The program MATERIAL

EUTEMPE-RX module 03

Monte Carlo simulation of x-ray imaging and dosimetry

Barcelona, June 2017

Program MATERIAL

PENELOPE's "pre-processor":

creates a file with tables of cross sections for a given material.

Compile **`material.f`** (needs **`penelope.f`**):

go to directory **`~/fsource/.`**

```
$ gfortran material.f -o material.exe -O
```

Move **`material.exe`** to **`~/pendbase/pdfiles/.`**

There are 280 predefined materials, listed in
`~/pendbase/pdfiles/pdcompos.pen`

1 - 99 are elements, ID = atomic number

100 - 280 are compounds, in alphabetical order

Lister - [c:\home\penelope2008\pendbase\pdfiles\pdcompos.p08]

File Edit Options Help 5 %

```
                                                    7 February, 2005
  This file contains composition data and physical parameters for
280 materials, taken from the database of the ESTAR program of
Berger (NISTIR 4999, 1992). The first 99 entries are the elements
Z=1-99, ordered by atomic number Z. Materials 100 to 280 are com-
pounds and mixtures, in alphabetical order. The data for each
material are:

 Identification no.      NAME
    No. of elements      Z/A      I(eV)      Density (g/cm**3)
    Element(Z)      Fraction by weight      Stoichiometric index
    Element(Z)      Fraction by weight      Stoichiometric index
    ...
            ****************************************

  1  HYDROGEN  (1)                                                  1
       1  9.92162E-01  1.92000E+01  8.37480E-05
       1  1.00000E+00  1.00000E+00
  2  HELIUM  (2)                                                    2
       1  4.99675E-01  4.18000E+01  1.66322E-04
       2  1.00000E+00  1.00000E+00
  3  LITHIUM  (3)                                                   3
       1  4.32214E-01  4.00000E+01  5.34000E-01
       3  1.00000E+00  1.00000E+00
  4  BERYLLIUM  (4)                                                 4
       1  4.43844E-01  6.37000E+01  1.84800E+00
       4  1.00000E+00  1.00000E+00
  5  BORON  (5)                                                     5
       1  4.62535E-01  7.60000E+01  2.37000E+00
       5  1.00000E+00  1.00000E+00
  6  AMORPHOUS CARBON  (6)                                          6
       1  4.99542E-01  8.10000E+01  2.00000E+00
       6  1.00000E+00  1.00000E+00
  7  NITROGEN  (7)                                                  7
       1  4.99761E-01  8.20000E+01  1.16528E-03
       7  1.00000E+00  1.00000E+00
  8  OXYGEN  (8)                                                    8
       1  5.00019E-01  9.50000E+01  1.33151E-03
       8  1.00000E+00  1.00000E+00
  9  FLUORINE  (9)                                                  9
       1  4.73724E-01  1.15000E+02  1.58029E-03
       9  1.00000E+00  1.00000E+00
 10  NEON  (10)                                                    10
       1  4.95565E-01  1.37000E+02  8.38505E-04
      10  1.00000E+00  1.00000E+00
 11  SODIUM  (11)                                                  11
       1  4.78474E-01  1.49000E+02  9.71000E-01
      11  1.00000E+00  1.00000E+00
 12  MAGNESIUM  (12)                                               12
       1  4.93726E-01  1.56000E+02  1.74000E+00
      12  1.00000E+00  1.00000E+00
 13  ALUMINUM  (13)                                                13
       1  4.81811E-01  1.66000E+02  2.69890E+00
      13  1.00000E+00  1.00000E+00
 14  SILICON  (14)                                                 14
       1  4.98478E-01  1.73000E+02  2.33000E+00
      14  1.00000E+00  1.00000E+00
 15  PHOSPHORUS  (15)                                              15
```

Running **`material.exe`**

- If your material is defined in **`pdcompos.pen`** its ID is the only information required.

- If your material is not in **`pdcompos.pen`**, you will need composition (atomic numbers and stoichiometric indices or fractions by weight) mean excitation energy, if available, and mass density.

In either case, you have to provide a file name, e.g., NaI.mat

- If the material is in **`pdcompos.pen`** it is highly recommended to define the material by using the information provided in PENELOPE's database.

Exercise: create the material file for liquid water, **`water.mat`**

Exercise:

Generate files for the following elements, compounds and alloys:

- Al
- NaI
- Fe
- W
- Stainless steel ANSI type 316L:
  1% Si, 17% Cr, 2% Mn, 68% Fe, 12% Ni
  mass density = 8.02 g/cm^3
- Spongiosa (approx. composition):
  8.3%H, 26.6%C, 2.7%N, 51.1%O, 4.0%P, 4.0%Ca
  mass density: 1.228 g/cm^3

Auxiliary program TABLES

Creates a file with tables of cross sections of the material of interest, ready to be visualized by a plotting program, e.g. gnuplot

Compile **`tables.f`** (needs **`penelope.f`**):

copy **`~/fsource/penelope.f`** to **`~/other/tables/.`**

go to **`~/other/tables/.`**

```
$ gfortran tables.f -o tables.exe -O
```

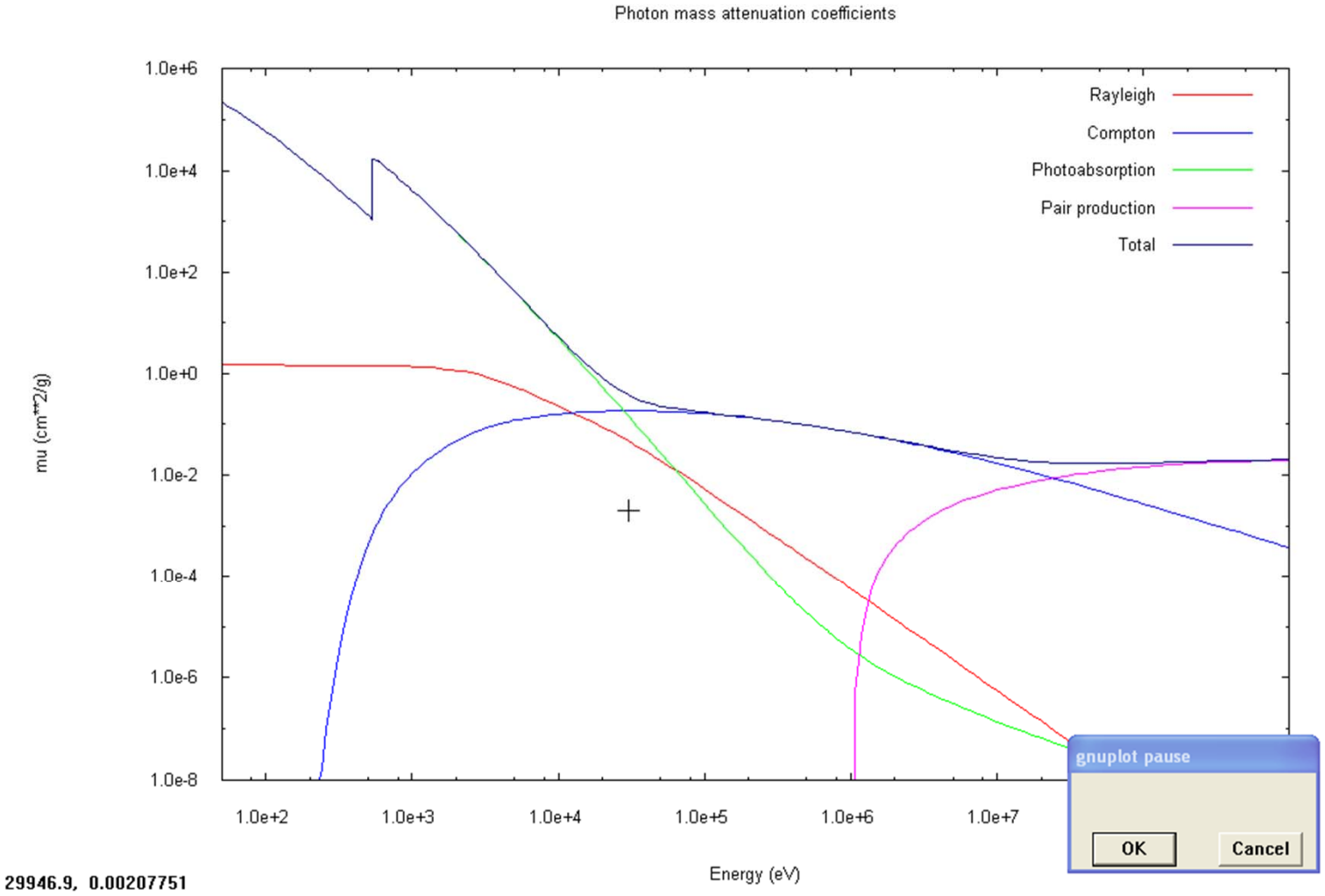
Copy **`water.mat`** to **`~/other/tables/.`**

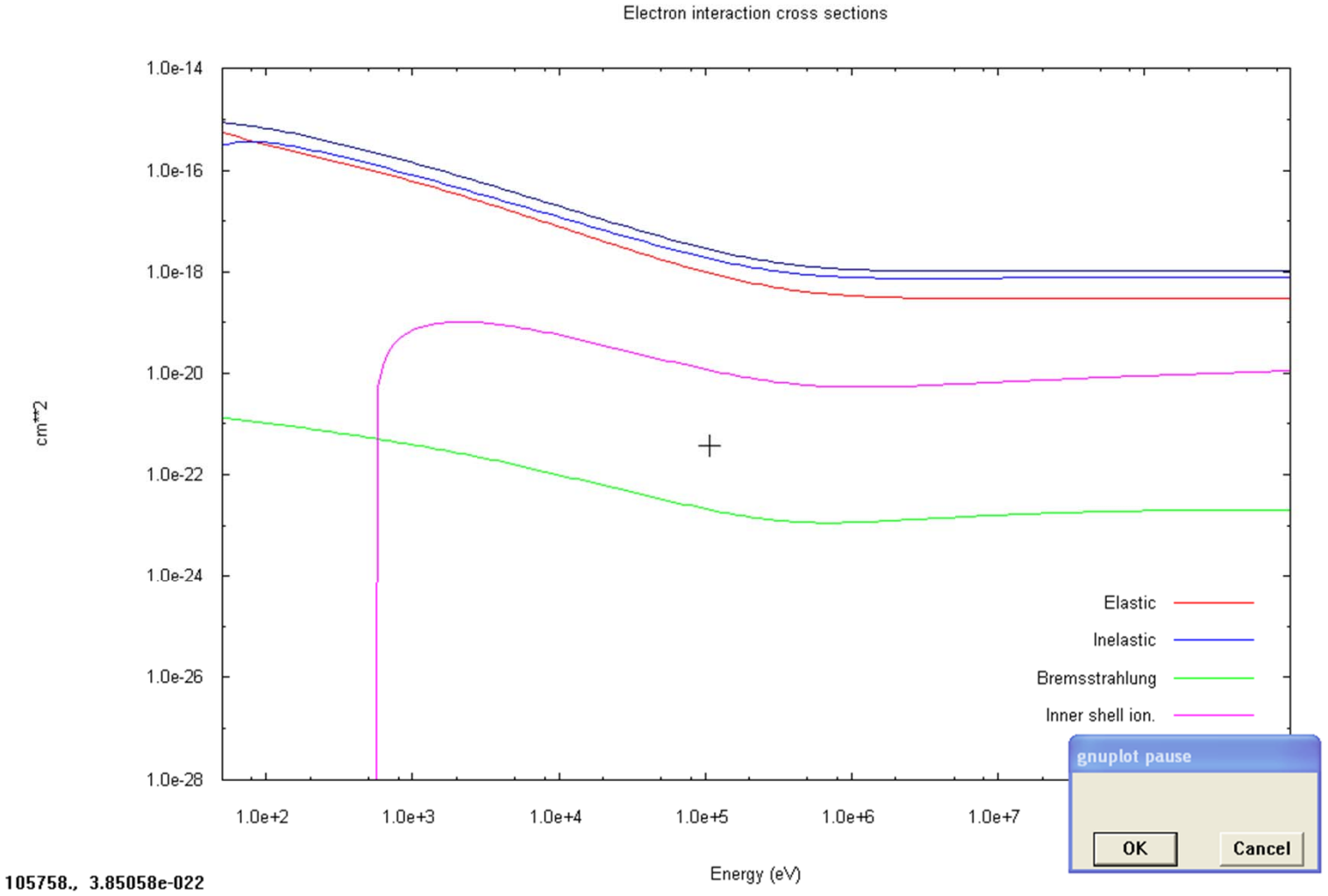
Run **`tables.exe`** for the material file **`water.mat`**

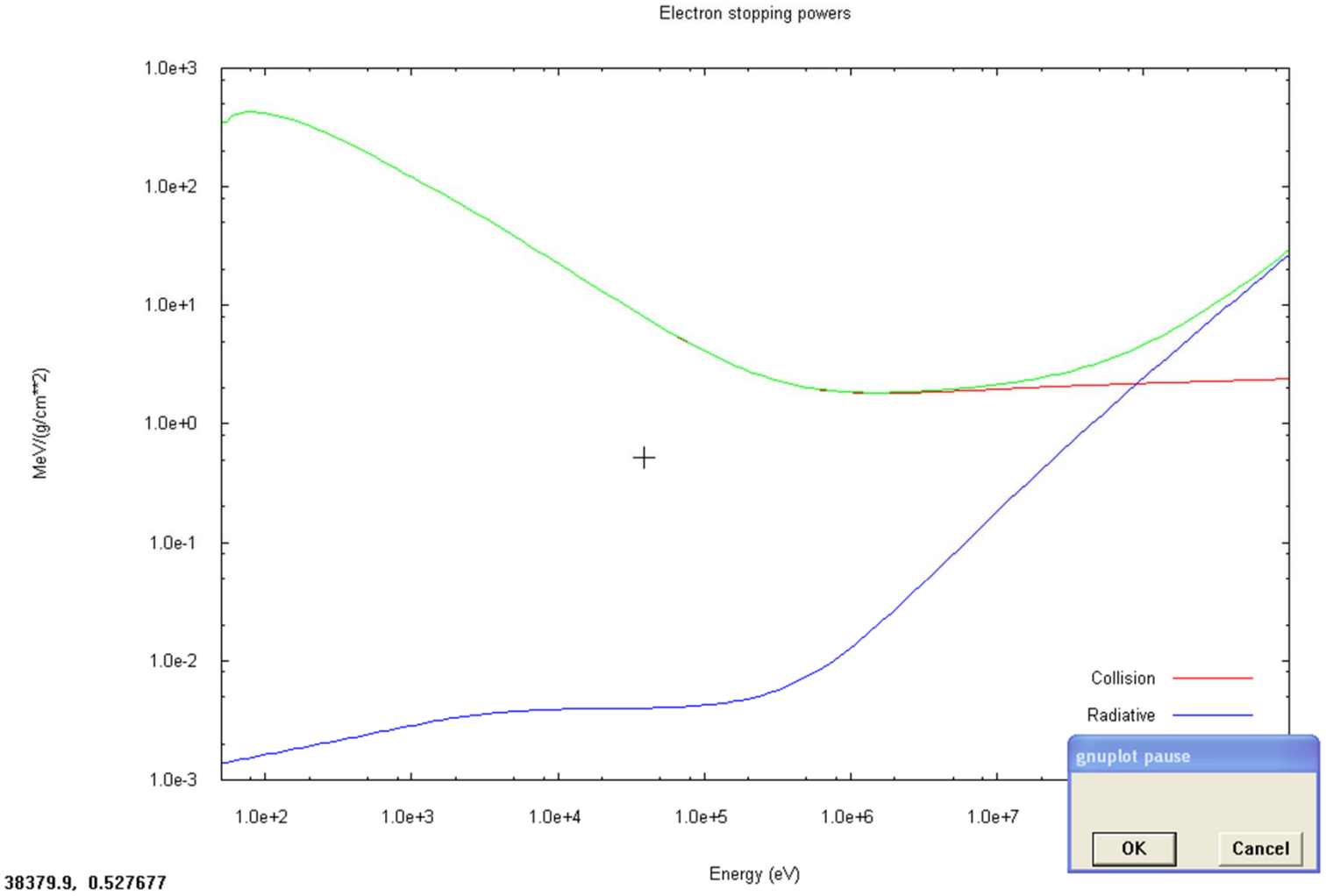
Browse the output file **`tables.dat`** and see what it contains.

Run gnuplot:

```
$ gnuplot tables.gnu
```


Photon mass attenuation coefficients
mu (cm**2/g)
1.0e+6
1.0e+4
1.0e+2
1.0e+0
1.0e-2
1.0e-4
1.0e-6
1.0e-8
1.0e+2
1.0e+3
1.0e+4
1.0e+5
1.0e+6
1.0e+7
Energy (eV)
Rayleigh
Compton
Photoabsorption
Pair production
Total
29946.9, 0.00207751
gnuplot pause
OK
Cancel


Electron interaction cross sections
1.0e-14
1.0e-16
1.0e-18
1.0e-20
1.0e-22
1.0e-24
1.0e-26
1.0e-28
cm**2
1.0e+2
1.0e+3
1.0e+4
1.0e+5
1.0e+6
1.0e+7
Energy (eV)
Elastic
Inelastic
Bremsstrahlung
Inner shell ion.
gnuplot pause
OK
Cancel
105758., 3.85058e-022


Electron stopping powers
1.0e+3
1.0e+2
1.0e+1
1.0e+0
1.0e-1
1.0e-2
1.0e-3
MeV/(g/cm**2)
1.0e+2
1.0e+3
1.0e+4
1.0e+5
1.0e+6
1.0e+7
Energy (eV)
Collision
Radiative
gnuplot pause
OK
Cancel
38379.9, 0.527677

Thank you.