NERS 590 – Monte Carlo Software Design
Winter 2017
Homework 2
Due at noon on Mar. 17, 2017

In this homework set, you will extend your 1-D slab Monte Carlo transport code from homework 1 to 3D. Your final code should, as before be in C++, be able to solve all of the provided problems. Problems 1-3 are the same as the previous homework with problems 4-5 being new.

A random number generator will be provided to you that you should use. Do not use the intrinsic C rand() function as it, depending upon the compiler implementation, may have a very short period and not be acceptable for scientific computing.

You should parse XML input in this assignment to receive full credit. Input files should be provided with the description. As before, internally, your code should be structured such that there is an initialization portion that handles problem setup and an execution phase that is coded generically (i.e., no references to problem definitions in this portion) to handle any problems within the scope. Your code should also build via a Makefile and be accessible from a Github repository.

To summarize, the design requirements are:

- 3-D geometry with one-speed transport,
- Multiple regions and constituent isotopes,
- Vacuum and reflecting boundary conditions,
- Isotropic and anisotropic scattering (see problems 1 and 4),
- Fission with a multiplicity distribution (see problem 3),
- Fixed sources with prescribed distributions in space and direction (see problems),
- Estimators for leakage (problems 1 and 2), support for counting the number of neutrons leaked out per history (problem 3), and reaction rate fluxes using track-length estimators (problems 4 and 5)
- Importance splitting for variance reduction (problem 5),
- Compilation with a Makefile,
- Accessible from a Github repository,
- User input to easily run any of the test problems.

You may work on this assignment in a group of up to 3 people, and I am happy to provide reference solutions and work with you to develop your code. Members of your group must still write all lines of code with the exception of the provided random number generator and other source codes I provide in class.

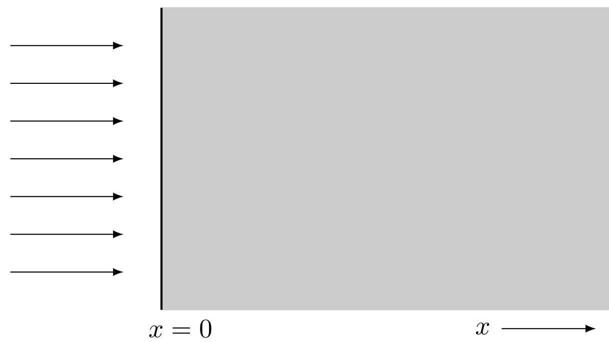
Turn in a document reporting the results of the given test problems and quantify their statistical uncertainties. Run each problems 1-4 for at least 10^7 histories and problem 5 for at least 10^8 histories. Problems 1-3 should be run as 3D, even though they are identical to the previous homework and technically 1D. Your code should be available on Github and include a Makefile.

The grading will be done as follows:

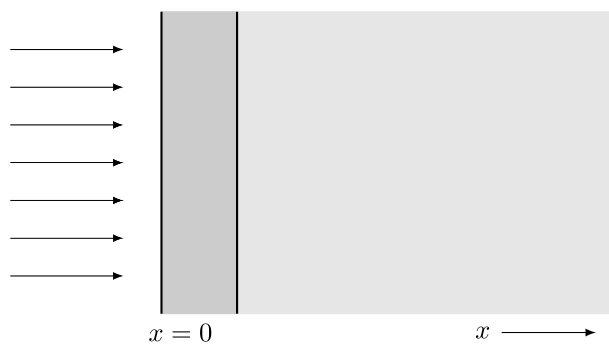
Item	Points
Report	50
Code clarity and style	50
Results: problems 1-3	30
Results: problems 4-5	40
XML input	20
Github checkout and Makefile	10

1. Suppose particles are normally incident upon a 1-D purely absorbing slab, as depicted in the following figures. Calculate the rate particles leak out of the right side of the slab both analytically and using your Monte Carlo code. Compare the result, quantifying the statistical uncertainty, with the analytical solution. Your code should handle the following cases:

   (a) Handle the case of a one-region slab with a constant cross section with two isotopes: $N_1 = 0.25$ $\text{b}^{-1}\cdot\text{cm}^{-1}$, $\sigma_{t1} = 2.0$ b and $N_2 = 0.75$ $\text{b}^{-1}\cdot\text{cm}^{-1}$, $\sigma_{t2} = 0.5$ b. The slab has a width is $0 \leq x \leq 5$ cm.

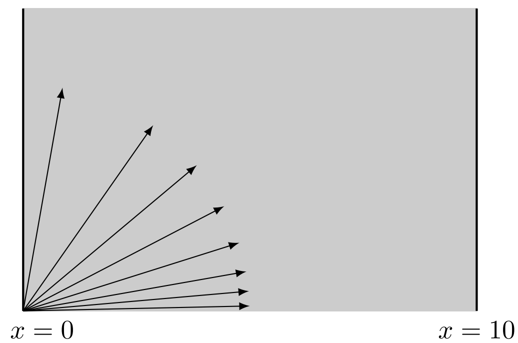


   (b) Handle the case of a two-region slab with constant cross sections in each region. The first region is $0 \leq x \leq 1$ cm with $N_1 = 1.0$ $\text{b}^{-1}\cdot\text{cm}^{-1}$ and $\sigma_{t1} = 2.0$ b and the second region is $1 \leq x < 5$ cm with $N_2 = 1.0$ $\text{b}^{-1}\cdot\text{cm}^{-1}$ and $\sigma_{t2} = 0.5$ b:



2. Handle the case of a finite, 1-D slab having scattering and width $0 < x < 10$ cm. The slab has an isotropic boundary flux at $x = 0$; this may be modeled as a point source at $x = 0$ source with a probability density for the direction cosine of $f(\mu) = 2\mu$ for $0 < \mu \leq 1$.

   The atomic density is 1.0 $\mathrm{b}^{-1}\cdot\mathrm{cm}^{-1}$, the total cross section is $\sigma_t = 1.00$ b and the scattering cross section is $\sigma_s = 0.98$ b. Using your Monte Carlo code, estimate the probability that a particle leaks out of the right side of the slab.



   (a) The scattering is isotropic:

$$p(\mu_0) = \frac{1}{2}.$$

   (b) The scattering follows the Henyey-Greenstein scattering density:

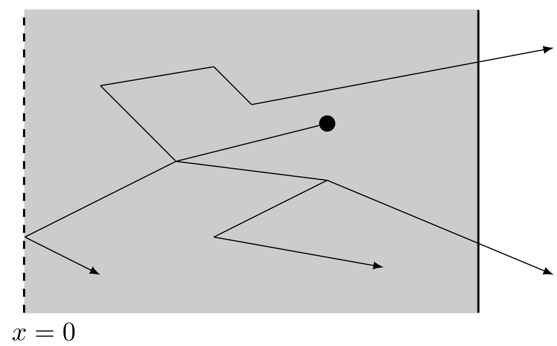
$$p(\mu_0) = \frac{1 - g^2}{2\left(1 + g^2 - 2g\mu_0\right)^{3/2}}.$$

   Give your result for anisotropy parameter $g = 0.25$.

   Discuss the results in your document. (Note that the Henyey-Greenstein distribution is commonly used in optical light transport.)

3. Handle the case of a 1-D, subcritical fissionable slab depicted below. The source is uniform and isotropic throughout the fuel. For the given fission multiplicity models, using your Monte Carlo code, calculate the probability mass function for the number of neutrons that leak out of the system per source neutron. Additionally, have your code report the mean and variance of this distribution.

   Model a bare slab with a reflecting boundary condition at $x = 0$ and a vacuum boundary condition at $x = 4$ cm. The fuel cross sections are $\sigma_c = 0.3$ b, $\sigma_f = 0.2$ b, $\sigma_s = 1.5$ b. The scattering is isotropic. The atom density of the fuel is 0.1 $\text{b}^{-1}\cdot\text{cm}^{-1}$.



   (a) Model the emission probability "on average" using the number of neutrons emitted from fission ν sampled by

   $$\nu = \lfloor \overline{\nu} + \xi \rfloor .$$

   Here $\overline{\nu}$ is the mean number of neutrons emitted per fission, which is 2.8, ξ is a uniform random number, and $\lfloor\cdot\rfloor$ is the floor operator that rounds down to an integer.

   (b) Model the emission probability explicitly. The probability of emitting ν neutrons from fission is approximately given by the semi-empirical Terrell cumulative distribution function

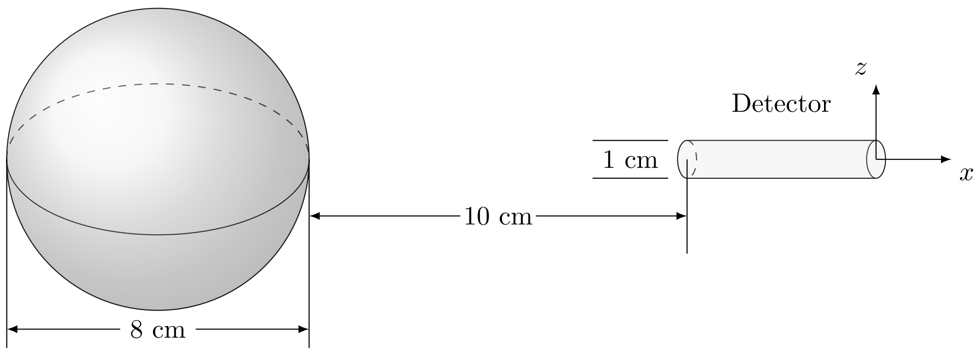
   $$P_\nu = \sum_{n=0}^{\nu} p_\nu = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{(\nu - \overline{\nu} + \frac{1}{2} + b)/\gamma} \exp\left(-\frac{t^2}{2}\right) dt.$$

   Fission with the provided isotope has the parameters $\overline{\nu} = 2.8$, $\gamma = 1.1$, $b = 1.41 \times 10^{-3}$.

   Compare the probability mass functions on a lin-log plot for at least 30 neutrons. Quantify uncertainties with error bars on the plot. You are not required to give an uncertainty for the computed mean and variance. Discuss the results in your document.

4. A sphere is centered at the origin having a radius of 4 cm and atomic density of 0.1 $\text{b}^{-1}\cdot\text{cm}^{-1}$ and containing two isotopes with respective atomic fractions 2/3 and 1/3. The first isotope has $\sigma_s = 19$ b, and $\sigma_c = 1$ b with linearly anisotropic scattering with $\overline{\mu}_0 = 1/3$. The second isotope has $\sigma_s = 4$ b, and $\sigma_c = 1$ b and isotropic scattering. Neither isotope is fissionable.

   A cylindrical detector with length of 5 cm and radius of 0.5 cm is placed with its planar surface facing the sphere at $x = 14$ cm centered along the x axis, i.e., the edge of the detector is 10 cm from the edge of the sphere. The detector material has an atomic density of 0.005 $\text{b}^{-1}\cdot\text{cm}^{-1}$, $\sigma_s = 1$ bm $\sigma_c = 59$ b, and isotropic scattering. The detector measures the absorption rate. The air outside the sphere and detector are vacuum.



   Find the absorption rate in the detector using a track-length estimator for the following sources:

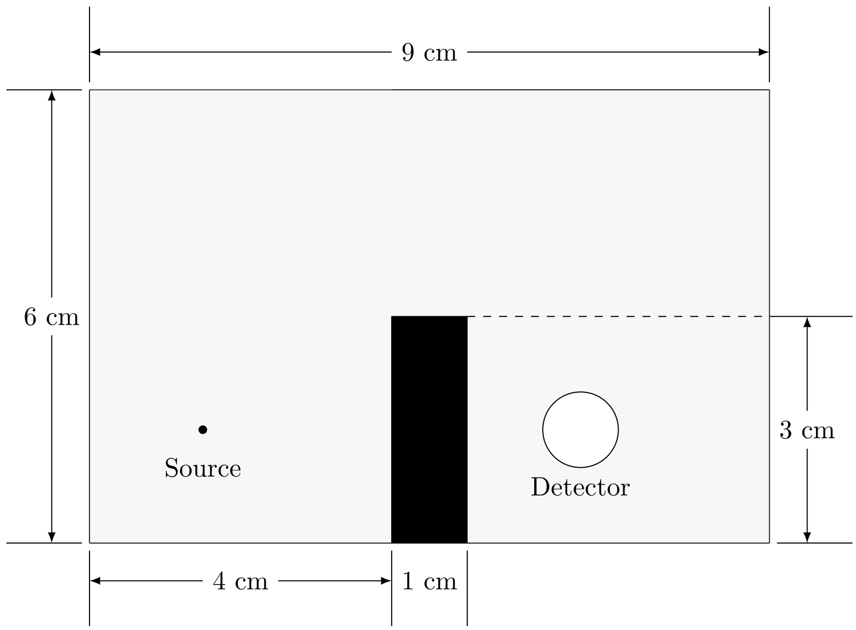
   (a) Three isotropic point sources located at the points $(1, 1, 2)$, $(-1, 0, -3)$, and $(0, -2, 1)$. The emission probabilities of each are 1/6, 1/3, and 1/2 respectively.

   (b) A spatially uniform (in volume) spherical shell source centered at the origin with inner radius of 1 cm and outer radius of 2 cm that emits particles isotropically.

   (c) A monodirectional beam source in the z direction emitted spatially uniform (in area) from a disk centered at $(-1, 0, -5)$ with a radius of 2 cm. The disk is oriented such that its outward normal points in the z direction.

5. The following problem is one that requires variance reduction techniques to get statistically significant results in a reasonable amount of time. Material A (in lighter gray on the figure) has an atomic density of 0.1 $\text{b}^{-1}\cdot\text{cm}^{-1}$, a microscopic capture cross section $\sigma_c = 10$ b, and microscopic scattering cross section $\sigma_s = 10$ b; scattering is isotropic. Material B (in darker gray on the figure) has an atomic density of 0.1 $\text{b}^{-1}\cdot\text{cm}^{-1}$, and is a pure absorber with microscopic capture cross section $\sigma_c = 100$ b. Neither material is fissionable. The system is infinite in the z direction and the region outside is vacuum.

   There is an isotropic point source located at $(1.5, 1.5, 0)$. An infinite (in z) cylindrical detector (in white on the figure) is centered at $(6.5, 1.5)$ with radius of 0.5 cm having the same materials in the previous problem: atomic density of 0.005 $\text{b}^{-1}\cdot\text{cm}^{-1}$, $\sigma_s = 1$ bm $\sigma_c = 59$ b, and isotropic scattering. As before, the detection measures absorption.



   Subdivide this problem into multiple cells and assign each region a cell importance such that the statistical uncertainty of the detector response estimator, a track-length estimate of absorption, is $< 10\%$ for 10^8 particles and the figure of merit is greater than 1×10^{-6}, where time is to be measured in the number of particle tracks in the entire simulation. (A particle track is defined as anytime the particle moves from one location to another, whether it be to the site of a collision or surface crossing.) Clearly report the final mean and variance and produce a figure illustrating how you subdivided the problem and what importances you ran.