Project 2: Photon-matter interaction — Monte Carlo simulation of X-ray imaging

Henning Goa Hugdal
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I. INTRODUCTION

X-rays are electromagnetic waves with energies approximately 0.1 keV to 100 keV. One of the uses of X-rays is in medical imaging, where differences in attenuation between materials can be used to produce for instance simple radiographs of bones and lungs, or more complex scans of the brain using computed tomography (CT). However, there are health risks associated with ionizing radiation such as X-rays, and one therefore seeks to minimize the energy deposited in the matter.

In this project we will simulate one-dimensional (1D) photon propagation and attenuation in matter using Monte Carlo methods. The simulations will then be used to study X-ray imaging, and the necessary conditions to get good contrast while considering the absorbed dose. Finally, we will image unknown objects, given by 3D arrays of attenuation coefficients.

II. PHOTON ATTENUATION IN MATTER

For medical imaging the X-ray energies typically lie in the energy range 10 keV to 100 keV. For photons in this energy range the most important interaction processes with matter are the photoelectric effect and Compton scattering, sketched in fig. 1. In the photoelectric effect a photon with energy E is absorbed by an atom, releasing an electron in the process. The scattering probability is proportional to the atomic number Z, and inversely proportional to the photon energy [1], leading to stronger scattering for heavier atoms and photons with low energy. Compton scattering is the interaction between a photon and an outer or free electron, leading to a change in the photon energy and direction.

When a photon beam is incident on a material, the beam intensity will be attenuated by the two above processes. For a single photon at location x, we assume that there is a probability p for it being absorbed or scattered when moving a small distance Δx to $x+\Delta x$. For a photon beam with intensity $I(x) = NE$ at x, where N and E is the photon count and energy respectively, the expected intensity at $x + \Delta x$ is therefore

$$I(x + \Delta x) = I(x)(1 - p) + p \cdot 0, \tag{1}$$

where we have assumed that absorbed or scattered photons do not contribute to the intensity at $x+\Delta x$. We also assume that the probability of absorption or scattering increases with increasing distance, to lowest order writing

$$p = \mu \Delta x, \tag{2}$$

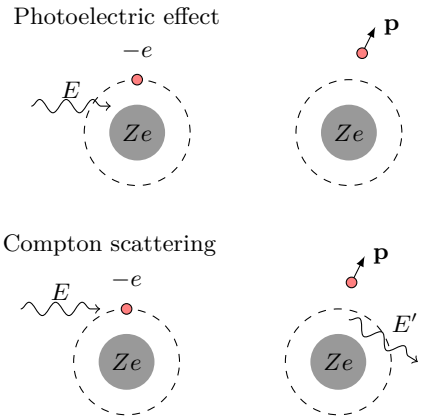

FIG. 1. Sketch of the photoelectric effect and Compton scattering.

where μ is called the attenuation coefficient. Inserting eq. (2) into eq. (1) and rearranging the terms, we get

$$\frac{I(x + \Delta x) - I(x)}{\Delta x} = -\mu I(x),$$

which for infinitesimal steps, $\Delta x \to 0$, results in

$$\frac{dI(x)}{dx} = -\mu I(x). \tag{3}$$

Solving this equation, we get

$$I(x) = I_0 e^{-\mu x}, \tag{4}$$

where we see from fig. 2 that higher μ, corresponding to higher absorption or scattering probability, leads to faster attenuation of the intensity.

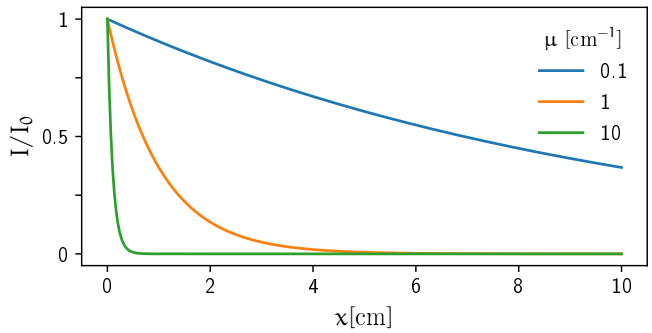

FIG. 2. Plot of intensity $I(x)$ for different values of the attenuation coefficient μ.

The attenuation coefficient varies with energy, for instance as shown in fig. 3 for air, soft tissue and bone [2].

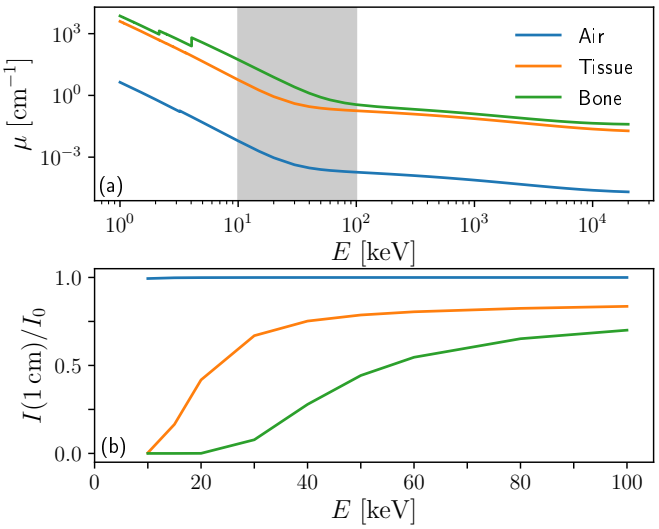

FIG. 3. (a) Plot of attenuation coefficient μ as a function of photon energy E for air, soft tissue and bone. The shaded area shows the energy interval used for medical imaging. (b) Intensity when passing through 1 cm of matter as a function of energy for different materials.

III. X-RAY RADIOGRAPHY

When using X-rays for medical imaging, there are certain conditions that have to be met to get a good image [3]. First, the intensity of the photon beam has to be sufficient when reaching the detector to get a good signal. Second, the difference in attenuation between tissue types should be large enough to give good contrast. In addition to this, one wants to minimize the absorbed dose to minimize health risks.

We will not consider the signal strength here. However, in order to detect for instance a small object placed inside a larger object, see fig. 4, we have to have a sufficient difference between the signals going through the different materials, that is, we want any differences in attenuation to be as visible as possible. We define the relative contrast as

$$C = \frac{I_1 - I_2}{I_1}, \tag{5}$$

where we assume $I_2 \leq I_1$ such that $0 \leq C \leq 1$. The highest contrast, and thus the best visibility, is obtained when $I_2 = 0$ and $I_1 \neq 0$, corresponding to a full attenuation only for the beam going through the smaller object.

The health risk associated with X-ray radiation increases with the energy absorbed, and thus on both how many photons are absorbed and the energy of the photons. It also depends on how much matter this energy is distributed over, i.e. the mass [4]. These considerations are quantified by the dose, for which we will use the simple definition

$$D = \frac{\text{absorbed energy}}{\text{mass}} = \frac{N_{\text{att}} E}{V\rho} \tag{6}$$

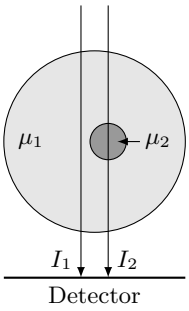

FIG. 4. Sketch of a small object placed inside a larger object, with attenuation coefficients μ_2 and μ_1 respectively, with $\mu_1 < \mu_2$. The two beams have intensities I_1 and I_2 when hitting the detector.

where N_{att} is the number of attenuated electrons, ρ is the density of the material, and $V = AL$ is a volume element with cross-section A and length L.

IV. MONTE CARLO METHODS

Monte Carlo methods are numerical methods which rely on random samples [5], and can for instance be used to perform integrals numerically (see e.g. Ref. [6]) or simulate stochastic processes. To illustrate the principle, we will calculate that area of a unit circle using random samples. We generate N random coordinates (x, y) with $-1 \leq x, y \leq 1$, and check if the points fall inside the circle by determining if $r = \sqrt{x^2 + y^2} \leq 1$. We call the total number of points inside the circle n. For large enough N we expect the relation

$$\frac{A_{\text{circle}}}{A_{\text{square}}} = \frac{n}{N}, \tag{7}$$

to hold. The area of the unit circle can therefore be calculated from $A_{\text{circle}} = A_{\text{square}} n/N$. This is illustrated in fig. 5, showing that the value of the calculated area stabilizes around the exact value π for increasing N.

One can also use Monte Carlo to simulate other processes, e.g. backscattering of a particle in 1D. If the scattering probability is p for each time step, this process can be simulated by generating a random number z for each step. If $z \leq p$ the particle's direction is reversed, otherwise it continues in the same direction. A similar approach will be used when simulating photon propagation in matter.

V. PROBLEMS

The following problems should be addressed in the report, including comments on your code. It might be useful to read all the problems before you start, as this can help you build up the code in such a way that it is easily expanded for each new task.

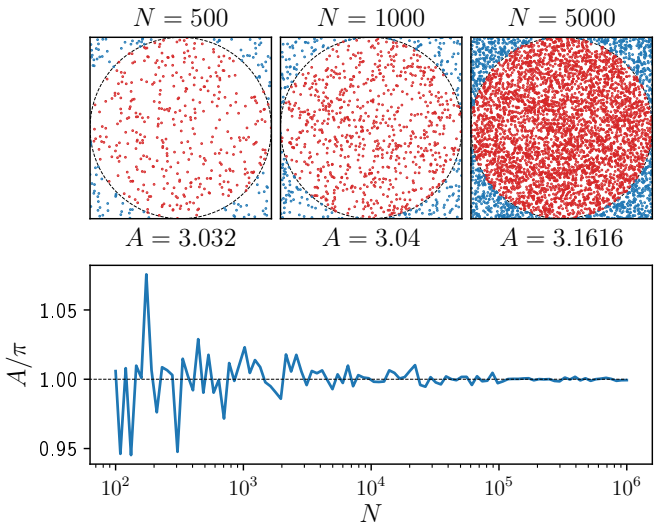

FIG. 5. Upper panel: calculated circle areas based on N random coordinates for $N = 500$, 1000, and 5000. Lower panel: calculated circle area normalized to analytical value for increasing number of random coordinates.

Overall requirements:

- The report should be written in Norwegian or English, and handed in as a Python Notebook (either `.ipynb`, `.pdf` or `.html` format). Be sure to check that the file looks as intended and displays your work properly before handing it in. A Python Notebook that can be used as a starting point can be found on Blackboard.
- You should complete all the below tasks and answer all the questions.
- Try to make the code clean and well commented. The answers, however, should be fully understandable without reading the code.
- It should not be necessary to re-run any of the code when grading the project.
- Include figures when asked for/necessary and at the appropriate place, with appropriate labels and comments.

You do not need to repeat theory from this text in the report, and can assume that the reader has the knowledge contained in this project text. If you use additional sources, these must be cited in the report.

Problem 1: We will now use Monte Carlo methods to simulate the attenuation of photons. The specific tasks are:

- Simulate the one-dimensional (1D) propagation of a photon in a material by dividing the trajectory into discrete steps of step size Δx. At each step, use a random number to determine if the photon is absorbed or scattered based on the attenuation coefficient μ. For concreteness you can use material thickness $t = 10\,\text{cm}$ and $\mu = 0.1\,\text{cm}^{-1}$.
- If you repeat the calculation a few times, does the photon always reach the end of the material? Approximately how often do you expect the photon to reach the end of the material based on the intensity curves in fig. 2?
- What considerations do you have to make when choosing the step size (Hint: What happens if $\mu = 100$)?
- Expand the code to simulate the propagation of N photons inside the material. For each discrete step record the number of photons still present in the material. Plot the results for different N together with the analytical curve in eq. (4). Is the result as expected? How do the results depend on N and the step size Δx? If the simulations deviate significantly from the analytical curve even for high N, make changes to the code to get better agreement. More or less perfect agreement is possible [8].

Problem 2: Simulating the attenuation of photons allows us to study X-ray imaging of objects. We will here study the necessary conditions to get good contrast and limiting the absorbed dose by considering two paths through a system such as the one sketched in fig. 4, where one object is embedded in another. Throughout this problem we will assume that the larger object is soft tissue, while the smaller object is bone. The attenuation coefficients are given in the two files `tissue.txt` and `bone.txt` [2]. The first column gives the energy in MeV. The second column contains the mass-attenuation coefficient μ/ρ in cm^2/g, and therefore has to be multiplied with the density ρ in order to get the attenuation coefficient. Use $\rho_{\text{tissue}} = 1.02\,\text{g/cm}^3$ and $\rho_{\text{bone}} = 1.92\,\text{g/cm}^3$ [2].

For concreteness, we will consider only the two beams shown in the figure, and set the thickness of the tissue to be 3 cm, and the thickness of the bone to be 1 cm, with 1 cm of tissue at each side. Hence, both beams go through 3 cm of matter.

- Write the necessary code to read the files `tissue.txt` and `bone.txt` in such a way that you can easily access the the energy-attenuation coefficient pairs. Plot the resulting attenuation coefficients as a function of energy.
- Make adjustments to the code from Problem 1 such that it handles spatial variations in the attenuation coefficient μ.
- Calculate the output intensity $I = NE$ at the detector for the two beams in fig. 4 for energies in the range 10 keV to 100 keV, and plot the resulting intensities as a function of energy.

TABLE I. Data for the two objects to be imaged in Problem 3.

Object no.	Energies (keV)	$N_x \times N_y \times N_z$	Dimensions (cm)
Object 1 [7]	20, 50 and 100	$13 \times 128 \times 128$	$6.5 \times 44.6 \times 44.6$
Object 2	25, 50 and 75	$60 \times 60 \times 50$	$12 \times 12 \times 10$

- Calculate and plot the contrast [eq. (5)] as a function of energy in the range 10 keV to 100 keV. What energies give the best contrast?
- Assume that the detector requires an intensity of 10 MeV from the I_1 beam in order to detect a signal. Determine how many photons are required to be emitted from the source (N_0) in order to achieve this intensity for each energy E in the range 10 keV to 100 keV. Plot the resulting intensities for the two beams, and the number of photons N_0 required as a function of energy. (Note that for some energies this threshold might never be reached, so beware of infinite loops.)
- Using the required number of photons for each energy, calculate the total dose [eq. (6)] absorbed along the two beams ($D_1 + D_2$), and plot it as a function of energy. Approximately what energy range should be used to obtain both good contrast and a low dose?

Problem 3: The files with names similar to `objectN_E.npy` contain 3D $N_x \times N_y \times N_z$ arrays of attenuation coefficients for different energies, see table I for details. To read these files use the `numpy` function `numpy.load(filename)`, which returns a `numpy` array. Your task is to image the objects described by the 3D arrays for the different energies given. We will assume that the photon beams only travel in a straight line along 1D paths as before.

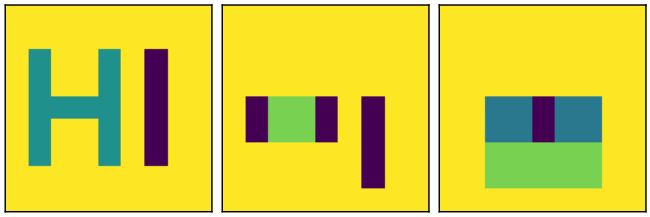

FIG. 6. Approximate view of imaging along the three directions of the cube given in `test_array.npy`.

- Expand your code to allow for propagation along all the $N_i \times N_j$ paths in one direction, and record the intensities for each path. For each object: Make contour plots (using for instance `pyplot.imshow`) of the intensity for the different energies when imaging in the three perpendicular directions.
- Comment on the differences between the plots. What energy would you use to image the objects? Include plots for all three imaging directions and energies for easy comparison. Can you tell what objects the 3D array of attenuation coefficients describe?

To help with the implementation of this task, the file `test_array.npy` contains a $9 \times 9 \times 9$ test array of a cube with sides of length 0.5 cm which can be used to test the code. The result for the three imaging directions should look similar to fig. 6.

[1] P. C. Hemmer. *Kvantemekanikk*. Tapir akademisk forlag, Trondheim, 2005.

[2] J. H. Hubbell and S. M. Seltzer. X-Ray Mass Attenuation Coefficients. NIST Standard Reference Database 126, 2004.

[3] Pål Erik Goa. TFY4320 Physics of Medical Imaging Compendium. 2018.

[4] https://en.wikipedia.org/wiki/Absorbed_dose Accessed Feb. 27, 2021.

[5] https://en.wikipedia.org/wiki/Monte_Carlo_method. Accessed Feb. 22, 2021.

[6] Tor Nordam. Monte Carlo Integration in 1 Dimension. Module on numfys.net.

[7] Ke Yan, Xiaosong Wang, Le Lu, Ronald M. Summers. Journal of Medical Imaging 5, 036501 (2018). doi: 10.1117/1.JMI.5.3.036501

[8] A small comment: In our current Monte Carlo simulation, we reproduce the analytical result in eq. (4), which is a necessary test of the method. However, we will not go much further than what we have already done in simulating the photon beam due to the two-week time frame, meaning we can in principle use the analytical results all along. However, in a more involved modeling of the system, this would not necessarily be the case, and the benefits of Monte Carlo simulation would become more apparent.