NRC-CNRC

Using PEGS4

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Introduction

- Primary purpose of PEGS4 is to create material data sets for subsequent use by EGSnrc (and EGS4, of course)
- Operations necessary to accomplish this task include:
  - Selection of materials
  - Selection of energy cutoffs
  - Piecewise linear fitting
  - Creation of output data set for direct use by EGSnrc

…Introduction (cont.)

- PEGS4 can provide other services too, such as:
  - Production of print plots of selected functions
  - Evaluation of functions at selected points
  - Comparison of functions with sampled spectra
- In this lecture we will learn how to create media data sets
- We will also take a quick look at some other PEGS4 services

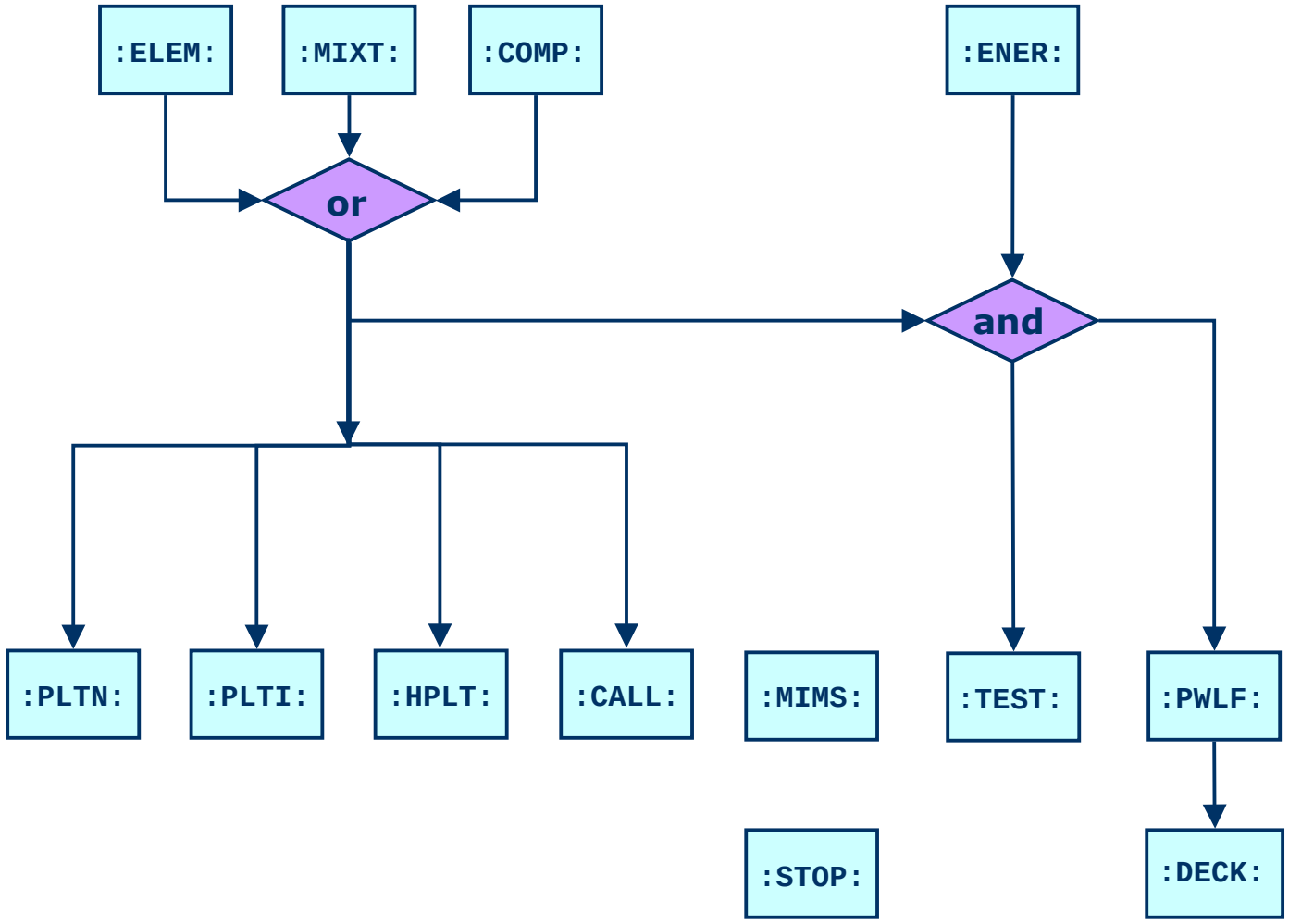
The PEGS4 Connection to EGSnrc

- PEGS4 has been modified very little for use with EGSnrc
- However, the EGSnrc code has new features that
  - require considerably more data than provided by the PEGS4 code, and
  - this data is read in directly by means of the EGSnrc version of SUBROUTINE HATCH

PEGS4 Documentation

- The PEGS4 User Manual is provided in Chapter 6 of the EGSnrc manual
- It is essentially a reprint of the original PEGS4 manual for the EGS4 Code System—i.e., Appendix 3 of SLAC265
- However, a few additions have been made to PEGS4 since 1985 and these are explained at the beginning of Chapter 6
- Of particular note is the documentation for the parameters IUNRST, EPSTFL and IAPRIM

Logical Relationship Between the Options of PEGS4



The ELEM, COMP and MIXT Options

- The purpose of the ELEMent, COMPound and MIXTure options is to specify the material(s) used by the PEGS4 functions
- Parameters needed to specify a material are:
  - Density (RHO)
  - Number of different kinds of elements (NE)
  - Atomic number of each kind (Z(I))
  - Atomic weight of each kind (WA(I))
  - Proportion of each kind:
    - By number (PZ(I)) for compounds
    - By weight (RHOZ(I)) for mixtures
- PEGS4 has tables for for elements I=1 through 100:
  - The atomic symbol(ASYM(1:100))
  - The atomic weight(WATBL(1:100))
- PEGS4 also has a table of the densities of the elements (RHOTBL(1:100))
- For each option there is an associated table that we will discuss, in turn, next.

The ELEM Option (1 of 3)

CARD	FORMAT	VARIABLES READ	COMMENTS
ELEM1	(4A1)	OPT(1:4)	'ELEM'. Means "select material that is an element."
ELEM2	NAMELIST/INP/	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 unity to included Rayleigh output.
		IUNRST	Optional. Set to unity for unrestricted collision stopping power.
		ISSB	Optional. Set to unity to use own density effect parameters (see text below).
		EPSTFL	Optional. Set to unity for ICRU-37 collision stopping power.
		IAPRIM	Optional. Set to unity to normalize bremsstrahlung cross section to ICRU-37 radiative stopping power.

The ELEM Option (2 of 3)

CARD	FORMAT	VARIABLES READ	COMMENTS
ELEM3	(24A1, 6X,24A1)	MEDIUM(1:24)	Identifier assigned to data set to be produced.
		IDSTRN(1:24)	Optional. Identifer of medium name under which desired Sternheimer-Seltzer-Berger coeffcients are given in PEGS. If not specified, the identifier in MEDIUM(1:24) is used.
ELEM4	(24(A2,1X))	ASYM(1)	Atomic symbol for element.

[It should be noted that when setting **EPSTFL=1** in **NAMELIST/INP/**, the NRC scripts require that a file containing the ICRU-37 collision stopping powers be identified on the command line invoking the script]

The ELEM Option (3 of 3)

- The following card setup illustrates how to use the **ELEM** option

```
                                Column
     12345678911234567892123456789312345678941234567 8..etc.
1    ELEM
2     &INP IAPRIM=1,IRAYL=1 &END
3    PB (10 KEV TO 100 MEV)        PB
4    PB
```

- **IAPRIM** set to unity—invokes option to normalize the bremsstrahlung cross section (radiative stopping power will be same as ICRU-37)
- **IRAYL** is set to unity — Rayleigh scattering included in PEGS4 output (note: user must still turn it on/off in User Code)
- The 24-character string: **'PB (10 KEV TO 100 MEV) '** is selected to be the ***identifier*** used in subsequent EGS runs
- PEGS4 will search for any Sternheimer-Seltzer_Berger coefficients identified by the 24-character string **'PB '**
- Since no other quantities have been added to the **NAMELIST/INP/**—i.e., between the **&INP** and **&END** delimiters—the default values for **RHO**, etc., will be used for the element **PB**

Sternheimer-Seltzer-Berger (SSB) Coefficients

- The **density effect** in the *dE/dx* (Bethe-Bloch) formula
  - Treated extensively for many years by Sternheimer
  - A general formula is used and is given in terms of Sternheimer parameters
- A set of density-effect parameters have been created by SSB
  - They are tabulated for 73 materials in PEGS4 (see Table 2.13.2 of SLAC-265 (p.71-72))
- The string **`IDSTRN(1:24)`** is used in order to make use of SSB density-effect parameters
  - If **`IDSTRN(1)`** is blank, then **`IDSTRN(1:24)`** is given the same name as **`MEDIUM(1:24)`**
  - If **`IDSTRN(1:24)`** cannot be found in the **`BLOCK DATA,`** the density effect is calculated from another general formula by Sternheimer and Peierls.
- Users can also supply their own SSB parameters by setting **`ISSB`** to unity

The COMP Option (1 of 3)

CARD	FORMAT	VARIABLES READ	COMMENTS
COMP1	(4A1)	OPT(1:4)	'COMP'. Means "select material that is a compound."
COMP2	NAMELIST/INP/	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 ELEM2.
		IUNRST	Same as for ELEM2.
		ISSB	Same as for ELEM2.
		EPSTFL	Same as for ELEM2.
		IAPRIM	Same as for ELEM2.

The COMP Option (2 of 3)

CARD	FORMAT	VARIABLES READ	COMMENTS
COMP3	(24A1, 6X,24A1)	MEDIUM,IDSTRN	Same as for ELEM3.
COMP4	(24(A2, 1X))	(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).

The COMP Option (3 of 3)

- The following card setup illustrates how to use the **COMP** option

```
                                  Column
     12345678911234567892123456789312345678941234567 8..etc.
1    COMP
2     &INP NE=2,PZ=2,1,RHO=1.0,IAPRIM=1 &END
3    WATER                              H2O
4    H  O
```

- The number of elements in the compound (NE) is 2
- The relative number of atoms in H_2O is **PZ=2,1** (we also could have written this out more specifically in the form **PZ(1)=2,PZ(2)=1**)
- The density is the standard **RHO=1.0** …but you must state what it is (i.e., it is not optional)
- The 24-character string: **'WATER ' ** is selected to be the ***identifier*** used in subsequent EGS runs
- PEGS4 will search for any Sternheimer-Seltzer_Berger coefficients identified by the 24-character string **'H2O ' **
- The atomic symbols are **H** and **O** --- note the ***order*** and the format **24(A2,1X))**

The MIXT Option (1 of 2)

CARD	FORMAT	VARIABLES READ	COMMENTS
MIXT1	(4A1)	OPT(1:4)	'MIXT'. Means "select material that is a mixture."
MIXT2	NAMELIST/INP/	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	Optional. Set to unity to included Rayleigh output.
		IUNRST	Same as for ELEM2.
		ISSB	Same as for ELEM2.
		EPSTFL	Same as for ELEM2.
		IAPRIM	Same as for ELEM2.
MIXT3	(24A1, 6X,24A1)	MEDIUM,IDSTRN	Same as for ELEM3.
MIXT4	(24(A2, 1X))	(ASYM(I),I=1,NE)	Same as for COMP4.

The MIXT Option (2 of 2)

- The following card setup illustrates how to use the **MIXT** option

```
                                  Column
      12345678911234567892123456789312345678941234567 8..etc.
1     MIXT
2      &INP NE=7,RHO=2.26,RHOZ=49.83,1.71,4.56,31.58,1.92,8.26,1.22 &END
3     CONCRETE
4     O  NA AL SI K  CA FE
```

- There are **7** elements and the density is 2.26 g/cm^3
- The relative amount of each atom by weight is written in the simple form **RHOZ=49.83,1.17**, …etc.
- The 24-character string: **'CONCRETE '** is selected to be the ***identifier*** used in subsequent EGS runs
- No character string was chosed for the Sternheimer identifier, so PEGS4 will set **e**qual to **'CONCRETE '** and this will **not** be found in the SSB table, so the approximation scheme will be used
- The atomic symbols for the elements are specified in the fourth **MIXT** card (again, pay attention to the format: **24(A2,1X)**

Additional Examples

```
------------------------------------------------------------------
  Material - Element is liquid Helium-3.  Density and atomic
             weight overridden by user.  Note that HELIUM-3
             will not be found in SSB tables.
------------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..etc.
ELEM1   ELEM
ELEM2    &INP RHO=0.178,WA(1)=3 &END
ELEM3   HELIUM-3
ELEM4   HE


------------------------------------------------------------------
  Material - Compound is Nitrogen gas (a diatomic molecule).
             Density and gas pressure overridden by user.
------------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..etc.
COMP1   COMP
COMP2    &INP NE=2,PZ=1,1,RHO=0.808,GASP=2 &END
COMP3   NITROGEN (2 ATM)              N2-GAS
COMP4   N  N
```

…Additional Examples (cont.)

```
------------------------------------------------------------
  Material - Compound is sodium iodide with IDSTRN(1:24)
             defaulting to MEDIUM(1:24)....but NAI will
             be found in SSB tables.
------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..etc.
COMP1   COMP
COMP2    &INP NE=2,RHO=3.667,PZ(1)=1,PZ(2)=1 &END
COMP3   NAI
COMP4   NA I


------------------------------------------------------------
  Material - Compound is Pilot-B scintillator.  Data taken from
             Physics Letters B204, April 1988 (density=1.032,
             atomic ratio H/C=1.10).  Material is in SSB table.
------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..etc.
COMP1   COMP
COMP2    &INP NE=2,RHO=1.032,PZ(1)=1,PZ(2)=1.10 &END
COMP3   PILOT-B                        POLYSTYRENE
COMP4   C  H
```

…Additional Examples (cont.)

```
------------------------------------------------------------
  Material - Mixture is lead glass, consisting of five specified
             elements (1 per cent trace elements unspecified).
             Density effect calculated by Sternheimer-Peierls.
------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..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

------------------------------------------------------------
  Material - Compound is Bismuth Germanate (BGO).
------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..etc.
COMP1   COMP
COMP2    &INP NE=3,RHO=7.13,PZ=4,3,12 &END
COMP3   BGO
COMP4   BI GE O

------------------------------------------------------------
  Material - Compound is Liquid Hydrogen.
------------------------------------------------------------
Card    12345678911234567892123456789312345678941234567 8..etc.
COMP1   COMP
COMP2    &INP NE=2,RHO=7.08E-2,PZ=1,1 &END
COMP3   LIQUID HYDROGEN              H2-LIQUID
COMP4   H  H
```

The ENER Option

CARD	FORMAT	VARIABLES READ	COMMENTS
ENER1	(4A1)	OPT(1:4)	'ENER'. Means "select energy limits."
ENER2	NAMELIST/INP/	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).

Note: If the user supplies negative values for the energy limits above, the absolute values given will be interpreted as in units of the electron rest mass energy. Thus, AE=-1 is equivalent to AE=0.511 MeV.

The following card setup illustrates how to use ENER option

```
        123456789112345678921234567893123456789412345678..etc.
    1   ENER
    2    &INP AE=0.521,UE=100.,AP=0.001,UP=100. &END
```

The Options: PWLF and DECK

- The minimal data setup for PEGS4 consists of choosing **ELEM** (or **MIXT** or **COMP**), followed by **ENER**, and then followed by **PWLF** and **DECK**
- For the general case, the **PWLF** and **DECK** options are very trivial (but necessary)–they consist of the option name followed by a blank **NAMELIST**-read card: **&INP &END**

The Options: PWLF and DECK (cont.)

- Together with one of the above examples, the ***entire*** card card setup might consist of the following ten cards (for BGO detector):

```
      123456789112345678921234567893123456789412345678..etc.
  1   COMP
  2    &INP NE=3,RHO=7.13,PZ=4,3,12 &END
  3   BGO
  4   BI GE O
  5   ENER
  6    &INP AE=0.521,UE=100.,AP=0.001,UP=100. &END
  7   PWLF
  8    &INP &END
  9   DECK
 10    &INP &END
```

- The **TEST** option is also available for obtaining plots of all functions that the **PWLF** option fits

Examples of PEGS4 Output

```
-------------------------------------------------------------------------------
MEDIUM=WOOD                      ,STERNCID=WOOD
COMP,RHO= 5.0000E-01,NE= 3
ASYM=C ,Z= 6.,A=   12.011,PZ= 6.00000E+00,RHOZ= 7.20669E+01
ASYM=H ,Z= 1.,A=    1.008,PZ= 5.00000E+00,RHOZ= 5.03985E+00
ASYM=O ,Z= 8.,A=   15.999,PZ= 5.00000E+00,RHOZ= 7.99970E+01
   7.65637E+01   5.21000E-01   1.00000E-02   5.05110E+01   5.00000E+01

    0  199    0  149    0    0    0    1    0
   9.99983E-01  -2.09272E-01   4.80231E-02   9.95902E-01  -2.24627E-01
                      500 or more cards follow
-------------------------------------------------------------------------------

-------------------------------------------------------------------------------
MEDIUM=AIR AT NTP                ,STERNCID=AIR-GAS
MIXT,RHO= 1.2050E-03,NE= 3,GASP= 1.0000E+00
ASYM=N ,Z= 7.,A=   14.007,PZ= 5.57090E+00,RHOZ= 7.80300E+01
ASYM=O ,Z= 8.,A=   15.999,PZ= 1.31442E+00,RHOZ= 2.10300E+01
ASYM=AR,Z=18.,A=   39.948,PZ= 2.35306E-02,RHOZ= 9.40000E-01
   3.05535E+04   1.50000E+00   1.00000E-01   1.00000E+05   1.00000E+05
    0  200    0  150    0    0    0    0    0
   9.99983E-01  -2.10279E-01   4.82540E-02   9.95882E-01  -2.25707E-01
                      500 or more cards follow
-------------------------------------------------------------------------------
```

…PEGS4 Output (cont.)

```
------------------------------------------------------------------------
   MEDIUM=ISOOCTANE               ,STERNCID=ISOOCTANE
   COMP,RHO= 6.9190E-01,NE= 2
   ASYM=C ,Z= 6.,A=   12.011,PZ= 8.00000E+00,RHOZ= 9.60892E+01
   ASYM=H ,Z= 1.,A=    1.008,PZ= 1.80000E+01,RHOZ= 1.81434E+01
      6.50520E+01   5.21000E-01   1.00000E-02   5.05110E+01   5.00000E+01
       0  199    0  149    0    0    0    0    0
      9.99983E-01  -2.04659E-01   4.69644E-02   9.95992E-01  -2.19675E-01
                         500 or more cards follow
------------------------------------------------------------------------
------------------------------------------------------------------------
    MEDIUM=AU (USING NEW PEGS4N)   ,STERNCID=AU
   ELEM,RHO= 1.9300E+01,NE= 1, IUNRST=0, EPSTFL=0, IAPRIM=1
   ASYM=AU,Z=79.,A=  196.987,PZ= 1.00000E+00,RHOZ= 1.96987E+02
      3.34846E-01   5.21000E-01   1.00000E-03   1.00000E+01   1.00000E+01
       0  199    0  150    0    0    0    1    0
      9.99979E-01  -2.53604E-01   5.81963E-02   9.95034E-01  -2.72211E-01
                         500 or more cards follow
------------------------------------------------------------------------
```

The CALL Option

```
-------------------------------------------------------------
CARD    FORMAT   VARIABLES READ          COMMENTS
-------------------------------------------------------------
CALL1   (4A1)       OPT(1:4)      'CALL'.  Means "Call the
                                  designated function and
                                  print value."

CALL2 NAMELIST/INP/  XP(1:4)      Values for up to four argu-
                                  ments of the function.
```

- The following card setup illustrates the **CALL** option:

```
          12345678911234567892123456789312345678941234567 8..etc.
    1     ELEM
    2      &INP &END
    3     PB
    4     PB
    5     CALL
    6      &INP XP(1)=49.99 &END
    7     GMFP
    8     CALL
    9      &INP XP(1)=50.01 &END
   10     GMFP
```

which produces the following PEGS4 output:

```
FUNCTION CALL:     1.95522     = GMFP   OF     49.9900
FUNCTION CALL:     1.97485     = GMFP   OF     50.0100
```