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Multi-Regional Delta-Tracking Method for Neutron Transport Tracking in Monte Carlo Criticality Calculation

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Abstract: The Monte Carlo method has been widely used as a standard method to perform neutron transport simulations in reactor physics. In conventional Monte Carlo codes corresponding to the neutron transport tracking with ray-tracing method, the distances to material boundaries must be computed frequently when the neutron changes its kinetic energy or moving into new material regions to determine the neutron transport length. However, if the neutron's mean free path length, to some extent, is greater than the macro size of the model, a huge amount of distances need to be computed. As a result, the computational efficiency of the neutron transport tracking will be degraded. An improved multi-regional delta-tracking method based on domain decomposition was introduced to solve this problem, in which the original heterogeneous model would be decomposed into many sub-regions and each sub-region was tracked using a local delta-tracking method. Consequently, the computational efficiency of the neutron transport tracking can be improved theoretically without the unnecessary distance calculations. The improved multi-regional delta-tracking method was incorporated into the MOSRT system, which is a multi-objective modeling and simulation platform for radiation transport system. Finally, the method was validated using the criticality benchmarks and its accuracy and efficiency were demonstrated in Monte Carlo criticality calculation. The results indicated that the new method was consistent with the conventional methods, but with a more competitive run-time performance.

Keywords: Monte Carlo; neutron tracking; multi-regional; delta-tracking; criticality calculation

1. Introduction

The Monte Carlo method has been widely used as a standard method to perform neutron transport simulations in reactor physics for its distinct features. The biggest advantages of the Monte Carlo method to simulate neutron transport in criticality calculation include essentially exact representation of geometrical configurations and physical phenomena that are important for reactor physics analysis. This means that the Monte Carlo method can perform complicated neutron transport problems in whole-core criticality calculation with arbitrary geometrical complexities and arbitrary physical complexities. These key features and advantages indicate that the Monte Carlo method is a very high-resolution and high-fidelity method for neutron transport simulations, which makes it a potential candidate for the next-generation advanced reactor physics methods [1,2]. However, one of the biggest disadvantages of the Monte Carlo method is that it is time-consuming for neutron transport simulations, especially for large scale whole-core analysis for realistic reactors. Actually, a large proportion of the runtime, typically accounting for 30–80% [3,4] of the total runtime, is consumed on the neutron

transport tracking process, which has been demonstrated to be one of the principle performance bottlenecks for modern Monte Carlo neutron transport simulations. Thus, the optimization methods for neutron transport tracking are of great significance to promote the computational efficiency of Monte Carlo simulations. To overcome this shortcoming and improve the efficiency of the conventional Monte Carlo method, an improved multi-regional delta-tracking method (MRDT) was proposed to solve this problem. Consequently, the computational efficiency of the neutron transport tracking can be improved theoretically without the unnecessary distance calculations. As the neutron transport tracking process was optimized with the MRDT method, some efficiency gains could be achieved in Monte Carlo simulations.

2. Conventional Neutron Transport Tracking Methods

2.1. Conventional Ray-Tracing Tracking (CRTT) Method

The basic principle [5] of the Monte Carlo method is to simulate a neutron from its birth (i.e., emitting from a neutron source) to eventual death (i.e., absorbed or escaping outside of the system), which is called a neutron history. When a neutron is simulated in a nuclear reactor with the Monte Carlo method, the neutron history can be specified with a series of status quantities. The status quantity can be denoted as $S = (r, E, \Omega)$, where $r = (x, y, z)$ is the spatial coordinate, E is the kinetic energy, and $\Omega = (u, v, w)$ is the flying direction of the neutron. Supposing that a source neutron emitting from a neutron source with its initial status $S_0 = (r_0, E_0, \Omega_0)$, the neutron will then transport in the system and interact with the materials, after m ($m \geq 1$) times interactions, the neutron status can be denoted as $S_m = (r_m, E_m, \Omega_m)$, where r_m is the spatial coordinate, E_m is the kinetic energy, and Ω_m is the flying direction of the m-th neutron status. Thus, a neutron history in a Monte Carlo simulation can be specified with a status sequence, that is, $S_0, S_1, S_2, \ldots, S_{M-1}, S_M$. As a result, the principle of the Monte Carlo neutron transport method is, given the m-th neutron status S_m, to determine the next status S_{m+1}, and then all the status quantities in a neutron history can be completely obtained with an analogy method. In Figure 1, given the status $S_m = (r_m, E_m, \Omega_m)(m = 0, 1, 2 \ldots)$, the neutron transport tracking needs to be done to determine the next status $S_{m+1} = (r_{m+1}, E_{m+1}, \Omega_{m+1})$. One of the most important tasks of the neutron transport tracking is to determine the transport length L, which is the distance between two successive collision sites r_m and r_{m+1}.

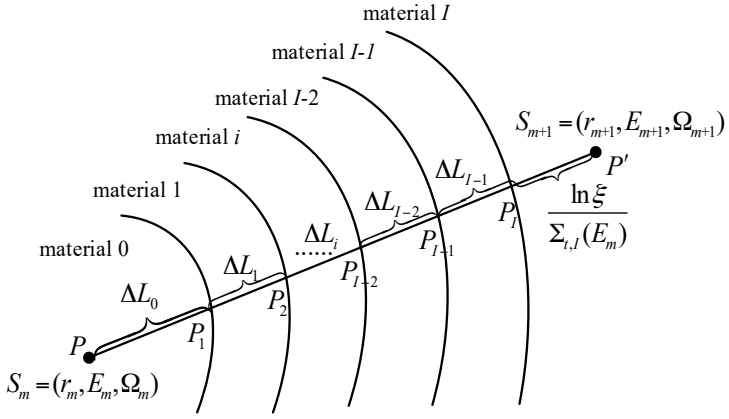


Figure 1. Conventional neutron transport tracking method in the Monte Carlo simulation.

The relationship between r_m and r_{m+1} can be denoted as $r_{m+1} = r_m + L\Omega_m$. In neutron transport theory, the distribution of neutron transport length satisfies the following probability density function (PDF):

$$f(L) = \Sigma_t(r_m, E_m) \cdot \exp\{-\int_0^L \Sigma_t(r_m + l\Omega_m, E_m)dl\} \quad L > 0 \tag{1}$$

where Σ_t is the macroscopic cross section and l is the neutron flying distance. As shown in Equation (1), when a neutron is simulated in a homogeneous material region, the neutron transport length L can be sampled randomly with the following equation:

$$L = -\frac{\ln \xi}{\Sigma_t(E_m)} \tag{2}$$

where ξ is a pseudo random number between 0 and 1. However, when a neutron transports in heterogeneous material regions, as shown in Figure 1, the neutron maybe cross over several material boundaries in one step. Under this circumstance, the neutron transport length should be determined using Equation (3), which is called conventional ray-tracing tracking (CRTT) method.

$$L = \sum_{i=0}^{I-1} \Delta L_i + \left(\frac{-\ln \xi}{\Sigma_{t,I}(E_m)} \right) \tag{3}$$

where ΔL_i is the traveled distance by the neutron in the I-th material region, and $\Sigma_{t,I}(E_m)$ is the total macroscopic cross section of the I-th material region for the neutron with kinetic energy E_m. Therefore, to determine the neutron transport length L, as given in Equation (3), for the Monte Carlo simulation in heterogeneous models (i.e., assemblies, realistic reactors), all the distances ΔL_i need to be calculated by solving a large amount of simultaneous equations, which are established by using the neutron's trajectory (i.e., ray-tracing) equation and the boundary surface equations. In the conventional neutron transport tracking method, when the neutron's mean free path length is greater than the macro size of the model, a large amount of distance calculations will degrade the run-time performance of the neutron transport tracking, which has been demonstrated to be one of the principle performance bottlenecks for the modern Monte Carlo simulations.

2.2. Single-Regional Delta-Tracking (SRDT) Method

To improve the run-time performance of the CNNT method, a new neutron transport tracking method called delta-tracking method was proposed by Woodcock [6] to optimize the neutron transport tracking for achieving some efficiency gains in the Monte Carlo simulation. In the conventional delta-tracking method, the heterogeneous model (i.e., reactor assembly), consisting of more than one material region, will be virtually homogenized into a single homogeneous model, not physically homogenized the model as that done in deterministic method, which is also called as the single-regional delta-tracking (SRDT) method. The basic principle of the SRDT method is that, for each material in the heterogeneous model, a part of virtual cross section will be added to the material's physical cross section, and then the total cross section will be equal to the maximum of all cross sections in the model. As a result, the neutron will see a virtual homogeneous model, in which the neutron transport length can be directly sampled using Equation (2) without unnecessary distance calculations, as those done in the CRTT method shown in Equation (3). Thus, some efficiency gains corresponding to the neutron transport tracking using SRDT method can be achieved in Monte Carlo simulations.

Figure 2 shows an example of neutron transport tracking process in the SRDT method. Supposing that a model consists of I kinds of materials, given the neutron energy E_m, the corresponding physical total cross sections for all materials can be denoted as $\Sigma_{t,1}$, $\Sigma_{t,2}$, $\Sigma_{t,3}$, ... , $\Sigma_{t,I}$. Then, the cross sections for all materials will be treated as follows:

$$\Sigma_{t,\max} = \max\{\Sigma_{t,1}, \Sigma_{t,2}, \Sigma_{t,3}, \ldots, \Sigma_{t,I}\} \tag{4}$$

$$\Sigma_{t,\max} = \Sigma_{t,1} + \Sigma_{1,\delta} = \Sigma_{t,2} + \Sigma_{2,\delta} = \ldots = \Sigma_{t,I} + \Sigma_{I,\delta} \tag{5}$$

where $\Sigma_{t,max}$ is the maximum of all total physical cross sections in the model. The added cross sections, $\Sigma_{1,\delta}$, $\Sigma_{2,\delta}$, $\Sigma_{3,\delta}$, ... , $\Sigma_{I,\delta}$, are virtual cross sections, which can be interpreted as the virtual reaction probabilities for neutrons tracked with the SRDT method. Consequently, the original heterogeneous

model can be treated as a homogeneous material region, in which the neutron transport length can be directly sampled using Equation (6):

$$L = -\frac{\ln \xi}{\Sigma_{t,\max}} \tag{6}$$

Comparing Equations (3) and (6), we can conclude that the run-time performance of the neutron transport tracking will be optimized for avoiding unnecessary distance calculations. However, as the virtual cross sections are added to the total cross sections, to guarantee the physical accuracy of the neutron's behavior, the nuclear reactions should be divided into virtual reactions and real reactions (i.e., physical reactions) when a neutron interacts with a specific nuclide at a collision site. When a virtual reaction takes place, the neutron's status will be not changed and it will continue moving forward without changing its flying direction and kinetic energy. The reject sampling technique (RST) will be utilized to distinguish the virtual and real reactions in the SRDT method. The basic procedures of SRDT method for neutron transport tracking are as follows:

(a) Given the neutron kinetic energy E, the maximum total cross section, $\Sigma_{t,max}$, for all materials in the model firstly should be calculated with Equation (4), and the corresponding virtual cross section for each material will be determined with Equation (5).

(b) The neutron transport length L will be calculated with Equation (6).

(c) When a neutron moves forward one step with a transport length L, the RST will determine whether the following condition is satisfied.

$$\xi_1 < \frac{\Sigma_{t,i}}{\Sigma_{t,\max}} \tag{7}$$

where $\Sigma_{t,i}$ is the physical total cross section of the i-th material, in which the neutron is currently located, and ξ_1 is a random number between 0 and 1. If Condition (7) is satisfied, a real reaction will be taken place at the current collision site, after that, the neutron will continue its transport for next step, and then return to Procedure (a).

(d) If Condition (7) is not satisfied, a virtual reaction will take place at the current site. Then, the neutron will continue its next transport step without changing its flying direction and kinetic energy, and then return to Procedure (b).

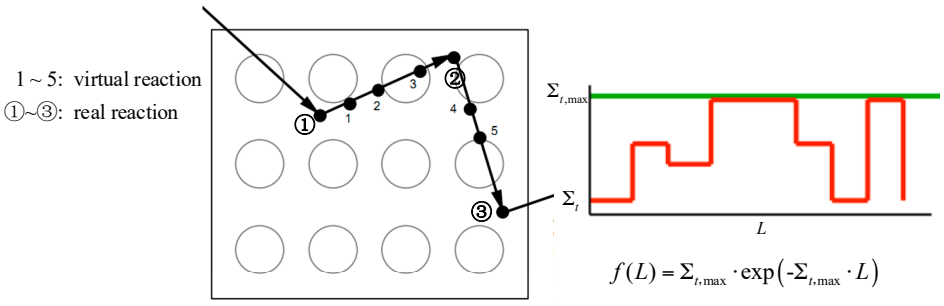


Figure 2. Neutron transport tracking based on the single-regional delta-tracking method.

3. Multi-Regional Delta-Tracking (MRDT) Method

3.1. Basic Principle

However, one of the biggest disadvantages of the SRDT method is that the run-time performance of the SRDT-based neutron transport tracking deteriorates [7,8] when the model has a high level of material heterogeneity, that is, when the material total cross sections differ significantly from each other. This is not a rare case for LWR (light water reactor), BWR (boiling water reactor), and HTGR (high temperature gas-cooled reactor) models. A typical example is an LWR fuel assembly that contains

localized heavy absorbers (i.e., specific materials with huge absorption cross sections for thermal neutrons), such as control rods or burnable absorber pins. The absorber cross section dominates the maximum total cross section $\Sigma_{t,max}$ at a low energy, even though the absorber material occupies a relatively small fraction of the total volume. Sometimes, the material physical total cross section $\Sigma_{t,i}$ outside the heavy absorber is two orders of magnitude below the maximum total cross section $\Sigma_{t,max}$ at a low energy, which will make the situation even worse. From a quantitative view, as the physical total cross section satisfies $\Sigma_{t,i} \ll \Sigma_{t,\max}$, the result is that Condition (8) will be satisfied approximately.

$$\frac{\Sigma_{t,i}}{\Sigma_{t,\max}} \approx 0 \tag{8}$$

As a result, the probability of sampling a real collision in the RST procedure becomes low outside the absorber. Meanwhile, the trajectory of the neutron will be cut into a greater number of short steps, which means that for each real collision, the neutron undergoes many virtual collisions that make no contribution to the results. Even worse, the computational time will be wasted in the re-sampling procedure, which will degrade the Monte Carlo simulation performance.

To overcome the shortcoming of the SRDT-based neutron transport tracking method, a novel improved multi-regional delta-tracking (MRDT) method was proposed in the paper. The basic idea of the MRDT method includes the following procedures. Firstly, the whole model is decomposed into multiple sub-regions using the geometrical surfaces bounding the sub-regions. Secondly, each sub-region will be treated as a virtual homogeneous region as that of done in the SRDT method. As a result, when the neutron is tracked in the k-th sub-region, a local $\Sigma^k_{t,\max}$ of the materials contained within the sub-region will be used to calculate the neutron transport length and perform the reject sampling process. We can see that the local $\Sigma^k_{t,\max}$ in one sub-region has no relationship with ones in other sub-regions, which will reduce the differences in physical total cross sections with the local $\Sigma^k_{t,\max}$. Consequently, the negative effect of the local heavy absorber on the neutron transport tracking will be decreased, and finally some efficiency gains will be achieved.

As an example illustrated in Figure 3a, there is a simplified reactor model consisting of four fuel assemblies, numbered 1, 2, 3, and 4. For k-th fuel assembly, it contains I_k (k = 1,2,3,4) materials. If the CRTT method is used, the original heterogeneous model, as shown in Figure 3a, will be used in the transport tracking process. If the neutron transport tracking is done using the SRDT method, the model will be virtually homogenized, as shown in Figure 3b. Therefore, the $\Sigma_{t,max}$ can be obtained with the following:

$$\Sigma_{t,\max} = \max\left\{\Sigma^1_{t,\max}, \Sigma^2_{t,\max}, \Sigma^3_{t,\max}, \Sigma^4_{t,\max}\right\} \tag{9}$$

If the neutron transport tracking is performed with the MRDT method, the model will be decomposed into four sub-regions, as shown in Figure 3c, according to the bounding surfaces of the assemblies. Then, the SRDT-based neutron transport tracking is performed in each sub-region, and the local $\Sigma^k_{t,\max}$ for each sub-region will be obtained with the following:

$$\begin{cases} \Sigma^1_{t,\max} = \max\left\{\Sigma^1_{t,1}, \Sigma^1_{t,2}, \Sigma^1_{t,3}, \ldots, \Sigma^1_{t,I_1}\right\} \\ \Sigma^2_{t,\max} = \max\left\{\Sigma^2_{t,1}, \Sigma^2_{t,2}, \Sigma^2_{t,3}, \ldots, \Sigma^2_{t,I_2}\right\} \\ \Sigma^3_{t,\max} = \max\left\{\Sigma^3_{t,1}, \Sigma^3_{t,2}, \Sigma^3_{t,3}, \ldots, \Sigma^3_{t,I_3}\right\} \\ \Sigma^4_{t,\max} = \max\left\{\Sigma^4_{t,1}, \Sigma^4_{t,2}, \Sigma^4_{t,3}, \ldots, \Sigma^4_{t,I_4}\right\} \end{cases} \tag{10}$$

where $\Sigma^k_{t,i}$ is the physical total cross section for i-th material contained within the k-th sub-region. We can see from Equations (7) and (8) that the MRDT method can decrease the negative effect of the local heavy absorbers that exist within some sub-regions on the neutron transport tracking process performed in other sub-regions, which is the central idea of the MRDT method, to optimize the run-time performance of the Monte Carlo simulations.

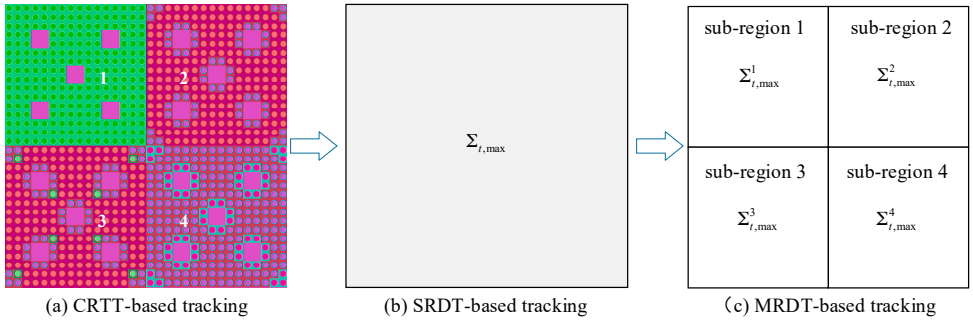


Figure 3. The model used in various neutron transport tracking methods. (**a**) CRTT—conventional ray-tracing tracking; (**b**) SRDT—single-regional delta-tracking; (**c**) MRDT—multi-regional delta-tracking.

3.2. MRDT-Based Tracking Scheme

The MRDT-based tracking scheme for the Monte Carlo neutron transport simulation is illustrated briefly in Figure 4.

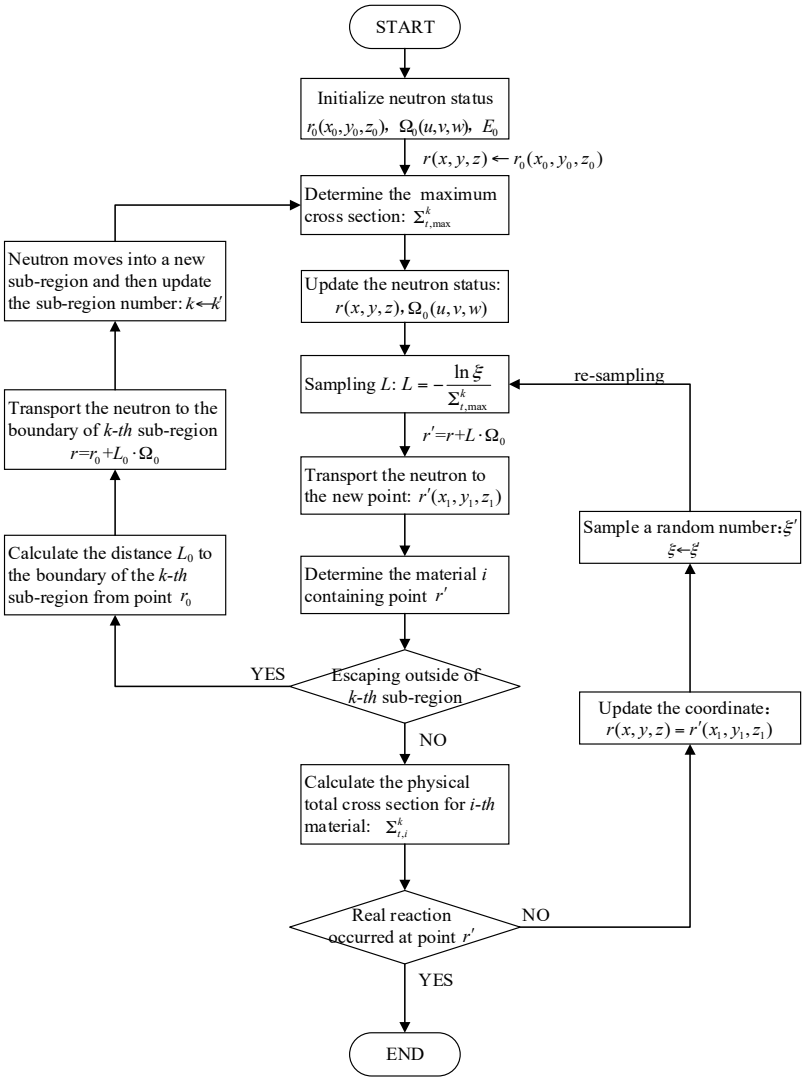


Figure 4. The MRDT-based neutron transport tracking scheme for the Monte Carlo simulation.

4. Validation and Results

The various neutron transport tracking methods, that is, CRTT, SRDT, and MRDT, are incorporated into the MOSRT system, which is a multi-objective modeling and simulation platform for radiation transport system developed by the NEAL (Nuclear Engineering and Application Laboratory) team in the University of South China [9]. To verify the accuracy and efficiency, the methods were verified using the criticality benchmarks and whole-core reactor models in Monte Carlo simulations. Firstly, forty simple criticality benchmarks introduced from the ICSBEP (International Criticality Safety Benchmark Evaluation Project) handbook were used to perform criticality calculations. Secondly, to further verify the applicability of the methods treating complicated models, three whole-core reactor models with detailed pin-by-pin configurations were also calculated. The effective multiplication factor (k_{eff}) of models were calculated and compared to show the accuracy of the methods, and the speedup ratios were given to demonstrate the efficiency.

4.1. ICSBEP Criticallity Benchmarks

The ICSBEP project was mandated through the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency's (NEA) Nuclear Science Committee (NSC) [10]. The purpose of the ICSBEP is to identify a comprehensive set of critical benchmark data for verifying the neutron transport calculation codes developed over different countries. To verify the capability of the methods for dealing with simple models, forty criticality benchmarks, which were typically critical facilities with simple geometrical configurations and material compositions, were selected from the ICSBEP handbook to perform the Monte Carlo simulations. The selected benchmarks are of models with various fuel enrichment (i.e., highly, intermediate, low), fuel type (i.e., metal, solution), and neutron spectrum (i.e., fast, thermal). According to the features of the facilities, the benchmarks were divided into four categories as follows:

(a) HMF benchmarks: highly-enrichment, metal-type fuel, fast spectrum systems.
(b) HST benchmarks: highly-enrichment, solution-type fuel, thermal spectrum systems.
(c) IMF benchmarks: intermediate-enrichment, metal-type fuel, fast spectrum systems.
(d) LST benchmarks: low-enrichment, solution-type fuel, thermal spectrum systems.

The comparisons of k_{eff} calculation results for the ICSBEP criticality benchmarks with various neutron transport tracking methods in the Monte Carlo simulation are given in Table 1. The calculation results with a standard Monte Carlo code MCNP (Monte Carlo N-Particle code) [11] were taken as the references. Meanwhile, the experimental results were also given in Table 1. From the aspect of accuracy, we can see that the results of the MRDT and SRDT method have good agreements with those of the CRTT method, and the two methods indicate 45 pcm and 121 pcm maximum deviations, respectively, compared with the CRTT method. Furthermore, Table 1 shows that the methods (i.e., MRDT, SRDT, and CRTT) incorporated in this paper give 53 pcm, 69 pcm, and 64 pcm maximum deviations, respectively, compared with the MCNP references, and the errors of the three methods compared with the references are all less than one standard deviation (i.e., σ^{MCNP}), which indicates that the testing results are consistent with the standard reference results. This means that the accuracy of the methods is demonstrated preliminarily.

Table 1. Validation of the accuracy for the International Criticality Safety Benchmark Evaluation Project (ICSBEP) benchmarks k_{eff} criticality calculations. CRTT—conventional ray-tracing tracking; SRDT—single-regional delta-tracking; MRDT—multi-regional delta-tracking.

Benchmark	Experiment	MRDT	SRDT	CRTT	MCNP
	$k_{eff}^{EXP}(\sigma^{EXP})$	$k_{eff}^{MRDT}(\sigma^{MRDT})$	$k_{eff}^{SRDT}(\sigma^{SRDT})$	$k_{eff}^{CRTT}(\sigma^{CRTT})$	$k_{eff}^{MCNP}(\sigma^{MCNP})$
hmf001	1.0000(0.00100)	0.99909(0.00055)	0.99924(0.00063)	0.99901(0.00058)	0.99907(0.00056)
hmf004	1.00200(0.00050)	1.00260(0.00060)	1.00278(0.00060)	1.00257(0.00064)	1.00250(0.00058)
hmf008	0.99890(0.00160)	0.99556(0.00057)	0.99553(0.00058)	0.99557(0.00055)	0.99590(0.00057)
hmf011	0.99890(0.00150)	0.99864(0.00054)	0.99817(0.00060)	0.99892(0.00062)	0.99854(0.00059)
hmf013	0.99900(0.00150)	0.99709(0.00056)	0.99659(0.00054)	0.99739(0.00057)	0.99692(0.00056)
hmf015	0.99960(0.00170)	0.99426(0.00055)	0.99448(0.00058)	0.99413(0.00059)	0.99455(0.00056)
hmf019	1.00000(0.00280)	1.00671(0.00062)	1.00706(0.00059)	1.00650(0.00056)	1.00699(0.00059)
hmf02611	1.00000(0.00380)	1.00437(0.00060)	1.00428(0.00060)	1.00442(0.00062)	1.00384(0.00063)
hmf034	0.99900(0.00120)	0.99818(0.00060)	0.99822(0.00063)	0.99816(0.00061)	0.99807(0.00056)
hmf069	0.99950(0.00130)	0.99921(0.00058)	0.99900(0.00056)	0.99933(0.00053)	0.99881(0.00057)
hst001	1.00040(0.00600)	0.99730(0.00074)	0.99718(0.00074)	0.99737(0.00068)	0.99735(0.00070)
hst004	1.00000(0.00320)	0.99719(0.00060)	0.99686(0.00068)	0.99739(0.00067)	0.99693(0.00063)
hst009	0.99900(0.00430)	1.00107(0.00073)	1.00166(0.00072)	1.00073(0.00067)	1.00128(0.00070)
hst010	1.00000(0.00290)	1.00106(0.00068)	1.00182(0.00066)	1.00061(0.00065)	1.00113(0.00071)
hst011	1.00000(0.00230)	1.00398(0.00067)	1.00442(0.00065)	1.00374(0.00067)	1.00438(0.00068)
hst012	0.99990(0.00580)	1.00093(0.00065)	1.00127(0.00061)	1.00073(0.00057)	1.00070(0.00061)
hst013	1.00120(0.00260)	0.99745(0.00059)	0.99682(0.00059)	0.99794(0.00058)	0.99738(0.00059)
hst020	0.99660(0.01160)	0.99099(0.00071)	0.99120(0.00071)	0.99087(0.00068)	0.99097(0.00069)
hst032	1.00150(0.00260)	0.99864(0.00050)	0.99876(0.00052)	0.99834(0.00053)	0.99827(0.00052)
hst042	0.99570(0.00390)	0.99582(0.00052)	0.99596(0.00058)	0.99574(0.00054)	0.99597(0.00055)
imf00101	1.00000(0.00090)	1.00030(0.00059)	1.00016(0.00057)	1.00039(0.00056)	1.00052(0.00059)
imf00102	1.00000(0.00090)	1.00046(0.00055)	1.00064(0.00057)	1.00035(0.00057)	1.00057(0.00057)
imf00103	1.00000(0.00030)	1.00133(0.00059)	1.00091(0.00056)	1.00158(0.00054)	1.00124(0.00058)
imf002	1.00000(0.00300)	0.99884(0.00046)	0.99847(0.00048)	0.99905(0.00049)	0.99888(0.00048)
imf00302	1.00000(0.00020)	1.00214(0.00050)	1.00191(0.00056)	1.00227(0.00052)	1.00201(0.00049)
imf00402	1.00000(0.00020)	1.00749(0.00057)	1.00778(0.00057)	1.00732(0.00057)	1.00763(0.00057)
imf00502	1.00000(0.00020)	1.00198(0.00056)	1.00141(0.00055)	1.00237(0.00050)	1.00189(0.00050)
imf00602	1.00000(0.00020)	0.99608(0.00057)	0.99543(0.00055)	0.99653(0.00052)	0.99598(0.00058)
imf00704	1.00450(0.00070)	1.00438(0.00048)	1.00479(0.00045)	1.00402(0.00048)	1.00433(0.00050)
imf009	1.00000(0.00530)	1.00999(0.00062)	1.01007(0.00066)	1.00995(0.00065)	1.01009(0.00061)
lst001	1.00000(0.00290)	1.01223(0.00069)	1.01238(0.00066)	1.01214(0.00069)	1.01244(0.00064)
lst002	1.00380(0.00400)	1.00048(0.00062)	1.00011(0.00058)	1.00076(0.00058)	1.00052(0.00056)
lst00301	1.00070(0.00390)	1.00066(0.00064)	1.00056(0.00066)	1.00072(0.00069)	1.00055(0.00060)
lst00302	1.00030(0.00420)	0.99990(0.00060)	0.99954(0.00061)	1.00012(0.00060)	0.99987(0.00060)
lst00401	0.99940(0.00080)	0.99906(0.00062)	0.99892(0.00063)	0.99914(0.00063)	0.99886(0.00061)
lst00429	0.99990(0.00090)	1.00251(0.00068)	1.00223(0.00061)	1.00267(0.00062)	1.00281(0.00062)
lst00714	0.99610(0.00090)	0.99466(0.00063)	0.99418(0.00066)	0.99494(0.00062)	0.99437(0.00063)
lst00730	0.99730(0.00090)	0.99716(0.00057)	0.99648(0.00059)	0.99756(0.00060)	0.99707(0.00063)
lst016105	0.99960(0.00130)	1.00542(0.00065)	1.00592(0.00061)	1.00512(0.00062)	1.00547(0.00064)
lst016113	0.99990(0.00130)	1.00558(0.00060)	1.00554(0.00065)	1.00561(0.00066)	1.00603(0.00067)

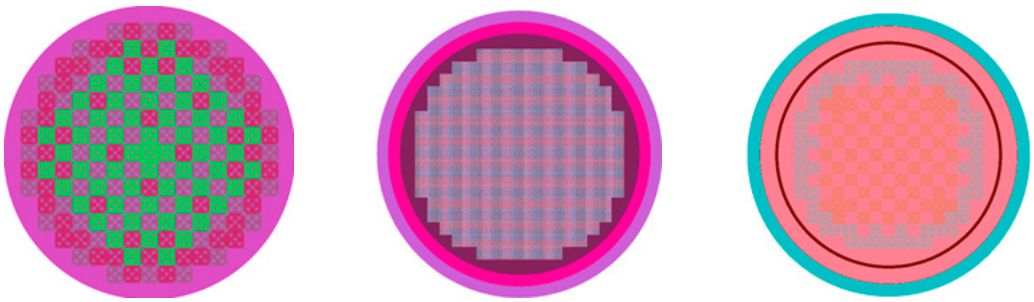
The main purpose of our work is to attempt to improve the run-time performance of the Monte Carlo simulation. The speedup ratios of MRDT and SRDT method, by comparing the total elapsed runtime with those of consumed in CRTT method, were achieved as shown in Table 2. In general, the delta-tracking method can greatly promote the Monte Carlo simulation performance in most cases, and the maximum speedup ratio achieved is approximately 1.8. It's interesting to find that the speedup ratios of MRDT method are comparable or somewhat greater than those of the SRDT method, which indicates the feasibility of the methods to achieve preliminarily efficiency gains.

Table 2. Verification of the efficiency for the ICSBEP benchmarks k_{eff} criticality calculations.

Benchmark	Speedup Ratio		Benchmark	Speedup Ratio	
	MRDT	SRDT		MRDT	SRDT
hmf001	1.18	1.12	imf00101	1.42	1.32
hmf004	1.01	1	imf00102	1.29	1.2
hmf008	1.18	1.12	imf00103	1.04	1
hmf011	1.02	1	imf002	1.42	1.32
hmf013	1.07	1.02	imf00302	1.54	1.43
hmf015	1.21	1.15	imf00402	1.41	1.31
hmf019	1.06	1	imf00502	1.25	1.17
hmf02611	1.44	1.36	imf00602	1.3	1.21
hmf034	1.08	1.02	imf00704	1.46	1.36
hmf069	1.32	1.25	imf009	1	1
hst001	1.24	1.21	lst001	1.8	1.74
hst004	1.06	1.03	lst002	1.5	1.45
hst009	1.02	1	lst00301	1.39	1.35
hst010	1.15	1.12	lst00302	1.13	1.09
hst011	1.26	1.23	lst00401	1.24	1.19
hst012	1.01	1	lst00429	1.26	1.21
hst013	1.57	1.53	lst00714	1.22	1.18
hst020	1.09	1.05	lst00730	1.12	1.08
hst032	1.58	1.54	lst016105	1.12	1.08
hst042	1.1	1.07	lst016113	1.18	1.14

4.2. Whole-Core Pin-by-Pin Reactors

To further verify the applicability of the methods treating complicated models, three whole-core reactor models with detailed pin-by-pin configurations were also calculated. The first model is of an optimized power reactor 1000 (OPR) like reactor [12], which is characterized by utilization of the combustion engineering type fuel assemblies having large water holes. There are five types of 16 × 16 fuel assemblies and 177 fuel assemblies are loaded into the core, as shown in Figure 5a. The second model is the Hoogenboom Martin (HM) model that is proposed to stimulate improvements in Monte Carlo codes and measure the performance of whole-core Monte Carlo simulations [13]. The model, as shown in Figure 5b, consists of 241 fuel assemblies arranged in a regular pattern with a maximum of 17 fuel assemblies in the X and Y directions. The third one, as shown in Figure 5c, is the most famous enchmark for evaluation and validation of reactor simulations (BEAVRS) model which is a high-detailed whole-core PWR (Pressurized-Water Reactor) model proposed by Massachusetts Institute of Technology [14]. The core lattice is made up of 193 Westinghouse optimized fuel assemblies (OFA) that each contain 264 fuel rods, 24 guide tubes, and 1 instrument tube arranged in a 17 × 17 square lattice.



(a) OPR reactor (b) HM reactor (c) BEAVRS reactor

Figure 5. The whole-core pin-by pin reactor models. (**a**) OPR—optimized power reactor; (**b**) HM—Hoogenboom Martin; (**c**) BEAVRS—benchmark for evaluation and validation of reactor simulations.

The calculation results of k_{eff} for the whole-core reactors with various tracking methods are given in Table 3 and compared with the MCNP standard reference results. The MRDT and SRDT methods give 15 pcm and 47 pcm maximum deviations, respectively, compared with the CRTT method, which indicates that the results of the two methods have good agreements with those of the CRTT method. Furthermore, Table 3 indicates that the incorporated methods (i.e., MRDT, SRDT, and CRTT) give 18 pcm, 46 pcm, and 33 pcm maximum deviations, respectively, compared with the MCNP references, and the errors of the three methods compared with the MCNP references are all less than one standard deviation (i.e., σ^{MCNP}), which indicates that the testing results are consistent with the standard reference results. This means that the accuracy of the methods is further demonstrated and the applicability of dealing with the complicated whole-core reactor models is approved to be feasible.

Table 3. Validation of the accuracy for the whole-core reactor k_{eff} criticality calculations. OPR—optimized power reactor; HM—Hoogenboom Martin; BEAVRS—benchmark for evaluation and validation of reactor simulations.

Reactor Model	MRDT	SRDT	CRTT	MCNP
	$k_{eff}^{\mathrm{MRDT}}(\sigma^{\mathrm{MRDT}})$	$k_{eff}^{\mathrm{SRDT}}(\sigma^{\mathrm{SRDT}})$	$k_{eff}^{\mathrm{CRTT}}(\sigma^{\mathrm{CRTT}})$	$k_{eff}^{\mathrm{MCNP}}(\sigma^{\mathrm{MCNP}})$
OPR	1.00610(0.00085)	1.00595(0.00105)	1.00623(0.00091)	1.00624(0.00082)
HM	1.00128(0.00059)	1.00158(0.00068)	1.00116(0.00057)	1.00112(0.00064)
BEAVRS	1.00505(0.00072)	1.00537(0.00084)	1.00490(0.00072)	1.00523(0.00068)

Meanwhile, the verification of the efficiency for the whole-core reactor models is illustrated in Table 4. We can see that the run-time performance of the MRDT method is obviously better than that of the SRDT and CRTT methods. From the quantitative view, the MRDT method gives average speedup factors of 1.4, 1.5, and 1.6 for the OPR, HM, and BEAVRS models, respectively. Furthermore, the results in Table 4 indicate that the more complicated the model is, the more competitive run-time performance will be achieved. Therefore, the applicability of the MRDT method to optimize the Monte Carlo simulation performance for complicated whole-core reactor models is demonstrated effectively.

Table 4. Verification of the efficiency for the whole-core reactor k_{eff} criticality calculations.

Reactor Model	Method	Tracking Rate (neutron/s)	Elapsed Runtime (s)	Speedup Ratio [1]	Speedup Ratio [2]
OPR	CRTT	6811	4.11×10^3	1.00	1.00
	SRDT	8823	3.21×10^3	1.30	1.28
	MRDT	9973	2.87×10^3	1.46	1.43
HM	CRTT	2532	1.09×10^4	1.00	1.00
	SRDT	3429	8.38×10^3	1.35	1.30
	MRDT	3917	7.13×10^3	1.55	1.53
BEAVRS	CRTT	2322	1.20×10^4	1.00	1.00
	SRDT	3450	8.30×10^3	1.49	1.45
	MRDT	3833	7.41×10^3	1.65	1.62

[1] The speedup ratio of the corresponding tracking rate to that of the CRTT method. [2] The speedup ratio of the corresponding elapsed runtime to that of the CRTT method.

5. Discussion

5.1. The Advantages of the MRDT Method

The MRDT method was proposed to optimize the run-time performance of the neutron transport tracking process in the Monte Carlo simulation. As we can conclude from Tables 2 and 4 that the run-time performance of MRDT method is competitive compared with that of the SRDT and CRTT methods. In the MRDT method, as the neutron transport length is sampled with Equation (6), which means that the transport step of the neutron can be continued over material boundaries.

As a result, besides sampling the neutron transport length with Equation (6), the MRDT-based tracking routine in a Monte Carlo code is reduced to determining which material fills the space at each reaction point, which must be computationally less expensive than calculating the surface distances, as done in the CRTT method. Thus, the MRDT-based tracking is usually more efficient in dealing with complex geometries, and complicated objects and surface types are easier to handle. As shown in Equation (3), we can find that easier handling of the complicated surfaces seems to be the main reason why the method is approved to be efficient in Monte Carlo simulations. Furthermore, the results given in Tables 2 and 4 indeed indicate that the speedup ratios are problem-dependent, which means that the more complicated the model is, the more competitive run-time performance will be achieved. Consequently, the MRDT method is approved to be more efficient compared with the CRTT method.

Meanwhile, as we mentioned that one of the biggest disadvantages of SRDT method is that the run-time performance will be degraded when the model has a high level of material heterogeneity, that is, when the material total cross sections differ significantly from each other. A typical example is an LWR fuel assembly, which contains localized heavy absorbers, such as control rods or burnable absorber pins. The absorber cross section dominates the maximum total cross section at low energy, even though the absorber material occupies a relatively small fraction of the total volume. Thus, the MRDT method was proposed to overcome the shortcoming of the SRDT-based method. In the MRDT method, the whole model is decomposed into multiple sub-regions and each sub-region has its own local maximum total cross section. As a result, the method can decrease the negative effect of the local heavy absorbers that exists within some sub-regions on the neutron transport tracking process performed in other sub-regions, which indicates a more competitive run-time performance will be achieved compared with the SRDT method. Furthermore, the results given in Tables 2 and 4 indeed indicate that the run-time performance of the MRDT method is better than that of SRDT method.

5.2. The Disadvantages of the MRDT Method

In Monte Carlo codes, the response quantities (i.e., neutron flux, surface current, reaction rate, etc.) are commonly calculated using the track-length estimator. However, in the MRDT-based tracking method, the neutron is tracked in a virtual homogeneous model. As a result, the main disadvantage of the method is that the surface crossings are not recorded at all, so the neutron's tracks in a specific material region are not known. The resulting penalty is that the most commonly-used track-length estimator of the neutron flux will be not available any more. Consequently, the neutron flux must be calculated using an alternative method, named a collision estimator, which is a less-efficient and error-prone method especially for tallies scored in small or thin regions. Furthermore, the surface flux and current estimates can be calculated only at the outer geometry boundaries, meaning that the quantities on the internal surfaces cannot be scored any more. Therefore, the MRDT-based tracking method is mainly used to perform Monte Carlo criticality calculations for the moment as indicated in the paper. If the MRDT method is to be extended to fixed source Monte Carlo calculations, a more efficient and accurate flux estimator needs to be studied further. For the moment, an improved neutron flux estimator is still under development and will be established in the near future.

6. Conclusions

To improve and optimize the run-time performance of the neutron transport tracking in Monte Carlo simulations, an improved multi-regional delta-tracking method (MRDT) was proposed. The corresponding methodologies, principles, schemes, verifications, and discussions were illustrated in detail. The MRDT method was verified using the simple criticality benchmarks and the complicated whole-core reactor models. Comparisons of the accuracy and efficiency results were given in the paper. Its accuracy and efficiency for the neutron transport tracking process were demonstrated in Monte Carlo criticality calculation. The results indicated that the new method was well consistent with the conventional methods, but with a more competitive run-time performance. Furthermore, the verifications showed that the new method was not only feasible to simple criticality benchmarks,

but also applicable for complicated whole-core reactor models. Generally, though the speedup ratios may be problem-dependent depending on the complexities of the geometrical configurations and material compositions, we can conclude that the method will achieve a more competitive run-time performance when performing Monte Carlo simulations for more complicated models.

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