NENG 685 Fall 2017
HW 4 Due Nov. 29, 2017

Name:

On homework:

- Well organized and documented work scores better. If I cannot figure out what is going on, then I am less likely to "intuit" what you intended, and the score will be reflective of this fact.
- If you work with anyone else, document what you worked on together.
- Show your work.
- Always clearly label plots (axis labels, a title, and a legend if applicable).
- Homework should be done "by hand" (i.e. not with a numerical program such as MATLAB, Python, or Wolfram Alpha) unless otherwise specified. You may use a numerical program to check your work.
- If you use a numerical program to solve a problem, submit the associated code, input, and output.
- ***I should not have to run your code to see your answers.*** The attached code is an additional form of feedback for me and a method to give partial credit. If you want full credit, then include the outputs (plots, tables, answers, etc.) in your write-up.

Do not write in the table to the right.

Problem	Points	Score
1	30	
2	30	
3	15	
4	25	
Total:	100	

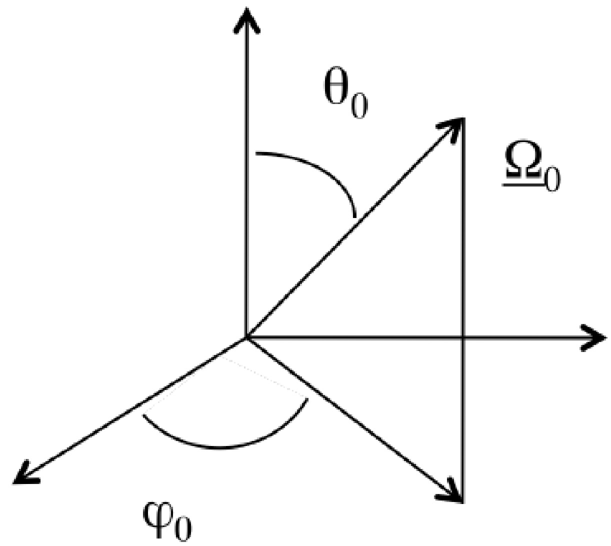
1. (30 points) Using the direct inversion of CDF sampling method, derive sampling algorithms for

   (a) The neutron direction in 3D if the neutron source is isotropic. *Note: each unit direction should have a specified sampling.*

   (b) The distance to the next collision in the direction of neutron motion if the neutron is in the center of the spherical volume that consists of three concentric layers with radii R_1, R_2, and R_3, each made of different materials with total cross sections Σ_{t1}, Σ_{t2}, and Σ_{t3}, respectively. *Note: Do not use the mfp algorithm to determine the distance; sample the distance explicitly.*

   (c) The type of collision if it is assumed that the neutron can have both elastic and inelastic scattering, and can be absorbed in fission or (n,gamma) capture interactions. Assume monoenergetic neutron transport.

Solution:



$$\underline{\Omega}_0 = \Omega_{x,0}\underline{i} + \Omega_{y,0}\underline{j} + \Omega_{z,0}\underline{k}$$

where

$$\Omega_{x,0} = \sin\theta_0\cos\varphi_0$$
$$\Omega_{y,0} = \sin\theta_0\sin\varphi_0 \,.$$
$$\Omega_{z,0} = \cos\theta_0$$

In order to develop a sampling method, we need to determine the PDF for angle sampling:

$$f(\underline{\Omega})d\underline{\Omega} = \frac{d\underline{\Omega}}{4\pi} = \frac{\sin\theta\, d\theta\, d\varphi}{4\pi} = -\frac{d(\cos\theta)d\varphi}{4\pi} = -\frac{d(\cos\theta)}{2} \times \frac{d\varphi}{2\pi}$$

Thus, the PDF for solid angle sampling could be presented as a product of two simpler PDFs, one for the polar angle cosine, and the other for azimuthal angle:

$$f(\underline{\Omega}) = g(\cos\theta) \times h(\varphi) = \frac{1}{2} \times \frac{1}{2\pi};$$

$$g(\cos\theta) = \frac{1}{2}; \quad h(\varphi) = \frac{1}{2\pi}$$

Now, check if these PDFs satisfy requirements to be PDFs:

$$g(\cos\theta) = \frac{1}{2} \geq 0; \quad \int_{-1}^{1} \frac{1}{2} d(\cos\theta) = 1.$$

$$h(\varphi) = \frac{1}{2\pi} \geq 0; \quad \int_{0}^{2\pi} \frac{1}{2\pi} d\varphi = 1.$$

We apply the direct inversion of CDF sampling method:

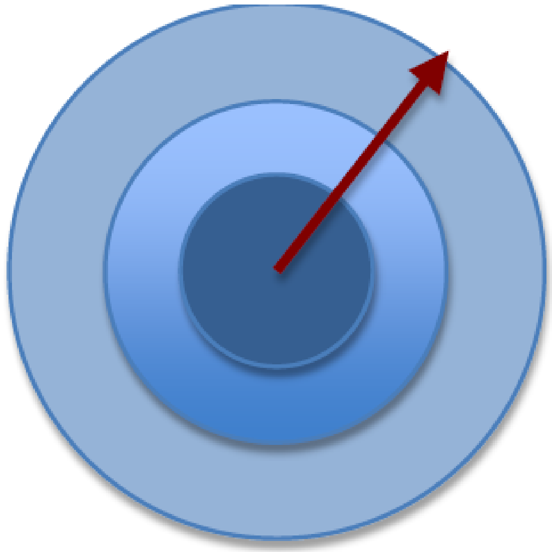
$$g(\cos\theta) = \frac{1}{2}; \quad G(\cos\theta) = \int_{-1}^{\cos\theta} \frac{1}{2} d(\cos\theta') = \xi_1 \quad \Rightarrow \quad \cos\theta = 2\xi_1 - 1$$

$$h(\varphi) = \frac{1}{2\pi}; \quad H(\varphi) = \int_{0}^{\varphi} \frac{1}{2\pi} d\varphi' = \xi_2 \quad \Rightarrow \quad \varphi = 2\pi\xi_2$$

We can now determine the x, y and z components of the unit directional vector $\underline{\Omega}_0$:

$$\vec{\Omega}_0 = \begin{bmatrix} \Omega_{0x} \\ \Omega_{0y} \\ \Omega_{0z} \end{bmatrix} = \begin{bmatrix} \sin\theta_0 \cos\varphi_0 \\ \sin\theta_0 \sin\varphi_0 \\ \cos\theta_0 \end{bmatrix} = \begin{bmatrix} \sqrt{1-\cos\theta_0}\cos\varphi_0 \\ \sqrt{1-\cos\theta_0}\sin\varphi_0 \\ \cos\theta_0 \end{bmatrix} = \begin{bmatrix} \sqrt{1-(2\xi_1-1)^2}\cos(2\pi\xi_2) \\ \sqrt{1-(2\xi_1-1)^2}\sin(2\pi\xi_2) \\ (2\xi_1-1) \end{bmatrix}.$$

(b) The distance to the next collision in the direction of neutron motion, if the neutron source is in the center of the spherical volume that consists of 3 concentric layers with radii R_1, R_2, and R_3, made of different materials with total cross sections $\Sigma_{t1}, \Sigma_{t2}, and\ \Sigma_{t3}$.



In order to determine the next collision site in the direction of neutron motion, we use the corresponding PDF:

$$f(s) = e^{-\Sigma_t s}\Sigma_t; \quad f(s) \geq 0; \quad \int_0^\infty \Sigma_t e^{-\Sigma_t s} ds = 1.$$

We use the direct inversion of CDF sampling method to determine the distance to the next collision site, starting from the center of the spheres:

$$F(s) = \int_0^s \Sigma_t e^{-\Sigma_t s'} ds' = 1 - e^{-\Sigma_t s} = \xi_3$$

$$s = -\frac{1}{\Sigma_t}\ln(1-\xi_3) = -\frac{1}{\Sigma_t}\ln(\xi_3)$$

However, we have 3 nested spheres, so the algorithm to determine the first collision location, if a neutron is emitted from the center of the spheres is more complicated. We first start from the innermost sphere and use the first cross section in the sampling algorithm:

$$s = -\frac{1}{\Sigma_{t1}}\ln(\xi_3)$$

If s is smaller or equal to R_1, that we have our collision location. However, if s is large that R_1, we have to place our neutron on the boundary between region 1 and 2 and repeat sampling of the distance to the collision with a new cross section for material 2:

$$s_1 = -\frac{1}{\Sigma_{t1}}\ln(\xi_3)$$

If $s_1 \le R_1$*, it is the location of the collision*

If $s_1 > R_1$:

$$s_2 = -\frac{1}{\Sigma_{t2}}\ln(\xi_4)$$

If $R_1 + s_2 \le R_2$*, then* $(R_1 + s_2)$ *is the location of the collision*

If $s_2 > R_2$:

$$s_3 = -\frac{1}{\Sigma_{t3}}\ln(\xi_5)$$

If $R_2 + s_3 \le R_3$*, then* $(R_2 + s_3)$ *is the location of the collision*

If $s_3 > R_3$ *: the neutron leaked out without a collision.*

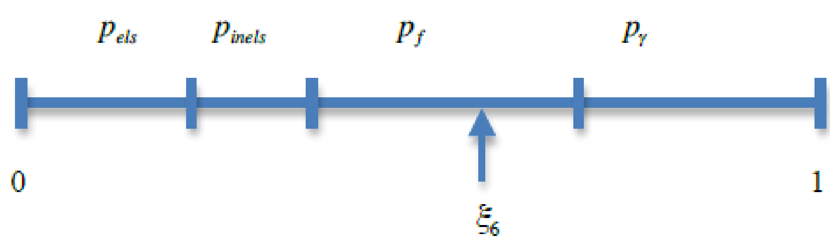
(c) The type of the collision, if it is assumed that the neutron can have both elastic and inelastic scattering, and can be absorbed in fission or (n,gamma) capture interactions. Assume monoenergetic neutron transport.

SOLUTION:

$$\Sigma_t = \Sigma_{els} + \Sigma_{inels} + \Sigma_f + \Sigma_\gamma$$

$$1 = \frac{\Sigma_{els}}{\Sigma_t} + \frac{\Sigma_{inels}}{\Sigma_t} + \frac{\Sigma_f}{\Sigma_t} + \frac{\Sigma_\gamma}{\Sigma_t} = p_{els} + p_{inels} + p_f + p_\gamma$$

We place all of these probabilities on a single segment:



We now select a new random number and depending on which segment the random number fells in, it will be the sampled collision type.

(1) If $0 \le \xi < p_{s,el}$, the collision type was elastic scattering,

(2) If $p_{s,el} \le \xi < p_{s,el} + p_{s,inel}$, the collision type was inelastic scattering,

(3) If $p_{s,el} + p_{s,inel} \le \xi < p_{s,el} + p_{s,inel} + p_f$, the collision type was fission,

(4) If $p_{s,el} + p_{s,inel} + p_f \le \xi < p_{s,el} + p_{s,inel} + p_f + p_\gamma = 1$, the collision type was (n, gamma) absorption.

2. A sample of MCNP input is given below:

```
PWR Single Pin
1 1 -10.41 -1 -10 20 imp:n=1
2 0 1 -2 -10 20 imp:n=1
3 3 -6.55 2 -3 -10 20 imp:n=1
4 4 -0.7 3 -5 6 -7 8 -10 20 imp:n=1
5 0 5:-6:7:-8:10:-20 imp:n=0

c Rods dimensions
1 cz 0.41
2 cz 0.42
3 cz 0.48
c Basic lattice cell
*5 px 0.63
*6 px -0.63
*7 py 0.63
*8 py -0.63
c Axial limits
*10 pz 200.0
*20 pz -200.0

c Material 1
m1 8016.73c 2.0
92235.73c 0.05
92238.73c 0.95
c Material 4
m4 1001.71c 2
8016.71c 1
mt4 lwtr.04t
c Material 3
m3 40000.58c 1.
c ——— Tallies ———
fc4 Tally 4
f4:n 1 3 4
e4:n 1e-6 1. 20.
fc14 Tally 14
f14:n 1
fm14 (1 1 (-2) (-6))
c ————————————
kcode 1000 1.00 50 250
ksrc 0. 0. 0.
print
mode n
VOL 12j 345.510821 j
```

(a) (10 points) Next to each line in this sample input add a short explanation what that line represents.

(b) (5 points) Using so-called reverse engineering determine the dimensions, material properties (isotopic composition, enrichment, densities), and cross-section data used for this fuel pin. Specify corresponding units when appropriate.

(c) (15 points) Prepare the MCNP/SERPENT input for this case (using reflective boundary conditions) and determine:

1. k_{inf}.

2. The average neutron flux in the fuel, clad and moderator (the actual onegroup scalar flux!).

3. The average one-group absorption and fission rates in the fuel zone.

4. The neutron flux spectra in the fuel and water zones, separately, with a minimum of 20 energy groups (structure should be fine enough to see resonance capture regions). Plot the neutron spectra. Also determine the two-group neutron flux in the fuel and water zones.

5. Plot the spatial distribution of a two-group flux (fast and thermal) along the central line of the fuel pin. You might want to add more cylindrical zones in the fuel region, and more zones in the water region. Explain why additional spatial subdivision is needed?

6. Comment of the spectral and energy distribution of neutron flux in the fuel pin.

Solution:

(a) See HW4_2a.in

(b) COMPOSITION: FUEL (m1, cell1): UO2, with 5 a/o (atom percent) 235U and 95 a/o 238U, with density of 10.41 g/cm3, (31.65 a/o 238U, 1.69 a/o 235U and 66.66 a/o 16O) CLAD (m3, cell 3): Zr (Zirconium), with density of 6.55 g/cm3

MODERATOR (m4, cell 4): Water, with density of 0.7 g/cm3, the input also specifies S- $\alpha - \beta$ data from the lwtr library.

DIMENSIONS: Pellet radius 0.41 cm, clad inside radius 0.42 cm, clad outside radius 0.48 cm, pin-cell pitch 2x0.63 cm = 1.26 cm, 400 cm long

TEMPERATURES: .69c cross-sections at 558 K, .94c cross sections at 1100 K, .70c 300K libraries for water, 600K libraries for the cladding (.71c), and 1200K libraries for the fuel (.73c). If you do not specify any library, it will use the default library (.70c 300K continuous energy).

(c) See HW_2c.in and HW_2c.out for the input deck and raw output.

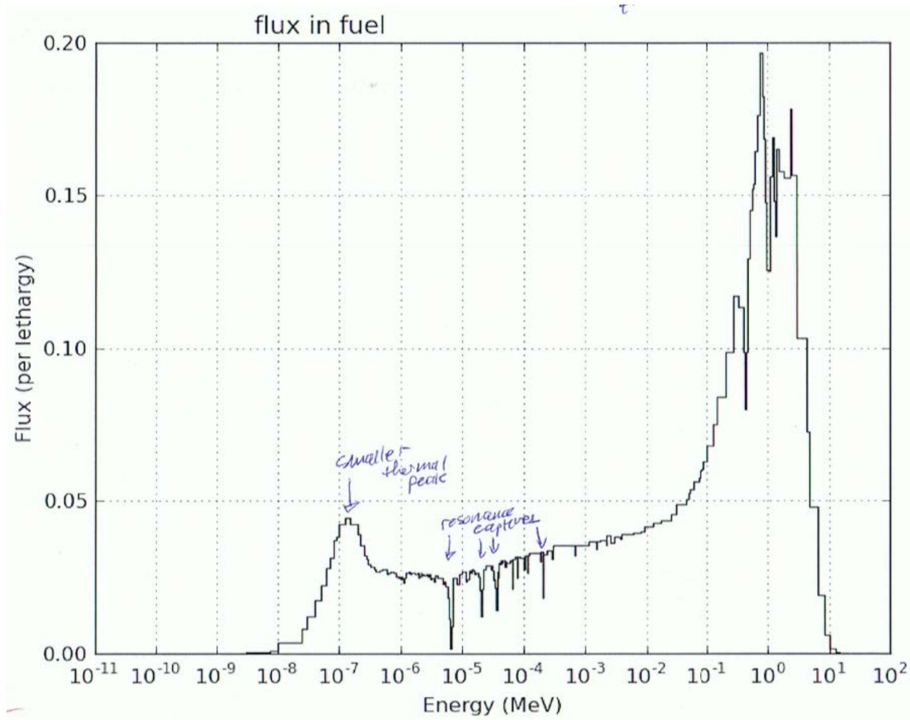
1. 1.38485 ± 0.00158

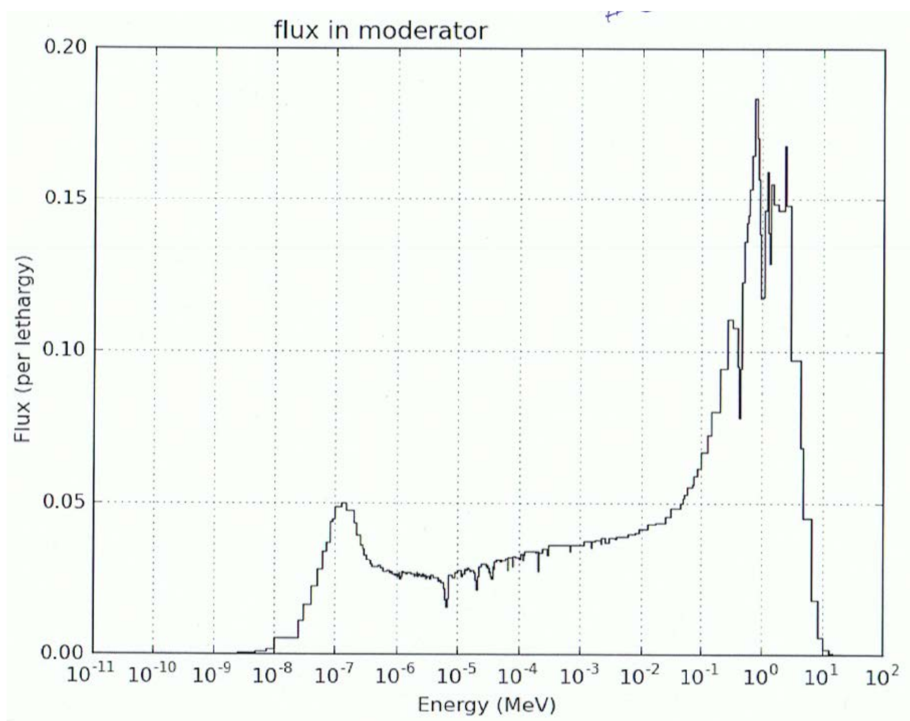
2. The average neutron flux in fuel: 6.93286E-02 ± 0.0010 n/cm^2/source neutron
   The average neutron flux in clad: 6.94431E-02 ± 0.0010 n/cm^2/source neutron
   The average neutron flux in moderator: 6.94438E-02 ± 0.0009 n/cm^2/source neutron

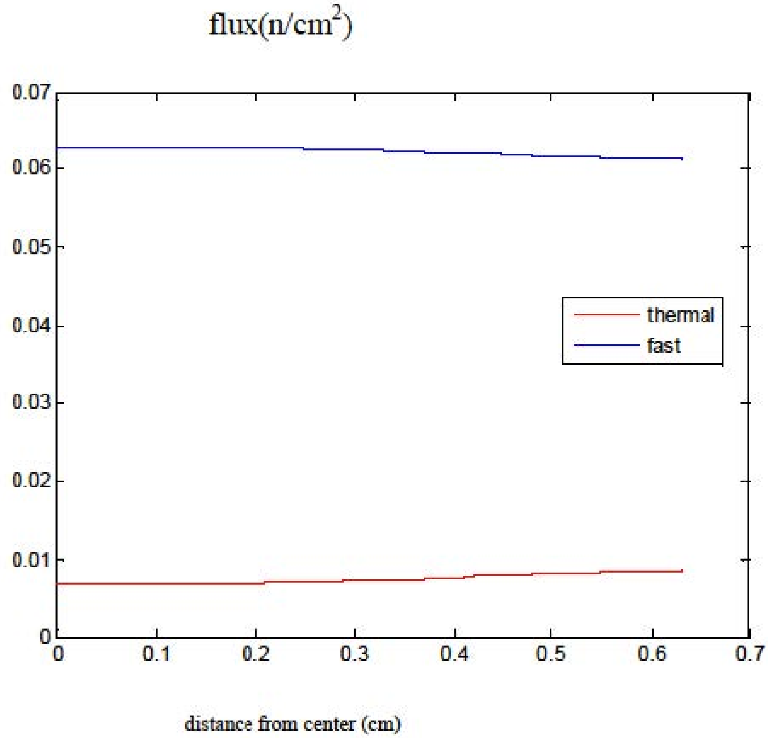
3. Fission rate in fuel: 2.66208E-03 ± 0.0022 fission/s
   Capture rate in fuel: 1.90964E-03 ± 0.0019 fission/s

4. Fuel
   THERMAL: 7.45888E-03 ± 0.0026
   FAST: 6.18697E-02 ± 0.0011

   Moderator
   THERMAL: 8.60499E-03 ± 0.0026
   FAST: 6.08388E-02 ± 0.0010


flux in fuel
Flux (per lethargy)
0.00
0.05
0.10
0.15
0.20
10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}
Energy (MeV)
smaller thermal peak
resonance captures


flux in moderator
Flux (per lethargy)
0.00
0.05
0.10
0.15
0.20
10^{-11} 10^{-10} 10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2}
Energy (MeV)



5.

6. From the spatial distribution plot, we notice that the fast flux is greater than the thermal flux. This is due to the fact there is not enough moderator/neutron path length to thermalize a large fraction of the neutrons. This is expected given the relative size of the fuel region compared to the moderator region. Furthermore, we notice that the thermal flux tends to increase in the moderator region and decrease in the fuel region. This too makes sense, since neutrons in the moderator region will tend to be thermalized contributing to the thermal flux, while thermal neutrons in the fuel region are more likely to be capture, leading to a depression of thermal flux in the fuel region (spatial selfshielding effects). The opposite is true for the fast flux, which is greater in the fuel region than in the moderator region.

   The general shapes of the energy spectra in the fuel and moderator regions are very similar, with some noted differences. The thermal flux is depressed for the fuel region compared to the moderator region. This is due to the capture of thermal neutrons by the fuel, which doesnt occur nearly as frequently in the moderator region. Similarly, there is a greater peak for fast neutrons in the fuel region due to fast neutrons being born from fission. The fast neutron peak is less pronounced in the moderator region because many neutrons in this region undergo collisions and begin to slow down. The epithermal part of the spectrum is nearly identical for the fuel and moderator region.

3. In Lesson #9, an outline was created for a simple 1D MC transport program. In class a

notebook was started to implement the MC algorithm, but it was not fully completed. Complete the code by:

(a) (5 points) Adding in the algorithm to transport the particle if $s_b < s_c$ in the transport function

(b) (5 points) Writing the main controller program to use the functions and classes defined in the notebook and transport N number of particles.

(c) (5 points) Outputting the flux tally in each cell in units of n/cm^2/src particle. Include the relative error for each flux.

Solution: See HW4-3_1D-MC_soln.ipynb

4. In lesson 14, a miniature city was created and exposed to neutrons from a fission weapon (nw_effects.in). The small scale of the city made it easy to get reasonable statistics. Now let's investigate something closer to reality:

   (a) (5 points) Add in a ground made of asphalt. Make the internal volume of the buildings 30% wood, 20% aluminum, 20% steel, and 30% air by mass (this should be one homogenized material).

   (b) (5 points) Scale the geometry by a factor of 10 and determine the flux for a car located between each block (use the previous definition of a "car"). Report the FOM and flux spectrum with errors (plot) for each.

   (c) (10 points) Use ADVANTG to create weight windows for the problem considered in part b). Run the MCNP with the ADVANTG weight windows with the same number of particles and report the FOM and flux spectrum with errors (plot) for each car.

   (d) (5 points) Comment on your findings regarding the FOM and uncertainties between the analog and ADVANTG variance reduction models.

Solution: See nw_effects.out

BONUS (5 points): submit your code by providing read/clone access to an online version control repository where your code is stored (e.g. github or bitbucket).