Information to run PENELOPE using Penmain

PENELOPE, an acronym for "PENetration and ENergy LOss of Positrons and Electrons" is developed by the University of Barcelona and was initially dedicated to the transport of electrons and positrons in the matter. Since then, it has been completed by the addition of photon transport, for an energy range from 100 eV to 1 GeV (Salvat, 2015, Salvat and Fernández-Varea, 2009). PENELOPE is programmed in FORTRAN77 and can be started by two predefined main programs: PENCYL or PENMAIN. The main difference between these is that the geometry of PENCYL is only cylindrical while PENMAIN allows a more complete set of three-dimensional surfaces to be used. The simulation details and the geometry are described in separate files: the materials files, the one with the extension ".geo" contains the geometrical model and the input file, with the extension ".in", includes the information about the source, materials and geometry characteristics, the requested output files and the simulation conditions.

Practical use:

One should have first compiled the "material" and "penmain" files to get executable versions, which depend on the computer operating and exploitation system.

There are 3 preliminary steps to prepare the simulation:

- First, it is necessary to prepare the "material" files (with extension ".mat"), according to the materials used in the geometry definition. These are prepared with the "material.exe" program, and the files structure depends on the version you are using.
- Second, the geometry file (with extension ".geo") must be prepared, according to the specific rules (some slight differences may exist depending on the PENELOPE version). In the recent release of the code, a graphical user Interface, PenGeomJar, developed under Java facilitates geometry preparation and its two- and three-dimensional viewing. For the exercise, a general scheme of the geometries (Detector-source-Geometry.pptx), together with an excel sheet (Detector-source-input-data) was prepared to summarize the input data. In any cases, it is necessary to check the geometry files using the viewing tool.

- Third, the "input" file includes all the information required for running the simulation:

  Source definition include:
  - Type of particle (SKPAR)
  - Energy (SENERG)
  - Source position (SPOSIT)

  Remark: For a volume source, there are two more information to include:
  - *Size of a "box" (SBOX) that will contain the volume*
  - *Number of the active body (source) in the geometry file (SBODY)*
  - Emission direction and angle (SCONE): here we define 360° emission angle

Material data include the list of all materials. Here, we included all the materials necessary for the exercise, even if these are not used in all geometries. In the geometry files, materials are defined by numbers, thus germanium (Ge.dat) will be identified as "1", aluminum (Al.mat) will be "2", lead (Pb.mat)' will be "6".
For each material with name (MFNAME), the simulation parameters (MSIMPA) are specified. Here, we used 1 keV as absorption energy for both electrons and photons (first two parameters) and kept the default values for the other parameters.

Geometry definition: the name of the dedicated geometry must be given there “AP.GEO” (GEOMFN)

Energy deposition detector: specifies the energy window and number of channels (ENDETC) and the number of the body that is the detector (here “2” represents the active germanium in the geometry file)

Job properties indicated the maximum number of showers (NSIMSH) **or maximum time (**TIME), together with the simulation seeds (RSEED)

Typical input file:

```
TITLE  DETECTOR A WITH POINT SOURCE
    .
    >>>>>>>> Source definition.
SKPAR 2                 [Primary particles: 1=electron, 2=photon, 3=positron]
SENERG 5.0E4            [Initial energy, in eV]
SPOSIT 0 0 0.1          [Source position: X0, Y0, Z0 in cm]
SCONE 0 0 180           [Beam direction: THETA, PHI in deg]
    .
    >>>>>>>> Material data and simulation parameters.
MFNAME Ge.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Al.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Water.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Polyeth.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Air.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Pb.mat
MSIMPA 1.0e3 1.0e3 1.0e4 0.1 0.1 1e4 1e3    [EABS(1:3),C1,C2,WCC,WCR]
    .
    >>>>>>>> Geometry definition file.
GEOMFN AP.geo           [Geometry file name, 18 characters]
    .
    >>>>>>>> Energy deposition detectors (up to 25).
ENDETC 1e3 5.1E4 1000   [Energy window and number of channels]
EDBODY 2                [Active body; one line for each body]
    .
    >>>>>>>> Job properties.
NSIMSH 10000000         [Desired number of showers, max=2**31-1]
TIME 50000              [Allotted simulation time, in sec]
RSEED 54321 12345       [Random number generator seeds]
```

When this material is ready, to run the simulation, one should open a “Command” window and type “penmain<input.in” (“input” being AP, BP, AS, etc.).

Once the simulation is complete, PENELOPE provides several output files, the results being summarized in “penmain-res.dat”.
The file of interest for determining the detection efficiencies is “spc-enddet-01.dat” which corresponds to the normalized energy spectrum and includes 3 columns:

1st column: deposited energy (eV).
2nd column: probability density (1/(eV*particle)).
3rd column: statistical uncertainty (3 sigma).

The full-energy peak efficiency is obtained as the value of # 2nd column at the energy of incident photons (as determined by SENERG in the input file) multiplied by the number of simulated primary particles (this is quoted in the “penmain-res.dat” file).
The total efficiency is obtained as the sum of the values of # 2nd column multiplied by the number of simulated primary particles . This is also calculated in the “penmain-res.dat” file, as the “spectral areas (energy deposition detectors”.

Results of the simulations:

This table displays the mean value and standard deviation of the PENELOPE participants results for the eight study cases:

	AP		BP		AW		BW		AF		BF		AS		BS	
E (keV)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)	Mean value	Standard deviation (%)
Full-energy peak efficiency																
50	0.0244	0.87	0.3171	0.18	0.0056	0.85	0.0629	0.35	0.0127	0.40	0.1778	0.11	0.0110	0.72	0.1113	0.41
100	0.1979	0.13	0.3262	0.13	0.0406	0.30	0.0673	0.30	0.1009	0.24	0.1786	0.16	0.0810	0.19	0.1293	0.19
200	0.1887	0.36	0.2315	0.22	0.0407	0.37	0.0506	0.53	0.0991	0.05	0.1261	0.09	0.0763	0.34	0.0939	0.13
500	0.0849	0.72	0.1008	0.19	0.0208	0.56	0.0247	0.38	0.0469	0.33	0.0567	0.44	0.0367	0.21	0.0437	0.38
1000	0.0478	0.28	0.0563	0.14	0.0126	0.44	0.0149	0.65	0.0271	0.44	0.0323	0.30	0.0215	0.76	0.0254	0.44
Total efficiency																
50	0.0270	0.86	0.3451	0.21	0.0077	0.63	0.1015	0.37	0.0143	0.40	0.1999	0.06	0.0137	0.53	0.1509	0.17
100	0.2302	0.10	0.3665	0.19	0.0657	0.35	0.1164	0.32	0.1229	0.13	0.2107	0.26	0.1178	0.11	0.1941	0.17
200	0.2709	0.59	0.3138	0.46	0.0826	0.47	0.1015	0.70	0.1509	0.29	0.1813	0.48	0.1406	0.43	0.1684	0.44
500	0.2270	0.53	0.2502	0.28	0.0730	0.51	0.0822	0.30	0.1321	0.59	0.1484	0.50	0.1203	0.42	0.1343	0.36
1000	0.1939	0.28	0.2128	0.27	0.0633	0.19	0.0706	0.25	0.1151	0.12	0.1288	0.17	0.1031	0.14	0.1142	0.12

References:

Salvat, F., 2015. PENELOPE-2014: A code System for Monte Carlo Simulation of Electron and Photon Transport, OECD/NEA Data Bank, NEA/NSC/DOC(2015)3. Issy-les-Moulineaux, France. Available from: http://www.nea.fr/lists/penelope.html
Salvat, F., Fernández-Varea, J. M., 2009.Overview of physical interaction models for photon and electron transport used in Monte Carlo codes. Metrologia 46, S112–S138.