Appendix C

PEGS USER MANUAL

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C.1   Introduction

PEGS (Preprocessor for EGS) is a set of FORTRAN subprograms which generate material data for use with the EGS5 Monte Carlo shower code and which also provide utilities for researchers studying electro-magnetic interactions. The active operations of PEGS are functionals; that is, they are operations whose arguments are functions (the functions related to physics interactions). Included among these operations are:

- Fitting of functions by means of piecewise linear fits.

- Production of printed plots of selected functions.

- Evaluation of functions at selected points.

- Comparison of functions with sampled spectra.

Associated with these active functionals are other operations:

- Selection of material to which the functions refer.

- Selection of energy cutoffs for fits.

- Printing of fitted data.

This manual describes the full general functionality of PEGS. Users interested only in preparing data sets for EGS5 can proceed directly to section C.3.

C.2   Structural Organization of PEGS

Beginning with version 5 of the EGS code system, MORTRAN is no longer supported, and PEGS is no longer a stand-alone program, but rather a subroutine to be called by EGS user code. The main PEGS subroutine (called `PEGS5`), however is essentially the same as the `MAIN` program in previous versions of PEGS, and EGS and PEGS are still quite distinct in EGS5.

The full PEGS5 system consists of almost 7000 of FORTRAN source code that make up over 100 subprograms, plus an additional 610 lines of FORTRAN in 40 files containing `COMMON` blocks accessed by the various PEGS subprograms through `include` statements. New to version 5 of PEGS, all floating point variables are declared as `double precision`.

Despite its size, PEGS has a simple structure. Figures C.1 and C.2 below contain a schematic flowchart of main subroutine (`PEGS5`) of PEGS. After the once-only initializations, an option loop

is entered. On each pass through this loop, an option is read (option names are four characters and are read as 4A1), numeric control parameters are read (using the FORTRAN `NAMELIST` I/O extension), and then the option name is looked up in the option table. If an option name is not found, the job is aborted. When an option name is found, the appropriate code is executed and the program returns to the beginning of the option loop. Normal exit from the loop is by selection of the STOP option or detection of an End-of-File condition on the input file. Detailed descriptions of the use of the options are contained in section C.3 of this manual.

Figures C.3 and C.4 show some of the subprogram relationships of PEGS[1]. Boxed items in the figures are subprograms, and option names (identified by ":" delimiters, as in ":CALL:") are used to show which subprograms correspond to which options. The general structure of PEGS is clearly evident. Subprograms which compute physical quantities are accessed directly by the PWLF option, but when the utility options TEST, PLTN, PLTI, HPLT, or CALL are invoked, physics routines are referenced using the function `FI`, the so-called "function multiplexer." The function multiplexer `FI` has five arguments. The first argument (`I`) tells which physical function to invoke, and the other four arguments (`X1, X2, X3, X4`) are used as needed as arguments for the called function. Calls to `FI` return values returned to `FI` by the called function specified by `I`. The full list of physical functions which can be called by `FI` is given in Figure C.4.

It should also be noted that there are relationships between the PEGS functions shown in Figure C.3 which are not indicated there. We show the most complicated of these in Figures C.5 and C.6 (Bremsstrahlung Related Functions) and in Figures C.7 and C.8 (Pair Production Related Functions). One reason for the complexity of these particular subprograms is that higher level forms of the relevant cross sections must be obtained by numerical integration of the more differential forms.

Tables C.1 and C.2 list the subroutines used in PEGS and provide brief descriptions of their functions. All of the subroutines in Table C.2 are new to PEGS5 and deal with either the calculation of the Goudsmit-Saunderson multiple scattering distribution or the determination of electron energy loss steps. Note that in the current implementation, when the Goudsmit-Saunderson distribution is requested, the routines which prepared the data are actually called by EGS during the set up operations performed in `HATCH`. We nevertheless refer to these new subprograms as part of PEGS, as they do involve pre-processing of data.

Tables C.3 through C.6 list the FORTRAN `FUNCTIONS` used in PEGS along with their mathematical symbols and definitions if appropriate. The names of most of the functions have been chosen in a mnemonic way. The first three or four letters suggest the process being considered. The last letter designates the form of the cross section (Z for element, M for mixture, and R for run-time mixture). The next to last letter describes either the particular form of the cross section (such as D for differential, T for total or R for range-integrated), or it indicates that only the secondary energy is to vary, with other data being passed through a common. The letter F is used in such cases and the data in common is initialized using the corresponding function that has a next to last letter of D. If the function word begins with an I through N (i.e., the FORTRAN integer

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[1]Subprograms involving the low energy physics and the multiple scattering models new to PEGS with the release of EGS5 are not included in the diagrams.
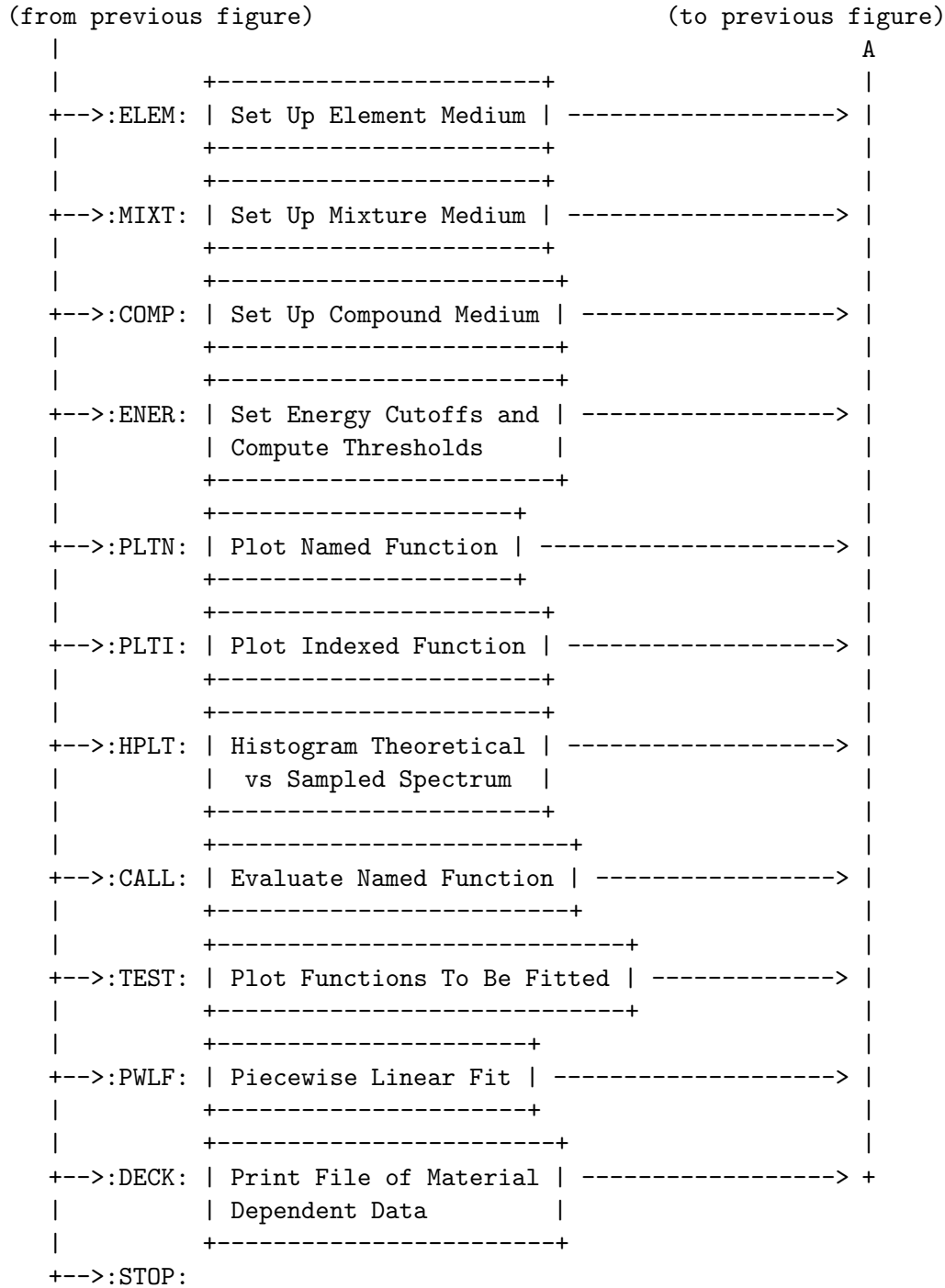
```
                          +------+
                          | PEGS |
                          +------+
                           |  |         +-------------+
                initialize |  +------>| OPTION LOOP |<---+
               +-------------+          +-------------+    A
               |                              |           |
               V                              V           |
   +----------------------+        +----------------+    |
   |   Compute Physical & |        |   Read Option  |    |
   | Mathematical Constants |      |    Name (4A1)  |    |
   +----------------------+        |        &       |    |
               |                   |   Read Control |    |
               |                   |    Parameters  |    |
               V                   | (NAMELIST/INP/)|    |
   +----------------------+        +----------------+    |
   | Read Pair Production, |               |            |
   |   Photoelectric, and |               |            |
   |   Rayleigh Data from |               |            |
   ! PGS5PEPR and PGS5FORM |              |            |
   +----------------------+               |            |
                                          V            |
          +------+      Yes       +--------------+    |
          | Stop |<------------ | End of File? |    |
          +------+               +--------------+    |
                                        |            |
                                        | No         |
                                        V            |
   +----------------------+       +--------------+    |
   | Illegal Option---Stop |<----- | Select Option |  |
   +----------------------+       +--------------+    |
                                        |            |
                                        V            |
     +<------------------------------------ +        |
     |                                               |
     V                                               |
  (to next figure)                       (from next figure)
```
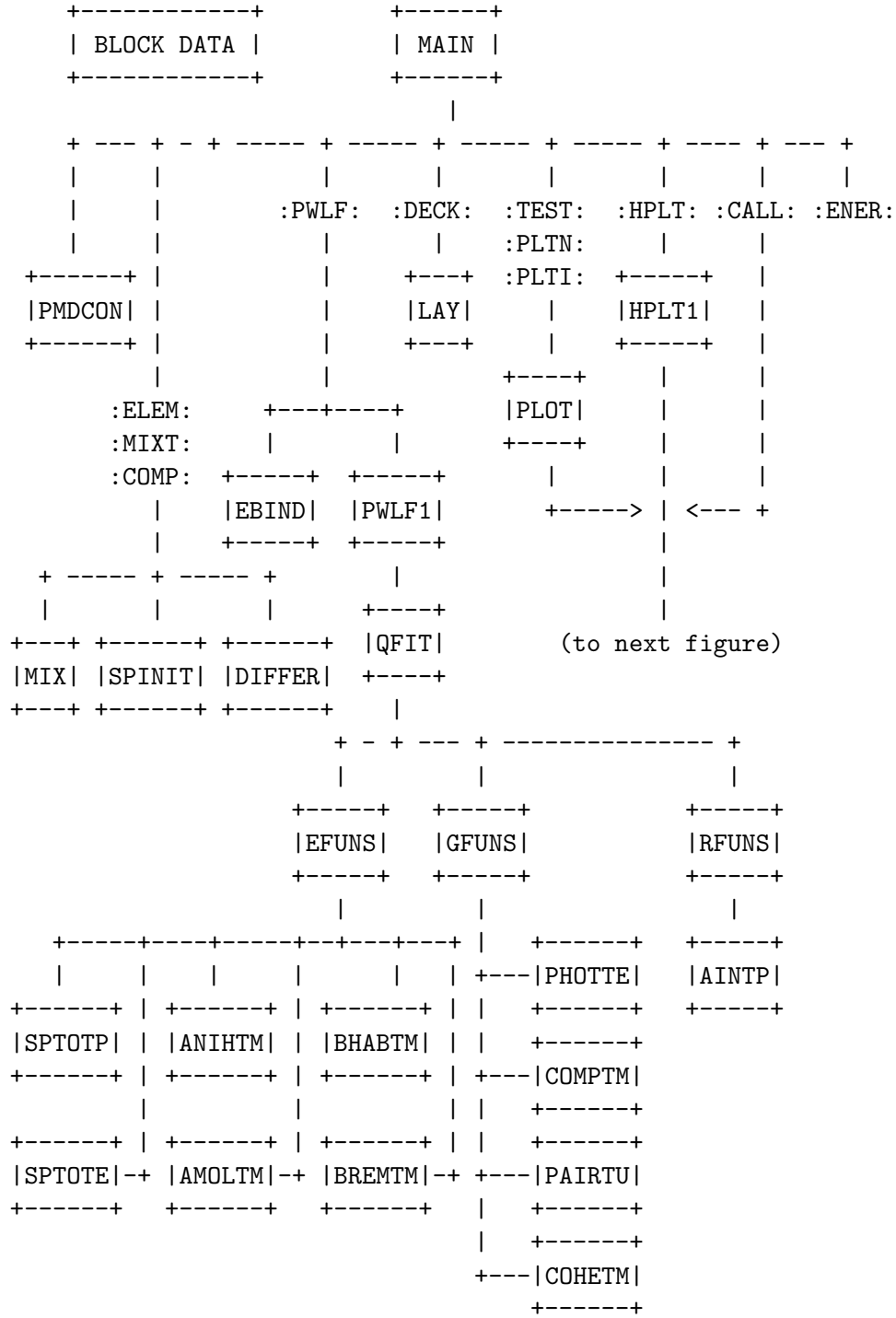
Figure C.1: Flowchart of the PEGS5 subprogram of PEGS, part 1.

```
(from previous figure)                        (to previous figure)
     |                                                  A
     |           +----------------------+               |
  +-->:ELEM: | Set Up Element Medium | ----------------->  |
     |           +----------------------+               |
     |           +----------------------+               |
  +-->:MIXT: | Set Up Mixture Medium | ----------------->  |
     |           +----------------------+               |
     |           +----------------------+               |
  +-->:COMP: | Set Up Compound Medium | ---------------->  |
     |           +----------------------+               |
     |           +----------------------+               |
  +-->:ENER: | Set Energy Cutoffs and | ----------------->  |
     |           | Compute Thresholds     |               |
     |           +----------------------+               |
     |           +--------------------+               |
  +-->:PLTN: | Plot Named Function | ----------------->  |
     |           +--------------------+               |
     |           +----------------------+               |
  +-->:PLTI: | Plot Indexed Function | ----------------->  |
     |           +----------------------+               |
     |           +----------------------+               |
  +-->:HPLT: | Histogram Theoretical | ----------------->  |
     |           |  vs Sampled Spectrum  |               |
     |           +----------------------+               |
     |           +------------------------+               |
  +-->:CALL: | Evaluate Named Function | ---------------->  |
     |           +------------------------+               |
     |           +--------------------------+               |
  +-->:TEST: | Plot Functions To Be Fitted | ------------->  |
     |           +--------------------------+               |
     |           +--------------------+               |
  +-->:PWLF: | Piecewise Linear Fit | ----------------->  |
     |           +--------------------+               |
     |           +----------------------+               |
  +-->:DECK: | Print File of Material | ---------------->  +
     |           | Dependent Data         |
     |           +----------------------+
  +-->:STOP:
```

Figure C.2: Flowchart of the PEGS5 subprogram of PEGS, part 2.

```
    +------------+          +------+
    | BLOCK DATA |          | MAIN |
    +------------+          +------+
                                |
    + --- + - + ----- + ----- + ----- + ----- + ---- + --- +
      |     |         |        |       |        |       |     |
      |     |       :PWLF:   :DECK:  :TEST:   :HPLT: :CALL: :ENER:
      |     |         |        |     :PLTN:     |       |
    +------+ |        |      +---+   :PLTI:   +-----+    |
    |PMDCON| |        |      |LAY|     |      |HPLT1|    |
    +------+ |        |      +---+     |      +-----+    |
             |        |             +----+      |       |
         :ELEM:     +---+----+      |PLOT|      |       |
         :MIXT:       |      |      +----+      |       |
         :COMP:     +-----+  +-----+   |        |       |
             |      |EBIND|  |PWLF1|   +----->  | <--- +
             |      +-----+  +-----+            |
    + ----- + ----- +          |               |
      |       |       |      +----+            |
    +---+ +------+ +------+   |QFIT|    (to next figure)
    |MIX| |SPINIT| |DIFFER|  +----+
    +---+ +------+ +------+     |
                    + - + --- + -------------- +
                      |       |                |
                  +-----+   +-----+          +-----+
                  |EFUNS|   |GFUNS|          |RFUNS|
                  +-----+   +-----+          +-----+
                      |        |                |
    +-----+----+-----+--+--+---+ |   +------+  +-----+
      |    |    |     |     |   | +---|PHOTTE|  |AINTP|
    +------+ | +------+ | +------+ | | +------+  +-----+
    |SPTOTP| | |ANIHTM| | |BHABTM| | | +------+
    +------+ | +------+ | +------+ | +---|COMPTM|
             |          |        | |  +------+
    +------+ | +------+ | +------+ | |  +------+
    |SPTOTE|-+ |AMOLTM|-+ |BREMTM|-+ +---|PAIRTU|
    +------+   +------+   +------+  |  +------+
                                   |  +------+
                                   +---|COHETM|
                                      +------+
```

Figure C.3: Subprogram relationships in PEGS, part 1.

```
              (from previous figure)
                       |
                       |
            + --------------------- +
            |           FI          |
            | "Function Multiplexer" |
            + --------------------- +
                       |
    + ------------------------------------ +
    |                                      |
    |   ALIN     APRIM    COMPFM   PAIRTE   |
    |   ALINI    BHABDM   COMPRM   PAIRTM   |
    |           BHABFM   COMPTM   PAIRTR   |
    |   ADFMOL   BHABRM   CRATIO   PAIRTU   |
    |   ADIMOL   BHABTM   EBIND    PAIRTZ   |
    |   ADDMOL   BREMDR   EBR1     PBR1     |
    |   DLOG     BREMFR   EDEDX    PBR2     |
    |   DEXP     BREMDZ   ESIG     PDEDX    |
    |   AREC     BRMSDZ   FCOULC   PHOTTZ   |
    |   ALKE     BREMFZ   GBR1     PHOTTE   |
    |   ALKEI    BRMSFZ   GBR2     PSIG     |
    |   AMOLDM   BREMRR   GMFP     SPIONE   |
    |   AMOLFM   BREMRM   PAIRDR   SPIONP   |
    |   AMOLRM   BREMRZ   PAIRFR   SPTOTE   |
    |   AMOLTM   BREMTM   PAIRDZ   SPTOTP   |
    |   ANIHDM   BREMTR   PAIRFZ   TMXB     |
    |   ANIHFM   BRMSRM   PAIRRM   TMXS     |
    |   ANIHRM   BRMSRZ   PAIRRR   TMXDE2   |
    |   ANIHTM   BRMSTM   PAIRRZ   XSIF     |
    |           COHETM   EEITM            |
    |           COHETZ                    |
    |           COMPDM                    |
    + ------------------------------------ +
```

Figure C.4: Subprogram relationships in PEGS, part 2.

```
    +------+              +------+
    |BREMTM|---------->|BREMRM|
    +------+              +------+
                              |
                              V
 +------+              +------+  initialize  +------+
 |  QD  |<------------ |BREMRZ|------------> |BREMDZ|
 +------+              +------+    BREMFZ     +------+
    |                                            |
    V                                            V
 +------+  +------+    +------+              +------+
 |DCADRE|-->|BREMFZ|--->|BRMSFZ|<------------- |BRMSDZ|
 +------+  +------+    +------+              +------+
                          A                     A |
                          |                     | |  +------+
              +--------------+                  | +-->|APRIM |
              |                                 | |  +------+
          +------+      +------+  initialize    | |
          |DCADRE|   +----|BRMSRZ|-------------> +  |   +------+
          +------+   |    +------+    BRMSFZ     +-->|  XSIF |
             A       |       A                  |   +------+
             |       |       |                  |
          +------+   |    +------+              |   +------+
          |  QD  |<--+    |BRMSRM|              +-->|FCOULC|
          +------+        +------+                  +------+
                             A
                             |
    +------+              +------+              +------+
    |SPTOTE|----------> |BRMSTM|<----------- |SPTOTP|
    +------+              +------+              +------+
       |                                          |
       V                                          V
    +------+              +------+              +------+
    |SPIONE|----------> |SPIONB|<----------- |SPIONP|
    +------+              +------+              +------+
```
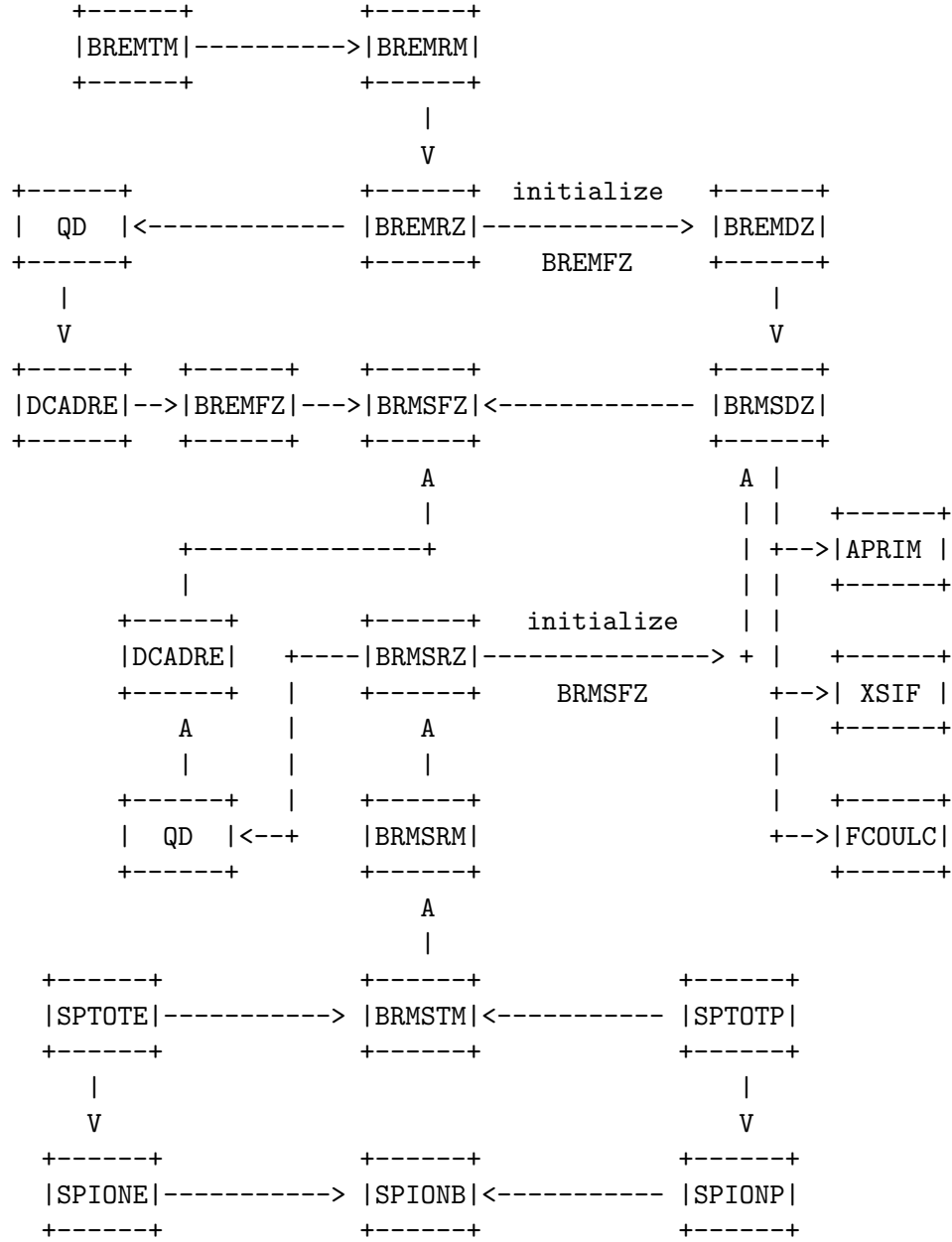
Figure C.5: Bremsstrahlung related functions—most accurate form (used to produce the total cross sections and stopping power).

```
                +------+
                |BREMTR|
                +------+
                    |
                    V
                +------+
                |BREMRR|
                +------+
                    |
          initialize V
        + <---------+-------> +
        |   BREMFR           |
        V                    V
   +------+             +------+
   |BREMDR|             |  QD  |
   +------+             +------+
       |                    |
       |                    V
       |                +------+
       |                |DCADRE|
       |                +------+
       |     +------+       |
       + ---> |BREMFR| <---- +
             +------+
```
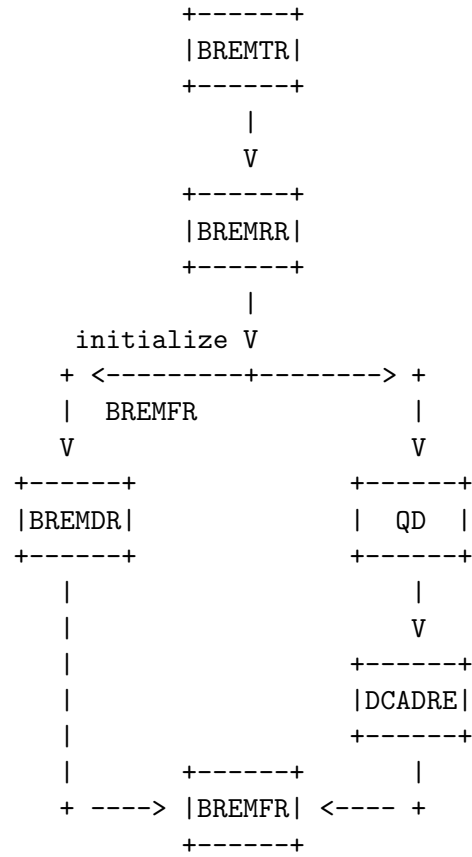
Figure C.6: Bremsstrahlung related functions—with run-time approximations (for comparison with sampled spectra).

9

```
                        +------+
                        |PAIRTU|
                        +------+
                          |  |
      + <---------------- +  + ----------------> +
      |                                          |
      V                                          V
    +------+                                  +------+
    |PAIRTM|                                  |PAIRTE|
    +------+                                  +------+
       |                                         |
       V                                         V
    +------+                                  +------+
    |PAIRRM|                                  |PAIRTZ|
    +------+                                  +------+
       |                                         |
       V                                         V
    +------+   initialize                     +------+
    |PAIRRZ|-------------> +                  |AINTP |
    +------+     PAIRFZ    |                  +------+
       |                   |
       V                   V
    +------+            +------+            +------+
    | QD   |            |PAIRDZ|-----+----> | XSIF |
    +------+            +------+     |      +------+
      |                   |         |      +------+
      |                   |         +----> |FCOULC|
      V                   V                +------+
    +------+            +------+
    |DCADRE|----------> |PAIRFZ|
    +------+            +------+
```
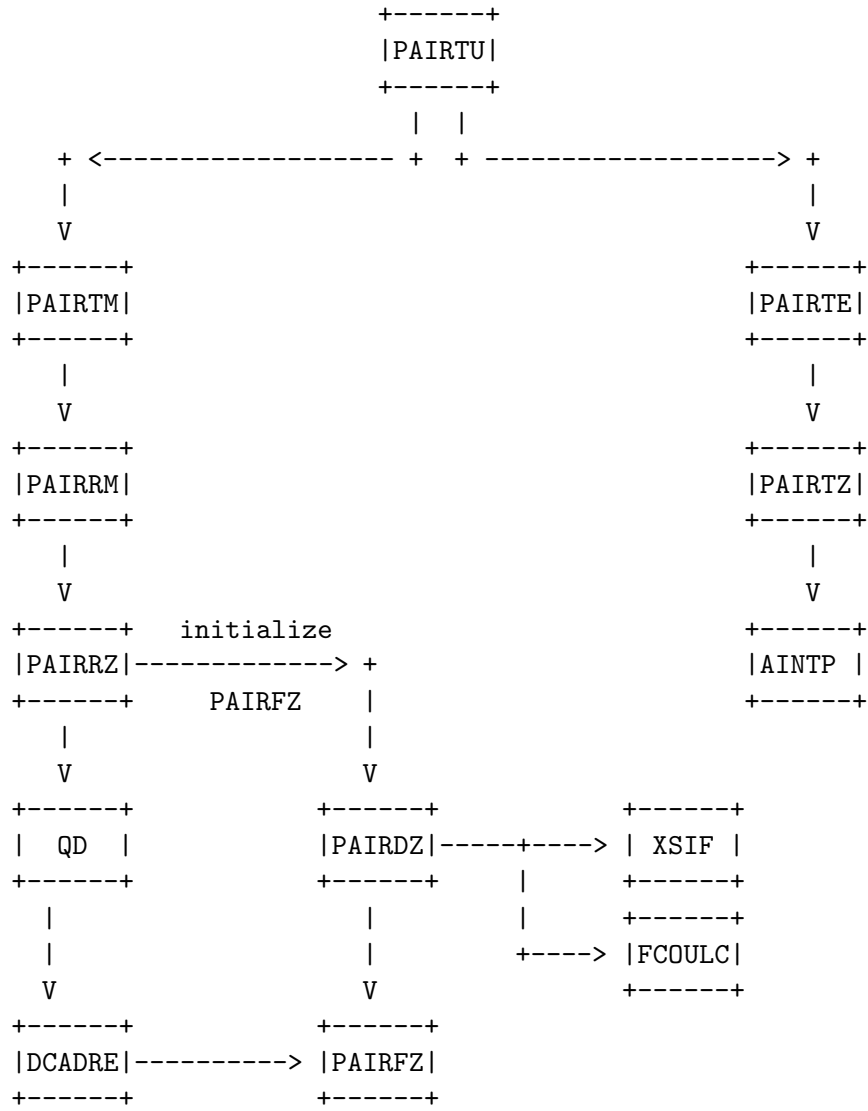
Figure C.7: Pair production related functions—most accurate form (used to produce the total cross sections and stopping power).

```
                    +------+
                    |PAIRTR|
                    +------+
                       |
                       V
                    +------+
                    |PAIRRR|
                    +------+
                       |
            initialize V
          + <-------- + ------> +
          |   PAIRFR            |
          V                     V
      +------+              +------+
      |PAIRDR|              |  QD  |
      +------+              +------+
         |                     |
         |                     V
         |                  +------+
         |                  |DCADRE|
         |                  +------+
         |     +------+        |
         + ---> |PAIRFR| <---- +
               +------+
```
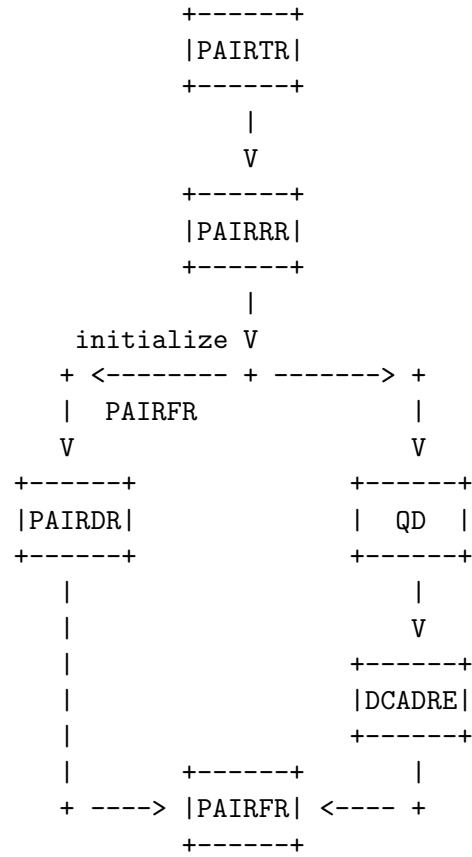
Figure C.8: Pair production related functions—with run-time approximations (for comparison With sampled spectra).

Table C.1: Subroutines in PEGS.

Name	Description
DIFFER	Determines the various parameters needed for bremsstrahlung and pair production energy sampling.
EFUNS	Subprogram to compute electron functions to be fit in a way that avoids repetition.
GFUNS	Subprogram to compute photon functions to be fit in a way that avoids repetition.
HPLT1	Creates line printer plot comparisons of EGS-sampled data (UCTESTSR User Code) and theoretical functions of PEGS.
LAY	Subprogram to produce a file of material dependent data (for subsequent use by EGS).
MIX	Computes Z-dependent parameters that reside in COMMON/MOLVAR/.
PLOT	Subprogram to plot a given function (referenced by number).
PMDCON	Determines the physical, mathematical, and derived constants in a very mnemonic way.
PWLF1	Subprogram to piecewise linearly fit up to 10 functions simultaneously on an interval (XL,XU).
RFUNS	Subprogram to compute Rayleigh scattering functions to be fit in a way that avoids repetition.
SPINIT	Initializes stopping power functions for a particular medium.
SFUNS	Subroutine to compute incoherent scattering functions to be fit.
CFUNS3	Subroutine to compute c.d.f. of shell-wise Compton profile to be fit.
CFUNS4	Subroutine to compute shell-wise Compton profile to be fit.
EIIFUNS	Subroutine to compute EII/Møller ratio to be fit.
MAKEK1	Prepares tables of initial scattering strength to be fit.

Table C.2: Goudsmit-Saunderson-related subroutines in PEGS.

Name	Description
DCSLOAD	Loads molecular elastic differential cross sections tables for multi-material PEGS runs.
DCSSTOR	Stores molecular elastic differential cross sections tables for multi-material PEGS runs.
DCSTAB	Computes tables of the molecular elastic differential cross sections for electrons and positrons.
ELASTINO	Prepares cumulative Goudsmit-Saunderson multiple scattering distributions on problem dependent energy and scattering strength grids.
ELINIT	Reads differential elastic scattering cross section data for electrons and positrons.
ESTEPLIM	Computes the maximum electron energy hinge step (in units of fractional energy loss) which assures a given error tolerance (currently fixed at 0.1%) in the total energy loss and total scattering power accumulated over the step.
FINDI	Does table look-up.
FITMS	Prepares special fit to Goudsmit-Saunderson multiple scattering data for fast sampling in EGS.
GAULEG	Provides abscissas and weights for Gauss-Legendre quadrature.
GSCOEF	Computes Goudsmit-Saunderson transport coefficients.
GSDIST	Computes Goudsmit-Saunderson multiple scattering probability density functions.
INIGRD	Initializes energy and scattering strength grid tables.
INTEG	Integrates cubic spline data.
LEGENP	Computes Legendre polynomials.
PRELASTINO	Writes multiple scattering grid parameters for later consistency checks.
SPLINE	Computes cubic splines.
WMSFIT	Writes fitted Goudsmit-Saunderson multiple scattering data parameters.

convention) the word is prefixed with the letter A. A few examples are given below:

AMOLDM	is the differential Møller cross section for a mixture of elements.
BREMDR	is the differential bremsstrahlung cross section for a run-time mixture of elements.
BREMRM	is the bremsstrahlung cross section, integrated over some energy range, for a mixture of elements.
BRMSTM	is the soft bremsstrahlung total cross section for a mixture of elements.
PAIRRR	is the pair production cross section, integrated over some energy range, for a run-time mixture of elements.
PAIRTZ	is the total cross section for pair production for an element.

Note that this method of naming is not strictly adhered to, however. For example, SPIONE is the ionization stopping power for an electron, PBR1 and PBR2 are positron branching ratios, and GMFP is the gamma-ray mean free path.

C.3 PEGS Options and Input Specifications

C.3.1 Interrelations Between Options

Figure C.9 illustrates the logical relationship between options of PEGS. For example, in order to be able to use the PLTN option, one of the material specification options (ELEM, MIXT, COMP) must have already been processed. The PWLF option requires that both the ENER option and one of the material specification options precede it. To use the DECK option, it is sufficient to have validly invoked the PWLF option. The STOP option is seen to be independent of the others.

In the following sections we give for each option its function, parameters which control it, the format of the data lines in a PEGS input file needed to invoke it, and an explanation of the routines (if any) that are used to implement it. The data lines for a given option are named with the first part of their name being the option name, and the last part the line number. For example, "MIXT2" is the name of the second line needed for the MIXT option. The information is summarized in Tables C.7 through C.18. The single line referred to as being read by NAMELIST may in fact be several lines, provided that the proper convention for continuing NAMELIST lines is followed. Once the first line (indicating the option) has been read in, however, the second line (i.e., NAMELIST/INP/) must follow (see examples at the end of the next section). It should also be noted that different compilers may require different formats for NAMELIST data.

Table C.3: Functions in PEGS, part 1.

Name	Description
AFFACT	Atomic form factor (squared) for an element or mixture of elements.
AINTP	Linear or log interpolation function.
ALKE	Log of kinetic energy (`LOG(E-RM)`), used as a cumulative distribution function for fits and plots.
ALKEI	Inverse of ALKE (`=EXP(X)+RM`).
ALIN	Linear cumulative distribution function for plots (`ALIN(X)=X`).
ALINI	Inverse of ALIN (=same as ALIN). Used as inverse cumulative distribution function in plots.
ADFMOL	Approximate cumulative distribution function for Møller and Bhabha cross sections (`ADFMOL(E)=-1/(E-RM)`).
ADIMOL	Inverse of ADFMOL.
ADDMOL	Derivative of ADFMOL.
AMOLDM	Møller differential cross section for a mixture of elements.
AMOLFM	One argument form of AMOLDM.
AMOLRM	Møller cross section, integrated over some energy range, for a mixture of elements.
AMOLTM	Møller total cross section for a mixture of elements.
ANIHDM	Annihilation differential cross section for a mixture of elements.
ANIHFM	One argument form of ANIHDM.
ANIHRM	Annihilation cross section, integrated over some energy range, for a mixture of elements.
ANIHTM	Annihilation total cross section for a mixture of elements.
APRIM	Empirical correction factor in bremsstrahlung cross section.
AREC	Reciprocal function (=derivative of `ALOG(X)`). Used as probability density function in log plots (`AREC(X)=1/X`).
BHABDM	Bhabha differential cross section for a mixture of elements.
BHABFM	One argument form of BHABDM.
BHABRM	Bhabha cross section, integrated over some energy range, for a mixture of elements.
BHABTM	Bhabha total cross section for a mixture of elements.

Table C.4: Functions in PEGS, part 2.

Name	Description
BREMDR	Bremsstrahlung differential cross section for a run-time mixture of elements.
BREMFR	One argument form of BREMDR.
BREMDZ	Bremsstrahlung differential cross section for an element.
BREMFZ	One argument form of BREMDZ.
BREMRM	Bremsstrahlung cross section, integrated over some energy range, for a mixture of elements.
BREMRR	Bremsstrahlung cross section, integrated over some energy range, for a run-time mixture of elements.
BREMRZ	Bremsstrahlung cross section, integrated over some energy range, for an element.
BREMTM	Bremsstrahlung total cross section for a mixture of elements.
BREMTR	Bremsstrahlung total cross section for a run-time mixture of elements.
BRMSDZ	Soft bremsstrahlung differential cross section for an element.
BRMSFZ	One argument form of BRMSDZ.
BRMSRM	Soft bremsstrahlung cross section, integrated over some energy range, for a mixture of elements.
BRMSRZ	Soft bremsstrahlung cross section integrated over some energy range, for an element.
BRMSTM	Soft bremsstrahlung total cross section for a mixture of elements.
COHETM	Coherent (Rayleigh) total cross section for a mixture of elements.
COHETZ	Coherent (Rayleigh) total cross section for an element.
COMPDM	Compton differential cross section for a mixture of elements.
COMPFM	One argument form for COMPDM.
COMPRM	Compton cross section, integrated over some energy range, for a mixture of elements.
COMPTM	Compton total cross section for a mixture of elements.
CPRFIL	Shell-wise Compton profiles.
CRATIO	Coherent (Rayleigh) cross section ratio.
CSDAR	Returns previously computed and stored values of CSDA range for electrons and positrons.
ESIG	Determines the total electron(-) interaction cross section (probability per radiation length).
DCADRE	Quadrature routine to integrate f(x) between a and b using cautious Romberg extrapolation.
DCSEL	Computes differential elastic scattering cross sections from data which has been fitted by cubic splines.
DCSN	Computes arbitrary Goudsmit-Saunderson elastic scattering transport coefficients from cross section data which has been fitted by cubic splines.
EBIND	Function to get an average photo-electric binding energy.
EBR1	Function to determine the electron(-) branching ratio (brem/total).
EDEDX	Evaluates SPTOTE with cutoff energies of `AE` and `AP`.

Table C.5: Functions in PEGS, part 3.

Name	Description
EIITM	K shell EII cross section
ESTEPMAX	Returns previously computed and stored values of maximum electron energy hinge steps.
FCOULC	Coulomb correction term in pair production and bremsstrahlung cross sections.
FI	Function multiplexer.
G1E	Computes scatter powering for positrons and electrons from either splines of partial wave cross sections or analytical form of Molière cross section.
G1EDEDX	Computes product of first elastic transport cross section and inverse stopping power for electrons.
G1PDEDX	Computes product of first elastic transport cross section and inverse stopping power for positrons.
GBR1	Function to determine the gamma-ray branching ratio (pair/total).
GBR2	Function to determine the gamma-ray branching ratio ((pair+Compton)/total).
GMFP	Function to determine the gamma-ray mean free path.
K1E	Computes scattering strength for electrons and positrons from spline data.
IFUNT	Given PEGS function name, it looks it up name in table and returns the function index. Used by options that specify functions by name.
PAIRDR	Pair production differential cross section for a run-time mixture of elements.
PAIRDZ	Pair production differential cross section for an element.
PAIRFR	One argument form of PAIRDR.
PAIRFZ	One argument form of PAIRDZ.
PAIRRM	Pair production cross section, integrated over some energy range, for a mixture of elements.
PAIRRR	Pair production cross section, integrated over some energy range, for a run-time mixture of elements.
PAIRRZ	Pair production cross section, integrated over some energy range, for an element.
PAIRTE	Empirical total pair production production cross section for a mixture (=SUM(PZ(I)*PAIRTZ(Z(I)))).
PAIRTM	Pair production total cross section for a mixture of elements, obtained by numerical integration of differential cross section.
PAIRTR	Pair production total cross section for a run-time mixture of elements.
PAIRTU	Pair production total cross section actually used. Same as PAIRTE for primary energy less than 50 MeV; otherwise, same as PAIRTM.
PAIRTZ	Computes contribution to empirical pair production total cross section for an element assuming one atom per molecule. It is obtained by log-linear interpolation of Storm-Israel data.

Table C.6: Functions in PEGS, part 4.

Name	Description
PBR1	Function to determine the positron branching ratio (brem/total).
PBR2	Function to determine the positron branching ratio ((brem+Bhabha)/total).
PDEDX	Evaluates SPTOTP with cutoff energies of `AE` and `AP`.
PHOTTE	Determines the proper mix of PHOTTZ's for a mixture.
PHOTTZ	Determines the interpolated total photoelectric cross section from tabulated data.
PSIG	Determines the total positron interaction cross section (probability per radiation length).
QD	Driver function for DCADRE, the numerical integration routine.
QFIT	Utility logical function for the piecewise linear fit subroutine, PWLF1. It returns `.TRUE.` if a given partition gives a good fit.
SUMGA	Integrates a function using a 20-point Gauss quadrature method with an adaptive bipartition scheme.
SPIONB	Does the work for SPIONE and SPIONP. One argument tells whether to compute stopping power for electron or positron.
SPIONE	Calculates the stopping power due to ionization for electrons(-).
SPIONP	Calculates the stopping power due to ionization for positrons.
SPTOTE	Calculates the total stopping power (ionization plus soft bremsstrahlung) for electrons(-) for specified cutoffs.
SPTOTP	Calculates the total stopping power (ionization plus soft bremsstrahlung) for positrons for specified cutoffs.
TMXB	Determines the maximum total step length consistent with Bethe's criterion.
TMXS	Determines the minimum of TMXB and 10 radiation lengths.
TMXDE2	Included for possible future modification purposes (`TMXDE2 = TMXB / (E**2 * BETA**4)`). It might be easier to fit this quantity than to fit TMXB and then apply the denominator in EGS at run-time.
XSIF	Function to account for bremsstrahlung and pair production in the field of the atomic electrons.
ZTBL	Given the atomic symbol for an element, it returns the atomic number.

```
+------+       +------+      +------+           +------+
|:ELEM:|       |:MIXT:|      |:COMP:|           |:ENER:|
+------+       +------+      +------+           +------+
   |              |             |                  |
   |              V             |                  |
   + ------> OR <-------- +                        |
                  |                                 V
        +-------------------------> AND ----+
                  |                   |      |
                  V                   |      |
     + ------+----+----+------- +     |      |
     |       |         |        |     |      |
     V       V         V        V     |      |
 +------+ +------+ +------+ +------+ +------+  |      |
 |:PLTN:| |:PLTI:| |:HPLT:| |:CALL:| |:TEST:|<---+    |
 +------+ +------+ +------+ +------+ +------+        V
                                             +------+
                                             |:PWLF:|
                                             +------+
                                                |
                                                V
 +------+                                    +------+
 |:STOP:|                                    |:DECK:|
 +------+                                    +------+
```
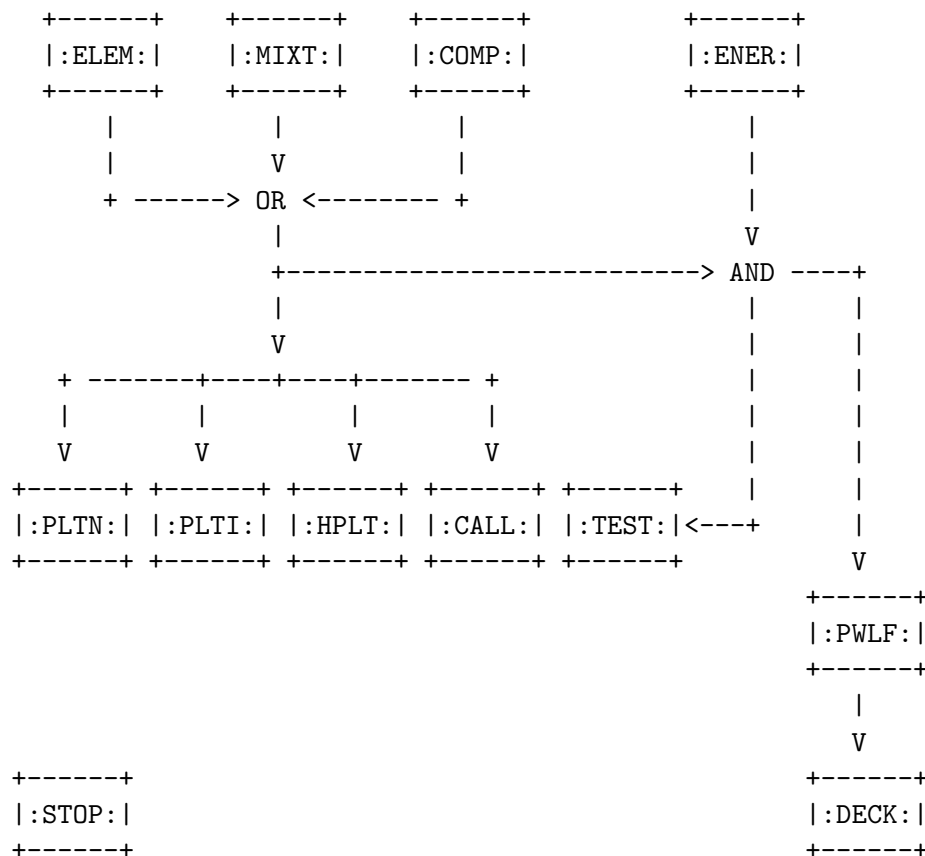
Figure C.9: Logical relationship between the options of PEGS.

C.3.2 The ELEM, MIXT, COMP Options

The purposes of the ELEMent, MIXTure, and COMPound options are to specify the materials used by the PEGS functions. The parameters needed to specify a material are its density (RHO), the number of different kinds of atoms (NE), and, for each different kind of atom, its atomic number (Z(I)), its atomic weight (WA(I)), and its proportion either by number (PZ(I)) for a compound or by weight (RHOZ(I)) for a mixture. PEGS has tables for the atomic symbol (ASYMT(1:100)) and the atomic weight (WATBL(1:100)) for elements I=1 through I=100, so the type of atom is specified by giving its atomic symbol (ASYM(I)). PEGS also has a table of the densities of the elements (RHOTBL(1:100)).

The ELEMent option is used if the material being used has only one type of atom. In this case PEGS defines that NE=1, takes the density from its internal data table, sets PZ(1)=1, and deduces Z(1) and WA(1) from ASYM(1). Thus the atomic symbol (ASYM(1)) is the only information that the user need supply. If either RHO or WA(I) are specified by the user, they override the table values in PEGS. This allows the different atoms to be non-standard isotopes and/or allows the overall density to be adjusted to the experimental state.

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Table C.7: ELEM option input data lines in PEGS, part 1.

Line and format	Variables	Comments
ELEM1 (4A1)	OPT(1:4)	'ELEM'. Means "select material that is an element."
ELEM2 NAMELIST	RHO	Optional. If given, this overrides the PEGS default density (g/cm^3) for the element.
	WA(1)	Optional. Atomic weight of element. If given, this overrides the PEGS default.
	IRAYL	Optional. Set to 1 (or 2, which requires additional data, see below) to model Rayleigh scattering. (default=0, ignore).
	IUNRST	Optional. For printing stopping powers (default = 0, restricted stopping powers, for EGS runs). 1 unrestricted collision only 2 unrestricted collision and radiative 3 unrestricted collision, restricted radiative . 4 restricted collision, unrestricted radiative 5 unrestricted radiative only 6 restricted radiative only 7 restricted collision only
	IAPRIM	Optional. For correction to bremsstrahlung cross section. Default (=1), normalizes integrated cross section to ICRU-37 radiative stopping power; set to 0 uses Motz *et al.*empirical; set to 2 uses no correction.
	ISSB	Optional. Set to 1 to use user-supplied density effect parameters (see below).
	EPSTFL	Optional. Set to 1 to use user-supplied density effect corrections (see below).
	FUDGEMS	Optional. Constant in $Z(Z + \xi_{MS})$ which describes the contribution of soft electron collisions to multiple scattering (default = 1.0).
	IBOUND	Optional. Set to 1 to use bound total Compton cross section (default = 0, use free Compton cross section).
	INCOH	Optional. Set to 1 to use incoherent scattering function to model electron binding effect on Compton scattering angles (default = 0, ignore).
	ICPROF	Optional. Set to 3,4,-3 or -4 (see below) to use shell-wise Compton profiles to get Compton scattering energies. (default = 0, ignore).

Table C.8: ELEM option input data lines in PEGS, part 2.

Line and format	Variables	Comments
ELEM2 (cont) NAMELIST	IMPACT	Optional. For selecting electron impact ionization cross section (default = 0, ignore): 1 Casnati's formula 2 Kolbenstvedt's rev. formula 3 Kolbenstvedt's formula 4 Jakoby's formula 5 Gryziński's formula 6 Gryziński's relativistic. formula
	NLEGO	Optional. Number of Legendre coefficients in computing Goudsmit-Saunderson distribution (default = 1000).
	EFRACH	Optional and not recommended. Fractional energy loss over a multiple scattering step at $E = $ UE (default = 0.05).
	EFRACL	Optional and not recommended. Fractional energy loss over a multiple scattering step at $E = $ AE (default = 0.20).
ELEM3 (24A1,6X,24A1)	MEDIUM	Identifier assigned to data set to be produced.
	IDSTRN	Optional. Identifier of media name of desired Sternheimer-Seltzer-Berger density effect coefficients in PEGS (see Table 2.3 of SLAC-R-730/KEK-2005-8 for a list of default media supplied with the EGS5 distribution.) If not specified, MEDIUM(1:24) is used.
ELEM4 (24(A2,1X))	ASYM(1)	Atomic symbol for element.

Table C.9: COMP option input data lines in PEGS.

Line and Format	Variables	Comments
COMP1 (4A1)	OPT(1:4)	'COMP'. Means "select material that is a compound."
COMP2 NAMELIST	NE	Number of elements in compound.
	RHO	Density (g/cm^3) of compound (at NTP for gases).
	(PZ(I),I=1,NE)	Relative numbers of atoms in compound.
	GASP	Optional. Defines state of compound: zero (default) for solid or liquid, otherwise value gives gas pressure (atm).
	(WA(I),I=1,NE)	Optional. May be used to override default atomic weights (e.g., to allow for special isotopes).
	IRAYL	Same as for ELEM, line 2.
	IUNRST	Same as for ELEM, line 2.
	IAPRIM	Same as for ELEM, line 2.
	ISSB	Same as for ELEM, line 2.
	EPSTFL	Same as for ELEM, line 2.
	FUDGEMS	Same as for ELEM, line 2.
	IBOUND	Same as for ELEM, line 2.
	INCOH	Same as for ELEM, line 2.
	ICPROF	Same as for ELEM, line 2.
	IMPACT	Same as for ELEM, line 2.
	NELGO	Same as for ELEM, line 2.
	EFRACH	Same as for ELEM, line 2.
	EFRACL	Same as for ELEM, line 2.
COMP3 (24A1,6X,24A1)	MEDIUM	Same as for ELEM, line 3.
	IDSTRN	Same as for ELEM, line 3.
COMP4 (24(A2,IX))	(ASYM(I),I=1,NE)	Atomic symbols for the atoms in the compound. Duplicates are allowed if several isotopes of the same element are present, or may be required for diatomic molecules (e.g. nitrogen gas).

Table C.10: MIXT option input data lines in PEGS.

Line and Format	Variables	Comments
MIXT1 (4A1)	OPT(1:4)	'MIXT'. Means "select material that is a mixture."
MIXT2 NAMELIST	NE	Number of elements in mixture.
	RHO	Density (g/cm^3) of mixture (at NTP for gases).
	(RHOZ(I),I=1,NE)	Relative amount of atom in mixture (by weight).
	GASP	Optional. Defines state of mixture: zero (default) for solid or liquid, otherwise value gives gas pressure (atm).
	(WA(I),I=1,NE)	Optional. May be used to override default atomic weights.
	IRAYL	Same as for ELEM, line 2.
	IUNRST	Same as for ELEM, line 2.
	IAPRIM	Same as for ELEM, line 2.
	ISSB	Same as for ELEM, line 2.
	EPSTFL	Same as for ELEM, line 2.
	FUDGEMS	Same as for ELEM, line 2.
	IBOUND	Same as for ELEM, line 2.
	INCOH	Same as for ELEM, line 2.
	ICPROF	Same as for ELEM, line 2.
	IMPACT	Same as for ELEM, line 2.
	NELGO	Same as for ELEM, line 2.
	EFRACH	Same as for ELEM, line 2.
	EFRACL	Same as for ELEM, line 2.
MIXT3 (24A1,6X,24A1)	MEDIUM	Same as for ELEM, line 3.
	IDSTRN	Same as for ELEM, line 3.
MIXT4 (24(A2,1X))	(ASYM(I),I=1,NE)	Same as for COMP, line 4.

Table C.11: ENER option input data lines in PEGS. Note that if the user supplies negative values for the energy limits above, the absolute values given will be interpreted as being given in units of the electron rest mass energy. Thus, AE=-1 is equivalent to AE=0.511 MeV.

Line and Format	Variables	Comments
ENER1 (4A1)	OPT(1:4)	'ENER'. Means "select energy limits."
ENER2 NAMELIST	AE	Lower cutoff energy (total) for charged particle transport (MeV).
	UE	Upper limit energy (total) for charged particle transport (MeV).
	AP	Lower cutoff energy for photon transport (MeV).
	UP	Upper limit energy for photon transport (MeV).

Table C.12: PWLF option input data lines in PEGS. Note: The PWLF parameters above (see section C.3.4 for longer descriptions) are optional and may be overridden by the user. The default values (assigned in `BLOCK DATA`) are indicated above, and all of the parameters are elements of both `NAMELIST/PWLFNM` and `NAMELIST/INP`.

Line and Format	Variables	Comments
PWLF1 (4A1)	OPT(1:4)	'PWLF'. Means "perform piecewise linear fit."
PWLF2 NAMELIST	EPE/0.01/	Electron EP parameter.
	EPG/0.01/	Gamma EP parameter.
	EPR/0.01/	Rayleigh scattering EP parameter.
	EPSF/0.01/	Incoherent scattering function EP parameter.
	EPCP/0.03/	Compton profile EP parameter.
	ZTHRE(1:8)/8*0./	Electron ZTHR parameter.
	ZTHRG(1:3)/0.,.1,0./	Gamma ZTHR parameter.
	ZTHRS(1:40)/40*0./	Incoherent scattering function ZTHR parameter.
	ZTHRR(1:40)/40*0./	Rayleigh scattering ZTHR parameter.
	ZTHRC(1:200)/200*0./	Compton profile ZTHR parameter.
	ZEPE(1:8)/8*0./	Electron ZEP parameter.
	ZEPG(1:3)/0.,.01,0./	Gamma ZEP parameter.
	ZEPS(1:40)/40*0./	Incoherent scattering function ZEP parameter.
	ZEPR(1:40)/40*0./	Rayleigh scattering ZEP parameter.
	ZEPC(1:200)/200*0./	Compton profile ZEP parameter.
	NIPE/20/	Electron NIP parameter.
	NIPG/20/	Gamma NIP parameter.
	NIPS/20/	Incoherent scattering function NIP parameter.
	NIPR/20/	Rayleigh scattering NIP parameter.
	NIPC/20/	Compton profile NIP parameter.
	NALE/150/	Electron NIMX parameter.
	NALG/1000/	Gamma NIMX parameter.
	NALR/100/	Rayleigh scattering NIMX parameter.
	NALS/100/	Incoherent scattering function NIMX parameter.
	NALC/2000/	Compton profile NIMX parameter.

Table C.13: DECK option input data lines in PEGS.

Line and Format	Variables	Comments
DECK1 (4A1)	OPT(1:4)	'DECK'. Means "print fitted data and other useful parameters."
DECK2	NAMELIST	No parameters, but &INP and &END tags must be present.

Table C.14: TEST option input data lines in PEGS.

Line and Format	Variables	Comments
TEST1 (4A1)	OPT(1:4)	'TEST'. Means "Prepare data for plotting the fitted functions."
TEST2 NAMELIST	NPTS	Optional. Number of points to plot per function (Default=50).

Table C.15: CALL option input data lines in PEGS.

Line and Format	Variables	Comments
CALL1 (4A1)	OPT(1:4)	'CALL'. Means "Call the designated function and print value."
CALL2 NAMELIST	XP(1:4)	Values for up to four arguments of the function.
CALL3 (6A1)	NAME(1:6)	Name of function to be evaluated.

Table C.16: PLTI option input data lines in PEGS.

Line and Format	Variables	Comments
PLTI1 (4A1)	OPT(1:4)	'PLTI'. Means "Plot function given its index and the index of the distribution function."
PLTI2 NAMELIST	IFUN	The index of the function to be plotted.
	XP(1:4)	Values for the static arguments (parameters).
	IV	Variable telling which argument is to be varied (e.g., IV=2 means plot function vs. its second argument).
	VLO	Lower limit for argument being varied.
	VHI	Upper limit for argument being varied.
	NPTS	Number of points to plot.
	IDF	Index of distribution function used to select independent variable.

Table C.17: PLTN option input data lines in PEGS.

Line and Format	Variables	Comments
PLTN1 (4A1)	OPT(1:4)	'PLTN'. Means "Plot the named function."
PLTN2 NAMELIST	XP(1:4), IV, VLO, VHI, NPTS, IDF, MP	Same as PLTI2.
PLTN3 (2(6A1))	NAME(1:6)	Name (6 characters) of function to be plotted.
	IDFNAM(1:6)	Name of distribution function to be used.

Table C.18: HPLT option input data lines in PEGS.

Line and Format	Variables	Comments
HPLT1 (4A1)	OPT(1:4)	'HPLT'. Means "Plot histogram to compare the sampled spectrum with the range-integrated and the differential theoretical values."
HPLT2 NAMELIST	EI	Test particle total energy (MeV).
	ISUB	Variable telling which function is being tested: 1=PAIR 2=COMPT 3=BREMS 4=MOLLER 5=BHABHA 6=ANNIH 7=MSCAT (not implemented).
HPLT3: FORMAT(' TEST DATA FOR ROUTINE=',12A1,',#SAMPLES=',I10,',NBINS=',I5)		
	NAMESB(1:12)	Name of subroutine tested.
	NTIMES	Number of samples.
	NBINS	Number of histogram bins.
HPLT4: FORMAT(' IQI=',I2,',RNLO,RNHI=',2F12.8,',IRNFLG=',I2)		
	IQI	Charge of test particle.
	RNLO,RNHI	Lower and upper limits to random number preceding call to test function.
	IRNFLG	Non-zero means to "apply above limits to preceding random number to test for correlation." Zero value means "don't do this."
HPLT5...etc, (9I8)	NH(1:NBINS)	Sampled data (from User Code UCTESTSR).

The COMPound option is used when there is more than one different kind of atom and it is desired to give the proportions by relative number of atoms (`PZ(I)`). The only required data is `NE`, `ASYM(I)`, and `PZ(I)` (for `I=1,NE`). Optionally, any of the values of `WA(I)` taken from the default PEGS tables can be overridden if specified by the user.

The MIXTure option is similar to the COMPound option except that the relative atomic proportions are given by weight (`RHOZ(I)`) rather than by number. When the `PZ(I)` values have been specified, PEGS obtains values of `RHOZ(I)` using `RHOZ(I)=PZ(I)*WA(I)`. Otherwise, `PZ(I)` values are obtained from `PZ(I)=RHOZ(I)/WA(I)`. The absolute normalization of the `PZ(I)` and `RHOZ(I)` values is not important because of the way the quantities are used. For example, the macroscopic cross sections contain factors like `PZ(I)/SUM(PZ(I)*WA(I))` where the denominator is the molecular weight.

Users may supply values for the various parameters used in calculating the density effect correction by setting the flag `ISSB` to 1 and specifying the six parameters, `AFACT, SK, X0, X1, CBAR`, and `IEV`) in the `NAMELIST/INP` input in ELEM, MIXT, or COMP. Note that if one only wants to override `IEV`, one must still input all six parameters.

Alternatively, users may request values of the density effect correction taken from the NBS (now NIST) database EPSTAR, in which case collision stopping powers calculated by PEGS will correspond with values from the ICRU-37 standard. To invoke this option, the flag `EPSTFL` in `NAMELIST/INP/` should be set to 1, and the appropriate data file from either the **elements** or the **compounds** subdirectory of the **density_corrections** directory of the EGS5 distribution data files should be copied or linked to a file called "epstar.dat" in the working user code directory. Note that when this option is employed and multiple materials are being processed, all of the appropriate data files from **density_corrections** must be concatenated onto **epstar.dat** in the order in which the materials are referenced in the PEGS input file.

Rayleigh (coherent) scattering data will be appended to the normal PEGS output data if the `IRAYL` flag is set to 1 or 2 in `NAMELIST/INP/`. An `IRAYL` value of 2 indicates that interference effects in coherent scattering are to be modeled, the user must supply pre-computed values of the coherent scattering cross section and coherent scattering form factors for the material in question. This is done by copying or linking the appropriate data files to files named "ics.dat" and 'iff.dat" in the working user code directory. Sample data files in the appropriate format for several materials are included in the **int_coherent_cs** and **int_form_factor** directories of the EGS5 distribution data set. As with the use of the `EPSTFL` flag, when multiple materials are being used all of the relevant material data files must be concatenated together in the proper order. Note that an option `IRAYL=3` exists in which PEGS will print the Form Factors themselves, rather than cumulative distributions for sampling in EGS runs, when the user wishes to study this data. Note that EGS will abort if it encounters a PEGS data file prepared with `IRAYL=3`.

Altering the value of the `NAMELIST/INP/` flag `IUNRST` causes different versions of the stopping power to be computed and printed in place of the default required by EGS (*i.e.*, the sum of the restricted collision and radiative stopping powers). This functionality is most useful in extracting data sets from PEGS-only user codes for comparison with publish results, and should *not* be

invoked when preparing data files for EGS runs. The available options and their effects are given in Table C.7.

Users may specify the way in which PEGS normalizes bremsstrahlung cross sections by altering the value of the `NAMELIST/INP/` flag `IAPRIM`, which has a default value of 1 (see Chapter 2 of SLAC-R-730/KEK-2005-8 for a complete discussion). Since radiative stopping powers calculated by default in PEGS comply with ICRU standards, changing `IAPRIM` is not recommended except during the development of and testing of new bremsstrahlung cross sections.

Users may input values of the empirical constant which is to be used to represent the contribution of soft electron collisions to multiple nuclear elastic scattering distributions by specifying the value of the parameter `FUDGEMS` in `NAMELIST/INP/`. The default of `FUDGEMS` is 1, which corresponds to approximating angular deflection due to electron scattering by replacing the Z^2 term in the nuclear elastic cross section with $Z(Z+1)$. See Chapter 2 of SLAC-R-730/KEK-2005-8 for a full discussion.

When the parameter `IBOUND` is set to 1 in `NAMELIST/INP/`, the effect of electron binding on the total Compton scattering cross section is taken into account, as described in Chapter 2 of SLAC-R-730/KEK-2005-8. In the default case (`IBOUND = 0`), atomic electrons are considered to be free and at rest for the purpose of modeling Compton scattering.

The effects of electron binding on the angular distribution of Compton scattered photons are modeled when, in conjunction with setting `IBOUND` to 1, the user also sets the parameter `INCOH` to be 1 in `NAMELIST/INP/`.

The effects of atomic electron motion on the energy distribution of photons Compton scattered through given angles (this is often referred to as "Doppler broadening") can be explicitly treated by specifying the value of the parameter `ICPROF`. Currently, `ICPROF` may be set to only 3 (in which case the user must supply values of shell-by-shell Compton profiles) or -3, in which case shell-wise Compton profile data is read from data files provided with the EGS5 distribution. When `ICPROF` is set to 3, the user must copy or link the input profile data to a file named "scp.dat" in the working user code directory. If multiple materials are being processed, data for all materials must concatenated to **scp.dat** in the order in which the materials are specified in the PEGS input file. In PEGS-only user codes designed to generate physics data for examination and study, users may request that PEGS output raw Compton profile data by specifying `ICPROF` to be 4 (for user supplied profile data) or -4 (for PEGS generated profile data). In almost all instances, users wishing to model Compton Doppler broadening should use `ICPROF=-3`. Note that EGS requires that `IBOUND` and `INCOH` be set to 1 when modeling of Doppler broadening is requested, and that EGS will not accept PEGS data sets prepared with `ICPROF` values of 4 or -4.

If electron impact ionization is to be explicitly treated, the user must specify which cross section is to be used by defining a non-zero value for the parameter `IMPACT` in `NAMELIST/INP`. The list of available cross sections and the values of `IMPACT` needed to invoke them is given in Table C.8. The user is referred to Chapter 2 of SLAC-R-730/KEK-2005-8 for a discussion of the derivations and limitations of the various cross sections.

Electron and positron multiple scattering step sizes to be taken in EGS run may be specified by the user when the parameters `EFRACH` and `EFRACL` are defined in `NAMELIST/INP` in a PEGS input file. Including these EGS-related quantities in PEGS arises from the need to compute electron multiple scattering step sizes in terms of scattering strength for the new EGS5 transport mechanics. The parameters `EFRACH` and `EFRACL` refer to the fractional energy loss which occurs over the step at energies corresponding to `UE` and `AE` respectively. See Chapter 2 of SLAC-R-730/KEK-2005-8 for a detailed description of multiple scattering step-size selection. Note that it is strongly recommended that users *not* use `EFRACH` and `EFRACL` to control electron step sizes, but instead specify problem "characteristic dimensions," as described in the EGS User Manual and Chapter 2 of SLAC-R-730/KEK-2005-8.

In addition to physically specifying the material being used, a unique name must be supplied (`MEDIUM(1:24)`) for identification purposes. This name is included in the output file when the DECK option is selected. One useful feature of this implementation is that different names can be used for data sets created with the same materials but different parameters. For example, one might produce PEGS output using a particular material but different energy limits (or fit tolerances, density effect parameters, etc.), with separate identification names for each (e.g., FE1, FE2, etc.).

The quantity `IDSTRN(1:24)` is used to identify the Sternheimer-Seltzer-Berger density effect parameters that are tabulated in `BLOCK DATA` (see Chapter 2 of SLAC-R-730/KEK-2005-8 for a complete list of identifier names and a general discussion of the density effect). If `IDSTRN(1)` is blank, then `IDSTRN` is given the same value as `MEDIUM`. If this name is not identifiable with any of those in `BLOCK DATA`, the Sternheimer density effect scheme is replaced with a general formula by Sternheimer and Peierls. Note that the options for computing stopping powers and the density effect invoked by either `ISSB` or `EPSTFL` take precedence over the specification of `IDSTRN`.

After reading the input data for these options, subroutine `MIX` is called in order to compute the Z-related parameters that reside in `COMMON/MOLVAR/`, subroutine `SPINIT` is called to initialize the stopping power routines for this material, and subroutine `DIFFER` is called to compute run-time parameters for the pair production and bremsstrahlung sampling routines.

The following are examples of sets of input data lines that can be used with the ELEM, MIXT, and COMP options:

1. Material - Element is Iron with defaults taken.

```
                          Column
    Line    12345678911234567892123456789312345678941234678..etc.
    ELEM1   ELEM
    ELEM2   &INP &END
    ELEM3   IRON                                FE
    ELEM4   FE
```

2. Material - Element is Helium-3 with the density and atomic weight overridden by user.

```
                          Column
 Line    1234567891123456789212345678931234567894123456 78..etc.
 ELEM1   ELEM
 ELEM2   &INP RHO=1.E-2,WA(1)=3 &END
 ELEM3   HELIUM-3                         HE
 ELEM4   HE
```

3. Material - Compound is sodium iodide, and `IDSTRN(1:24)` defaults to `MEDIUM(1:24)`.

```
                          Column
 Line    1234567891123456789212345678931234567894123456 78..etc.
 COMP1   COMP
 COMP2   &INP NE=2,RHO=3.667,PZ(1)=1,PZ(2)=1 &END
 COMP3   NAI
 COMP4   NA I
```

4. Material - Compound is polystyrene scintillator (e.g., PILOT-B or NE-102A) with data taken from: "Particle Properties Data Booklet, April 1982" (Physics Letters 111B, April 1982). Sternheimer-Peierls default.

```
                          Column
 Line    1234567891123456789212345678931234567894123456 78..etc.
 COMP1   COMP
 COMP2   &INP NE=2,RHO=1.032,PZ(1)=1,PZ(2)=1.1 &END
 COMP3   POLYSTYRENE SCINTILLATOR
 COMP4   C  H
```

5. Material - Mixture is lead glass, consisting of five specified elements (and 1 per cent of the trace elements unspecified). Sternheimer-Peierls default.

```
                          Column
 Line    1234567891123456789212345678931234567894123456 78..etc.
 MIXT1   MIXT
 MIXT2   &INP NE=5,RHO=3.61,RHOZ=41.8,21.0,29.0,5.0,2.2 &END
 MIXT3   LEAD GLASS
 MIXT4   PB SI O  K  NA
```

6. Material - Mixture is U-235, U-238, and carbon (not a real material). Sternheimer-Peierls default.

```
                          Column
 Line    1234567891123456789212345678931234567894123456 78..etc.
 MIXT1   MIXT
 MIXT2   &INP NE=3,RHO=16,WA=235,238,RHOZ=50,30,10 &END
 MIXT3   JUNK
 MIXT4   U  U  C
```

7. Material - Element is Iron with shell-wise Compton profile.

```
                             Column
Line    12345678911234567892123456789312345678941234567 8..etc.
ELEM1   ELEM
ELEM2   &INP IBOUND=1,INCOH=1,ICPROF=-3 &END
ELEM3   IRON                             FE
ELEM4   FE
```

8. Material - Element is Iron with EII cross section by Casnati's formula.

```
                             Column
Line    12345678911234567892123456789312345678941234567 8..etc.
ELEM1   ELEM
ELEM2   &INP IMPACT=1 &END
ELEM3   IRON                       FE
ELEM4   FE
```

C.3.3 The ENER Option

The ENERgy option is used to define the electron and photon energy intervals over which it is desired to transport particles, and hence, over which fits to total cross sections and branching ratios must be made. The electron energy interval is (`AE,UE`) and the photon interval is (`AP,UP`). If any of these parameter is entered by the user with a negative value, it is multiplied by -0.511 MeV; that is, the absolute magnitude of the input energy is assumed to be in units of the electron rest mass energy. The quantities `TE=AE-RM`, `TET2=2*TE`, and `TEM=TE/RM`, as well as the bremsstrahlung and Møller thresholds (`RM+AP` and `AE+TM`, respectively), are then computed and printed out.

The following are examples of sets of input data lines that can be used with the ENER option:

1. Electron and photon cutoff energies are 1.5 MeV and 10 keV, respectively. The upper energy limit for both is set at 100 GeV. (Note: All energies are in MeV and are total energies).

```
                             Column
Line    12345678911234567892123456789312345678941234567 8..etc.
ENER1   ENER
ENER2   &INP AE=1.5,UE=100000.,AP=0.01,UP=100000. &END
```

2. Same as above, except AE=3*RM.

```
                             Column
Line    12345678911234567892123456789312345678941234567 8..etc.
ENER1   ENER
ENER2   &INP AE=-3,UE=100000.,AP=0.01,UP=100000. &END
```

C.3.4 The PWLF Option

The PieceWise Linear Fit option performs a simultaneous piecewise linear fit (vs. $\ln(E - RM)$) of ten or twelve electron functions over the energy interval (AE,UE) and a simultaneous piecewise linear fit (vs. $\ln E$) of three or four photon functions over the energy interval (AP,UP). Each simultaneous fit over several functions is accomplished by a single call to subroutine PWLF1, once for the electrons and once for the photons. (By simultaneous fit we mean that the same energy sub intervals are used for all of the functions of a set.)

The PWLF1 subroutine is an executive routine that calls the function QFIT. Function QFIT tries to perform a fit to the vector function by doing a linear fit with a given number of subintervals. It returns the value .TRUE. if the fit satisfies all tolerances and .FALSE. otherwise. Subroutine PWLF1 starts out doubling the number of subintervals until a successful fit is found. Additional calls to QFIT are then made to determine the minimum number of subintervals needed to give a good fit. Sometimes, because of discontinuities in the functions being fitted, a fit satisfying the specified tolerances cannot be obtained within the constraints of the number of subintervals allowed by the array sizes of EGS. When this happens, PEGS prints out the warning message (for example):

```
NUMBER OF ALLOCATED INTERVALS(=  150) WAS INSUFFICIENT
TO GET MAXIMUM RELATIVE ERROR LESS THAN        0.01
```

Even in this case a fit is produced which is sufficient most of the time. Suppose NFUN is the number of components to the vector function F(IFUN,E(J)) (where IFUN runs from 1 to NFUN) and E(J) is a sequence of points (with J from 1 to NI) covering the interval being fitted. The number of points NI must be about ten times the number of fit intervals NINT so that the fit will be well tested in the interiors of the intervals. If FEXACT(IFUN,J) and FFIT(IFUN,J) are the exact and fitted values of the IFUNth component at E(J), then the flow of the logical function QFIT may be shown as follows:

```
LOGICAL FUNCTION QFIT(NINT)
(commons and declarations)
QFIT=.TRUE.
REM=0.0
NI=10*NINT
DO J=1,NI
 DO IFUN=1,NFUN
  AER=ABS(FEXACT(IFUN,J)-FFIT(IFUN,J))
  AF=ABS(FEXACT(IFUN,J))
  IF(AF.GE.ZTHR(IFUN)) THEN
    IF(AF.NE.0.0) REM=AMAX1(REM,AER/AF)
  ELSE
    IF(AER.GT.ZEP(IFUN)) QFIT=.FALSE.
  END DO
END DO
```

```
QFIT=QFIT.AND.REM.LE.EP
RETURN
END
```

Thus we see that `EP` is the largest allowed relative error for those points where the absolute computed value is above `ZTHR(IFUN)`, and `ZEP(IFUN)` is the largest allowed absolute error for those points where the absolute computed value is less than `ZTHR(IFUN)`.

Other features of the `QFIT` routine include provisions for aligning a subinterval boundary at a specified point in the overall interval (in case the fitted function has a discontinuous slope such as at the pair production or Møller thresholds), and computing fit parameters in bins flanking the main interval to guard against truncation errors in sub-interval index computations.

The net result of the fit is the determination of coefficients `AX`, `BX`, `AF(IFUN,J)`, and `BF(IFUN,J)` such that

```
FVALUE(E)=AF(IFUN,INTERV)*XFUN(E) + BF(IFUN,INTERV)
```

is the value of the `IFUN`th function, and where

```
INTERV=INT(AX*XFUN(E) + BX).
```

`XFUN` is called the distribution function and is $\ln(E - RM)$ for electrons and $\ln(E)$ for photons.

Note that the coding of EGS is designed to allow a "mapped PWLF" in which we have `AX`, `BX`, `AF(IFUN,J)`, `BF(IFUN,J)`, and `M(I)`, such that when `I=INT(AX*XFUN(E)+BX)` and `J=M(I)`, then

```
FVALUE(E)=AF(IFUN,J)*XFUN(E) + BF(IFUN,J)
```

for the `IFUN`th function. This kind of fit has the advantage that it yields a better fit with a smaller amount of stored data than the default fit computed by `PWFL1`. Such a scheme has never been implemented in PEGS, however, despite that more data than necessary is currently used in describing the functions at higher energies where they vary quite smoothly.

The following is an example of the input data lines that can be used with the PWLF option:

```
                        Column
 Line     12345678911234567892123456789312345678941234567 8..etc.
 PWLF1    PWLF
 PWLF2    &INP &END
```

C.3.5   The DECK Option

The DECK option, with the aid of subroutine `LAY`, prints the data needed to specify the current material, the energy intervals specified, various computed molecular parameters (e.g., the radiation length), the run-time parameters for pair production and bremsstrahlung, and the fit data produced by the PWLF option. In other words, DECK prints anything that might be of use to EGS in simulating showers or to users in analysis routines. Subroutines `LAY` (in PEGS) and `HATCH` (in EGS) are a matched pair in that `HATCH` reads what `LAY` writes (PEGS "lays" and EGS "hatches"). Thus when users alter `LAY` to write additional material data to PEGS output files, `HATCH` must be be updated appropriately.

   DECK should be invoked when either ELEM, MIXT, or COMP and ENER and PWLF have been run for the current material and before any of these have been executed for the next material (see Figure C.9). The following is an example of the input data lines that can be used with the DECK option:

```
                        Column
 Line     12345678911234567892123456789312345678941234578..etc.
 DECK1    DECK
 DECK2    &INP &END
```

C.3.6   The TEST Option

The TEST option is used as an easy way to obtain data for plots of some of the functions (not the fits) that the PWLF option fits. Output is printed to a file "pgs5job.pegs5plot" in the working user code directory, and includes sequential sets of data from PEGS functions `ESIG`, `PSIG`, `EDEDX`, `PDEDX`, `EBR1`, `PBR1`, `PBR2`, `TMXS`, `TMXDE2`, `GMFP`, `GBR1`, `GBR2` and `CRATIO`. Thus the TEST option provides yet another useful PEGS tool for examining and studying raw physics data.

   The following is an example of the input data lines that can be used with the TEST option:

```
                        Column
 Line     12345678911234567892123456789312345678941234578..etc.
 TEST1    TEST
 TEST2    &INP NPTS=50 &END
```

C.3.7   The CALL Option

The CALL option is used whenever one desires to have PEGS evaluate a particular function and print out the results. The following is an example of the input data lines that can be used with

the CALL option in order to test for discontinuities in GMFP (Gamma Mean Free Path) near 50 MeV. (Note: In this example we have included the (necessary) ELEM option data lines for Lead).

```
                        Column
 Line    123456789112345678921234567893123456789412345678..etc.
 ELEM1   ELEM
 ELEM2   &INP &END
 ELEM3   PB
 ELEM4   PB
 CALL1   CALL
 CALL2   &INP XP(1)=49.99 &END
 CALL3   GMFP
 CALL1   CALL
 CALL2   &INP XP(1)=50.01 &END
 CALL3   GMFP
```

The resulting output from a user code accessing PEGS would be:

```
 OPT = CALL
 Function call:    1.95522    = GMFP   OF    49.9900
 OPT = CALL
 Function call:    1.97485    = GMFP   OF    50.0100
```

C.3.8 The PLTI and PLTN Options

The PLTI and PLTN options may be used to obtain printer plots of any of the functions in the PEGS function table. These options are somewhat analogous to the TEST option in that they call the same PEGS output routine (subroutine PLOT) and write output data in the same format to the same file ('pgs5job.pegs5plot' in the working user code directory). However, the information which can be extracted using the TEST option is restricted to the energy-dependent default functions over the ranges from AE to UE and AP to UP, while PLTI and PLTN can access arbitrary PEGS functions and produce physics data over arbitrary ranges. The PLTI option is rather primitive in that the functions involved must be specified by number, so we shall instead concentrate on the PLTN option in which the functions are specified by name.

Consider the function BRMSRZ(Z,E,K1,K2), which is the soft bremsstrahlung cross section (for an electron of total energy energy E and element Z) integrated over the photon energy range (K1,K2). Suppose we would like to see a plot of BRMSRZ(2,E,0.0,1.5) for values of E from 5 to 100 MeV. Also assume we want the data points evenly spaced in $\ln(E)$. Then (see Table C.17) the function name we would use is BRMSRZ, the distribution function name to be specified is IDFNAM=ALOG, the static arguments needed are XP(1)=2., XP(3)=0.0, XP(4)=1.5, the independent variable to be accessed is the second argument (*i.e.*, IV=2), and its limits are VLO=5.0 and VHI=100.0. If we want

Table C.19: Distribution functions available with PLTI and PLTN.

IDFNAM	Purpose
ALIN	Linear plot.
DLOG	Natural log plot.
ALKE	Natural log of electron kinetic energy plot.
ADFMOL	Approximation to Møller and Bhabha distributions

100 points on the data set we specific `NPTS=100`. The input data lines necessary to accomplish this are:

```
                      Column
 Line     123456789112345678921234567893123456789412345678..etc.
 PLTN1    PLTN
 PLTN2    &INP XP(1)=2.,XP(3)=0.0,XP(4)=1.5,IV=2,VLO=5.,
           VHI=100.,NPTS=100 &END
 PLTN3    BRMSRZALOG
```

Distribution functions that are available are listed and described in Table C.19.

C.3.9   The HPLT Option

The Histogram PLoT option is designed to be used in conjunction with UCTESTSR (User Code to TEST Sampling Routine), which is provided with the EGS5 distribution. This option provides a way to test the EGS methods used to sample differential distributions functions by looking for discrepancies between actual differential physics data and histograms of sampled data during simulations.

Suppose that a probability density function, $PDF(X)$ (see Chapter 2 of SLAC-R-730/KEK-2005-8), is to be sampled by EGS (note: $PDF(X)$ will have other static arguments which we ignore for this discussion). Let $CDF(X)$ be the cumulative distribution function associated with $PDF(X)$. If $PDF(X)$ drops sharply with increasing X, we will not get many samples in the bins with large X unless we make the bins themselves larger in such regions. We accomplish this by finding another p.d.f.and c.d.f., $PDG(X)$ and $CDG(X)$, respectively, such that $PDG(X)$ approximates $PDF(X)$. If we want N bins, we then pick the $X(I)$ such that

```
CDG(X(I+1))-CDG(X(I))=(CDG(X(N+1))-CDG(X(I)))/N.
```

For all I this implies that

```
X(I)=CDGI((CDG(X(N+1))-CDG(X(1)))*I/(N+1) + CDG(X(1)))
```

where $CDGI$ is the inverse function of CDG. Thus, if $PDG(X)$ is a reasonable approximation, the histogram bins at large X should have the same order of magnitude of counts as those at lower X. The function $CDG(X)$ is called the "distribution function" in the context of the HPLT option. $CDG(X), CDGI(X)$, and $PDG(X)$ are used by the UCTESTSR user code and `HPLT1` subroutine in PEGS. If we let $SPDF(X)$ and $SCDF(X)$ be the "sampled" data, and $PDF(X)$ and $CDF(X)$ be the theoretical data, then the routine `HPLT1` can be summarized by the pseudo-code:

```
DO I=1,N
PLOT((SCDF(X(I+1))-SCDF(X(I)))/(CDG(X(I+1))-CDG(X(I))))
PLOT((CDF(X(I+1))-CDF(X(I)))/(CDG(X(I+1))-CDG(X(I))))
DO....X(I) at 10 points in the interval (X(I),X(I+1))
  PLOT(d(SCDF)/d(CDG)=PDF(X)/PDG(X))
END DO
RETURN
END
```

All of the input data lines for a specified HPLT option are printed directly by UCTESTSR to standard output. This data can then be used in a subsequent run of PEGS to produce line-printer style plots of the actual and sample functions . Users should refer to the listing for UCTESTSR and comments therein for a better understanding of the HPLT option (see also Chapter 6 of SLAC-210).

C.4 Concluding Remarks

In the previous sections we have seen the various uses for PEGS. We summarize by giving the option sequences most generally used:

1. Minimal options for a material data set creation (for later use by EGS):

    ```
    1.   ELEM (or MIXT, or COMP)
    2.   ENER
    3.   PWLF
    4.   DECK
    ```

2. Same as above, with default data dumps of functions for which the PWLF option provides fits:

    ```
    1.   ELEM (or MIXT, or COMP)
    2.   ENER
    3.   TEST
    4.   PWLF
    5.   DECK
    ```

3. Comparison of theoretical and sampled distributions by means of the HPLT option:

```
1.   ELEM (or MIXT, or COMP)
     Note: Data lines should agree with those used
           with the UCTESTSR run that generated the HPLT input.
2.   HPLT
     Note: Output data from UCTESTSR run.
```

4. Selective plotting of various functions:

```
1.   ELEM (or MIXT, or COMP) - for material 1
2.   PLTN  -  for function 1
3.   PLTN  -  for function 2,....etc.
4.   ELEM (or MIXT, or COMP) - for material 2,....etc.
5.   PLTN  -  for function 1
6.   PLTN  -  for function 2,....etc.
```