Simulation of radiation transport with the Monte-Carlo simulation code system PENELOPE

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Preliminaries

Radiation transport is a broad area of materials science which concerns itself with the transport of electrons, photons, protons, positrons, and other kinds of particles in material media. These phenomena are interesting both from a fundamental and from an applied point of view. On the one hand, examining the energy and angular spectrum of emitted particles allows one to examine fundamental aspects of radiation-matter interaction and to explicitly test the validity of the employed interaction cross sections and transport theories. On the other hand, having a solid knowledge of radiation transport in matter allows one to address a series of technological problems, in areas as diverse as detectors technology, medical imaging, radiotherapy,

sterilization of medical equipment and food, biotechnology, and radiation shielding, to name a few [1].

In this computer-lab exercise we aim at presenting a general overview of basic aspects of the simulation of radiation transport with the Monte-Carlo simulation code system PENELOPE [2, 3, 4]. In order to obtain the code and the required tools and documentation to carry out the exercises below, make an appointment due diligence via e-mail with me. Gnuplot is recommended to visualize the simulation output data.

1 Introduction

Electrons, photons, positrons, and other kinds of particles passing through matter lose energy and are deflected in the course of subsequent individual collisions. Each interaction mechanism is governed by a differential cross section, which prescribes the probability of being deflected by a given angle and of losing a certain energy in a collision of the considered type. A detailed quantitative knowledge of these interaction cross sections allows one to simulate the transport of radiation through matter. On the basis of a solid and quantitative knowledge of the relevant interaction cross sections, Monte-Carlo sampling techniques can be used to simulate an ensemble of particle trajectories, and thus to effectively solve the transport problem. The code system PENELOPE adopts this strategy to simulate the passage of electrons, positrons, and photons through complex material geometries.

The user's manual for PENELOPE can be readily downloaded from `http://www.oecd-nea.org/dbprog/courses/nsc-doc2011-5.pdf` and contains not only an explanation of the mode of operation, but also a fairly detailed account of the physics involved in the employed interaction cross sections. The manual is not intended to be read from beginning to end, as this is way beyond the scope of the present computer-lab exercise. The following sections are needed to address the present exercises:

- Section 1.1 reviews basic elements of probability theory.
- Section 1.2 is an optional read for technical aspects of random-sampling techniques, used in the code to sample energy losses and deflections of the probing particles at each collision for the considered interaction mechanisms.
- Section 1.4 describes the Monte-Carlo simulation of particle trajectories.
- Section 1.5 discusses the calculation of results affected by statistical uncertainties.
- Sections 2 and 3 discuss in detail the different interaction mechanisms of photons, electrons, and positrons with matter. For the present exercise it suffices to have a general overview of the interaction mechanisms included in the simulation and to have a general idea of the behavior of the interaction cross sections.
- Section 6 should be read, as it discusses how to define the material geometry in the simulation.

- Finally, Section 7.1 describes the program flow and how the input and output works. Section 7.1.1 can be skipped, as material files will be provided.

After this preliminary reading, the following exercises should be doable. For the third exercise, an additional set of slides will be provided, to better put the exercise in context.

2 Energy losses of non-relativistic electrons in homogeneous and isotropic media

Although it is not envisaged in this introductory lab exercise to go in depth into the derivation of the cross sections for all considered interaction mechanisms, we do take some time here to elucidate how the distribution of energy losses of non-relativistic electrons (energies below the 10-keV range) in homogeneous and isotropic media can be derived, as this can be readily done on the basis of a semiclassical theory and provides a simple interaction picture. The model employed in the simulation reduces to the presented scheme for non-relativistic projectiles.

We will describe the stopping of a swift charged projectile in a medium within the so-called semiclassical dielectric theory, whose main tenet is readily stated as follows. The presence of the charged projectile in the medium polarizes the material. An induced electric field is therefore generated, which is assumed to act on the charged projectile as a stopping force. It is then a matter of deriving a distribution of energy losses per unit path length which can be used by the Monte Carlo simulation, as described in section 1.4 of the Penelope user's guide. We use cgs units below.

We assume here an infinite medium with a dielectric function $\epsilon(\mathbf{q},\omega)$, where $\mathbf{q}$ and ω are the Fourier-conjugate variables of the position $\mathbf{r}$ and time t. The charge distribution of the external projectile with charge Z_0 moving along a straight line with velocity $\mathbf{v}$ reads

$$\rho(\mathbf{r},t) = Z_0 e\delta(\mathbf{r}-\mathbf{v}t). \tag{1}$$

The Poisson equation yields the electric displacement $\boldsymbol{\mathcal{D}}(\mathbf{r},t)$ as a function of $\rho(\mathbf{r},t)$,

$$\nabla\cdot\boldsymbol{\mathcal{D}}(\mathbf{r},t) = 4\pi\rho(\mathbf{r},t). \tag{2}$$

Taking the Fourier transform of this expression we obtain

$$\mathrm{i}\mathbf{q}\cdot\boldsymbol{\mathcal{D}}(\mathbf{q},\omega) = 4\pi\rho(\mathbf{q},\omega). \tag{3}$$

At this instance, two approximations are made:

1. We assume that the response of the medium to the passage of the projectile is directly proportional to the electric field $\boldsymbol{\mathcal{E}}(\mathbf{r},t)$. This linearity can be expressed in a more general fashion in Fourier space:
$$\boldsymbol{\mathcal{D}}(\mathbf{q},\omega) = \epsilon(\mathbf{q},\omega)\boldsymbol{\mathcal{E}}(\mathbf{q},\omega). \tag{4}$$
This approximation has been shown in practice to work for projectile kinetic energies above the 100-eV domain.

2. The electric field has a contribution from the scalar potential $V(\mathbf{r},t)$ and from the vector potential $\mathbf{A}(\mathbf{r},t)$:

$$\boldsymbol{\mathcal{E}}(\mathbf{r},t) = -\nabla V(\mathbf{r},t) - \frac{1}{c}\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}. \tag{5}$$

Here we will disregard the second term. A posteriori it can be shown that this amounts to restricting the domain of validity of the calculation to non-relativistic projectiles (velocities $v \ll c$). We therefore take

$$\boldsymbol{\mathcal{E}}(\mathbf{r},t) = -\nabla V(\mathbf{r},t), \tag{6}$$

which in Fourier space takes the form

$$\boldsymbol{\mathcal{E}}(\mathbf{q},\omega) = -\mathrm{i}\mathbf{q}V(\mathbf{q},\omega). \tag{7}$$

Combining Eqs. (3), (4), and (7) we can obtain an expression for the total electric field in terms of the external charge density:

$$\boldsymbol{\mathcal{E}}(\mathbf{q},\omega) = -\mathrm{i}4\pi\frac{\mathbf{q}}{q^2}\frac{1}{\epsilon(\mathbf{q},\omega)}\rho(\mathbf{q},\omega). \tag{8}$$

In order to obtain the *induced* electric field we need only to subtract the field that the projectile would create in vacuum [$\epsilon(\mathbf{q},\omega) = 1$]:

$$\boldsymbol{\mathcal{E}}_{\mathrm{ind}}(\mathbf{q},\omega) = -\mathrm{i}4\pi\frac{\mathbf{q}}{q^2}\rho(\mathbf{q},\omega)\left[\frac{1}{\epsilon(\mathbf{q},\omega)} - 1\right]. \tag{9}$$

We can then derive the rate of energy loss per unit path $s = vt$. This quantity is known as the stopping power (even though its dimensions are actually those of force) and can be readily derived as

$$\begin{aligned} S &= -\frac{\mathrm{d}E}{\mathrm{d}s} \\ &= -\frac{1}{v}\frac{\mathrm{d}E}{\mathrm{d}t} \\ &= -\frac{1}{v}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}m\mathbf{v}\cdot\mathbf{v}\right) \\ &= -\frac{1}{v}\mathbf{v}\cdot\left(m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}\right) \\ &= -\left.\frac{Z_0}{v}\mathbf{v}\cdot\boldsymbol{\mathcal{E}}_{\mathrm{ind}}(\mathbf{r},t)\right|_{\mathbf{r}=\mathbf{v}t}. \end{aligned}$$

It is now a matter of carrying out the inverse Fourier transform of $\boldsymbol{\mathcal{E}}_{\mathrm{ind}}(\mathbf{q},\omega)$, whereby we use symmetrical normalization factors of $1/\sqrt{2\pi}$, to obtain

$$S = \frac{2(Z_0 e)^2}{\pi}\frac{1}{v^2}\int_0^\infty \mathrm{d}q\frac{1}{q}\int_0^{qv}\mathrm{d}\omega\ \omega\mathrm{Im}\left[-\frac{1}{\epsilon(q,\omega)}\right], \tag{10}$$

where we have assumed a homogeneous and isotropic medium, so that $\epsilon(\mathbf{q},\omega)$ depends on $\mathbf{q}$ only through its modulus.

Up to this point, the stopping of the charged projectile is continuous, whereas in reality, energy losses occur in the course of discrete inelastic interactions. We therefore have to reconcile the present classical description of the process with its actual quantum nature. This is done by what in this context is known as the semiclassical approximation, which consists in assigning a physical meaning to the Fourier variables $\mathbf{q}$ and ω. The quantities $\hbar\mathbf{q}$ and $\hbar\omega$ are respectively understood as a momentum transfer from the projectile to the material and as an energy loss of the projectile. The corresponding integrals should now be restricted to the kinematically allowed domain, *i. e.*, $\omega \in [0, E]$ and $q \in [q_-, q_+]$, where

$$q_\mp = \sqrt{2E} \pm \sqrt{2(E-\omega)} \tag{11}$$

follows from energy and momentum conservation rules. The stopping power now reads

$$S = \frac{2(Z_0 e)^2}{\pi} \frac{1}{\hbar^2 v^2} \int_0^E \mathrm{d}\omega\, \omega \int_{q_-}^{q_+} \mathrm{d}q\, \frac{1}{q} \mathrm{Im}\left[-\frac{1}{\epsilon(q,\omega)}\right]. \tag{12}$$

Recalling the definition of the stopping power (average energy loss per unit path length), this expression can be understood as the first moment of a distribution of energy losses per unit path length, $\mathrm{d}\mu/\mathrm{d}\omega$:

$$S = \int_0^E \mathrm{d}\omega\, \omega \frac{\mathrm{d}\mu}{\mathrm{d}\omega}. \tag{13}$$

Thus, we can identify the so-called differential inelastic inverse mean free path (DIIMFP),

$$\frac{\mathrm{d}\mu}{\mathrm{d}\omega} = \frac{2(Z_0 e)^2}{\pi} \frac{1}{\hbar^2 v^2} \int_{q_-}^{q_+} \mathrm{d}q\, \frac{1}{q} \mathrm{Im}\left[-\frac{1}{\epsilon(q,\omega)}\right], \tag{14}$$

a quantity which indeed yields the distribution of energy losses $\hbar\omega$ per unit path length. Its inverse integral is the inelastic inverse mean free path,

$$\lambda_i = \left\{ \frac{2(Z_0 e)^2}{\pi} \frac{1}{\hbar^2 v^2} \int_0^E \mathrm{d}\omega \int_{q_-}^{q_+} \mathrm{d}q\, \frac{1}{q} \mathrm{Im}\left[-\frac{1}{\epsilon(q,\omega)}\right] \right\}^{-1}, \tag{15}$$

the average distance between consecutive inelastic interactions.

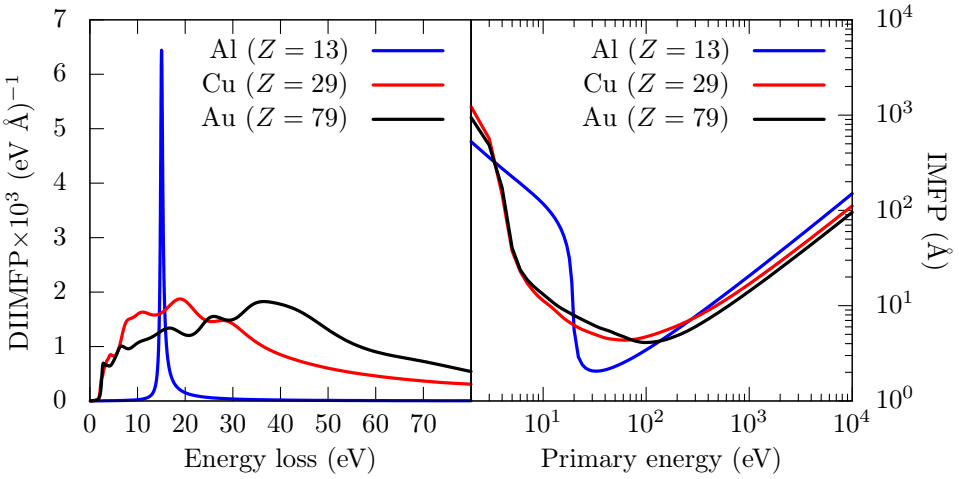

Figure 1: Differential inelastic inverse mean free path for 500-eV electrons (left) and inverse mean free path as a function of electron energy (right) for electrons in Al, Cu, and Au.

In order to have a certain feel for these quantities, Fig. 1 displays in its left panel the DIIMFP for 500-eV electrons in Al, Cu, and Au. In the case of Al (a nearly-free-electron material), the DIIMFP is dominated by an energy loss at 15 eV, corresponding to the excitation energy of a bulk plasmon (collective response of the electron gas). For Cu and Au, materials with a more intricate electronic structure, the DIIMFP exhibits a broader energy-loss spectrum. The right-hand panel of Fig. 1 displays the inelastic inverse mean free path of electrons as a function of their energy in Al, Cu, Au.

The DIIMFP and the IMFP are the quantities needed to include energy losses in a simulation of electron transport through matter. In the case of relativistic projectiles, further corrections appear to the expressions derived above.

For each interaction mechanism of the considered projectile with matter, a differential cross section and a mean free path is derived (usually involving quantum mechanics), which can are constructively added to the Monte-Carlo simulation scheme to provide further detailed modelling of radiation transport.

3 Exercises

You are requested to turn in a report where your solution to each exercise is briefly sketched.

3.1 Exercise 0 - Warm-up

Follow the Penelope tutorial to get acquainted with the different main programs (pencyl, penmain, geometry viewers, etc.) Skip the compilation steps. You are most welcome to examine the examples (x-ray tube, particle detectors, electron accelerator, etc.) You do not have to report on this exercise.

3.2 Exercise 1 - Interactions of photons in matter

Using the visualization software `shower`, simulate 25 photon trajectories of 10 MeV in a slab of 10 cm of lead. Identify, if found, an example of the following events:

- an electron-positron pair-production event,
- a Compton scattering event.

Hint: take a screenshot of the simulation window and identify each of the events with an ellipse (color code up to you), added with a image-editing software of your choice.

3.3 Exercise 2 - Radiation shielding

Estimate the width of a slab in order to absorb photons of 1.5 MeV. Compare the situation for the following materials: lead, concrete, aluminium.

3.4 Exercise 3 - Spectrum of electrons backscattered from an Al sample

In this exercise you are asked to calculate the spectrum of 10-keV electrons backscattered from a polycrystalline Al sample, which can be considered as a semi-infinite medium (region below a plane).

- Generate a Penelope geometry file consisting of a plane at $z = 0$.
- Generate a Penelope input file. Let $z < 0$ be Al (material file provided) and let $z > 0$ be vacuum.
- Define an impact detector consisting of the region $z > 0$.
- Consider only the first 500 eV of energy loss (no need to follow trajectory to energies below 4.5 keV).

Plot the spectrum of electrons backscattered from the sample and provide an explanation of the different peaks that appear. Hint: consider the DIIMFP for Al shown in the additional slides.

3.5 Exercise 4 - Energy deposition in the human body for radiotherapy applications

Consider a beam of photons impinging in the human body (Penelope-geometry definition file `male0` available). Compare the energy deposited in the thyroid gland by photons of 1 keV, 10 keV, 100 keV, and 1 MeV.

References

[1] "Uses of radiation (US Nuclear Regulatory Commission)." `http://www.nrc.gov/about-nrc/radiation/around-us/uses-radiation.html`.

[2] F. Salvat, J. M. Fernández-Varea, and J. Sempau, PENELOPE-*2011: A code System for Monte Carlo Simulation of Electron and Photon Transport.* Issy-les-Moulineaux, France: OECD/NEA Data Bank, 2011. Available in PDF format from http://www.nea.fr/lists/penelope.html.

[3] J. Baro, J. Sempau, J. Fernández-Varea, and F. Salvat, "Penelope: An algorithm for monte carlo simulation of the penetration and energy loss of electrons and positrons in matter," *Nucl. Instrum. Meth. B*, vol. 100, pp. 31–46, 1995.

[4] J. Sempau, J. M. Fernández-Varea, E. Acosta, and F. Salvat, "Experimental benchmarks of the Monte Carlo code PENELOPE," *Nucl. Instrum. Meth. B*, vol. 207, pp. 107–123, 2003.