NRE7203 Homework 1
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Neutron Transport with Monte Carlo Assignment

Problem 1: List the three main disadvantages of delta tracking (DT) compared to the surface tracking method. Provide two distinct examples (related to specific reactors, fuel, etc.) on the deterioration in performance of the DT approach.

Solution: The delta tracking (DT) approach for Monte Carlo simulations develops disadvantages in situations to be discussed below.

1. Considering a heterogenous domain with largely dissimilar macroscopic cross sections, it is likely that the majorant cross section is much larger than the average macroscopic cross sections in the domain. To accept a collision as a real collision, the following inequality must be satisfied,
$$\xi_2 < \frac{\Sigma_{t,m}}{\Sigma_{t,maj}} \tag{1}$$
where $\xi_2 \in unif[0,1]$. Therefore, if the majorant cross section is significantly larger than the total macroscopic cross sections in the domain, the number of virtual collisions required for a real collision to occur increases. Thus, the efficiency of the method is reduced.
2. The DT method is unlike the surface tracking (ST) method in that it does not track surface crossings. As a result, the DT method is incapable of calculating the Track Length Estimator (TLE) given by
$$R_x = \sum_i L_i \Sigma_x(E_i) \tag{2}$$
where L_i is the i^{th} neutron pathlength and Σ_x is the specific reaction. However, this calculation requires knowledge of the pathlength of the neutron through each material crossed. Thus, the DT method is unable to calculate this quantity and must rely on the Collision Flux Estimator (CFE).
3. DT tends to underestimate integral flux and overestimate the homogenized total cross section. The integral flux is underestimated because DT methods must use the CFE, which fails to account for neutrons that do not undergo reactions in a given volume. Therefore, variance in the neutron flux tends to be higher, especially in regions where interaction probabilities are low (e.g. transparent materials, voids).

These disadvantages manifest in regions where large voids are present or in the presence of heavy absorbers. For example, Prismatic HTGR designs have helium coolant channels which are represented as voids. In regions near the void, one expects the CFE to underestimate integral flux while using DT methods. Similarly, benefits of the DT method depreciate in a region with a heavy absorber such as near a control rod in a fuel element.

Problem 2: Provide a more rigorous explanation of how implicit absorption preserves a fair game.

Solution: Implicit absorption implies explicit absorption is removed from the Monte Carlo simulation. However, interactions that would have resulted in an absorption, thus terminating the neutron, are treated by a reduction in the neutron's statistical weight. In an analog game, the tally for interactions directly accounts for neutron absorption in a binary scoring system. If the neutron is absorbed, its history is terminated and the next neutron random walk is considered.

With implicit absorption, applied in a weighted delta tracking routine, the tally is not considered to be binary. A score is added to the tally based on the "weight" of the neutron in the given region. Since the neutron does not undergo explicit absorption, the only mechanism to terminate the neutron is via leakage. To prevent this, neutrons with statistical weight below a set threshold are subject to Russian Roulette to determine survival. By using Russian Roulette, the survival of the neutron is determined in an unbiased way thus preserving the fair game. Furthermore, upon the neutron surviving Russian Roulette the neutron's weight is restored to provide higher weight to those neutrons that survive.

Problem 3: Use the workshop and implement the weighted delta tracking routine (with Russian Roulette). Describe the methodology (for weighted delta tracking) and compare the results of weighted delta tracking with surface tracking and delta tracking results.

Solution: Weighted delta tracking utilizes the majorant cross section as defined in the delta tracking algorithm. The majorant cross section takes the form of

$$\Sigma_{maj} = \max(\Sigma_{t,i}) \tag{3}$$

where the *i* index represents the material region. For the specified problem, it is assumed that the neutrons are born from a point source at the origin. Each neutron is thus born with an initial position of $\boldsymbol{x} = (0, 0, 0)$. In the nonanalog game, the neutron is born with a weight of unity.

With the initial neutron position and weight specified, the neutron streams a distance given by

$$S = -\frac{\ln(\xi)}{\Sigma_{maj}} \tag{4}$$

before a collision occurs. The direction in which the neutron traveled is determined by randomly sampling for the polar and azimuthal direction as

$$\begin{gathered} \theta = \cos^{-1}(1 - 2\xi) \\ \phi = 2\pi\xi \end{gathered} \tag{5}$$

and then calculating the new components of the neutron position following streaming as

$$\begin{gathered} x = r\sin(\theta)\cos(\phi) + S\sin(\theta')\cos(\phi') \\ y = r\sin(\theta)\sin(\phi) + S\sin(\theta')\cos(\phi') \\ z = r\cos(\theta) + S\cos(\theta') \end{gathered}$$

The random numbers are uniformly distributed in the range $\xi \in [0,1]$ and each random variable sampled is sampled using a different random number. Separate random numbers are also used to sample the direction in which the neutron streams a distance of *S*. Unlike the DT algorithm, each time the neutron travels a distance *S*, part of the neutron is implicitly absorbed while the remainder is considered scattered. After each distance *S*, the neutron's weight is reduced by

$$w_{i+1} = w_i\left(1 - \frac{\Sigma_t}{\Sigma_{maj}}\right) \tag{6}$$

while the neutron weight that contributes to the flux tally is given by

$$w_i\left(\frac{\Sigma_t}{\Sigma_{maj}}\right) \tag{7}$$

To account for the regions the neutron passes between collisions, two indices are tracked. First, an index is used to track the region in which the neutron started streaming. The second index represents the region where the collision occurred.

As the neutron weight is reduced through collisions, a check is performed based on a predetermined threshold weight. Below this threshold weight, Russian Roulette is played. A survival probability is calculated as

$$P_{survive} = \frac{w_{i+1}}{w_o} \tag{8}$$

and a random number is drawn between zero and one. If the random number is less than $P_{survive}$ the neutron weight is restored to unity (w_o) and the neutron continues a random walk. Otherwise, the neutron will terminate.

For those neutrons that survive Russian Roulette, the neutron position is updated and the cycle is repeated. If at any time the neutron's position places it outside of the defined regions, the neutron's weight is added to the flux tally for all regions.

Using this methodology, three cases are examined to assess the performance of weighted delta tracking (WDT) compared to ST and DT. This first case considers ten concentric spherical regions each with a randomized macroscopic total cross section between 0.10 and 0.25 cm^{-1}. For the first case, the cross sections are shown in the Figure 1 below.

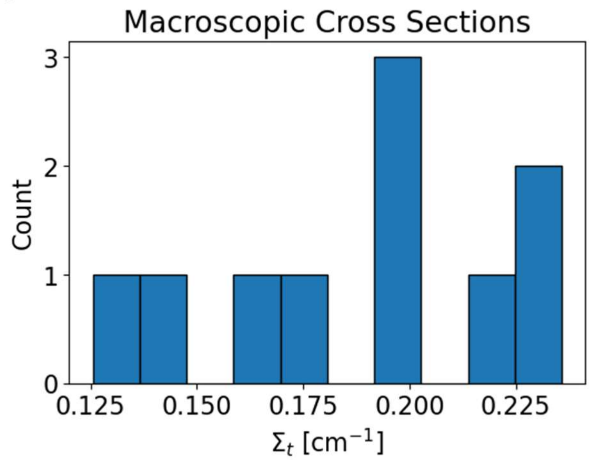


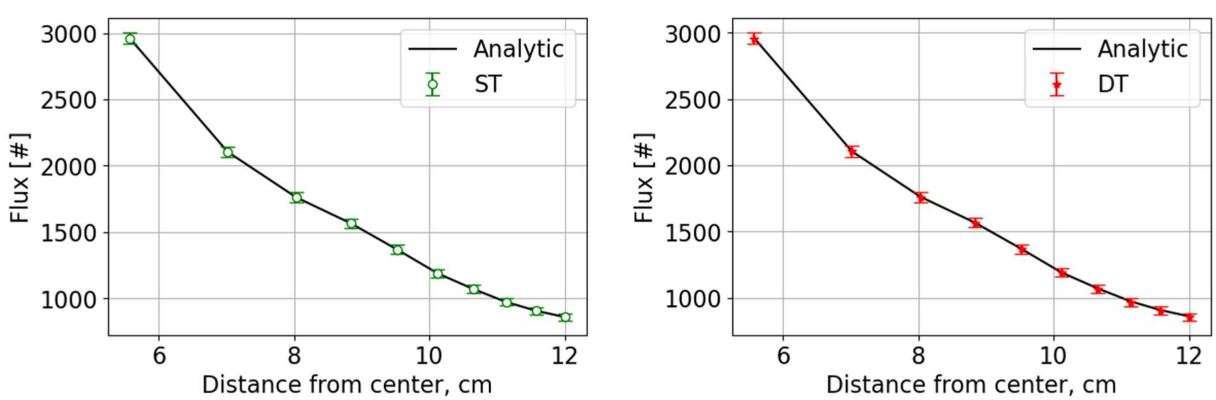
Figure 1. Case 1 macroscopic cross sections.

An analytical solution is developed to provide comparison between the Monte Carlo algorithms. Each algorithm performs the Monte Carlo simulation with the same cross sections, regions, radii, source, and number of simulations performed. The first case is performed using the following simulation conditions.

Table 1. Case 1 and 2 Simulation Conditions.

Simulations	Regions	External Radius [cm]	Source [# neutrons]
100	10	12.0	10000

The resulting flux for ST, DT, and WDT are plotted with the analytical solution with associated error for the simulated flux in each region. The ST and DT algorithms are in good agreement with the analytical flux throughout all regions. The WDT algorithm appears to converge to the analytical solution in the outer regions but tends to underpredict the flux near the source. Flux distributions are provided in Figure 2.



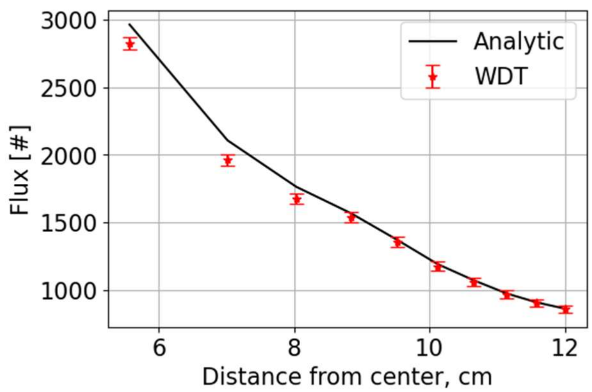


Figure 2. Case 1 flux plots for ST (top left), DT (top right), and WDT (bottom).

In the second case, a cross section of 3 cm^{-1} is defined for the seventh region while the other regions maintain their random uniform distribution between 0.1 and 0.25 cm^{-1}. The same conditions as described by Table 1 are implemented for all algorithms. The cross sections used are shown in Figure 3.

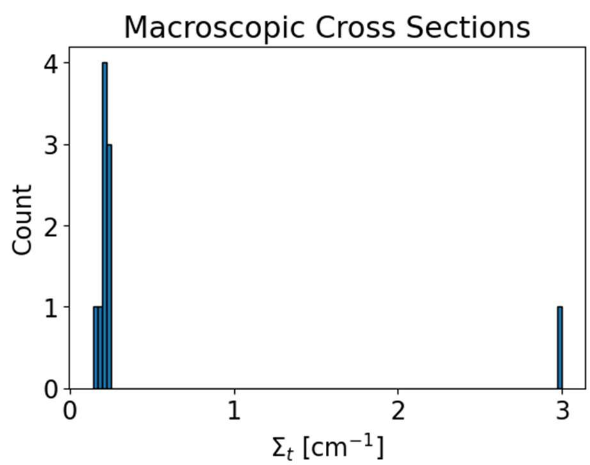
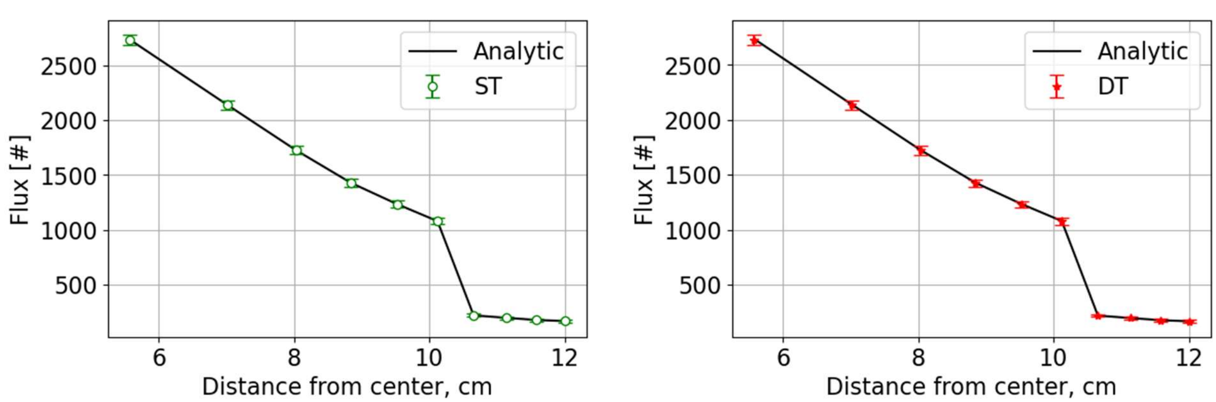


Figure 3. Case 2 macroscopic cross sections.

The resulting flux distributions are shown in Figure 4. A large reduction in neutron flux is seen across the seventh region which is consistent with expectations. Neutrons have a higher probability of absorption through this region thus reducing the flux in subsequent regions. This is captured by the analytic solution. Both the ST and DT algorithms capture this reduction in flux. The WDT algorithm significantly underpredicts the flux prior to the large cross section region and then converges toward the analytic solution.



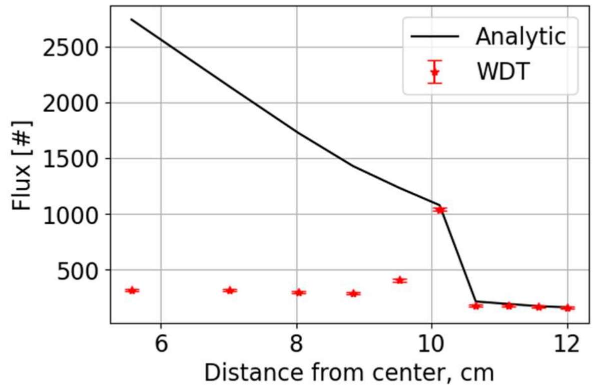


Figure 4. Case 2 flux plots for ST (top left), DT (top right), and WDT (bottom).

The third case considers 30 regions over which the cross sections are randomized between 0.1 and 0.25 cm^{-1}. The simulation conditions used are provided in Table 2. The cross sections used are provided in Figure 5. Both the ST and DT methods track well with the analytic solution. The WDT method again underpredicts flux in the inner regions but then converges to the analytic solution in the outer regions. The flux plots for case three are provided in Figure 6.

Table 2. Case 3 Simulation Conditions.

Simulations	Regions	External Radius [cm]	Source [# neutrons]
100	30	12.0	10000

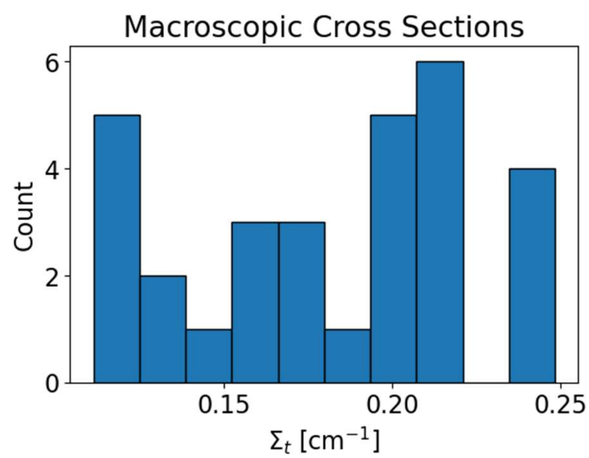


Figure 5. Case 3 macroscopic cross sections.

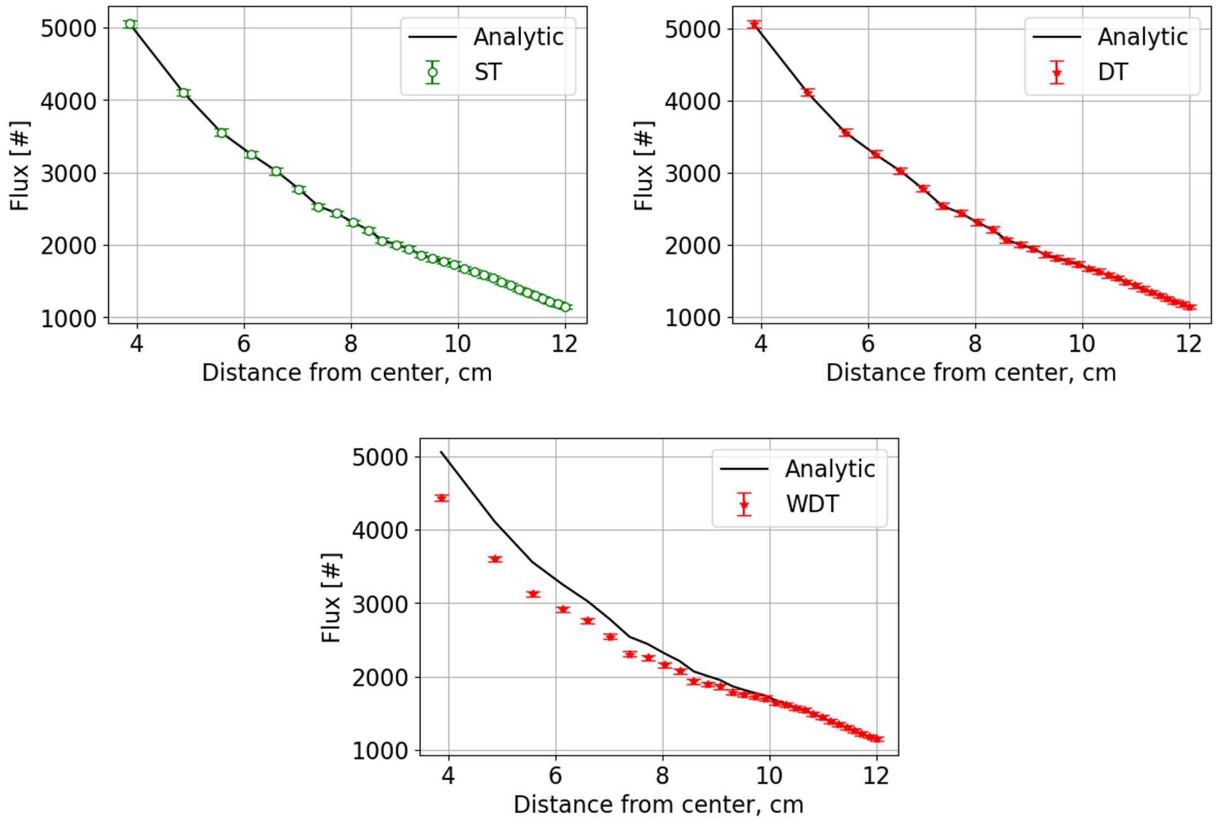


Figure 6. Case 3 flux plots for ST (top left), DT (top right), and WDT (bottom).

A summary of results is provided in Table. The figure of merit (FoM) is calculated as

$$FoM = \frac{1}{\sigma_{flux}^2 T} \tag{9}$$

The variance, σ_{flux}^2, is measured between successive simulations to measure spread in flux data. The time, T, is the time required to complete all simulations using a given algorithm.

Table 3. Comparison of ST, DT, and WDT results across cases.

Case 1	ΔLeakage [%]	Runtime [s]	σ_{flux}	FoM
ST	0.01	22.85	45.48	2.12E-5
DT	0.04	20.54	45.42	2.36E-5
WDT	0.02	25.58	44.49	1.98E-5
Case 2				
ST	0.00	21.33	46.12	2.20E-5
DT	0.00	89.64	46.62	5.13E-6
WDT	0.00	203.66	9.62	5.31E-5
Case 3				
ST	0.03	39.01	50.44	1.01E-5
DT	0.01	22.20	53.69	1.56E-5
WDT	0.04	27.75	40.69	2.18E-5

The leakage difference above is calculated based on the analytic leakage for each case. In case 2, the large macroscopic cross section in the seventh region clearly impacts the efficiency of the DT and WDT algorithms. This is consistent with the expectation that DT performance is degraded near heavy absorbers. The number of virtual collisions reduces simulation efficiency. Similarly, the WDT algorithm is significantly impacted by the heavy absorber. Since the majorant cross section directly impacts the neutron weight reduction many neutrons undergo Russian Roulette in the inner shells, thus reducing the flux tally. The DT and WDT algorithms perform well in case 3. The ST algorithm requires calculating new positions and random numbers at every surface crossed, therefore reducing the efficiency. The DT and WDT algorithms have improved speed and FoM when compared to the ST algorithm. In comparison, the ratio of FoM between DT and ST is 1.54 and the ratio between WDT and ST is 2.16.

The WDT and DT routines perform well for case 1 and 3 but have reduced efficiency and inaccurate results. Specifically, the WDT method underestimates the flux tally in the inner regions before reaching the region with the large cross section. It is possible that this is caused by the large majorant cross section developing conditions where neutrons in the inner regions as terminated early before having a chance to contribute to the tally. A possible improvement could be reducing the weight threshold or restoring neutron weights to a higher value for those that survive roulette. An additional unexpected result is the low FoM across all cases. The variance in flux across all simulations is consistently on the order of 10^3 which drives the FoM low values. The variance could be reduced by performing more Monte Carlo simulations, thus increasing the sample size for the variance calculation.

In summary, surface tracking, standard delta tracking, and weighted delta tracking were analyzed against analytic solutions to neutron transport through concentric spherical shells with heterogenous macroscopic cross sections. By varying the number of shells and the macroscopic cross sections, the differences between solution methods were identified. Delta tracking and weighted delta tracking were penalized in case 2 due to the insertion of a large macroscopic cross section. Surface tracking was penalized when the number of regions, therefore surfaces, was increased. From these results, the times in which one uses different algorithms is dependent on the physical system modeled.