NERS 544 Winter 2015 Class Project Due at 12:30 PM on Apr. 30, 2015

Course project requirements are as follows:

- 1. involve Monte Carlo theory and methods in a significant way;
- 2. involve some amount of coding on the part of the student involving Monte Carlo (running an existing Monte Carlo code and analyzing data is NOT acceptable);
- 3. be new to the student, i.e., work already done may not be turned in;
- 4. be accompanied by a written report with convincing results.

Students may work individually or in a group. The amount of work expected scales with the size of the group. You should meet with me to discuss your project so we can come to an understanding of what is expected.

To receive credit, at or prior to the end of the term (see due date above), the student(s) must submit a written report and their source code. Except under unforeseen and extreme circumstances, late projects will not be accepted. Both the report and source code must be submitted electronically to me. The project is worth a maximum of 400 points. The grade will be assigned based upon (1) the difficulty of the project and (2) the overall quality of the report and source code. Based on my discretion, I will assign a percentage based upon both criteria, take their product, and multiply by 400 to obtain your project grade. The scale for grading either is roughly as follows relative to what is typically expected of students in graduate courses in the NERS department:

100%	Exceptional
90%	Superior
80%	Average
70%	Acceptable
50%	Minimally Acceptable

The written report should:

- 1. clearly document the problem the project is solving and how the approaches used involve Monte Carlo methods:
- 2. give a detailed explanation of the methods, algorithms, and data structures used in the program, preferably showing relevant parts of code;
- 3. discuss testing and provide results (with quantified uncertainties if feasible) demonstrating that the method is working as intended;
- 4. provide references to background materials as appropriate.

The source code will also be graded based on clarity, commenting, and correctness. In other words, any reasonably knowledgable person who has read your report should be able to read your code and, without too much effort, understand what it is attempting to do.

Example Project

This project represents a "superior" project for a group of two students.

Write a Monte Carlo neutron transport problem to solve for the effective multiplication factor in an infinite lattice of reactor fuel pins with vacuum boundaries on top and bottom.

Geometry

The geometry is a cylinder containing fuel (uranium dioxide) centered at the origin. The fuel has a radius of 1.5 cm (larger than a typical reactor). Surrounding the fuel is a box containing water. In the x and y directions, the edges of the box are reflecting. The fuel pin is uniform, but finite in extent in z with a height of 100 cm. You may neglect the cladding. The pitch is variable and its impact on k will be studied using the results of this program.

Students may optionally support more complicated geometry for additional credit.

Material Compositions

The fuel is roughly 4% enriched uranium dioxide and the moderator is water. The materials are taken to be at room temperature, T = 293 K. The atomic densities (in atoms per barn-cm) are given in Table 1.

 $\begin{array}{|c|c|c|c|c|c|c|c|c|} \hline Material & ^{1}H & ^{16}O & ^{235}U & ^{238}U \\ \hline Fuel & 0.0 & 4.7284 \times 10^{-2} & 9.4567 \times 10^{-4} & 2.2696 \times 10^{-2} \\ \hline Moderator & 6.6911 \times 10^{-2} & 3.3455 \times 10^{-2} & 0.0 & 0.0 \\ \hline \end{array}$

Table 1: Material Data for the Fuel Pin

Nuclear Physics

The nuclear interactions modeled are radiative capture, elastic scattering (no inelastic scattering), and fission. Elastic scattering is assumed to be isotropic in the center-of-mass frame, but not the lab frame, and free-gas thermal motion of the nuclei ($T=293~\rm K$) should be taken into account. Emission of fission neutrons is assumed to be isotropic in the lab frame with energies sampled from a Watt fission spectrum with $a=0.988~\rm MeV$ and $b=2.249~\rm MeV^{-1}$ for $^{235}\rm U$ The number of mean number neutrons per fission is $\nu=2.45~\rm for$ $^{235}\rm U$. Fission in $^{238}\rm U$ is going to be neglected in this model.

In reality, the cross sections are complicated functions of energy represented with large sets of tabular data; however, this project will use simplified means of generating them as described below. A further simplification is that the cross sections will be taken at 0 K, i.e., no Doppler broadening, although the scattering kinematics will be at 293 K. For simplicity, the cross sections are given by a semi-emprical approximate functional form

$$\sigma(E) = \left(c_1 + \frac{c_2}{\sqrt{E}}\right) \exp\left(c_3\sqrt{E}\right) + \sum_j \sigma_{res,j}(E),\tag{1}$$

with parameters given in Table 2. The units are: c_1 is b, c_2 is MeV^{1/2}·b, and c_3 is MeV^{-1/2}·b.

Capture in ²³⁸U (no other isotopes or reactions for our model) has additional resonances (three in this very simplified model) given by the following formula:

$$\sigma_{res,j}(E) = \sigma_{0,j} \sqrt{\frac{E_{0,j}}{E}} \frac{1}{1+y^2}, \quad y = \frac{2}{\Gamma_j} (E - E_{0,j})$$
 (2)

The three resonances are described in Table 3.

Table 2: Cross Section Parameters for Approximate Model

		c_1	c_2	c_3
$^{1}\mathrm{H}$	Scatter	2.0×10^{1}	3.0×10^{-3}	-1.2×10^{0}
	Capture	0.0	8.0×10^{-5}	0.0
¹⁶ O	Scatter	4.0×10^{0}	1.5×10^{-4}	-6.0×10^{-1}
	Capture	0.0	0.0	0.0
	Scatter	1.5×10^{1}	1.5×10^{-4}	-4.0×10^{-1}
$^{235}\mathrm{U}$	Capture	4.0×10^{-1}	2.5×10^{-3}	-1.0×10^{0}
	Fission	8.0×10^{-1}	6.0×10^{-2}	0.0
²³⁸ U	Scatter	9.0×10^{0}	1.0×10^{-4}	-1.6×10^{-1}
	Capture	1.8×10^{0}	4.0×10^{-4}	-1.5×10^{0}

Table 3: Resonance Parameters in $^{238}\mathrm{U}$

j	$E_{0,j}$ (MeV)	$\sigma_{0,j}$ (b)	$\Gamma_j \; ({ m MeV})$
1	6.6×10^{-6}	7.0×10^{3}	4.0×10^{-8}
2	2.2×10^{-5}	6.0×10^{3}	3.0×10^{-8}
3	3.8×10^{-5}	6.5×10^{3}	1.0×10^{-7}

Estimators

Three estimators in the problem are:

- 1. Collision estimate of the effective multiplication factor k.
- 2. Track-length estimate of the effective multiplication factor k.
- 3. Surface current estimate of neutrons leaking out of the top and bottom of the geometry.

Uncertainties in the mean for each estimator should be quantified. Show that the collision and track-length estimators for k are, on average, the same. Find k as a function of pitch.

For more credit, students may include more estimators, e.g., the neutron spectrum in the fuel and moderator.

Variance Reduction

For more credit, students may optionally include implicit capture and/or fission and include weight rouletting. Other variance reduction techniques are unlikely to be effective in this problem.

Criticality Calculation

The simulation should be performed based upon the power iteration method. An assessment of source convergence should be performed as well, and no scores should be made to estimators prior to convergence.