TRIMON: AN EFFICIENT MULTIGROUP MONTE CARLO NEUTRON TRANSPORT CODE FOR TRIGA REACTORS

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TRIMON: AN EFFICIENT MULTIGROUP MONTE CARLO NEUTRON TRANSPORT CODE FOR TRIGA REACTORS

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[[	Position vector within a nuclear system or a nuclear reactor core.
t	Infinitesimal volume within a nuclear system or a nuclear reactor core.
[[	Neutron energy.
[[	Neutron direction unit vector.
r r	Components of the neutron direction unit vector.
[[	Time.
h r r r i	Angular neutron density.
h r i[[	Neutron density.
	Angular neutron flux.
	Neutron flux.
	Angular neutron current density.
	Neutron current density.
	Neutron group flux vector.
[[	Microscopic neutron cross section.
	Macroscopic neutron cross section.
	Number density of a material.
	Neutron energy group index.
	Total number of neutron energy groups.
	A random number between 0 and 1.
||	Effective multiplication factor.
	Dominance ratio.
	Fission source entropy.
	Neutron batch size.
	Survive-to-search acceleration parameter.

	Number of transport stages per S2S cycle.
	Wielandt acceleration parameter.
	Monte Carlo fission cycle index.
	Fuel burnup level in percent.
\(	Fuel element power in kW.
	Nominal reactor core power in kW.

LIST OF ABBREVIATIONS

TRIGA	Training Research Isotope General Atomics
TRIMON	TRIGA Monte Carlo Code
MCNP	Monte Carlo N-Particle Transport Code
WIMS	Winfrith Improved Multigroup Scheme Lattice Code
IAEA	International Atomic Energy Agency
MNA	Malaysian Nuclear Agency
RTP	Reaktor TRIGA Puspati
OECD/NEA	Organisation for Economic Co-operation and Development of Nuclear Energy Agency
S2S	Survive-to-search method
AWM	Asymptotic Wielandt Method
ASM	Asymptotic Superhistory Method
LWR	Light Water Reactor

TRIMON: KOD PENGANGKUTAN NEUTRON MONTE CARLO PELBAGAI KUMPULAN YANG EFISIEN BAGI REAKTOR TRIGA

ABSTRAK

Dalam kajian ini, TRIMON, iaitu kod Monte Carlo pengurusan teras reaktor TRIGA Mark-II telah dibangunkan. TRIMON membolehkan pengiraan empirikal terhadap penyusutan bahan api nuklear secara langsung, di mana kesan tahap penyusutan bahan api terhadap keadaan genting pengoperasian sesebuah reaktor diambil kira tanpa memerlukan kod pengiraan penyusutan bahan api yang lain. Dengan keupayaan ini, TRIMON menggantikan kod Monte Carlo semasa yang tidak optimum dalam membuat pertimbangan tahap penyusutan bahan api secara langsung, pertimbangan reka bentuk teras dan prestasi pengiraan. Ujian pengesahan pertama TRIMON menunjukkan persetujuan yang baik dengan hasil eksperimen yang diperoleh dari kerja sebelumnya. Selain itu, eksperimen penanda aras prestasi yang dilakukan dalam kajian ini membuktikan bahawa penggunaan keratan rentas neutron terhomogen mampu mengurangkan masa simulasi. Pada peringkat kedua kajian ini, kod TRIMON telah menjadi alat untuk menilai masalah yang tidak dapat diselesaikan dalam kajian pengiraan tahap genting Monte Carlo. Masalah tersebut adalah berkenaan penumpuan yang perlahan terhadap taburan sumber pembelahan. Dalam masalah ini, para pengkaji Monte Carlo perlu menunggu masa yang lama untuk membenarkan taburan tersebut menumpu kepada taburan. Ini telah menyebabkan simulasi teras reaktor yang rumit dan bersaiz besar menjadi suatu tugas yang sukar. Maka, penyelidikan ini menghasilkan kaedah baharu untuk mempercepat penumpuan taburan sumber pembelahan yang dikenali sebagai kaedah *Survive-to-Search* (S2S). Ujian pengiraan kaedah S2S menggunakan TRIMON untuk pelbagai masalah penumpuan

perlahan terhadap taburan sumber pembelahan menunjukkan bahawa kaedah tersebut dapat mengurangkan sehingga 87% dari masa penumpuan yang asal.

TRIMON: AN EFFICIENT MULTIGROUP MONTE CARLO NEUTRON TRANSPORT CODE FOR TRIGA REACTORS

ABSTRACT

In this research, TRIMON, a multigroup Monte Carlo core management code for TRIGA Mark-II reactors has been developed. Furthermore, TRIMON enables direct empirical fuel burnup consideration, where the fuel burnup effect on reactor criticality is considered independently without the need for an external fuel depletion code. With these capabilities, TRIMON supersedes the current state-of-the-art Monte Carlo codes which are not optimal in the direct fuel burnup consideration, core design consideration and performance. The first validation test of TRIMON shows a good agreement with the experimental results obtained from previous experimental works. Plus, the performance benchmark experiment done in this research proves that the use of homogenized neutron cross section reduces the simulation time. At the second stage of this research, TRIMON code has become the tools to assess the unresolved problem of Monte Carlo criticality calculation. Such an unresolved problem is the slow fission source convergence. In this problem, Monte Carlo researchers must wait for a significant amount of time to let the fission source distribution to settle down and converge to a stationary distribution. This has made the simulation of large and complicated reactor cores become a difficult. As a result, this research results in the development of a new fission source convergence acceleration method which is called the Survive-to-Search (S2S) method. Numerical tests of the S2S method for various slow converging problems using TRIMON demonstrated that the method eliminates up to 87% of the convergence time.

CHAPTER 1: INTRODUCTION

When talking about nuclear reactor analysis with Monte Carlo method, physicists often fathomed that the simulated fission neutron random movements are tracked from the moment the neutron is created during a fission event until its death. Such a direct simulation is done repeatedly for a large number of trials using a powerful computer. As a result, the statistical assemble of the simulated neutronic behaviour within a nuclear reactor can be observed. Particularly, the simulated neutronic behaviour is analysed by counting the number of neutrons occupying various regions within a nuclear reactor core. This information will finally form a spatial distribution of neutrons count over the entire reactor core. Traditionally, the spatial distribution of neutrons count is calculated by solving a specialised partial differential equation rather than simulating a large number of actual neutron movements. Here, the former technique is formally known as the deterministic method and the latter is known as the Monte Carlo method. Each of these techniques entails several pros and cons in terms of problem-solving capability. And of course, the Monte Carlo method is a formidable tool in nuclear reactor analysis due to its ability to simulate neutron movements in various complicated reactor core geometries. In this research, several new computational techniques are proposed to circumvent the limiting issues in the Monte Carlo method. One of the remarkable initiatives proposed in this research includes the coupling of the deterministic method with the Monte Carlo method in attempt to improve the computational efficiency. Such an initiative is yet to be assessed by the nuclear reactor physicists. To begin with, this preliminary chapter provides a brief introduction to the Monte Carlo method and Monte Carlo codes, as well as the motivations, the objectives and the scope of this research.

1.1 Understanding Monte Carlo Simulation of Neutron Transport

At this level, it is convenient to briefly illustrate a simple Monte Carlo simulation of neutron movements within a typical system, say, a slab of fissile material. Among nuclear Monte Carlo physicists, such movements are recognized as neutron transport phenomenon. When a neutron travels from point *A*h m m i to point *B*h m m i, one can alternatively say that the neutron is being *transported* from point *A* to point *B*. Initially, a Monte Carlo physicist will routinely provide an initial guess of fission source locations. Each of these locations will be the starting point (or sometimes termed as the birth location) of a simulated fission neutron created in the computer memory. Afterwards, a fission neutron batch size, say, $=10^6$ is assigned and kept constant throughout the entire simulation. Subsequently, a queue which holds $=10^6$ fission neutrons awaiting to be simulated is created in the computer memory. Their birth locations are randomly picked from the initial guess of fission source locations initialized beforehand. A fission neutron is drawn from the queue and simulated. Conventionally, the starting locations of these fission neutrons form a spatial distribution which is known as the *fission source distribution*.

Fig. 1.1 depicts the random series of collisions of a fission neutron selected from the top of a queue. The neutron is programmatically ejected from its birth location at *A* and randomly transported within a slab of fissile material. Next, numbers between zero and unity are randomly generated by the computer. Later, these numbers are used to decide where the neutron collision takes place and what type of neutron-nucleus interaction occur at the collision location. Whether the neutron undergoes scattering reaction, or fission, or being captured by the nucleus at the collision site – it all depends on the fate dictated by the generated random numbers. And of course, these random choices are based on the rules of physics and probabilities represented by a quantity

known as the *neutron cross section*. The value of the neutron cross section for various types of materials and reactions are gathered and stored in a formatted data file. Such a data file is commonly identified as a nuclear data file. A nuclear data file is provided by various organizations. For example, ENDF (Evaluated Nuclear Data File) is provided by Los Alamos National Laboratory (LANL) (Chadwick *et al.*, 2011) and JENDL (Japanese Evaluated Nuclear Data Library) is provided by Japanese Atomic Energy Agency (Igarasi *et al.*, 1979).

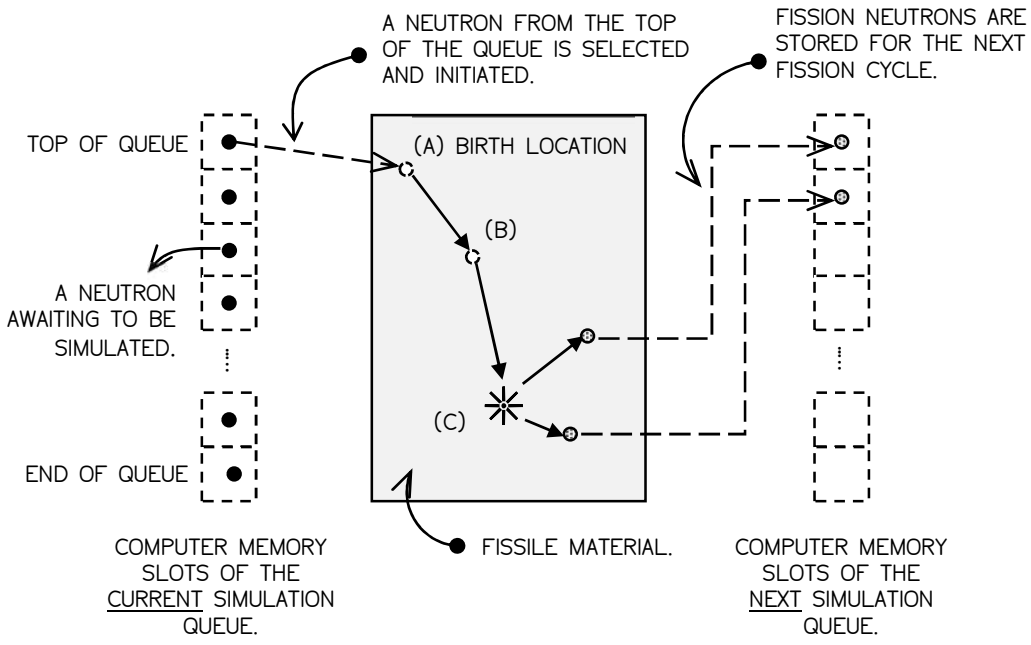

Figure 1.1: Overview of Monte Carlo neutron transport simulation.

Back to the neutron simulation, suppose the neutron collides at location *B*. After that, the neutron is scattered in the direction portrayed in Fig. 1.1. Plus, the scattering direction is randomly generated based on the physical scattering angle distribution. At collision point *C*, fission happens, ending in the death of the incoming neutron due to absorption and the birth of two outgoing fission neutrons. At this point, the simulation

is said to complete the first fission cycle of a single neutron. These two fission neutrons are not further tracked but they are saved in a new neutron queue for later tracking during the next fission cycle. This neutron history is now complete. The next neutron from the queue is ejected from its corresponding birth location and further tracked. This process continues until the neutron source queue is exhausted. As more histories are followed, the neutron distributions become favourably known. The quantities of interest, e.g. the neutron flux, track length or whatever the nuclear Monte Carlo physicist requests are tallied, simultaneously with the estimates of the statistical uncertainty of the tallies.

1.2 TRIGA Reactors

TRIGA is a commercial research reactor built by General Atomics, USA. Now, the reactor has been installed in 24 different countries. The reactor has been used for many diverse applications such as radioisotopes production, non-destructive testing, research on the properties of matter and for education and training. The reactor is a pool-typed water reactor and the reactor core is loaded with hydride fuel-moderator element, specifically U-ZrH. Most neutron moderations take place in the fuel element itself and the neutron moderation is mainly due to H in H-Zr (Henry *et al.*, 2017). The reactor utilises demineralized water as coolant and moderator, where the loaded fuels are cooled by the flow of the coolant through the reactor core through natural convection or by forced cooling which depends on the reactor design.

TRIGA reactors are well recognised for its built-in safety characteristic due to a physical property of U-ZrH fuel. Here, TRIGA reactors have large prompt negative temperature coefficient. This implies that it is adequate to control an unexpected large insertion of positive reactivity to the reactor core. The fuel meat is a solid,

homogeneous alloy of U-ZrH with the uranium enriched to 20% U-235. Also, the fuel meat is clad by a 0.051cm thick aluminium or stainless steel (SUS304) can.

Reaktor TRIGA Puspati (RTP) is a 1 MWth research reactor that has been installed in 1982 at Malaysian Nuclear Agency, Bangi, Malaysia. RTP core is an annular-shaped core holding 127 designated core locations to accommodate fuel elements and other non-fuel elements such as control rods and irradiation facilities. The reactor core and the reflector assembly are mounted at the bottom of an aluminium tank situated inside the concrete shielding. The reactor core and experimental facilities are enclosed by a high-density concrete shielding. The reflector is made up of graphite and the reactor assembly is equipped with four boron carbide control rods. To provide vertical shielding, water is filled about 5m above the reactor core. Each element is arranged in seven concentric rings designated as Ring-A, Ring-B, …, Ring-G with 1, 6, 12, 18, 24, 30 and 36 core locations, respectively. In addition, TRIGLAV is the currently available core management code that is designed for TRIGA reactors (Peršič *et al.*, 2017). The code implements four neutron energy groups and it represents the TRIGA core as a two-dimensional annular geometry.

1.3 Motivations

Nuclear Monte Carlo method has become an elegant computational tool for the neutronic calculation of a complex reactor geometry. The physics behind the neutronic process is well understood, and the knowledgebase of controlling the fission chain reaction is growing. However, the method still needs several improvements on certain aspects such as its computational performance and its practicability to be applied in the real engineering situation such as managing fuel configuration in the reactor core.

Undoubtedly, most current state-of-the-art Monte Carlo codes such as MCNP and Serpent are extremely powerful and commonly used in research reactor calculations. However, a majority of these codes are still not optimal in core design and fuel burnup management (Peršič *et al.*, 2017). For the case of core design, a TRIGA core consists of various fuel and non-fuel elements where their arrangement in the reactor core vary for every different reactor operation. Thus, the process of redefining the core arrangement and compositions of each reactor operation in a general multi-purpose code can be cumbersome. For instance, redefining the TRIGA core arrangement in MCNP requires redefinitions of materials within hundreds of individual geometrical cells defined in the input file.

When a nuclear fission fuel is used for a period of time, the amount of the fissile isotope within the fuel will deplete. Thus, it leads to a weak release of fission power. Such a physical phenomenon is called *fuel burnup*. In fuel burnup management, transferring the fuel burnup level information of the end of a reactor operational cycle (EOC) to correct the neutron cross-section data for the use of the next begin of a reactor operational cycle (BOC) can be tedious. Several pieces of research done by Alnour *et al.* (2013) and Zheng *et al.* (2014) attempted to provide a scheme for combining burnup codes with design code. However, it turns out that the scheme itself is complicated.

The standard power iteration method is the common strategy used in criticality calculation for neutron transport applications. The use of the power iteration method in Monte Carlo eigenvalue calculation involves faithful neutron history tracking from one iteration cycle to another. Plus, the term *iteration cycle* is coined as *Monte Carlo (MC) cycle* later in this text. In a single analog MC cycle, the real neutronic processes and their physics are simulated from the birth of a neutron at a fission source site until its termination after escape or disappearance reaction.

During power iteration, it is crucial for the fission source distribution to converge before any tallies are accumulated. In common practice, several MC cycles are skipped to ensure tallies accumulation starts after the fission source distribution over the entire fissile system has converged. Most Monte Carlo physicists acknowledged the existence of loosely coupled problems. These problems often require many MC cycles to reach the convergence of fission source distribution. Such problems include a system with weak mutual interactions of neutrons between fissile regions and large-scale problems involving an actual power supplying nuclear reactor core. Unfortunately, a slowly converging fission could lead to ambiguity when estimating the number of skip MC cycles required before begin accumulating neutronic quantities. To rectify this, many nuclear Monte Carlo physicists came up with various acceleration methods such as the Wielandt method and the Superhistory method. Unfortunately, these methods increase the computational time to reach fission source convergence, despite reducing the number of MC cycles to reach fission source convergence. Therefore, the formulation of a new fission source convergence acceleration technique that could reduce the number of MC cycles and computation time to reach fission source convergence is in demand.

1.4 Problem Statement

There is still no research done on assessing the feasibility of integrating homogenized neutron cross section data obtained using the deterministic method to a Monte Carlo code. There is also a practical possibility to boost the efficiency of the Monte Carlo simulation by properly introducing homogenized neutron cross section data to the Monte Carlo method. Here, the homogenized neutron cross section data are calculated using the deterministic method.

The current in-practice Monte Carlo method for neutron transport typically require several performance improvements including fission source convergence acceleration. The currently available acceleration methods are not efficient in terms of computational time, despite the observed reduction of the number of Monte Carlo iterations. A slowly converging simulation can possibly cause erroneous results which will tremendously affect the reliability of the simulation (X-5 Monte Carlo Team, 2005).

Finally, a three-dimensional core management code for TRIGA reactors is in demand since there is still no upgrade of the current reactor core management code. The currently available core management code is already obsolete and severely restricted to two-dimensional reactor geometry with four neutron energy groups.

1.5 Research Objectives

The overall aim of this thesis is to develop a next generation multigroup Monte Carlo core management code designed specifically for TRIGA Mark-II reactors, replacing the current state-of-the-art code. In order to improve the currently in-use Monte Carlo technique, this thesis also embarks on several specific objectives:

1) To advance the current practice of nuclear Monte Carlo method by constructing a clear methodology of using homogenized cross section data in the Monte Carlo method and to assess the feasibility of using this approach.
2) To improve the current strategy on considering fuel burnup in Monte Carlo calculation, that is, to outline a scheme that offers direct empirical fuel burnup correlation without the need of a tedious process of linking to a third-party fuel depletion code.

3) To provide a solution to the current unresolved slow fission source convergence issue in Monte Carlo method by developing a practical and low computational cost strategy for speeding up fission source convergence with minimum modification of the standard Monte Carlo power iteration scheme.

1.6 Research Scope and Gaps

The major work of this research will only focus on the development of a core management code for TRIGA Mark-II reactors. Correspondingly, the entire code modules will be written in Fortran90 language despite the availability of various modern codes such as C++ and Python. The decision on using Fortran90 is to ensure that the current code development is interoperable and reusable with the existing nuclear Monte Carlo algorithms that are mostly expressed using the legacy Fortran language. Even so, this research is tailored to bring two major advancements to the current Monte Carlo simulation practice. The first advancement is to improve the efficiency of the current in-practice Monte Carlo power iteration by introducing homogenized cross section data to it. The second advancement is to improve the currently unresolved slow fission source convergence issue. Even though this research focuses on TRIGA reactor systems, it is adapted to accommodate future application to different types of reactor systems. Correspondingly, the code to be developed will be organized so that its geometrical module can be modified in the future for different types of reactor geometry. However, the modification process can be a bit tedious and require major programming work.

The Monte Carlo power iteration method is the only main simulation technique that will be implemented in the newly developed core management code. Inevitably, the author of this thesis does not own any rights to modify any state-of-the-art codes.

Thus, it is impossible to implement any new improvised simulation method in these well-known codes for numerical verification. It is necessary to verify a new simulation method via numerical experiments that assess its performance and reproducibility. With the best efforts, the newly developed multigroup Monte Carlo code will be used to validate the newly established method. In this work, two benchmark experiments outlined by existing published works have been repeated, so that a convincing numerical result can be produced at its best. Furthermore, the fission source acceleration benchmark experiments conducted in this work involve the two prominent slow-converging problems defined by OECD/NEA. These problems include the fissile slabs case and the LWR pin case.

It is also worth to remark that the verification of the newly developed code was only carried out using RTP operational parameters and experimental data. It is best if the newly developed code is verified with the experimental data of other TRIGA reactors owned by various international organizations. However, obtaining the reactor operational parameters and experimental data from these international organizations is almost impossible due to confidentiality concern. Nonetheless, the outcome of this research indicates that the newly developed code works satisfactorily with numerous RTP operational test cases. Since the design of TRIGA reactors are not much different from one to another, this code has a high capability to reproduce the experimental data of other TRIGA reactors, provided that the correct TRIGA operational parameters are fed to the code.

1.7 Thesis Outline

This thesis consists of six chapters. Briefly, Chapter 2 is dedicated for the literature review whereas Chapter 3 contains the details of the essential theorems that need to be familiarized by the reader before jumping into the new theoretical development conveyed by this research. Followed by Chapter 4 and Chapter 5, they clarify the outcomes of this research. Finally, Chapter 6 contains the conclusion and recommendations drawn by this research. All of the six chapters are organized according to the following ways:

Chapter 1 – Introduction

An introduction to the research topic to be addressed by this thesis, including some introductory background of the methods used in this research, research limitations on the development of a multigroup Monte Carlo code for TRIGA reactors, problem statements, motivations and objectives of this research.

Chapter 2 – Literature Review

A detailed analysis of the existing published works focusing on the limitations of Monte Carlo techniques and codes are thoroughly discussed. This includes the limitations imposed by the current state-of-the-art codes when dealing with TRIGA reactors.

Chapter 3 – Preliminary Theorems and Neutron Transport Theory

This chapter is a primer of the basic concepts in neutron transport theory such as the neutron cross section, nuclear interaction rates, number density and etc. The basic neutron-nucleus interaction processes are introduced, and the neutron transport

equation is derived in detail. The theories and concepts that become the basis of the multigroup Monte Carlo method are also presented. These theories include neutron diffusion theory, the multigroup method and reactor -eigenvalue equation. The deterministic method of criticality calculation is also explained in detail.

Chapter 4 – The Development of TRIMON

This chapter outlines the details of the development of TRIMON (**TRI**GA **Mon**te Carlo Code), a new reactor core management code for TRIGA reactors that integrates diffusion-theory-type homogenized group cross sections into the Monte Carlo method. This chapter also discusses advanced Monte Carlo for neutron transport concepts that are implemented in TRIMON which include the criticality calculation, Monte Carlo random processes and etc.

Chapter 5 – Fission Source Convergence Acceleration in TRIMON

The development of TRIMON has led to the formulation of a new Monte Carlo power iteration scheme that speeds up fission source convergence. In this chapter, the fission source convergence behaviour of a Monte Carlo power iteration is further analysed, some state-of-the-art fission source convergence acceleration methods are introduced and the strategy on speeding up fission source convergence is also analysed. A detailed description of the newly developed fission source convergence acceleration scheme which is named as Survive-to-Search (S2S) method will be given. This chapter includes several reports on the numerical verification of the newly developed acceleration strategy.

Chapter 6 – Conclusions and Recommendations

This chapter concludes the outcome of this research and provides suggestions for possible future works based on the findings of this thesis.

CHAPTER 2: LITERATURE REVIEW

In this chapter, numerous published works have been thoroughly analysed to evaluate the limitations of the existing nuclear Monte Carlo codes in terms of their practicability on handling the actual reactor engineering issues. Also, readers may also learn that much of the limitations of the current Monte Carlo codes tend to be associated to the core design consideration, fuel burnup management (for the burned core problem) and also code performance concerns when applied to the real complex rector geometry. Furthermore, several research works done on the Monte Carlo calculation analysis of TRIGA reactors demonstrated the similar restrictions of the existing Monte Carlo method when applied to the real power producing reactors. Consequently, it is essential to uncover the ways of enhancing the capability of the Monte Carlo method to ensure the viability of the method when employed to the actual reactor analysis.

2.1 The Monte Carlo Method

The Monte Carlo method (Metropolis & Ulam, 1949) is utilized to reproduce a theoretically statistical phenomenon such as the way neutrons interact with materials. It is effective for simulating complex problems that cannot be modelled by computational codes that implement the standard numerical method. In the Monte Carlo method, the discrete probabilistic events that consist of realistic processes are simulated sequentially. Traditionally, neutrons behaviour is predicted by solving an integrodifferential equation identified as the neutron transport equation (Lamarsh & Baratta, 1955). The solution of the transport equation is the neutron flux distribution, which is a function of position, energy and time. The flux distribution is a useful piece of information in nuclear reactor analysis that enables nuclear engineers to design a practical and secure nuclear system. In the deterministic method, the neutron transport

problem is solved using unique mathematical techniques, such as the Greens' function method (Öztürk *et al.*, 2006) and the collision probability method (Lefvert, 1979; Raghav, 1977). In contrast, the Monte Carlo method inherently 'solves' the neutron transport equation via the actual simulation of neutron random walk movements.

2.2 Monte Carlo Codes for Nuclear Reactor Analysis

A nuclear Monte Carlo code is a set of computer instructions that simulates nuclear processes, typically the way neutrons behave and move inside a nuclear reactor (Duderstadt & Hamilton, 1976). Recall that the example of such a simulation has been briefly described in the previous section. The execution of a reactor code produces information such as the stability of a nuclear reactor. It helps nuclear engineers to properly design and control the nuclear system. Most importantly, simulating the way neutrons behave in a reactor allows a nuclear Monte Carlo physicist to estimate the number of neutrons within the reactor. The number of neutrons in a particular reactor is proportional to the amount of fission power produced by the reactor. Essentially, the stability of a nuclear system is quantified using the multiplication factor, . It assesses the rate of growth or decay of the total number of neutrons within the system. Briefly, the multiplication factor is defined as (Carter & Cashwell, 1975),

$$\pm \frac{\text{[illegible]}}{\text{[illegible]}} \qquad (2.1)$$

To illustrate, an unstable nuclear system will have a typical value of $\times r$, which can inadvertently lead to an exponential and uncontrollable growth of neutron population within the system. This will then increase the possibility of inducing an uncontrollable amount of fission reactions. Consequently, a tremendous amount of

fission energy is tapped and thus causing a nuclear disaster such as Fukushima Dai-ichi incident (Hirose, 2012) and Chernobyl incident (Beresford *et al.*, 2016).

In nuclear reactor analysis, there are two distinct types of nuclear code and they are the nuclear design code and the reactor core management code. The solving technique implemented in both codes can be categorized as the deterministic method or the Monte Carlo method. The purpose of a nuclear design code is to enable nuclear engineers to first design nuclear devices or even a nuclear reactor. Typically, a design code allows the user to define arbitrary geometries that compose of various different types of materials. For example, a design code can be used to design a radiation shielding wall (Cho *et al.*, 2004) or even to study the production of weapons-grade plutonium for military purpose (Glaser & Ramana, 2007). In contrast, a core management code is a code specifically designed for a specific nuclear reactor model. It allows nuclear engineers to make decisions on managing reactor core compositions such as fuel reshuffling, nuclear fuel replacements and allocation of various irradiation facilities inside the reactor core.

Several examples of the deterministic code are TRIGLAV (Peršič *et al.*, 2017) for generic TRIGA reactors, and APOLLO (Mathonniere & Stankovski, 1992) used by EDF Energy and Areva. Whereas some examples of the Monte Carlo nuclear system design code are MCNP by Los Alamos National Laboratory (LANL) (X-5 Monte Carlo Team, 2005), OpenMC by Massachusetts Institute of Technology (MIT) (Romano & Forget, 2013), Geant4 by The European Organization for Nuclear Research (CERN) (Allison *et al.*, 2016) and MONK by ANSWERS Software Service (Smith *et al.*, 2001).

It is also worth to mention that most legacy nuclear codes such as MONK and MCNP are written in the modern version of Fortran language, that is, Fortran90/95 (Goorley *et al.*, 2016; Smith *et al.*, 2001). In addition, several modern codes such as OpenMC, Geant4 and Apollo are written in C++ (Allison *et al.*, 2016; Mathonniere & Stankovski, 1992; Romano & Forget, 2013). Deliberately, legacy nuclear codes are still using the Fortran90/95 language architecture since most existing modules of these codes are written in Fortran77 which is old and obsolete. In order to aid the long-term practicability of these legacy nuclear codes, transformation effort has been done to upgrade the compiler of these codes from Fortran77 to Fortran90/95 (Forster *et al.*, 2004). Here, the modern version of Fortran grants for a more modular approach that facilitates in code maintenance, code reusability and addition of new programming language features. Fortunately, the advent of the modern-day Fortran 90/95 scientific language has commenced the path toward modern and higher-level programming techniques that can be implemented efficiently to create a contemporary version of the legacy nuclear codes (Talou *et al.*, 2005). This acceptably justifies the rationale of why some of the nuclear Monte Carlo codes are still using the Fortran architecture. This simply suggests that Fortran language is still relevant in nuclear industry. The new modular approach implemented in Fortran90/95 has also made itself an elegant programming language, plus, it is much easier for the user to add new mathematical models and physical models for further development (Wu *et al.*, 2010).

Criticality calculation, or sometimes called the eigenvalue calculation, is a well-known neutron transport simulation technique to determine the multiplication factor of a certain nuclear system (Duderstadt & Hamilton, 1976). Here, neutron productions via fission reaction are included in the simulation. Most nuclear design codes and core management codes have the capability of running criticality calculations. In a

deterministic criticality code, a modified neutron transport equation called the - eigenvalue equation is solved and computed by various mathematical methods available (Duderstadt & Hamilton, 1976). Also, a deterministic code is computationally less expensive since there are no random processes involved.

2.3 Issues with the State-of-the-art Nuclear Codes

Undoubtedly, most current state-of-the-art Monte Carlo codes such as MCNP and Serpent are extremely powerful and commonly used in research reactor calculations. However, a majority of these codes are still not optimal in core design and fuel burnup management (Peršič *et al.*, 2017). For the case of core design, a TRIGA core consists of various fuel and non-fuel elements where their arrangement in the reactor core vary for every different reactor operation. Thus, the process of redefining the core arrangement and compositions of each reactor operation in a general multi-purpose code can be cumbersome. For instance, redefining the TRIGA core arrangement in MCNP requires redefinitions of materials within hundreds of individual geometrical cells defined in the input file.

Fundamentally, one must note that the neutron cross sections of a fuel material are heavily affected by the burnup level of the fuel. It is essential to account the current fuel burnup effect by making corrections to these cross sections values before prescribing them to a core calculation code. To accomplish this, various strategies have been published by researchers on linking Monte Carlo to a fuel depletion code such as ORIGEN and CINDER (Goorley *et al.*, 2016). However, these strategies are poorly outlined and require intermediate linking codes that are inaccessible to all researchers. Furthermore, none of these attempts demonstrates core local burnup effect consideration into their calculations. Previous works only consider the burnup effect

of the whole fuel element, which in fact neglecting the effect of burnup variation along the fuel length.

Recently, most state-of-the-art Monte Carlo codes developers have introduced various impressive theoretical strategies for simulating changes in the composition of nuclear fuel over time (Maria, 2016; D. She *et al.*, 2012). In fact, these theoretical strategies have been integrated into their upgraded codes. Unfortunately, these strategies impose extra relevant parameters to the code input. Hence, their usage requires a deep theoretical understanding of nuclide depletion mechanisms. As a result, this leads to a dubious process of defining simulation problem among average code users. These strategies also complicate numerical calculation processes, thus, adding more computational load to the CPUs.

Suppose a reactor region consists of distinct volumes with each having a different type of material. Correspondingly, each of these materials has a specific set of cross section data. In deterministic reactor calculations, these distinct volumes can be represented with a single *effective* volume with a set of homogenized neutron cross section data (Duderstadt & Hamilton, 1976). Apparently, there is a lack of research on integrating homogenized cross section data with Monte Carlo method. Previous work done by Kuijper *et al.* (2007) involves modifying scripts to feed in homogenized cross section data into MCNP, a continuous energy Monte Carlo code. Yet, the validity and the theoretical aspect of the trial is poorly understood.

2.4 Slowly Converging Fission Source Distribution

Recall that the power iteration method is the common strategy used in eigenvalue calculation for neutron transport applications. Also, Monte Carlo power iteration

method necessitates faithful neutron history tracking from one MC cycle to another. Here, the real neutronic processes and their corresponding theoretical physics laws are implemented from the moment a neutron is born at a fission source site until its death due to a disappearance reaction. During power iteration, it is crucial for the fission source distribution to converge before any tallies are accumulated (X-5 Monte Carlo Team, 2005). In common practice, several MC cycles are skipped to ensure tallies accumulation starts after the fission source distribution over the entire fissile system has converged.

The *dominance ratio* (DR) is an effective mathematical quantity that characterizes the convergence behaviour of the fission source distribution (Ueki *et al.*, 2003). A simulation model with DR close to unity often suffers slow convergence, and this problem is always encountered in loosely coupled problems. The term *loosely coupled* here means the ability of a fission site in one region to cause the creation of another fission site on the other region is feeble. Such problems include a system with weak mutual interactions of neutrons between fissile regions and large-scale problems involving an actual power supplying nuclear reactor core. To rectify this, many nuclear Monte Carlo physicists came up with various acceleration methods such as the functional Monte Carlo (FMC) method (Larsen & Yang, 2008), the coarse-mesh finite difference (CMFD) method (Lee *et al.*, 2010), the stratified source sampling (Mohamed, 1998), the super-history powering (Brissenden & Garlick, 1986), Wielandt method (Yamamoto & Miyoshi, 2004), Asymptotic Wielandt method (AWM) and Asymptotic Superhistory method (ASM) (She *et al.*, 2012). Among these established methods, the super-history powering and Wielandt method are preferred since both strategies involve simple modifications to the conventional power iteration scheme

(She *et al.*, 2012). Hence, an acceleration method that provides simple modifications to the conventional power iteration scheme is preferred.

Unfortunately, some of the established methods impose certain restrictions which sacrifice the advantage of Monte Carlo method over deterministic method (She *et al.*, 2012). For instance, the FMC method is restricted to a regular geometrical mesh and the CMFD method necessitates the use of multigroup cross sections. Also, the previous work done by Yamamoto & Miyoshi (2004) demonstrated that Wielandt method substantially increases the source convergence time compared to the conventional non-accelerated method. According to She *et al.* (2012), even though the Wielandt method and the Superhistory method decrease the necessary number of inactive cycles to reach source convergence, they increase the time expense during each inactive MC cycle and the convergence time is not reduced. At this instance, we define the source convergence time as the CPU time required for the fission source distribution to converge. It is vital to ensure a correct fission source convergence and reducing the inter-generation correlations imposed by the standard method. Even if the CPU time is a remarkable concern, it is important to avoid false convergence. Also, reducing the number of MC cycles required to reach source convergence helps to avoid making wrong decisions for the source convergence.

2.5 Issues with Monte Carlo Analysis of TRIGA Cores

TRIGLAV is a state-of-the-art deterministic criticality and core management code specially designed for TRIGA reactors (Peršič *et al.*, 2017). It allows TRIGA engineers to manage the fuel loading configuration and reactor safety. The code categorizes neutrons into four discretized neutron energy groups and the four-group neutron diffusion equations are solved simultaneously via the finite element method (Peršič *et*

al., 1998). It represents the TRIGA reactor core as a two-dimensional cylindrical geometry. Hence, a criticality code that can handle the three-dimensional geometrical representation of a TRIGA core is desired and will be considered as an advancement of the existing code. TRIGLAV has been used extensively by some nuclear institutes such as Malaysian Nuclear Agency (Rabir *et al.*, 2017), Istanbul Technical University (Büke, 2008) and Józef Stefan Institute (Peršič *et al.*, 2017).

Solving a three-dimensional TRIGA problem via deterministic method is tedious and impractical since solving the tedious three-dimensional neutron transport equation is nearly impossible. It has been reported that currently a three-dimensional deterministic criticality and core management code, GNOMER (Trkov, 2019), has been developed earlier. However, the code imposes crude geometrical approximation which causes a dramatic impact on the calculation accuracy. Whereas the long-established MCNP code and Serpent (Leppänen *et al.*, 2015) are remarkably powerful in terms of reactor design. Unfortunately, they are not readily catered to the consideration of fuel depletion effect inside a reactor core and these codes are still not practical in reactor core management (Peršič *et al.*, 2017).

Due to the availability of high-end processors during recent years, the Monte Carlo method has become relevant and famous among nuclear engineers. It is also eminent that many researchers and engineers opted to analyse TRIGA cores using Monte Carlo codes that are available today. For instance, Rabir *et al.* (2016) used MCNP to investigate the reactor parameters affecting the core flux and power spectrum. In addition, numerous researchers also used MCNP to investigates the power peaking factors of TRIGA reactors (Britton & Wu, 2020; Rabir *et al.*, 2016; Rabir *et al.*, 2017). Here, the power peaking factor is an important parameter that helps

nuclear engineers to avoid significant power peaking, thus, ensuring uniform fuel power distribution within the reactor core.

Unfortunately, there are several issues on core design consideration and burnup management issues that are currently encountered by TRIGA researchers when using a general multipurpose Monte Carlo code. In the aspect of core design consideration, Yavar *et al.* (2012) stated that the user must change the positions of cell cards and surface cards in the MCNP input file according to new TRIGA core configuration. Correspondingly, Türkmen *et al.* (2015) utilized MCNP to investigates the optimum core loading which would maximize the fuel utilization and extend the fuel cycle length. Unfortunately, Türkmen *et al.* (2015) and Jeraj *et al.* (2002) demonstrated that fuel burnup consideration in the standard state-of-the-art code remains cumbersome. It has been revealed that they required to couple MCNP with an external burnup code, ORIGEN (Croff, 1983), to modify the macroscopic cross sections so that it is valid for the MC calculation of a burned core.

CHAPTER 3: PRELIMINARY THEOREMS AND NEUTRON TRANSPORT THEORY

In a reactor core, neutrons move in complicated trajectories due to constant collisions with nuclei. Typically, these recurring collisions cause the neutron trajectories to appear to be zigzag. For instance, source neutrons were originated from their corresponding birth locations, , moving with particular energy, , and direction . Afterwards, they appear at other positions, , at a later time, . These neutrons could also change its energy and direction into[′ and , respectively after a collision at . In that sense, these neutrons are said to have been transported from the current state h m m mi[to the next subsequent state h m m m i. Correspondingly, the study of such a process is coined as the neutron transport theory. In this chapter, an exact equation which describes the neutron transport phenomena will be introduced. Such an equation is recognized as *the neutron transport equation* and the key objective of this study is to solve the equation.

The readers will also be introduced with the basic concepts of the neutron transport theory before jumping into the battle of solving the equation. Also, the multigroup method will be introduced to simplify and reduce the general transport equation into the multigroup equations. Then, readers will be presented with the most vital calculation in reactor physics, that is, the criticality calculation. At this point, the criticality calculation of a nuclear system will allow us to evaluate the stability of the fission chain reaction. Briefly, a criticality calculation at first gathers all parameters related to the reactor design, nuclear fuel properties and the reactor core configuration. At the end of the calculation, nuclear engineers will be able to quantitatively estimate the stability of the reactor using the multiplication factor, .