Homework 1

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NUEN 629

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NUEN 629, Homework 1

Due Date Sept. 17

1 Ayzman

(10 points) Henyey and Greenstein (1941) introduced a function which, by the variation of one parameter, $-1 \leq h \leq 1$, ranges from backscattering through isotropic scattering to forward scattering. In our notation we can write this as

$$K(\mu_0, v' \to v) = \frac{1}{2} \frac{1-h^2}{(1+h^2-2h\mu_0)^{3/2}} \delta(v'-v).$$

Verify that this is a properly normalized $f(\mu_0)$ and compute $K_l(v' \to v)$ for $l = 0, 1, 2$ as a function of h.

2 Bolding

(20 points) In an elastic scatter between a neutron and a nucleus, the scattering angle in the center of mass system is related to the energy change as

$$\frac{E}{E'} = \frac{1}{2}\left((1+\alpha) + (1-\alpha)\cos\theta_{\mathrm{c}}\right),$$

where E is the energy after scattering and E' is the initial energy of the neutron and

$$\alpha = \frac{(A-1)^2}{(A+1)^2}.$$

The scattered angle in the center-of-mass system is related the lab-frame scattered angle as

$$\tan\theta_{\mathrm{L}} = \frac{\sin\theta_{\mathrm{c}}}{A^{-1} + \cos\theta_{\mathrm{c}}}.$$

Also, the distribution of scattered energy is given by

$$P(E' \to E) = \begin{cases} \frac{1}{(1-\alpha)E'}, & \alpha E' \leq E \leq E' \\ 0 & \text{otherwise} \end{cases}.$$

Derive an expression for $K(\mu_0, E' \to E)$, where μ_0 is $\cos\theta_{\mathrm{L}}$. What is the distribution in angle of neutrons of energy in the range $[0.05\,\mathrm{MeV}, 10\,\mathrm{MeV}]$ to energies below 1 eV if the scatter is hydrogen?

3

(70 points) Consider an infinite square lattice of infinitely tall cylindrical UO2 fuel pins in water. A quarter of a pin cell looks for a square lattice is shown in Fig. 1 and an infinite hex lattice in Fig. 2. The cross-section data for each is given in Table 1. The neutron transport equation for this problem is given simply by

$$\hat{\Omega} \cdot \nabla \psi(x,y,\hat{\Omega}) + \Sigma_{\mathrm{t}} \psi(x,y,\hat{\Omega}) = \frac{1}{4\pi} \Sigma_{\mathrm{s}} \phi(x,y) + \frac{Q}{4\pi}.$$

You may choose whichever lattice you wish – square or hex. For one or the other, perform the following:

Table 1: Data for Test Problem

	Fuel	Moderator
Σ_{t} (cm^{-1})	0.1414	0.08
Σ_{s} (cm^{-1})	0	0
Q (n/cm^3·s)	1	0

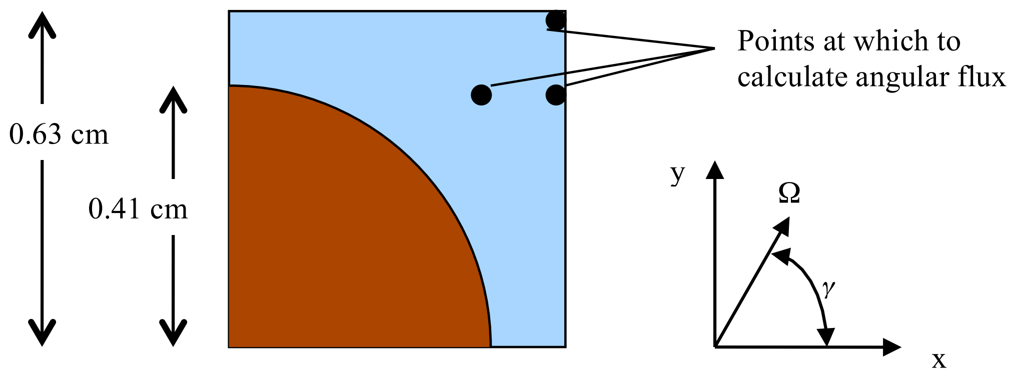


Figure 1: Quarter of a pin cell of infinite square lattice problem. The azimuthal angle φ is written as γ in the figure.

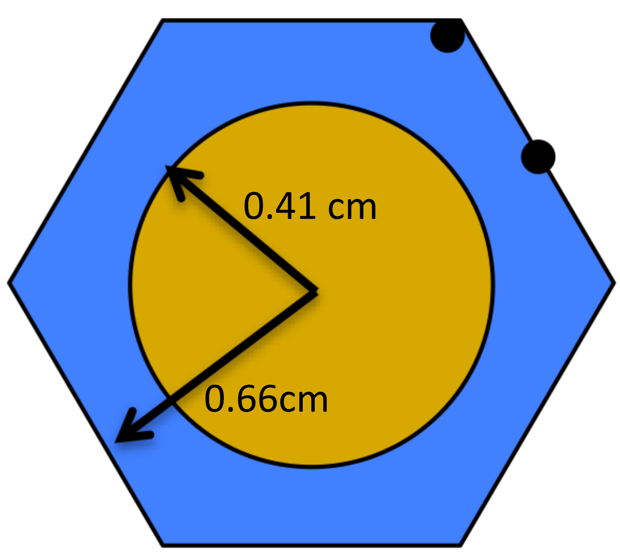


Figure 2: Pin cell of infinite hex lattice problem.

1. Calculate the angular flux as a function of the azimuthal angle, φ, at the spatial points indicated in the figure (two points for the hex lattice; three for the square). Use two different polar angles: $\pi/2$, which means the neutrons are traveling in the x-y plane, and $\pi/8$. Use the dimensions and cross sections from Table 1. Note that to simplify the problem we have abolished scattering. In the highest energy group of a fine-group set, there is very little within-group scattering, so it does not change the problem very much to ignore scattering. We have also assumed that the neutrons are born uniformly in the fuel – a flat radial profile. This isn't precisely true, but again, the simplification does not change the character of the solution that we wish to study. You will need to write a simple computer program for this in whatever language you'd like. You will need to trace rays and compute points of intersection. When you reach the boundary of a pin cell you use a periodic boundary condition to translate the ray across the cell, and then you continue. You will need a strategy to know how far a ray must be traced before you say "enough." Your code should accept as input:

   (a) the number of values of the azimuthal angle, φ at which to calculate the angular flux;

   (b) the precision to which to calculate the angular flux at a given spatial point and given φ. (This tells you when you can say "enough." You can say "enough" when you've traced through τ mean free paths, where $\exp(-\tau) =$ the requested precision.)

2. Convince me that your code calculates the angular flux correctly.

3. Plot the angular flux as a function of φ for each of the two polar angles, for each of the three spatial points (two if hex lattice). Use enough φ values to convince yourself that you have resolved all the significant bumps and wiggles in the angular flux. Discuss your plots, and in particular compare them against what was shown in the notes for square pins. Do the circles make things smoother? Be prepared to present your solutions to the class, and (see part above) be prepared to argue that they are correct.

Problem 1:

Henyey and Greenstein (1941) introduced a function which, by the variation of one parameter, $1 \leq h \leq 1$, ranges from backscattering through isotropic scattering to forward scattering. In our notation we can write this as

$$K(\mu_0, v' \to v) = \frac{1}{2} \frac{1 - h^2}{(1 + h^2 - 2h\mu_0)^{3/2}} \delta(v' - v). \tag{1}$$

Verify that this is a properly normalized $f(\mu_0)$ and compute $K_l(v' \to v)$ for $l = 0, 1, 2$ as a function of h.

Solution:

Solution:

- First, expand scattering kernel in Legendre Polynomials.
- Begin w/ Legendre generating fn:

$$\frac{1}{\sqrt{1-2xh+h^2}} = \sum_{n=0}^{\infty} P_n(x) h^n \qquad (1)\ [\text{wiki}]$$

- Take a derivative w.r.t. x

$$\frac{h}{(1-2xh+h^2)^{3/2}} = \sum_{n=0}^{\infty} P_n'(x) h^n \qquad (2)$$

- Multiply both sides by $\frac{(1-h^2)}{2h}$:

$$K(x) = \frac{1}{2} \frac{(1-h^2)}{(1-2xh+h^2)^{3/2}} = \frac{1}{2}\sum_{n=0}^{\infty} P_n'(x) h^{n-1}(1-h^2) \qquad (3)$$

- (3) is our scattering kernel. Now we need to eliminate the derivative in terms of $P_n(x)$. Rewrite sum by letting $n \to n+1$

$$\frac{1}{2}\sum_{n=0}^{\infty} P_n'(x) h^{n-1}(1-h^2) = \frac{1}{2}\sum_{n=0}^{\infty} P_{n+1}'(x) h^{n}(1-h^2) \qquad (4)$$

- Note that the sum still starts at zero because $P_0'(x)=0$, so we can trivially add this term. From Abromowitz:

$$P_{n+1}'(x) = \sum_{m\ \text{even}}^{n} (2m+1) P_m(x) \qquad (5)$$

- (5)→(4) and write as two sums:

$$K(x) = \frac{1}{2}\sum_{n=0}^{\infty} \sum_{\substack{m\\ \text{even}}}^{n} (2m+1) P_m(x) h^n - \frac{1}{2}\sum_{n=0}^{\infty} \sum_{\substack{m\\ \text{even}}}^{n} (2m+1) P_m(x) h^{n+2} \qquad (6)$$

* Note: Here orthogonality is defined as $\int P_m P_n = \frac{\delta_{mn}\, 2}{2n+1}$ *

- Shift the second infinite sum by $n' = n+2$

$$K = \frac{1}{2}\sum_{n=0}^{\infty}\sum_{\substack{m\\ \text{even}}}^{n}(2m+1)P_m(x)h^n - \frac{1}{2}\sum_{n'=2}^{\infty}\sum_{\substack{m\\ \text{even}}}^{n'-2}(2m+1)P_m(x)h^{n'}$$

- Combine the two series, writing out $n=0,1$ & letting $n' \to n$

$$K = \frac{1}{2}\sum_{n=0}^{1}(2n+1)P_n(x)h^n + \frac{1}{2}\sum_{n=2}^{\infty}\left(\sum_{\substack{m\\ \text{even}}}^{n}(2m+1)P_m(x) - \sum_{\substack{m\\ \text{even}}}^{n-2}(2m+1)P_m(x)\right)h^n$$

- For the inner sums all terms but n cancel, adding back energy:

$$\boxed{K(\mu_0, \nu' \to \nu) = \frac{1}{2}\sum_{n=0}^{\infty}(2n+1)P_n(\mu_0)h^n\delta(\nu'-\nu)} \qquad (7)$$

- Taking legendre moments:

$$K_\ell(\nu' \to \nu) = \frac{\delta(\nu'-\nu)}{2}\sum_{n=0}^{\infty}(2n+1)h^n\int_{-1}^{1}d\mu_0\, P_n(\mu_0)P_\ell(\mu_0)$$

$$K_\ell(\nu' \to \nu) = \delta(\nu'-\nu)\sum_{n=0}^{\infty}\left(\frac{2n+1}{2}\right)h^n\frac{\delta_{n\ell}2}{(2\ell+1)}$$

$$\boxed{K_\ell(\nu' \to \nu) = h^\ell}$$

- Noting $\int_0^\infty d\nu\int_{-1}^{1}d\mu_0(\cdot) = \int_0^\infty d\nu\int_{-1}^{1}P_0(\mu_0)(\cdot)$; $\int_0^\infty d\nu\int_{-1}^{1}d(\mu_0)\,K(\mu_0,\nu'\to\nu) = h^0 = 1$,

So normalization is correct.

$$\boxed{\begin{aligned} K_0 &= 1 \\ K_1 &= h \\ K_2 &= h^2 \end{aligned}}$$

Problem 2:

In an elastic scatter between a neutron and a nucleus, the scattering angle in the center of mass system is related to the energy change as

$$\frac{E}{E'} = \frac{1}{2}\left((1+\alpha) + (1-\alpha)\cos\theta_c\right) \tag{2}$$

where E is the energy after scattering and E' is the initial energy of the neutron and

$$\alpha = \frac{(A-1)^2}{(A+1)^2}. \tag{3}$$

The scattered angle in the center-of-mass system is related the lab-frame scattered angle as

$$\tan\theta_L = \frac{A\sin\theta_c}{1 + A\cos\theta_c} \tag{4}$$

Also, the distribution of scattered energy is given by

$$P(E' \to E) = \begin{cases} \frac{1}{(1-\alpha)E'} & E'\alpha \le E \le E' \\ 0 & \text{otherwise} \end{cases}. \tag{5}$$

Derive an expression for $K(\mu_0, E' \to E)$, where μ_0 is $\cos\theta_L$. What is the distribution in angle of neutrons of energy in the range [0.05 MeV, 10 MeV] to energies below 1 eV if the scatter is with hydrogen?

Solution:

Scattering Kernel Derivation

Due to Eq. (2), for a fixed A, a given value of E and E' fully define μ_c; the lab frame cosine of the scattering angle μ_0 is also fully defined through Eq. (4). As a result, the shape of the doubly differential scattering cross section is fully defined by the probability density function (PDF) $P(E' \to E)$. Thus, it is possible to write the scattering cross section in the COM frame as [1]

$$\Sigma_s(\mu_0, E' \to E) = \Sigma_s(E')P(E' \to E)\delta(\mu_c - f_\mu(E, E')) \tag{6}$$

where $f_\mu(E, E')$ is the value of μ_c that satisfies Eq. (2) for a given E, i.e.,

$$f_\mu(E, E') = \frac{2(\frac{E}{E'}) - (1+\alpha)}{(1-\alpha)} \tag{7}$$

Because we are interested in the scattering kernel as a function of the lab frame cosine μ_0, we define the scattering cross section in an equivalent form

$$\Sigma_s(\mu_0, E' \to E) = \Sigma_s(E')P(\mu_0)\delta(E - f_E(\mu_c(\mu_0), E')) \tag{8}$$

where $P(\mu_0)$ is a PDF for μ_0 given a certain value of E', f_E is defined as

$$f(\mu_0, E') = \frac{E'}{2}\left((1+\alpha) + (1-\alpha)\mu_c\right), \tag{9}$$

and μ_c as a function of μ_0 will be derived later in Eq. (21). The scattering kernel is defined as

$$K(\mu_0, E' \to E) = \frac{\Sigma_s(E' \to E, \mu_0)}{\int\limits_0^\infty \mathrm{d}E \int\limits_{-1}^{1} \mathrm{d}\mu_0 \, \Sigma_s(E' \to E, \mu_0)} \tag{10}$$

The denominator is evaluated as

$$\int\limits_{-1}^{1} \mathrm{d}\mu_0 \int\limits_0^\infty \mathrm{d}E \; \Sigma_s(E') P(\mu_0) \delta(E - f_E(\mu_c(\mu_0), E)) = \Sigma_s(E') \int\limits_{-1}^{1} \mathrm{d}\mu_0 P(\mu_0) = \Sigma_s(E') \tag{11}$$

where the first equality is true because the argument of the delta function is zero for the value of μ_0 and E' that satisfy f, which in this case gives the μ_0 that is the integration variable of the outer integral. The scattering Kernel is then just

$$K(\mu_0, E' \to E) = P(\mu_0)\delta(E - f_E(\mu_C(\mu_0), E)). \tag{12}$$

We now need to transform the PDF $P(E' \to E)$ into a density function $P(\mu_0)$. From Eq. (2), there is a one-to-one relationship between E and $\mu_c = \cos(\Theta_c)$ in the range of $E \in [\alpha E', E']$, thus

$$P(E' \to E)\mathrm{d}E = P(\mu_c)\mathrm{d}\mu_c \tag{13}$$

or

$$P(\mu_c) = P(E' \to E)\frac{\mathrm{d}E}{\mathrm{d}\mu_c}. \tag{14}$$

Multiplication of Eq. (2) by E', followed by differentiation, yields

$$\frac{\mathrm{d}E}{\mathrm{d}\mu_c} = \frac{1}{2}(1-\alpha)E' \tag{15}$$

Evaluating μ_c for E at the limits $\alpha E'$ and E' gives the support for $P(\mu_c)$, defined for $\mu_c \in [-1, 1]$. Substitution of the above equation and Eq. (5) into Eq. (14) gives the PDF in the COM frame

$$P(\mu_c) = \frac{1}{(1-\alpha)E'}\left(\frac{1}{2}(1-\alpha)E'\right) = \frac{1}{2}, \quad \mu_c \in [-1, 1] \tag{16}$$

We must now transform to the lab frame scattering cosine μ_0. First, we solve Eq. (4) for μ_0 in terms of μ_c as follows:

$$\tan^2\theta_L = \left(\frac{A\sin\theta_c}{1+A\cos\theta_c}\right)^2 \tag{17}$$

$$\sec^2\theta_L - 1 = \left(\frac{A\sin\theta_c}{1+A\cos\theta_c}\right)^2 \tag{18}$$

$$\mu_0^{-2} = \frac{A^2(\sin^2\theta_c+\cos^2\theta_c)+1+2A\mu_c}{(1+A\mu_c)^2} \tag{19}$$

$$\mu_0 = \frac{1+A\mu_c}{\sqrt{1+2\mu_c A+A^2}}. \tag{20}$$

Solution of the above equation for μ_c in terms of μ_L gives

$$\mu_c = -\frac{1}{A}(1-\mu_0^2)+\mu_0\sqrt{1-\frac{1}{A^2}(1-\mu_0^2)}\,. \tag{21}$$

Eq. (20) demonstrates a one-to-one relationship between μ_0 and μ_C. As before,

$$P(\mu_0) = P\left(\mu_C(\mu_0)\right)\frac{\mathrm{d}\mu_c}{\mathrm{d}\mu_0}. \tag{22}$$

Differentiation of Eq. (21) with respect to μ_0 and algebraic manipulation ultimately yields

$$\frac{\mathrm{d}\mu_c}{\mathrm{d}\mu_0} = \frac{2\mu_0}{A}+\frac{1-\frac{1}{A^2}(1-2\mu_0^2)}{\sqrt{1-\frac{1}{A^2}(1-\mu_0^2)}}. \tag{23}$$

Substitution of the above equation and Eq. (16) into Eq. (22) gives an expression for $P(\mu_0)$. The final expression for the scattering kernal is, for $A>1$

$$\boxed{K(\mu_0,E'\to E) = \begin{cases}\left[\frac{\mu_0}{A}+\frac{1-\frac{1}{A^2}(1-2\mu_0^2)}{2\sqrt{1-\frac{1}{A^2}(1-\mu_0^2)}}\right]\delta(E-f_E\left(\mu_c(\mu_0),E'\right)), & \mu_0\in[-1,1]\\ 0, & \text{otherwise}\end{cases}}. \tag{24}$$

where the support is from evaluation of Eq. (20) at $\mu_c=-1,1$. The case of $A=1$ must be treated separately. This can be seen, for instance, because evaluation of Eq. (20) at $\mu_c=-1$ results in an indeterminant $0/0$. Evaluation of Eq. (21) for $A=1$ gives a non-indeterminant expression for μ_0 as

$$\mu_0 = \sqrt{\frac{1+\mu_c}{2}} \tag{25}$$

Thus, the support becomes $\mu_0\in[0,1]$. The kernel also simplifies significantly at $A=1$. The final scattering kernel, for the case of $A=1$, is

$$\boxed{K(\mu_0,E'\to E) = \begin{cases}2\mu_0\,\delta(E-f_E\left(\mu_c(\mu_0),E'\right)), & \mu_0\in[0,1]\\ 0, & \text{otherwise}\end{cases}}. \tag{26}$$

which is PDF normalized over μ_0 and E.

Plots for A=1

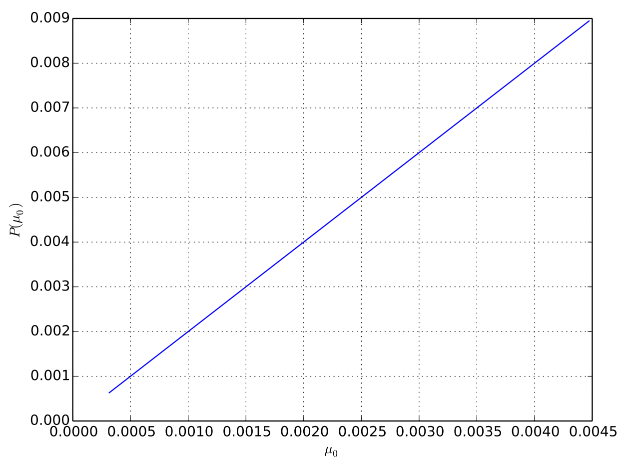
To plot in terms of energy, we evaluate Eq. (2) at $A = 1$, giving

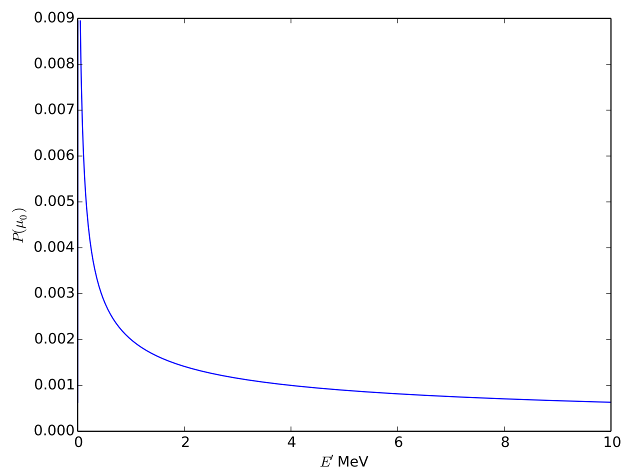
$$\frac{E}{E'} = \frac{1+\mu_c}{2}. \tag{27}$$

Then, using Eq. (25), μ_0 in terms of E and E' is

$$\mu_0 = \sqrt{\frac{E}{E'}}. \tag{28}$$

A plot of $P(\mu_0)$ vs μ_0 and $P(\mu(E', E))$ vs E' are given below. The values of E' range between 0.05 MeV to 10 MeV, with E fixed at 1 eV. As expected, lower energy neutrons are more likely to scatter to 1 eV.





References

[1] W.L. Dunn and J.K. Shultis, *Exploring Monte Carlo Methods*, 2012.

Problem 3:

The problem details are given on the second page.

Solution:

Description of code

The angular flux ψ is computed by tracing characteristics as discussed in class. To compute points of intersection, the ray and surfaces of intersection are written in parametric form. The position of a particle in the projected $x-y$ plane is denoted $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}}$. Since we want to trace upstream, the parametric equation for the particle position is given by

$$\mathbf{r} = (x_{i-1} - \Omega_x s)\hat{\mathbf{i}} + (y_{i-1} - \Omega_y s)\hat{\mathbf{j}} \tag{29}$$

where $\mathbf{r}_{i-1}$ is the previous location, s is a parameter that corresponds to the signed distance the particle has traveled, and

$$\Omega_x = \sin(\theta)\cos(\phi) \tag{30}$$

$$\Omega_y = \sin(\theta)\sin(\phi). \tag{31}$$

The parametric equation for each of the surfaces in the problem as a function of x and y are given in Table 1. These equations are then evaluated with $x = x_{i-1} - \Omega_x s$ and $y = y_{i-1} - \Omega_y s$ and solved for s algebraically. The smallest positive value of s from each equation, excluding surfaces where a solution does not exist, corresponds to the next point of intersection. If we were already at a surface, then that solution will give $s = 0$. Care is taken to exclude this solution, accounting for potential roundoff.

Table 1: Parametric equations for surfaces in problem.

Surface	$f(x, y) = 0$
Fuel	$x^2 + y^2 - R_{\text{fuel}}^2 = 0$
Left Boundary	$x - x_{\min} = 0$
Right Boundary	$x - x_{\max} = 0$
Bottom Boundary	$y - y_{\min} = 0$
Top Boundary	$y - y_{\max} = 0$

The particle is moved to the new location, and the number of mean free paths travelled $\tau_i = s_i \Sigma_t(x, y)$ along the i-th path is computed. The total number of MFP traveled up to the latest point s_i is accumulated as $\tau_{\text{tot},i} = \sum_{k=1}^{i} \tau_k$. Because the transport equation is linear, we can consider the contribution from each fuel element to the angular flux separately. If the i-th path traced to point $\mathbf{r}_i$ was across a fuel element, then a contribution is made to the flux. If the path of length s_i crossed the j-th fuel element, the contribution to the flux from that fuel element is computed as

$$\psi_j = \frac{Q e^{-\tau_{\text{tot},i-1}}}{4\pi \Sigma_{t,F}} \left(1 - e^{-\Sigma_{t,F} s_i}\right) \tag{32}$$

where $\tau_{\text{tot},i-1}$ does not include attenuation across the fuel because that attenuation was included in solution for the term in parenthesis.

Finally, if the particle had hit a boundary, the corresponding coordinate is translated to the opposing boundary, taking care to handle roundoff issues and corners. For example, if the right boundary is hit at point $\mathbf{r} = x_{\max}\hat{\mathbf{i}} + y_1\hat{\mathbf{j}}$, the particle is moved to $\mathbf{r} = x_{\min}\hat{\mathbf{i}} + y_1\hat{\mathbf{j}}$. The process outlined above is repeated for all directions Ω and positions of interest.