
"  ESPECIALLY WITH REGARD TO THE NEW UPPER AND LOWER LIMITS, SEE
"
"  'PRESTA-the Parameter Reduced Electron-Step Transport Algorithm-  "
"  for Electron Monte Carlo Transport' by A.F.Bielajew & D.W.O.Rogers,"
"  NRCC Internal Report PIRS-042 obtainable by contacting the above.  "
"                                                                    "
"  V01         DEC 10,1981 DAVE ROGERS NRCC                          "
"  V02         DEC 1984                       EGS4 VERSION           "
"  V03        JAN 1986  ALEX BIELAJEW NRCC   REVISED FOR PRESTA
"
"***********************************************************************"
;COMIN/ELECIN,MEDIA,USER/;

ESTEPE=ESTEP;

IF(MEDIUM > $MXMED)["ERROR"  OUTPUT MEDIUM;
(///'0********* MEDIUM=',I4,' IN FIXTMX IS TOO LARGE');RETURN;]

IF((ESTEPE = 0.) & (IOLDTM = 1)) RETURN; "USE THE CURRENT ALGORITHM "
IF(ESTEPE = 0.) ESTEPE=1.; "NEW VERSION DEFAULTS TO TOTAL ENERGY
LOSS"
IF(IOLDTM = 0)[BLCCC=BLCC(MEDIUM);XCC2=XCC(MEDIUM)**2; "NEEDED BY
ROOTMX"]
"SET UP SOME VARIABLES FOR FIRST PASS THROUGH LOOP"
EI =EXP( (1.-EKE0(MEDIUM))/EKE1(MEDIUM));"ENERGY OF FIRST TABLE
ENTRY"
EIL = ALOG(EI);  LEIL=1;
"THIS IS EQUIVALENT TO $SETINTERVAL EIL,EKE; BUT AVOIDS ROUNDOFF"
$EVALUATE EDEDX USING EDEDX(EIL);"GET THE ELECTRON STOPPPING AT
EI"
"NOW CALCULATE STEP REQUIRED TO CAUSE AN ESTEPE REDUCTION IN
ENERGY"
IF(IOLDTM = 1)[SI=ESTEPE*EI/EDEDX;]ELSE[SI=ROOTMX(EI,ESTEPE);]
"TABULATED ENERGIES ARE IN A FIXED RATIO - CALC LOG OF THE RATIO"
ERATIO=-1./EKE1(MEDIUM);

NEKE=MEKE(MEDIUM);"NUMBER OF ELEMENTS IN STORAGE ARRAY"
DO I=1,NEKE-1[
EIP1=EXP((FLOAT(I+1)-EKE0(MEDIUM))/EKE1(MEDIUM));"ENERGY AT I+1"
EIP1L=ALOG(EIP1);LEIP1L=I+1;"DESIGNED THIS WAY=$SETINTERVAL"
$EVALUATE EDEDX USING EDEDX(EIP1L);
IF(IOLDTM =
1)[SIP1=ESTEPE*EIP1/EDEDX;]ELSE[SIP1=ROOTMX(EIP1,ESTEPE);]


"NOW SOLVE THESE EQUATIONS                                      "
"  SI   = TMXS1 * EIL   + TMXS0                                 "
"  SIP1 = TMXS1 * EIP1L + TMXS0                                 "
"                                                               "
TMXS1(I,MEDIUM)=(SI-SIP1)/ERATIO;TMXS0(I,MEDIUM)=SI-TMXS1(I,MEDIUM)*
EIL;
"TRANSFER VALUES FOR NEXT LOOP"
EIL=EIP1L;SI=SIP1;]
"NOW PICK UP LAST TABLE ENTRY WHICH APPLIES ONLY TO LAST ENERGY"
TMXS0(NEKE,MEDIUM)=TMXS0(NEKE-1,MEDIUM);
TMXS1(NEKE,MEDIUM)=TMXS1(NEKE-1,MEDIUM);
RETURN;END;
%E
"******************************************************************************"
"                                  *        *                                 "
"                                  * ROOTMX *
"
"                                  *        *                                 "
"                                  **********                                 "
"                                                                             "
FUNCTION ROOTMX(EI,ESTEP);
"                                                                             "
"        THIS ROUTINE RETURNS MAX(TMIN,MIN(TMAX,ESTEPE*EI/DEDX))
WHERE         "
"    TMAX IS THE MAXIMUM STEP ALLOWED BY THE MOLIERE MULTIPLE
SCATTERING      "
"    THEORY, TMIN IS THE THE MINIMUN STEP AND ESTEPE*EI/DEDX IS THE
GREATEST   "
"    STEP ALLOWED DUE TO CONTINUOUS ENERGY LOSS PROCESSES.
"
"                                                                             "
"        NOTE THE USE OF ITS AUXILLIARY FUNCTION FTMX APPENDED TO
ROOTMX.      "
"    BECAUSE THE TMAX FUNCTION IS STRONGLY ENERGY DEPENDENT, IT
WAS FOUND      "
"    NECESSARY TO INCLUDE A CORRECTION FOR ENERGY LOSS IN IT.
```

```
OTHERWISE THE    "
"    UPPER LIMIT COULD BE GREATLY EXCEEDED - BY AS MUCH AS 50% IN
SOME CASES.  "
"    CORRECTING FOR ENERGY LOSS NECESSITATES USING A ROOT FINDING
METHOD TO    "
"    OBTAIN TMAX (HENCE THE NAME ROOTMX). TMIN IS ALSO STRONGLY
ENERGY         "
"    DEPENDENT BUT IT DOES NOT MATTER WITHIN THE LOGIC OF THE
CODE IF THIS     "
"    QUANTITY IS AS MUCH AS 50% HIGH SINCE NO PHYSICS CONSTRAINTS
WILL BE      "
"    VIOLATED.
"
"                                                                             "
"        THE ZERO-FINDING ROUTINE IS A CRUDE ONE BASED ON THE
ASSUMPTION THAT  "
"    THE FUNCTION FTMX IS MONOTONIC AND THAT THE FUNCTION
EVALUATED AT THE TWO "
"    STARTING POINTS RETURNS DIFFERENT SIGNS. IF THE SIGNS ARE THE
SAME THEN   "
"    EITHER THE ENERGY-LOSS STEP-SIZE IS MORE RESTRICTIVE OR THE
STEP-SIZE IS  "
"    BELOW TMIN.
"
"                                                                             "
"        ALTHOUGH THIS ROUTINE COMES WITH THE PRESTA PACKAGE IT IS
REALLY      "
"    INDEPENDENT OF IT AND IT IS AN IMPROVEMENT OVER THE PREVIOUS
TMXS METHODS."
"    THE OLD TMXS ROUTINE ALLOWED BOTH THE TMAX AND TMIN BOUNDS
TO BE VIOLATED."
"    EXCEEDING TMAX TAKES ONE OUT OF THE REGION OF VALIDITY OF
THE MOLIERE     "
"    THEORY STILL ALLOWING A MULTIPLE SCATTERING SELECTION BUT OF
UNPREDICTABLE"
"    WORTH. GOING LOWER THAN TMIN CAUSES THE MULTIPLE
SCATTERING TO GET        "
"    SWITCHED OFF (STARTING WITH THE LOWER ENERGIES). THIS CAN
SOMETIMES LEAD  "
"    TO CALCULATIONAL ARTIFACTS. ONE WORD OF CAUTION] USING THIS
ROUTINE AT    "
"    VERY LOW ELECTRON ENERGIES .LE.10 keV CAUSES NEGATIVE USTEP
ERRORS IF THE "
"    OLD EGS PATHLENGTH CORRECTION ALGORITHM (BASED ON
FERMI-EYGES THEORY) IS  "
"    USED. THE OLD EGS LESSENED THIS PROBLEM BY REDUCING THE
UPPER LIMIT TO    "
"    0.8 THE VALUE USED IN THIS ROUTINE. THE PRESTA PATHLENGTH
CORRECTION DOES "
"    NOT GIVE NEGATIVE USTEPS IN ANY OF THE CASES WE HAVE TESTED.
"
"                                                                             "
"            VERSION 1       ALEX BIELAJEW          JAN. 86
"
"            VERSION 1.1     ALEX BIELAJEW          OCT. 87
"
"                            Lower limit ESTEPE violation fixed               "
"                                                                             "
"*****************************************************************************"

;
COMIN/USEFUL,USER/;
ESTEPE=ESTEP;
TMIN=2.718282*EI*(EI+2.*RM)/(BLCCC*(EI+RM)**2); "LOWER LIMIT, eq.(2-8)"
X1=TMIN; "INITIAL LOWER STARTING POINT OF THE SEARCH"
X2=ESTEPE*EI/EDEDX; "INITIAL UPPER STARTING POINT OF THE SEARCH"

"THIS IS THE FIX-UP FOR THE MINIMUM STEP-SIZE"
IF( X2 <= X1 ) [ROOTMX=X1;RETURN;]

F1=FTMX(X1,EI);F2=FTMX(X2,EI);
AF1=ABS(F1);AF2=ABS(F2);
SF1=SIGN(1.,F1);SF2=SIGN(1.,F2);
```

```
"FIRST CHECK TO SEE IF EITHER OF THE STARTING POINTS IS ALREADY
GOOD ENOUGH."
 IF((AF1 <= $ROOTMX_PRECISION) | (AF2 <= $ROOTMX_PRECISION))[
    IF(AF1 <= AF2)[ROOTMX=X1;]ELSE[ROOTMX=X2;]]

"NOW CHECK TO SEE IF EITHER THE ENERGY LOSS IS MORE RESTRICTIVE
THAN THE       "
"UPPER LIMIT TMAX (TRUE FOR HIGH ENERGIES) OR IF IT MORE
RESTRICTIVE THAN      "
"TMIN (TRUE FOR LOW ENERGIES WITH A SMALL ENOUGH ESTEPE).
"
ELSEIF(SF1 = SF2)[ROOTMX=X2;]

"OTHERWISE A SEARCH FOR TMAX MUST BE UNDERTAKEN."
ELSE[ "ITERATE"
ITI=0; "NUMBER OF ITERATIONS COUNTER"
XL=X1; "LAST X FOUND"
:SEARCH-ROOT:LOOP[
ITI=ITI+1;
IF(ITI > 1000)[ "QUIT IF THIS HAPPENS"
OUTPUT;(' SEARCH FOR TMXS ABORTED. TOO MANY ITERATIONS');STOP;]
XT=(X1*F2-X2*F1)/(F2-F1);
IF(XT = XL)[ROOTMX=XT;EXIT:SEARCH-ROOT:;"CONVERGENCE OBTAINED"]
FT=FTMX(XT,EI);AFT=ABS(FT);
IF(AFT <=
$ROOTMX_PRECISION)[ROOTMX=XT;EXIT:SEARCH-ROOT:;"CONVERGENCE
OBTAINED"]
ELSE[ "RE-ITERATE"
SFT=SIGN(1.,FT);
IF(SFT =
SF1)[X1=XT;F1=FT;AF1=AFT;SF1=SFT;]ELSE[X2=XT;F2=FT;AF2=AFT;SF2=SFT;]
XL=XT; "UPDATE LAST X FOUND"
]
] "END OF SEARCH FOR ROOT LOOP"
] "END OF ITERATE ELSE"
RETURN;END;

FUNCTION FTMX(T,EI);
"When t=tmax as defined in eq.(2-10) this function returns 0. It is used by    "
"FUNCTION ROOTMX in the search for tmax.
"
COMIN/USEFUL,USER/;
"Energy dependent quantities are evaluated at the energy mid-point of the step."
"See section IV of the report PIRS-042.                                        "
EK=AMAX1(0.0001,EI-0.5*EDEDX*T);E=EK+RM;BETA2=EK*(E+RM)/E**2;
A=BLCCC/BETA2;G=XCC2/(E*BETA2)**2;
FTMX=1./ALOG(A/G)-G*T;
RETURN;END;
%E

SUBROUTINE RMARIN;
;
COMIN/RANDOM/;
;
IF((IXX.LE.0).OR.(IXX.GT.31328)) IXX=1802; "SETS MARSAGLIA DEFAULT"

" BUG. In the following line the assignment previous to 90/09/18  "
" was to IXX. This DID NOT upset the randomness of the sequence,  "
" just the initial starting point. BLIF 90/09/18.                 "

IF((JXX.LE.0).OR.(JXX.GT.30081)) JXX=9373; "SETS MARSAGLIA DEFAULT"

I = MOD(IXX/177,177) + 2;
J = MOD(IXX,    177) + 2;
K = MOD(JXX/169,178) + 1;
L = MOD(JXX,    169)    ;

DO II=1,97[
    S=0.0;T=0.5;
    DO JJ=1,24[
        M=MOD(MOD(I*J,179)*K,179);
        I=J;J=K;K=M;L=MOD(53*L+1,169);
        IF(MOD(L*M,64).GE.32) S=S+T;
        T=0.5*T;
        ]
    URNDM(II)=S;
    ]

CRNDM  =   362436./16777216.;
CDRNDM =  7654321./16777216.;
CMRNDM = 16777213./16777216.;

IXX = 97;
JXX = 33;

RETURN;END;
"******************************************************************"
"************************** ucbrempc.mor END **********************"
"******************************************************************"
```