DEVELOPMENT OF NEW SOURCE DIAGNOSTIC METHODS AND VARIANCE REDUCTION TECHNIQUES FOR MONTE CARLO EIGENVALUE PROBLEMS WITH A FOCUS ON HIGH DOMINANCE RATIO PROBLEMS

By

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A DISSERTATION PRESENTED TO THE GRADUATE SCHOOL OF THE UNIVERSITY OF FLORIDA IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

UNIVERSITY OF FLORIDA

2010
To my parents, who always believed in me even when I didn’t believe in myself
ACKNOWLEDGMENTS

I extend my thanks to my thesis advisor, Dr. Alireza Haghighat for his guidance over the years. I would also like to extend my gratitude to all of my committee, Dr. Glenn Sjoden, Dr. David Hintenlang, Dr. Alireza Entezari and Dr. John Wagner for their help and support.

I would also like to thank the many members of the University of Florida Transport Theory Group for their thoughtfulness and willingness to listen to discussions about my work. In particular, Dr. Benoit Dionne, Dr. Ce Yi, Mr. William Walters and Mr. Kevin Manalo who have provided valuable insight and also their friendship. I would like to thank all of my family and friends for their love and support over the years. I would not have been able to accomplish this without you. Finally, I would like to thank Jen for putting up with me through the difficult times of this work and encouraging me to finish what I had started.
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Obtaining the solution to the linear Boltzmann equation is often a daunting task. The time-independent form is an equation of six independent variables which cannot be solved analytically in all but some special problems. Instead, numerical approaches have been devised. This work focuses on improving Monte Carlo methods for its solution in eigenvalue form.

First, a statistical method of stationarity detection called the KPSS test adapted as a Monte Carlo eigenvalue source convergence test. The KPSS test analyzes the source center of mass series which was chosen since it should be indicative of overall source behavior, and is physically easy to understand. A source center of mass plot alone serves as a good visual source convergence diagnostic. The KPSS test and three different information theoretic diagnostics were implemented into the well known KENO.V.a code inside of the SCALE (version 5) code package from Oak Ridge National Laboratory and compared through analysis of a simple problem and several difficult source convergence benchmarks. Results showed that the KPSS test can add to the overall confidence by identifying more problematic simulations than without its usage. Not only this, the source center of mass information on hand visually aids in the understanding of the problem physics.
The second major focus of this dissertation concerned variance reduction methodologies for Monte Carlo eigenvalue problems. The CADIS methodology, based on importance sampling, was adapted to the eigenvalue problems. It was shown that the straight adaptation of importance sampling can provide a significant variance reduction in determination of $k_{eff}$ (in cases studied up to 30%?). A modified version of this methodology was developed which utilizes independent deterministic importance simulations. In this new methodology, each particle is simulated multiple times, once to every other discretized source region utilizing the importance for that region only. Since each particle is simulated multiple times, this methodology often slows down the final $k_{eff}$ convergence, but an increase coupling between source zones with important yet low probability interaction is observed. This is an important finding for loosely coupled systems and may be useful in their analysis.

The third major focus of this dissertation concerns the use of the standard cumulative fission matrix methodology for high dominance ratio problems which results in high source correlation. Source eigenvector confidence is calculated utilizing a Monte Carlo iterated confidence approach and shown to be superior to the currently used plus and minus fission matrix methodology. Utilizing the fission matrix based approach with appropriately meshing and particle density, it is shown that the fission matrix elements tend to be independent. As a result, the $k_{eff}$ and the source eigenvector can be calculated without bias, which is not the case for the standard methodology due to the source correlation. This approach was tested with a 1-D multigroup eigenvalue code developed for this work. A preliminary automatic mesh and particle population diagnostic were formulated to ensure independent and normal fission matrix elements. The algorithm was extended in parallel to show the favorable speedup possible with the fission matrix based approach.
CHAPTER 1
INTRODUCTION

Objective

Since the Boltzmann equation was first introduced, it has found application in many areas, such as the kinetic theory of gases (Alexev, 2004) and charged (Cercignani, 1975) and neutral particle transport (Bell and Glasstone, 1985; Lewis and Miller, 1993). Although very powerful, obtaining a solution to the Boltzmann Equation is often a daunting task. The time-independent form of Linear Boltzmann Equation (LBE) is an equation of six variables which cannot be solved analytically in all but some simplified problems.

Numerical approaches devised to solve the LBE can be broken into two distinct groups: deterministic and Monte Carlo methods. In the deterministic approach, the equation itself is discretized and then is either solved directly or via iteration schemes. There are a large variety of deterministic methods available due to the different discretization and approximations utilized, but some of the more common methods include the discrete ordinates ($S_N$) methods, nodal methods, method of characteristics (MOC), and the collision probability methods (CPM) (Lewis and Miller, 1993). Errors from these methodologies are systematic in nature since they arise out of the inability to represent the system as it is due to the different discretizations utilized. If the final solution is obtained iteratively, a convergence criterion is also utilized adding to the error.

In the Monte Carlo Method, a stochastic model is constructed and the expected value of a desired random variable, which can be an integral quantity of interest is calculated (Kalos and Whitlock, 1986; Metropolis and Ulam, 1949). The expected value is obtained by calculating the average of many independent samples. Often, the method is likened to performing “an experiment on a computer”. Given that the stochastic model utilized is accurate (i.e. the underlying physical characteristics of the system are well known), the approach is accurate.
Random numbers are used to sample from probability density functions (pdf’s) representing the basic physical phenomena to provide the desired independent samples. Alternatively, the Monte Carlo Method can be used to directly solve deterministic equations as a numerical integration tool.

Monte Carlo error is observed from an incorrect stochastic model and from the statistical uncertainties of the calculated results. The former is reduced by modeling the process as close to nature as possible, and the latter is estimated using principles of statistics to be reviewed later such as expectation values, variances, use of the Central Limit Theorem, etc. Recently, more researchers have begun to utilize both deterministic and Monte Carlo methods together to benefit from the strengths of each method.

Particle transport via the Monte Carlo Method has long been lauded for its ability to provide accurate solutions to some of the most challenging problems. Monte Carlo analysis of this type usually focuses on a specific local objective since the process is time consuming. With the ever increasing computer capabilities, problems of increasing complexity are being resolved like never before, but these problems pose new challenges and also bring to light some new issues. Problem specific objectives are no longer desired, and full phase space analysis is sought, with the idea that even 3-D burnup with Monte Carlo is now an obtainable goal. In addition, the solution of criticality (eigenvalue) problems via the Monte Carlo Method is standard practice, and although reliable eigenvalue estimates may be easily obtained in most cases, full phase space information is often much more difficult to obtain. Even with current computing technology, this can be a very time consuming process. In addition, source convergence difficulties have long plagued the solution of criticality problems, particularly for high dominance ratio (DR) problems, as has been pointed out for decades (Blomquist and Gelbard, 2000; Brissenden and
This work aims at providing additional information regarding source convergence and providing new techniques for difficult source convergence problems, such as those with high DR, while attempting to reduce variance and improve accuracy.

**Literature Review**

Current source convergence diagnostics have improved diagnostic ability with the introduction of several new approaches, however, none of the diagnostic tools are failsafe. Consequently, it is believed that a multilevel testing approach using a combined methodology may be best. One focus of this work is the addition of a new diagnostic test for any Monte Carlo eigenvalue problem with analysis indicating combined use of available diagnostics as the most tractable approach.

Source acceleration for criticality problems has not had the level of success that shielding problems have enjoyed. Nevertheless, some excellent ideas and success has been met with past and more recent methods such as stratified source sampling (Blomquist, 2000; Gelbard and Roussel, 1995), super-history powering (Blomquist, 2000; Brissenden and Garlick, 1986), fission matrix methods (Kadotani et al., 1991; Morton, 1956), and more recently some interesting ideas such as Wielandt’s method (Brown, 2007; Yamamoto and Miyoshi, 2004), the Vacation Matrix approach (Finch, 2006), a semi-fixed source fission matrix approach (Dufek, 2007), and a zero-variance scheme using importance sampling (Dufek, 2007). A good summary of their strengths and weaknesses (except vacation matrix approach) are summarized in “Accelerated Monte Carlo Eigenvalue Calculations” (Dufek, 2007). Source initialization via deterministic methods may also be utilized in conjunction with these approaches which in itself can accelerate convergence due to a much shorter period of source initialization (Wenner et al., 2000). Strengths and weaknesses are evident in these and other approaches, and the need still exists to improve these
calculations with regard to both accuracy (of the results and their confidence) and calculation time. In fact, many of these methods are in the “acceleration” category, but are really used to reduce bias and help with fission source convergence of high DR problems, due to their inherent poor convergence properties. The work in this dissertation also puts forth new methodologies addressing the aforementioned issues.

The multiplication factor \( k_{\text{eff}} \) or dominant eigenvalue of a fissile system without an external source can be interpreted physically as the number of neutrons in one generation divided by the number of neutrons in the previous generation. In order to calculate this parameter via the Monte Carlo Method, one starts with an initial source distribution (guess) of neutrons inside the fissionable material, since the source distribution is not known. Using the known interaction probability distribution functions, the events in the life of each neutron (e.g., free flight, absorption, scattering) are randomly sampled. Along the way the results of this process such as the number of fission neutrons produced, their location and direction are stored for future use.

When all of the original source particles are exhausted, one can determine the \( k_{\text{eff}} \) by tabulating the number of neutrons generated to the number of neutrons started. This should be the first estimate of the eigenvalue and is denoted the first generation (or cycle) \( k_{\text{eff}} \). This procedure is repeated for many generations until the source converges and then the “active” generations begin. Until this period has ended, the initial generations must be discarded. Once the source has converged, the final \( k_{\text{eff}} \) is taken as an average of the \( k_{\text{eff}} \) of all active generations. A numerical problem that arises out of this strategy is that if the eigenvalue is not 1.0, the source will eventually die out \( (k_{\text{eff}} < 1.0) \) or increase exponentially \( (k_{\text{eff}} > 1.0) \). In order to account for this, a normalization scheme is utilized to keep the approximate number of source particles constant using the current \( k_{\text{eff}} \) estimate as a normalization factor.
Many sources of bias can become evident during a Monte Carlo eigenvalue simulation. A bias of the fission source has been shown to be related to the normalization of the source population at the end of each generation and autocorrelation of the fission source (Brissenden and Garlick, 1986; Gelbard, 1991; Gelbard and Gu, 1994; Gelbard and Prael, 1974). This bias can be made insignificant for many problems; however, significant issues can still be prevalent depending on the problem simulated (especially high DR problems). Also, the variance estimators can also be biased for similar reasons (Gelbard, 1990; MacMillian, 1973). This bias can become more pronounced if $k_{eff}$’s from an unconverged source are utilized in the calculation of $k_{eff}$ or if the underlying source is not independent.

**Introduction to Monte Carlo Source Convergence**

Source convergence in Monte Carlo eigenvalue problems is one of the most important issues the analyst must deal with in regards to a criticality simulation. All tally information should be deferred until the source has converged. The identification of a converged source, however, is not always an easy task. Many widely-used codes such as MCNP (X-5 Monte Carlo Team, 2003) and KENO (SCALE, 2005) have multiple checks regarding any tally information, including the $k_{eff}$. These checks are not adequate though when pertaining to identification of a converged fission source. Most standard statistical tests for tallies are not adequate when applied to source convergence and may be biased for reasons previously discussed in this chapter. Most code developers have begun or have already implemented new source convergence algorithms.

The difficulty in identifying source convergence is that although the $k_{eff}$ may have acceptable sample variance, it may be inaccurate due to many reasons, not least of which an unconverged source (from poor initial guess) and or strong autocorrelation. Traditional variance estimators are not pertinent when independence of samples is not guaranteed. Since $k_{eff}$ is an
integral quantity over the entire phase space, these errors may be small or non-existent, yet other tallies may suffer dramatically from an improperly converged source. One major objective of this work is to provide a new diagnostic tool for detection of a converged source distribution for which bias will be reduced, and therefore overall accuracy improved for all tallies as a secondary result.

In order to understand current and past work for identifying source convergence, the concept of a time series is introduced. A time series is a random or non-deterministic function $x$ of an independent variable $t$ for which future behavior cannot be predicted exactly (Jenkins and Watts, 1968). The $k_{\text{eff}}$ series is a time series that is no more than a random variable of a complex stochastic process. One of the most important decisions (often assumptions) made is whether the time series is said to be stationary. If stationary, the stochastic process can be described by its mean, variance, covariance, and other related parameters (Jenkins and Watts, 1968). This is important, since a diagnosis of stationarity implies that the statistical properties of the series do not change with time (or generation in this case). Physically, without a stationary series, the source has not converged and reliable estimates of random variables such as flux, $k_{\text{eff}}$, neutron current, etc., are not attainable. Note that even with a diagnosis of stationarity, bias can still be present in both the tallies and their error estimation. Furthermore, a converged stationary source may not be the true source. For the remainder of this dissertation, however, a stationary source will be deemed converged unless otherwise stated.

General statistical tests for stationarity are difficult to find. Some of the more well known methodologies concerning source convergence diagnostics are as follows:

- Sandwich approach (Yang and Naito, 2004)
- Information (Shannon) entropy based diagnostics (Ueki, 2005)
- Intergenerational Correlation Length (Shim and Kim, 2007)
- Limiting Distribution Approach (Richet et al., 2003)
The sandwich method (Yang and Naito, 2004) utilizes two calculations, one for which all the source is started in the most reactive area (obtained through pre-calculations), and one with a completely flat initial guess. Provided the results of both simulations are within statistics of each other, it is assumed the calculation is successful. This approach suffers from several issues. For one, two calculations are needed instead of one. Second, both calculations may converge in $k_{\text{eff}}$; however, the source may not have converged. It is well known that $k_{\text{eff}}$ convergence does not guarantee fission source convergence further complicating the issue (Ueki et al., 2003).

The information (Shannon) Entropy approach utilizes concepts from information theory in order to characterize whether the fission source is changing in an unacceptable manner. The Shannon Entropy is a measure of the randomness associated with data. The Shannon Entropy of a probability density distribution gives the minimum number of bits for which a density function can be stored in a computer memory. A related definition called the relative entropy is a measure between two distributions in terms of the information they carry. Here, the idea is if the fission source is tallied over a finite binning structure, it can be characterized by its Shannon Entropy (Cover and Thomas, 1991; Ueki and Brown, 2002).

Several criteria have been developed to identify if the fission source is changing “too much”. To identify what is “too much”, one criterion (Ueki and Brown, 2002) relies on the concept of minimum descriptive length and the Kraft inequality to show that the source should be converged if the fluctuation of the relative entropy is insignificant relative to the fluctuation of the entropy itself through the use of their mean squares. A second criterion (Ueki and Brown, 2002) is derived from a large sample property and is another inequality comparing the difference between the entropy of the average source and the entropy of each generation with the relative entropy of each generation. A third criterion (Ueki and Brown, 2002) is derived from the
concavity of the Shannon Entropy and indicates that the difference between the Shannon Entropy of the average source and the average Shannon Entropy should be within a small tolerance (Cover and Thomas, 1991; Ueki, 2005).

The Shannon Entropy approach has proven fruitful for many problems; however, assumptions must be made in the convergence criterion, none more important than the use of the average source from the second half of the simulation as the “true” source. Also, convergence of the Shannon Entropy does not guarantee fission source convergence (Ueki et al., 2003), and the Shannon Entropy tests can suffer from a reduced diagnostic ability for problems which may exhibit symmetric oscillations (L’Abbate et al., 2007).

The intergeneration correlation length (Shim and Kim, 2007) approach attempts to modify the normal statistical testing procedure if the fission source had no autocorrelation. In order to do this, the equation must be modified to add the “intergeneration correlation length” (Shim and Kim, 2007). This term is the minimum number of calculation generations apart which separate two uncorrelated fission sources. This method aims at an “on the fly” determination of the skipped generations. Approximations to the variance of the binned fission source matrix and the covariance matrix between fission sources of different generations must be estimated. Good results have been published in the literature; nevertheless, as with all the other methods, estimators must be acquired which are problem dependent (Shim and Kim, 2007). Furthermore, problems exist with very strong and long lasting correlation which is compounded in the high DR problems.

The “limiting distribution approach” (LDA) uses “convergence of probability measures” (Billingsley, 1968), for which an autocorrelated time series is said to converge to the Brownian Bridge if the time series is stationary. This methodology was originally developed for
simulations in operations research (Heidelberger and Welch, 1983; Schruben, 1982). It was applied to the $k_{\text{eff}}$ time series which will converge to the Brownian Bridge identified through the use of significance tests applied to the $k_{\text{eff}}$ series (Richet et al., 2003). This approach suffers from several drawbacks in that it tests the $k_{\text{eff}}$ series which is not a good indicator of source convergence as previously mentioned. Also an estimate of a parameter called the “long run variance” must be determined which may be inadequate or impractical using the estimators derived from the work in operations research. Many different estimators have been used and proposed (Heidelberger and Welch, 1981; Heidelberger and Welch, 1983; Schruben, 1982). Further, stationarity is being indirectly tested for, which only preliminary statistical power and size analysis has been undertaken for the proposed significance tests.

A major issue with the LDA is obtaining a parameter which is closely related to the Monte Carlo source convergence in order to perform the diagnostic test. A first guess has been the use of the $k_{\text{eff}}$ series, which does not imply source convergence. A natural choice appears to be the use of the source center of mass (COM) (Wenner and Haghighat, 2007). The source COM is a single value at each generation which should closely follow the spatial behavior of the fission source. Given the source COM, it was desired to utilize this series with analysis similar to that of the LDA. In this dissertation, a formal testing procedure has been implemented which shows that the sum of residuals from a least squares fit of a time series should follow a Brownian Bridge related distribution, and a significance test has been implemented for this purpose called the Generalized KPSS test for stationarity (Kwiatkowski et al., 1992). Distinct differences exist between this approach and the LDA approach making it a novel approach when compared to the LDA. The statistical testing procedure has been formalized, and the COM series behavior has been chosen as the parameter to characterize source behavior. Also, estimation of the “long run
“variance” has been updated to provide more accurate testing. More details on this method will be given in Chapter 3.

**Introduction to Monte Carlo Source Acceleration**

Accuracy of solution is the first priority for a Monte Carlo eigenvalue simulation. Nevertheless, if computation of an accurate solution is not practical within a limited time, results are not useful. In order to overcome this, variance reduction techniques have been developed to speed up the calculation process. Variance reduction has enjoyed great success concerning fixed source problems where localized objectives are desired. In an eigenvalue simulation, however, all fissile regions are important, therefore many conventional variance reduction techniques are not effective.

Several methods have been proposed that are unique to the eigenvalue calculation. Some of these are as follows:

- Stratified Source Sampling (Gelbard and Roussel, 1995)
- Super-History Powering (Brissenden and Garlick, 1986)
- Vacation Matrix Approach (Finch, 2006)
- Wielandt’s Method (Brown, 2007; Yamamoto and Miyoshi, 2004)
- Importance Sampling Methodologies (Christoforou and Hoogenboom, 2006; Dufek, 2007; Wagner et al., 2007)

The stratified source sampling method attempts to force at least one fission neutron be in each fissile region (user defined). This method has the potential to improve both accuracy and simulation time. Success is limited since ensuring at least one fission neutron may not be enough, and at times it is still possible to lose the fission source entirely in a region (Blomquist, 2000; Gelbard and Roussel, 1995).

In super-history powering, cycles and generations are not equivalent. Super-history powering alters the source normalization scheme such that each cycle is not just one neutron
generation but \( l \) generations contained within a cycle. Instead of normalizing the weight for each cycle to the number of neutrons per generation, \( m \), it is normalized to the total source for that cycle and generation. The fission source for the first generation of each cycle is from the last generation in the previous cycle. Up to 10 generations per cycle is recommended. This approach can reduce source bias by increasing priority in highly multiplying regions, however, any localized information in less multiplying areas may be less reliable (Brissenden and Garlick, 1986; Dufek, 2007).

If the system is discretized spatially, a matrix equation can be formulated such that each element of the matrix (fission matrix) represents the transfer probability of fission from one cell to another (or itself). This information can be used to bias the source and achieve speedup. The fission matrix method has had some success, but problems in convergence of the fission matrix elements due to statistical noise has limited its usefulness. If the cumulative fission matrix is utilized; however, this problem may be reduced but not eliminated, and still contamination from unreliable source cycles becomes an issue (Dufek, 2007; Kaplan, 1958; Morton, 1956; Urbatsch, 1995).

Until recently, the fission matrix method has been the preferred method of fission source convergence acceleration. Statistical noise in computing the fission matrix elements, especially in those problems with loose coupling between different source areas has prohibited the method from widespread success. A new approach called the Vacation Matrix method has been devised by identifying which variables in the matrix are independent of one another and uses them to devise a new spatial binning, thereby reducing the noise associated with these variables. The variables are the leakage probability and the vacated source probability (Finch, 2006).
Wielandt’s method is a deterministic acceleration technique for problems with high dominance ratio causing slow convergence. In this approach, the eigenvalue in the transport equation is simply replaced by two components, and it can be shown that the dominance ratio of this equation will be reduced under certain conditions. In order to adapt this method to Monte Carlo eigenvalue simulations, the fission bank and fission site selection is modified to incorporate these two components which facilitates the tracking of all fission neutrons and their progeny (with respect to this new formulation). The method causes more neutrons to be followed per generation, yet there are less banked neutrons per collision for use with the next generation. This causes a larger dispersion of source neutrons inside each generation thereby reducing problems of loose coupling between fission sites. A drawback to this method is the fact that often the simulation time has been shown to increase (Brown, 2007; Yamamoto and Miyoshi, 2004).

A semi-fixed source fission matrix method has recently been devised which samples all regions equally since it is known that the sampling of fission matrix elements with different numbers of fission neutrons is one cause of instability in the fission matrix method. In order to achieve this, the spatial discretization must be done such that an equal number of source is in each volume. This discretization is not possible to know apriori; however, if the mesh is sufficiently small, bias caused from this approximation is minimal or eliminated. Difficulties arise due to the size of the fission matrix utilized (Dufek, 2007).

Importance sampling related methods include a zero-variance based scheme derived for eigenvalue calculations which can be implemented in a similar manner to conventional deterministic biasing. By looking at the components of the calculated $k_{eff}$, a “detector- response” like formulation can be derived and applied. Initial investigation in this dissertation shows
favorable speedup is possible as well as in (Christoforou and Hoogenboom, 2006) and (Dufek, 2007). This work is a straightforward extension of the zero-variance formulations for shielding calculations which were extended to Monte Carlo shielding problems by Wagner and Haghigat in their Consistent-Adjoint Driven Important Sampling (CADIS) methodology (Wagner and Haghigat, 1998). Recently, the CADIS methodology has been extended to provide a means to obtain a similarly converged global solution over the problem phase space and is known as Forward Weighted-CADIS (FW-CADIS) (Wagner et al., 2007).

Lastly, a fission matrix based Monte Carlo method has recently been devised related to the semi-fixed source method (Dufek, 2009). In this work it is shown that the operator in the eigenvalue problem is independent of the source, however when the operator is discretized to write the fission matrix algorithm, it gains its spatial dependence. Through the use of limit theorems it is shown that in the limit of fission matrix mesh sizes approaching zero, the fission matrix elements are independent of the source distribution (Dufek, 2009). This method shows some interesting characteristics of the fission matrix algorithm and is extended in this dissertation. A solution methodology is arrived at in this dissertation for difficult source convergence problems, including high DR problems via the use of the fission matrix algorithm with a deterministic obtained initialized source option, all included in a parallel algorithm. Under problem conditions which lead to a high DR, the distribution of fission matrix elements remain independent (and Gaussian) if a large enough particle density is utilized with a fine fission matrix mesh density. Utilization of a reasonable initialized source will assure that the bias is reduced, while parallelization provides added efficiency.

Also developed in this dissertation is a new source iteration strategy extending the CADIS methodology in an alternative fashion for reducing variance of the fission matrix elements. This
methodology requires multiple deterministic importance calculations to acquire an estimate of
the importance to fission for a user-defined coarse source region. Once obtained, the power
iteration method is modified such that each source in each region is transported to itself and
every other region in separate calculations reusing the same initial conditions. The weight-
window approach is utilized to control population weight as in the CADIS methodology instead
of biasing the actual sampling probabilities as in the zero-variance method. This methodology
can improve accuracy for loosely coupled systems, as well as help to mitigate some of the
difficulties seen with high DR problems.

Chapter 2 of this dissertation describes the general theory required encompassing this
work. Chapter 3 gives a detailed discussion of the methodology utilized for the KPSS test for
stationarity detection applied to Monte Carlo eigenvalue calculations, as well as a review of
some information theoretic diagnostics utilized for comparison. Chapter 4 discusses
implementation and testing of the diagnostics discussed in Chapter 3. Chapter 5 discusses the
new source acceleration methodologies based on the CADIS importance sampling methodology
and the fission matrix acceleration methodology. Chapter 6 discusses the implementation and
testing of the acceleration methodologies developed in chapter 5. Chapter 7 gives new revised
methodologies/algorithms for use in high dominance ratio problems by extending the fission
matrix based Monte Carlo (FMBMC) approach. Lastly, chapter 8 gives some conclusions and
suggestions for future work.
CHAPTER 2
GENERAL THEORY

A general description of the Monte Carlo eigenvalue problem in order to determine the multiplication factor $k_{\text{eff}}$ is given here. The eigenvalue form of the equation is derived from the time independent Boltzmann transport equation. Once the equation is obtained, its mathematical adjoint is discussed in relation to particle importance. After that, a brief discussion of Monte Carlo transport is given, followed by a short discussion of probability and statistics related to error estimation. Next, the estimators for $k_{\text{eff}}$ are given and the two most common Monte Carlo $k_{\text{eff}}$ algorithms are discussed. Furthermore, a discussion of stationary stochastic processes is given in the context of Monte Carlo source convergence. In addition, a short description of Monte Carlo variance reduction techniques is included. After that, a brief description of the deterministic $S_N$ method is discussed. Lastly, computer codes utilized in this dissertation are described.

Forward Transport

Neutral particle transport can accurately be described by the Linear Boltzmann transport equation. Since neutron kinetics parameters will not be important for this work, the time-independent form is utilized. The LBE is nothing more than a balance equation ensuring neutron conservation and can be derived from physical arguments. It does, however, contain six independent variables, making direct solution, except in special cases, not possible. The time-independent integro-differential form of the LBE is given by

$$
\Omega \cdot \nabla \psi(\vec{r}, E, \Omega) + \sigma_t(\vec{r}, E) \psi(\vec{r}, E, \Omega) = \\
\int_{4\pi} d\Omega' \int_0^\infty dE' \sigma_s(\vec{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) \psi(\vec{r}, E', \Omega') + \\
\frac{\chi(E)}{4\pi} \int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E') \sigma_f(E') \psi(\vec{r}, E', \Omega') + Q_{\text{ext}}(\vec{r}, E, \Omega),
$$

(2-1)

where
• \( \mathbf{r} \) = particle coordinate in space
• \( E \) = particle energy
• \( \mathbf{\hat{r}} \) = unit vector in direction of particle motion
• \( \psi \) = angular flux
• \( \sigma_t \) = total macroscopic cross section
• \( \sigma_s \) = double differential scattering cross section
• \( \chi \) = fission spectrum
• \( v \) = average number of neutrons produced during fission
• \( \sigma_f \) = fission cross section
• \( Q_{\text{ext}} \) = external independent source.

The first term ("streaming") represents leakage into or out of the system. The second term ("collision") is a loss term due to collision. The first term on the right hand side of the equation ("scattering") represents neutron scattering from all energies and angles \( dE' d\Omega' \) into \( dE \ d\Omega \).

Next is the "fission" term which gives the total rate at which fission neutrons are born at a position \( \mathbf{r} \), with an energy distribution given by the fission spectrum \( \chi(E) \). This term assumes all neutrons are prompt, and since neutron kinetics is not being studied, this is adequate. Lastly, \( Q_{\text{ext}}(\mathbf{r}, E, \mathbf{\hat{r}}) d\mathbf{r} dE d\Omega \) is the rate of neutrons appearing in \( d\mathbf{r} \) about \( \mathbf{r} \), \( dE \) about \( E \), and \( d\Omega \) about \( \mathbf{\hat{r}} \) from an external source.

Note that even though lowercase Greek symbols are utilized, it is still the macroscopic (as opposed to microscopic) cross sections in the equation as this follows convention of most textbooks concerning neutron transport theory. The solution to this equation will provide the angular flux throughout the phase space. Often, to simplify the writing of EQ. (2-1), operator notation is used. The operator \( H \) is defined as

\[
H = \mathbf{\hat{r}} \cdot \nabla + \sigma_t(\mathbf{r}, E) - \int_{4\pi} d\Omega' \int_0^\infty dE' \sigma_s(\mathbf{r}, E \rightarrow E', \Omega \rightarrow \mathbf{\hat{r}}'). \tag{2-2}
\]

Neglecting the fission source term, EQ. (2-1) can then be written as

\[
H\psi(\mathbf{r}, \mathbf{\hat{r}}, E) = Q_{\text{ext}}(\mathbf{r}, \mathbf{\hat{r}}, E). \tag{2-3}
\]
Adjoint Transport and Neutron Importance

Utilizing operator notation and neglecting dependencies, the adjoint property is shown in EQ. (2-4) (Bell and Glasstone, 1985). The dagger (†) in EQ. (2-4) identifies the adjoint, and the brackets, ⟨ ⟩, are referred to as Dirac Brackets and signify integration over all independent variables. It can be shown that in order for the adjoint property to hold, vacuum boundary conditions for the angular flux and its adjoint must be present as shown in EQ. (2-5) and EQ. (2-6).

\[
\langle \psi^\dagger H \psi \rangle = \langle \psi H^\dagger \psi^\dagger \rangle \tag{2-4}
\]

\[
\psi(\vec{r}, \Omega, E) = 0, \quad \vec{r} \in \Gamma, \hat{n} \cdot \hat{n} < 0 \tag{2-5}
\]

\[
\psi^\dagger(\vec{r}, \Omega, E) = 0, \quad \vec{r} \in \Gamma, \hat{n} \cdot \hat{n} > 0 \tag{2-6}
\]

\(\Gamma\) is the boundary surface and \(\hat{n}\) is an outward unit vector normal to the surface. Utilizing the adjoint property, the adjoint operator \(H^\dagger\) can be derived and shown to be

\[
H^\dagger = -\bar{\Omega} \cdot \bar{V} + \sigma_t(\vec{r}, E) - \int_{4\pi} d\Omega' \int_0^\infty dE' \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega}). \tag{2-7}
\]

Neglecting the fission term, the adjoint equation to the LBE can then be written as

\[
H^\dagger \psi^\dagger(\vec{r}, \Omega, E) = Q^\dagger_{\text{ext}}(\vec{r}, \Omega, E), \tag{2-8}
\]

subject to the boundary conditions of EQ’s (2-5) and (2-6).

Using physical arguments, however, it is possible to derive a balance equation for particle importance. This equation turns out to be the same as the adjoint transport equation, but is not subject to the vacuum boundary restriction (Bell and Glasstone, 1985). This implies that the solution to the adjoint LBE relates to the importance of a particle to an objective represented by the adjoint source \(Q^\dagger_{\text{ext}}\).
To illustrate the power of adjoint transport theory, the calculation of detector response for a fixed source problem is reviewed. Detector response \( R \) can be calculated from the angular flux and detector cross section \( \sigma_d(\vec{r}, E) \) as shown in EQ. (2-9).

\[
R = \langle \psi(\vec{r}, \vec{\Omega}, E) \sigma_d(\vec{r}, E) \rangle \tag{2-9}
\]

Forming a commutation relation by multiplying the LBE by the adjoint flux and the adjoint LBE by the angular flux and subtracting yields

\[
\langle \psi^\dagger H \psi \rangle - \langle \psi H^\dagger \psi^\dagger \rangle = \langle \psi^\dagger Q \rangle - \langle \psi Q^\dagger \rangle. \tag{2-10}
\]

Utilizing the adjoint property in EQ. (2-4), EQ. (2-10) is reduced to

\[
\langle \psi^\dagger Q \rangle = \langle \psi Q^\dagger \rangle. \tag{2-11}
\]

Considering the adjoint source to be the detector cross section, detector response can be determined alternately as

\[
R = \langle \psi^\dagger(\vec{r}, \vec{\Omega}, E) Q(\vec{r}, E) \rangle. \tag{2-12}
\]

Physically, the adjoint flux is the importance toward producing a detector count. Note that if only a single adjoint calculation is performed, the detector response can be calculated for any “forward” source without the need for another calculation. These results were obtained by neglecting the fission term. This does not affect the resulting formulation for detector response which was omitted for simplicity.

Understanding the concept of importance is necessary in utilizing it for biasing in the Monte Carlo method to be discussed later. Briefly, the neutron importance can be used to bias the different physical processes in order to sample more important events relating to the desired objective. It is easy to see that when the objective is localized, the method is very powerful. In a criticality problem though, the objective will be spread throughout the problem and utilizing the neutron importance to accelerate the solution will be more difficult.
The Eigenvalue Problem

In multiplying systems, a system is critical if it has a time-independent, nonnegative solution to eqn. EQ. (2-1). Since it is not easy to know apriori the combination of cross section and geometry necessary to achieve criticality, EQ. (2-1) is modified into the form of an eigenvalue problem. The eigenvalue that will be discussed in this work is the multiplication factor \( k_{\text{eff}} \) eigenvalue.

First, neglecting the external source, \( k_{\text{eff}} \) is introduced into EQ. (2-1) which will give a measure of the criticality of the system:

\[
\Omega \cdot \nabla \psi \big( \vec{r}, E, \Omega \big) + \sigma_t \big( \vec{r}, E \big) \psi \big( \vec{r}, E, \Omega \big) = \int_{4\pi} \frac{d\Omega'}{k_{\text{eff}} 4\pi} \int_0^\infty dE' \nu(E') \sigma_f \big( E' \big) \psi \big( \vec{r}, E', \Omega' \big) + \int_{4\pi} d\Omega' \int_0^\infty dE' \sigma_r \big( \vec{r}, E', \Omega' \big) \psi \big( \vec{r}, E', \Omega' \big) + \frac{\chi(E)}{k_{\text{eff}} 4\pi} \int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E') \sigma_f \big( E' \big) \psi \big( \vec{r}, E', \Omega' \big) \]

\( \text{(2-13)} \)

It is of interest to find the fundamental mode solution of EQ. (2-13). This eigenvalue is the multiplication factor \( k_{\text{eff}} \) of the system. The system is critical (self sustaining) if \( k_{\text{eff}} = 1 \), supercritical if \( k_{\text{eff}} > 1 \), and subcritical if \( k_{\text{eff}} < 1 \).

The form of the LBE in EQ. (2-13) is the integro-differential form of the equation. The equation can be transformed to the integral form using the Green’s function shown here, or the method of characteristics. If the Green’s function \( \mathcal{G}(\vec{r}' \rightarrow r, \vec{\Omega}' \rightarrow \Omega, E' \rightarrow E) \) is defined as the neutron angular flux at \( r, E, \Omega \) due to a unit point source at \( \vec{r}' \) emitting one neutron/sec in the direction \( \vec{\Omega}' \) with energy \( E' \), then the solution to the angular flux can be obtained by:

\[
\psi \big( \vec{r}, E, \Omega \big) = \int_V dr' \int_{4\pi} d\Omega' \int_0^\infty dE' \mathcal{G}(\vec{r}' \rightarrow \vec{r}, \vec{\Omega}' \rightarrow \Omega, E' \rightarrow E) \times \frac{\chi(E)}{k_{\text{eff}} 4\pi} \int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E') \sigma_f \big( E' \big) \psi \big( \vec{r}, E', \Omega' \big) \]

\( \text{(2-14)} \)

This is so because if one looks at the fission source density given by

\[
\int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E') \sigma_f \big( E' \big) \psi \big( \vec{r}, E', \Omega' \big) , \]

it is apparent that the Green’s function (whatever it may be) in EQ. (2-14) is like a transfer function for the source, providing its impact to the flux.
by effectively summing up all the point sources totaling the actual problem source. This is
important since the Monte Carlo Method is often said to solve the integral form of the LBE.
This is so because of the Fundamental Formulation of Monte Carlo discussed later.

Starting with either Eq. (2-13) or Eq. (2-14), the same matrix eigenvalue problem can be
derived. As previously stated, the transport equation is often written in operator form (Lewis and
Miller, 1993) where the transport operator \( H \) is as before, and the fission operator \( F \) is defined as

\[
F = \int_{4\pi} d\Omega' \int_0^\infty dE' \nu(E')\sigma_f(E') .
\]  

(2-15)

Without explicitly writing the dependencies then, Eq. (2-13) can be written as

\[
H\psi = \frac{1}{k_{\text{eff}}} \chi F\psi .
\]

(2-16)

Inverting \( H \) and operating by \( F \) on both sides of Eq. (2-16), the resulting form of the equation is

\[
F\psi = \frac{1}{k_{\text{eff}}} [FH^{-1}\chi]F\psi .
\]

(2-17)

Finally then, Eq. (2-17) can be rewritten as

\[
k_{\text{eff}}S = AS,
\]

(2-18)

where \( S = F\psi \) is the source and \( A = FH^{-1}\chi \). Since the operator \( A \) applied on \( S \) gives the next
generated fission source, with \( k_{\text{eff}} \) the eigenvalue, \( AS \) can then be defined as

\[
AS(\vec{r}) = \int_{\Omega'} a(\vec{r}' \rightarrow \vec{r})d\vec{r}'S(\vec{r}').
\]

(2-19)

Physically, one can think of \( a(\vec{r}' \rightarrow \vec{r}) \) as the expected number of fission neutrons produced per
unit volume at \( \vec{r} \) from fission neutrons at \( \vec{r}' \). Eq. (2-19) is solved using the power iteration
method (Bell and Glasstone, 1985; Lewis and Miller, 1993). If the system is discretized
spatially, the operator \( A \) can be approximated with the fission matrix \( (A)_{i,j} \) (Kaplan, 1958;
Morton, 1956). The fission matrix elements \( (A)_{i,j} \)'s, can be considered as the probability that a
neutron born in cell \( j \) will generate a fission neutron in cell \( i \) as
\[
(A)_{i,j} = \frac{\int_{V_i} d\vec{r} \int_{V_j} d\vec{r}' a(\vec{r}' \rightarrow \vec{r})S_0(\vec{r}')}}{\int_{V_j} d\vec{r}' S_0(\vec{r}')}}
\]

(2-20)

where \(S_0(\vec{r}')\) is the fundamental mode source. Of course \(S_0(\vec{r}')\) is not known apriori and an approximation is used with biasing methods to be discussed in chapter 5.

**The Monte Carlo Method**

The Monte Carlo method is a statistical method to solve mathematical and/or physical problems. Unlike deterministic methods, such as the discrete ordinates (\(S_N\)) method, which explicitly solves the LBE (Lewis and Miller, 1993), Monte Carlo methods do not explicitly solve any equation. Instead, the average particle behavior is determined from simulating individual particles (Metropolis and Ulam, 1949; X-5 Monte Carlo Team, 2003).

Many in the nuclear engineering discipline point out that Monte Carlo solves the integral form of the LBE. Depending on your viewpoint, this may or may not be the case. First, Monte Carlo solves a transport problem by simulating individual particle histories for which an equation doesn’t need to be written. In this way nothing must be said of the LBE. However, the Monte Carlo Method can be used as a mathematical tool to solve complex integrals (or simple ones). Since the transport equation can be written in integral form, many say that Monte Carlo is used to solve this integral equation. This statement is unclear since the exact pdf of the complex process needed in the integral analysis such as transporting particles through a 3-D geometry is not known. Instead it is sampled by tracking all the microscopic events (which constitute the complex process) in the histories of a large number of particles, thus solving the integral equation by Monte Carlo methods (Dionne, 2007; X-5 Monte Carlo Team, 2003). Because of this fact, importance sampling can be effectively utilized through the use of an approximate importance function.
Random Variable

All elementary physical processes appear to be random at the microscopic level. Individual process behavior cannot be determined with any certainty, but these random events can often be characterized by their macroscopic effects which represent average behavior of a physical system. In general, every outcome of an experiment can be associated with a number by specifying a rule of association. This rule can then be called a random variable since different numerical values are possible and because the observed value depends on the possible experimental outcome (Devore, 2000).

Two functions are defined for any random variable. These are the probability density function (pdf) and the cumulative distribution function (cdf). For a continuous random variable, the pdf is the probability that the outcome of a random process is $x$ within $x$ and $x + dx$. For example, for a cubical die, the probability of a particular event to occur is 1/6 because there are six sides and the cube is fair. The pdf ($p(x)$) is normalized as

$$\int_{a}^{b} p(x)dx = 1 \quad a \leq x \leq b. \quad (2-21)$$

The cdf is the probability that the outcome of the random process has a value not exceeding some value $x$. The cdf ($P(x)$) is then defined by

$$P(x) = \int_{a}^{x} p(x)dx \quad a \leq x \leq b. \quad (2-22)$$

Random Numbers and the Fundamental Formulation of Monte Carlo (FFMC)

Random numbers are a sequence of numbers for which the occurrence of each number is unpredictable. Commonly, random numbers ($\eta$) are defined in the range of [0,1] and their pdf is given by

$$p(\eta) = 1 \quad 0 < \eta < 1. \quad (2-23)$$

This leads to a cdf given by

38
\[ P(\eta) = \int_{\eta_0}^{\eta} p(\eta') \, d\eta' = \eta. \]  

(2-24)

Assuming that the basic physics associated with a problem are known, i.e., obtaining the pdf’s associated with the physical properties; it is then coherent to desire to simulate the problem. Assuming that random numbers can be generated, it is desired to obtain a random variable \( x \) relating to a random process with pdf \( p(x) \) by relating the random variable to a random number \( \eta \) as

\[
\int_a^x p(x) \, dx = \int_0^\eta p(\eta) \, d\eta \quad a \leq x \leq b \quad \text{and} \quad 0 \leq \eta \leq 1.
\] (2-25)

Substituting Eq. (2-23) into Eq. (2-25) the result is

\[
\int_a^x p(x) \, dx = \int_0^\eta d\eta = \eta \Rightarrow P(x) = \eta.
\] (2-26)

EQ. (2-25) is given the name the Fundamental Formulation of Monte Carlo (FFMC) (class notes on Monte Carlo Methods by Alireza Haghighat).

**Particle Transport with Monte Carlo Methods**

Using the concept of the FFMC, individual particles can be simulated from their birth to death. This assumes that the pdf’s associated with the particle behavior are known, such as particle interaction data, which are given through interaction cross sections. Even particle “birth” is a random process that has an associated probability.

Consider the events that are possible in the life of a particle. The first event that must be present is the birth of a particle. Using a density function to represent the spatial distribution of source one can sample this density function to give birth to source particles. Alternatively, in an eigenvalue equation, once an initial starting source distribution is given, subsequent generations of neutron births are a direct result of fission from the previous generation. This takes care of the
spatial distribution of source, but similarly, initial particle direction and energy must be determined. These as well can be determined similarly to the spatial distribution.

Aside from particle birth, interactions may occur. This creates several physical phenomena which must be characterized. First, how far does the particle travel between interactions? To show how the basic physics are represented utilizing the FFMC, the equation for free flight between collisions is derived here. From basic particle physics it is known that the probability of no collision in a distance \( r \) is \( e^{-\Sigma t r} \), and that the probability of collision in \( dr \) is \( \Sigma t dr \). This leads to EQ. (2-27).

\[
p(r) dr = \Sigma_t e^{-\Sigma_t r} dr
\]  

(2-27)

Utilizing the FFMC, it can be written that

\[
P(r) = \int_0^r \Sigma_t e^{-\Sigma_t r'} dr' = \eta.
\]  

(2-28)

Performing the integration and rearranging terms, the particle free flight length between interactions is determined by

\[
r = \frac{-\ln \eta}{\Sigma_t}.
\]  

(2-29)

All of the physical phenomena are sampled using this technique (analytical inversion) or by using another sampling technique (such as the rejection technique) when direct analytical inversion is not possible or practical.

Knowing the original particle location, its initial direction of travel, and the distance to collision, the interaction site location is determined and the material or isotope of interaction is determined. Selection of interaction type can be performed by forming a cumulative distribution function relating different interactions. This ensures that each interaction is statistically chosen according to its interaction probability \( \left( \frac{\Sigma x}{\Sigma t} \right) \), where \( x \) represents a generic interaction of type \( x \). If the particle has been absorbed, its life has been ended, however, if the absorption event created
new particles (e.g., (n,γ), (n,2n), (n,fission), etc.), its/their initial position(s), energy/energies, and
direction(s) are then temporarily stored, or banked. Once the original source particle has been
terminated, transport of the secondary particle(s) is performed. If the calculation is for neutrons
only, gammas, electrons or other particles that are generated are not banked and are ignored.

If the particle is not absorbed, a new energy and direction of travel are determined from
random sampling of the physics of the interaction type and a new distance to collision calculated.
The governing physics equation utilized in selection of a scattering angle and energy after
collision is the differential scattering cross section of interest and subsequent kinematics
information. Continuing then with the original particle, this process is repeated until the particle
is either absorbed, or exits the problem boundaries. Upon particle termination, any secondary
particles generated by that particle are transported until termination (except for neutrons in an
eigenvalue problem). At this time a new source particle is generated until a user defined number
of histories have been simulated (Wagner, 1997).

In an eigenvalue problem, fission neutrons are stored instead of transported. Upon
completion of all particles in the initial batch (generation) of starting neutrons, the banked source
particles are started as if they were the original source particles. Eventually, the source
distribution will settle and a user defined number of “active” cycles of source generations are
simulated.

To obtain observable results from the system, tally regions are set up to “score” any
contribution a particular particle has toward an objective. Since each particle is simulated, an
adequate number of trials are necessary to obtain a statistically reasonable average. To estimate
the reliability of the results, the relative error of each tally is evaluated. In an eigenvalue
problem, all scoring is deferred until a sufficient number of generations have been run such that
the source has converged. These deferred generations are commonly called skipped generations.

**Statistics for Monte Carlo Analyses**

Since the information obtained from Monte Carlo simulations is average quantities, it is
desirable that these averages are within a specified precision. To achieve this, a basic review of
pertinent probability and statistics is given. The expected value of a function of a random
variable \( x \) is the true mean of the function. If a function \( g(x) \) is defined on an interval \([a,b]\), then
the expected value of the function is given as

\[
E[g(x)] = \int_a^b g(x) p(x) dx.
\]  
(2-30)

For a continuous random variable, where \( g(x) = x \), the true mean of \( x \) is given by

\[
m = E(x) = \int_a^b x p(x) dx,
\]  
(2-31)

and its variance is given by

\[
\sigma^2 = E[(x - m)^2] = \int_a^b (x - m)^2 p(x) dx.
\]  
(2-32)

It is of interest, however, to obtain averages and their associated variances when sampling
from unknown populations, whereas the above formulae are from known populations. Similar to
the above equations, the sample mean and sample variance can be defined respectively as

\[
\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i,
\]  
(2-33)

and

\[
s_x^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2.
\]  
(2-34)

Since inferential statistics is utilized, an unbiased estimate of the population parameters is sought
through the use of the sample parameters. Care must be taken to ensure that the parameters are
unbiased estimators of the population parameters. To accomplish this, the expected values of the
sample mean and sample variance are computed. The expected value of the sample mean is given by

$$E[\bar{x}] = E \left[ \frac{1}{N} \sum_{i=1}^{N} x_i \right] = \frac{1}{N} E \left[ \sum_{i=1}^{N} x_i \right] = E(x) = m. \quad (2-35)$$

As a result, EQ. (2-33) is an unbiased estimator of the true mean. For the sake of brevity, only the result of the expected value of the sample variance is written as

$$E[s^2] = E \left[ \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2 \right] = \frac{N - 1}{N} \sigma^2. \quad (2-36)$$

This demonstrates that the EQ. (2-34) is not an unbiased estimator of the true variance. Hence, a new unbiased estimator is defined as

$$S^2 = \frac{1}{N - 1} \sum_{i=1}^{N} (x_i - \bar{x})^2. \quad (2-37)$$

To proceed from here, the Central Limit Theorem (CLT) and its validity is discussed. The CLT deals with a random sample of $x_1, x_2, \ldots, x_n$ from a random distribution with mean $\mu$ and variance $\sigma^2$. It states that $\bar{x}$ has a normal distribution with $\mu_\bar{x} = \mu$ and $\sigma^2_\bar{x} = \frac{\sigma^2}{N}$ if $N$ is sufficiently large. This statement is true even when the original population distribution is not normal. Extending this to the sample variance, the relative error for $\bar{x}$ is then given by

$$R = \frac{S_\bar{x}}{\bar{x}} = \frac{s}{\bar{x} \sqrt{N}}. \quad (2-38)$$

This discussion assumes independence of samples. If samples are dependent, then the formulae for mean, variance and relative error become biased since one value will influence another and this correlation must be accounted for in proper error estimation. This will not be dealt with explicitly in this dissertation.
Tallying in a Monte Carlo Simulation

Now that the tools necessary for transport of particles and statistics analysis have been discussed, a review of tallying (scoring) is given. The calculation of physical quantities such as neutron flux, neutron current, reaction rates, gamma heating or other quantities of interest are often desired. In order to determine any quantities in a localized phase space, a discretization of space, energy, angle or time must be undertaken according to the desired information. Recall also that results from Monte Carlo tallies are normalized per source particle. This should be apparent from an understanding of the method. If actual physical results are desired, the tally information must be multiplied by the total source strength.

Another quantity of interest is the effective multiplication factor $k_{eff}$. Here, the parameter in question is not localized and will be dependent on the entire fissionable region. $k_{eff}$ estimators are also discussed later. In an eigenvalue calculation, the average of the $k_{eff}$ estimators over all active cycles is often utilized. Some standard computer codes use more than one estimator combined, while others utilize only the collision estimator. Time dependence is not important in this dissertation and will be neglected. The tallies discussed are algorithmic in nature.

Collision estimators

A counter is set up in order to estimate the number of collisions in a certain discretized volume element $\Delta V_i$, with direction $\hat{\Omega}$ within a solid angle $\Delta \Omega_k$, with energy $E$ within $\Delta E_j$. This counter can be represented with the counter in EQ. (2-39).

$$C(i, j, k) = C(i, j, k) + \frac{w}{\Sigma_t(E)}$$

(2-39)

The parameter $w$ is the particle weight, and for an unbiased simulation $w=1$. The reason the counter is divided by the total cross section at each score will be discussed.
Physically, if the total number of collisions in a region were counted and normalized per simulation source particle, what would be obtained is the total reaction rate in that volume. Knowing that the relationship between neutron flux and reaction rate first introduced in EQ. (2-9) and repeated here with the scalar flux $\phi$ and macroscopic cross section $\Sigma$ in EQ. (2-40) is

$$R(\bar{r}) = \int E \, dE \Sigma(E) \phi(\bar{r}, E), \quad (2-40)$$

recall the relationship between angular flux and scalar flux is

$$\phi(\bar{r}, E) = \int_{4\pi} d\Omega \psi(\bar{r}, E, \bar{\Omega}). \quad (2-41)$$

The counter in EQ. (2-39) can be utilized to yield the angular flux, scalar flux and reaction rate of interest. First, the angular flux is given by

$$\psi(\bar{r}_i, E_j, \bar{\Omega}_k) = \frac{C(i, j, k)}{H \Delta V_i \Delta E_j \Delta \Omega_k}, \quad (2-42)$$

where $H$ is the number of histories. If the counter in EQ. (2-39) did not include the total cross section, EQ. (2-42) would be nothing more than the total collisions within the phase space unit $\Delta V_i \Delta E_j \Delta \Omega_k$, and is in effect a discretized reaction rate. To estimate the angular flux, a factor of the total cross section must be included in accordance with EQ. (2-40), which is energy dependent. As a result the counter must be divided by the cross section at the time of collision.

Following from EQ. (2-42), the scalar flux can be shown to be

$$\phi(\bar{r}_i, E_j) = \sum_{k=1}^{K} \psi(\bar{r}_i, E_j, \bar{\Omega}_k) \Delta \Omega_k \frac{\sum_{k=1}^{K} C(i, j, k)}{H \Delta V_i \Delta E_j}. \quad (2-43)$$

Lastly, concerning localized data, the reaction rate collision estimator is written as

$$R(\bar{r}_i) = \sum_{j=1}^{L} \frac{C(i, j)}{H \Delta V_i}, \quad (2-44)$$

where
Path length estimators

The concept of the path length estimator has its origin in the physical interpretation of the definition of the scalar flux as the total path length of particles per unit volume. As before, discretization is necessary and a counter sums particle path lengths within volume element \( \Delta V_i \), with direction \( \Omega \), within a solid angle \( \Delta \Omega_k \), with energy \( E \) within \( \Delta E_j \) and can be expressed as

\[
p(i, j, k) = p(i, j, k) + w \cdot p,
\]

where \( p \) is the path length. The angular and scalar flux can then be written in EQ.'s (2-47) and (2-48) respectively as

\[
\psi(\vec{r}_i, E_j, \bar{\Omega}_k) = \frac{p(i, j, k)}{H \Delta V_i \Delta E_j \Delta \Omega_k}
\]

and

\[
\phi(\vec{r}_i, E_j) = \frac{\sum_{k=1}^{K} p(i, j, k)}{H \Delta V_i \Delta E_j}.
\]

The reaction rate is then given by

\[
R(\vec{r}_i) = \frac{\sum_{j=1}^{J} \Delta P(i, j)}{H \Delta V_i},
\]

where

\[
CC(i, j) = CC(i, j) + w \Sigma_c(E) * p.
\]

Surface crossing estimators

Surface crossing estimators lend themselves to easy calculation of the partial currents since they are associated with a surface in their definition. Simple counters can be set up for this task. It is still possible, however, to calculate the flux using a surface crossing estimator as well. The end result for the flux, equivalent to a volume estimator in a thin foil that approaches a zero thickness, is shown in EQ. (2-51) as
\[ \phi(\vec{r}, E_j) = \frac{FS(i, j)}{H \Delta A_i \Delta E_j}, \quad (2-51) \]

where

\[ FS(i, j) = FS(i, j) + \frac{w}{\cos(\theta)}, \quad (2-52) \]

and the area \( \Delta A_i \) is the area of the surface being crossed. A difficulty will arise as \( \theta \) approaches 90\(^\circ\) since the formulation will approach infinity. In order to overcome this problem, an exclusion region must be utilized.

**Other estimators**

Other estimators may exist where an analytical formulation is utilized to improve the tallying process. These tally estimators must be used with caution as biased results may occur since actual Monte Carlo transport is not done for all of the particle history.

**\( k_{\text{eff}} \) estimators**

Several \( k_{\text{eff}} \) estimators can be devised. The collision estimator for \( k_{\text{eff}} \) for a single generation of neutrons is easily obtained. In a single region problem the equation to calculate \( k_{\text{eff}} \) for a single generation is given by

\[ k_{\text{eff}}^{c,n} = \frac{1}{N} \sum_i w_i \nu \frac{\sigma_f}{\sigma_t}, \quad (2-53) \]

where

- \( n = \) current generation
- \( i = \) collision number for all collisions in an entire generation
- \( N = \) source particles in current generation
- \( w_i = \) source particle weight before collision.

For algorithms without implicit capture (variance reduction technique), the absorption estimator can be written as
where \( i \) is analog capture. Last, a track length estimator can be written as

\[
k_{\text{eff}}^{t,n} = \frac{1}{N} \sum_{i} \frac{w_i \nu \sigma_f}{\sigma_t},
\]

(2-55)

where \( i \) is every path length segment in a fissionable region for all particles in a generation. A combination of these estimators can be used as in the MCNP code, or a single estimator (usually the collision estimator) may be used. This procedure is easily extended to multi-region problems as one only needs to modify the interaction cross sections as a particle moves from region to region.

**Non-Analog Monte Carlo**

Quite often results from a Monte Carlo calculation require significant computation time and some results are even impractical to obtain. In order to make these simulations viable, techniques have been developed to reduce the variance associated with the tallies. In an apropos manner, these techniques are referred to as variance reduction techniques. They range from very simple (and often effective) to the very elaborate. Usually, the effectiveness of variance reduction is measured using the figure of Merit (FOM) discussed later in this chapter.

**Common Variance Reduction Techniques**

Variance reduction techniques deal with the concept of particle weight. One can think that in an analog (standard) Monte Carlo simulation, each particle has a weight of unity. Utilizing variance reduction techniques, a particle's weight may be adjusted. Biasing should not be introduced, however, and the weight adjustments will follow physical arguments. The weight is usually modified according to the following strategy shown in EQ. (2-56).

\[
w * \text{biased pdf} = w_0 * \text{unbiased pdf}
\]

(2-56)
\(w\) is the biased weight after biasing and \(w_0\) is the weight before biasing. A list of some of the most common variance reduction techniques follows:

1. **Cutoff Methods**: Cutoff methods take advantage of the fact that particles at some locations, energies and/or times may not be important. Using this fact, particles can be selectively “killed”.
   
a. **Spatial Cutoff**: The spatial cutoff would typically be the problem boundaries. Particles that go outside of this region are terminated. It is possible to set any region of space as a region to terminate particles if so desired.

b. **Energy Cutoff**: Particles whose energies are not in the range of interest are not tracked and effectively “killed”.

c. **Time Cutoff**: Particles not in the range of time of interest are not tracked.

2. **Splitting Methods with Russian Roulette**: These methods involve splitting particles in regions of high importance to lower weight particles since the probability of contributing to the desired result is high. The more particles that contribute, the faster the variance is reduced. Here, the word region may be geometric as in geometric spitting, energy regions for energy splitting, or certain angular bin for angular splitting. Time splitting is also possible for time dependent problems. If available, the neutron importance function can be utilized. For instance, if the importance map is known in space, a particle moving from region of lower importance \(I_1\) to higher importance \(I_2\) should be split into \(n = I_2/I_1\) particles (any fractions are kept by comparing a random number to their weight and killing the particle if the random number is higher than the weight). For moving to lower
importance regions, Russian Roulette is performed which always accompanies splitting methods. After a particle has fallen below a chosen weight cutoff, a random number ($\eta$) is generated and compared to $1/d$ where typically $d$ is between 2 and 10. If $\eta < 1/d$ the history is terminated, else the particle survives and is given a weight $d^*w$. This ensures that particles whose weight has fallen too low to be of consequence are not tracked and, as a result, simulation time not wasted on their behalf. This action conserves the total particle weight so that a “fair game” is still being played.

3. Weight-window: The weight-window is a set of lower and upper weights for which a particle weight must be maintained, outside of this window, splitting or Russian Roulette is applied to keep the particle within this “weight-window”.

4. Survival Biasing (Implicit Capture): Here, each collision is treated as a fraction of individual interactions according to their interaction probability. The particle then continues after interaction with a weight modified by its scattering probability (effectively, the fraction of the particle that scatters, survives). If the weight falls below the weight cutoff, Russian Roulette is performed.

5. Exponential Transform: To transport particles long distances, the distance between collisions in a preferred direction is artificially increased utilizing an exponential transformation (and decreased in the opposite direction) and the weight is correspondingly adjusted according to EQ. (2-56).

6. Source Biasing: Source particles that have a higher importance are sampled more than those with a lower importance. To account for this, they are given a lower
weight to preserve the physics (conserve total particle weight). This can be angle, energy or space dependent, or any combination thereof.

7. Forced Collision: For very optically thin media, particles may be split into two components, an uncollided component and a collided component. This forces interactions to occur in the region of interest.

8. Analytical Biasing: Involves deterministically transporting particles on collision to the neighborhood of a tally and then calculating contributions to the tally from these particles. Care must be taken here to be certain the deterministic transport is accurate or severely biased (yet precise) results may be obtained.

9. Importance sampling: Importance sampling utilizes known importance information (or estimated information) to sample particles that may contribute more to the objective with higher frequency. Many of the methods already shown touch on this idea. More will be said about this technique in Chapter 5.

These are many of the most widely used variance reduction techniques. Specific acceleration methods for criticality problems were introduced earlier and more detail will be given in Chapter 5.

**Efficiency of a Monte Carlo Simulation**

In general, a Monte Carlo tally relative error square ($R^2$) should be proportional to $1/N$, the total number of particles simulated, if the Central Limit Theorem is valid. This is easily confirmed for the eigenvalue as well where generations of particles are simulated. Also, the computer simulation time $T$ is proportional to the total number of particles simulated $N$. This implies that the factor $R^2T$ should remain approximately constant. A “good” simulation will result in a reliable tally in a short time thus desiring a minimal relative error in a short time. As a result, the Figure-of-Merit (FOM) is utilized as a measure of efficiency of the simulation,
whereby the larger figure of merit the more effective the calculation concerning the tally, and is given by

\[ FOM = \frac{1}{R^2 T}. \]  

(2-57)

To compare two different techniques (or variance reduction), speedup can be obtained by comparing the FOM from two different simulations as

\[ \text{speedup} = \frac{FOM_2}{FOM_1}. \]

(2-58)

If the same relative error is achieved in both simulations, the speedup reduces to a ratio of simulation times \((T_1/T_2)\).

**Monte Carlo \(k_{\text{eff}}\) Solution Strategies**

For simplicity, the formulations are written in 1-D with a uniform material. Note that these formulations can easily be expanded to 3-D and multi-region problems.

**Source Iteration Method**

The power iteration method solves for the \(k_{\text{eff}}\) eigenvalue as the ratio of two successive neuron generation sources as

\[ k_{\text{eff}} = \frac{\int S^{(n)}(x) dx}{\int S^{(n-1)}(x) dx} \]

(2-59)

where \(S^{(n)}(x)\) is the source distribution related to the \(n^{th}\) generation. Final results are calculated through a recursive procedure that starts with an initial guessed spatial source distribution \(S^{(0)}(x)\).

The simulation is assumed to have \(N\) neutrons per generation. Survival biasing is assumed combined with Russian Roulette. The procedure is as follows:

1. Either from the initial source or the previous generation source, \(N\) source neutrons are transported.
2. At each collision within the generation (for all particles) several things must occur (recall this problem is a 1 region problem so all collisions are in a fissile region)
   a. The contribution to fission is calculated by one of the $k_{eff}$ estimators such as the collision estimator using the counter

   \[ Ck(n) = Ck(n) + w \frac{\nu \Sigma_f}{\Sigma_t}, \]  
   \[ (2-60) \]

   where

   \[ w = \text{the weight of the particle at the time of collision and} \]

   \[ n = \text{the current generation number}. \]

   b. Store information of fission neutrons:
      i. Update the fission storage bank with the number of fission neutrons to include for the next generation source. In order to keep the particle population stable, a normalization factor of $1/k_{eff}$ is utilized as follows:

   \[ \text{neutrons} = \text{neutrons} + \text{int} \left( w \frac{1}{k_{eff}} \frac{\nu \Sigma_f}{\Sigma_t} + \eta \right), \]  
   \[ (2-61) \]

   where \( \eta = \text{random number between 0 and 1}. \) This is done to conserve the weight from fractional particles, i.e. if \( \text{neutrons}=2.2, \)

   20% of the time three fission neutrons are generated and 80% of the time two fission neutrons.

   ii. Store the location of the fission neutrons.

   iii. Sample the fission spectrum in order to provide the energy of the fission neutron(s) and store the/their energy/energies.

   iv. Sample and store the fission neutron(s) initial direction of travel.

   c. Calculate the weight of the initial particle after collision.
d. Apply Russian Roulette as needed.

e. Sample the scattered particle direction.

f. Repeat until the particle is terminated.

NOTE: If splitting techniques are utilized, a run bank must be utilized to store split particles, when the original split particle is terminated, particles are taken from the run bank (other parts of the original split particle) until exhausted, whereupon the next particle is selected.

3. Repeat for all particles in the generation.

4. Calculate the generation $k_{\text{eff}}$ as:

$$k_{\text{eff}}(n) = \frac{Ck(n)}{npg}.$$  \hspace{1cm} (2-62)

5. Normalize the weight of ALL the fission neutrons to the input number per generation ($npg$) as (This number should be close to 1 as the formulation should generate close to $npg$ neutrons.)

$$w = \frac{\text{neutrons}}{npg}.$$ \hspace{1cm} (2-63)

6. Repeat process for all generations.

7. Calculate the final $k_{\text{eff}}$ and associated relative error.

**Fission Matrix Method**

The fission matrix method does nothing different in the transport of particles, or the storage of the fission source for each generation. An addition to the algorithmic logic must be the discretization of the source into spatial regions. To this end, only the following modifications to the source iteration method are needed.

1. Store the number of source particles in each discretized spatial region as $(\mathcal{C})_j$. 

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2. At each collision for every particle in the generation, increment a fission neutron
counter to add to the proper fission matrix element as:

\[(B)_{i,j} = (B)_{i,j} + w \frac{\nu \Sigma_f}{\Sigma_t} \]  \hspace{1cm} (2-64)

3. After all histories for the current generation have been exhausted, the fission matrix
elements are approximated as shown in EQ. (2-65).

\[(A)_{i,j} = \frac{(B)_{i,j}}{(C)_{j}} \]  \hspace{1cm} (2-65)

4. Calculate \(k_{eff} (n)\) as the dominant eigenvalue of the fission matrix \((A)_{i,j}\).

Two different approaches for formulating the fission matrix solution are available. The
elements of \((A)_{i,j}\) can be zeroed after every generation resulting in a cycle-wise fission matrix,
or a cumulative fission matrix can be utilized where the elements of \((A)_{i,j}\) are obtained using
cumulative data from all active generations.

**Deterministic S_N Method**

For deterministic analysis, since the LBE is too complex to solve analytically in all but a
few special cases, numerical methods are utilized. One of the most widely used methods of
solving the LBE is the so called \(S_N\) method. Some of the work performed for this dissertation
utilizes results of deterministic \(S_N\) calculations to perform variance reduction; therefore a brief
background on the method is given. The discrete ordinates \((S_N)\) method has its origin in the \(S_N\)
method that was proposed by Carlson (Carlson, 1953). The discrete ordinates method
approximates a solution to the transport equation by solving the transport equation along a
discrete number of directions using a numerical quadrature. The directions and their associated
weights define a numerical quadrature set. Discretization over energy and space are also
required and are discussed.
Multigroup Energy Approximation

In order to solve the LBE numerically with the discrete ordinates method, the energy variable is discretized. This discretization is performed by dividing the energy domain into a discrete number of intervals \((G)\) called groups starting from high energy at \(g=1\), to the lowest energy group \(g=G\). The procedure is known as the multi-group approximation. To obtain the multigroup form of the LBE, EQ. (2-1) (with the eigenvalue \(k_{\text{eff}}\) included, and noting that the scattering cross section is only dependent on the scattering angle, \(\hat{\Omega}' \cdot \hat{\Omega}\)) is integrated over the energy intervals, resulting in

\[
\Omega \cdot \vec{v} \psi_g (\bar{r}, \hat{\Omega}) + \sigma_g (\bar{r}, E) \psi_g (\bar{r}, \hat{\Omega}) = Q_{\text{ext}, g} (\bar{r}, \hat{\Omega})
\]

\[
\sum_{g'=1}^{G} \int_{4\pi} d\Omega' \sigma_{g' \to g} (\bar{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi_g (\bar{r}, \hat{\Omega}') + \frac{\chi_g}{4\pi k} \sum_{g'=1}^{G} \int_{4\pi} d\Omega' \nu \sigma_{f g'} (\bar{r}) \psi (\bar{r}, \hat{\Omega}'),
\]

for \(g=1, \ldots, G\).

Particles in group \(g\) are considered to be at one energy between \(E_g\) and \(E_{g+1}\). The group angular flux is defined by

\[
\psi_g (\bar{r}, \hat{\Omega}) = \int_{E_g}^{E_{g+1}} dE \psi (\bar{r}, E),
\]

and the multigroup cross sections are defined as

\[
\sigma_g (\bar{r}) = \frac{\int_{E_g}^{E_{g+1}} dE \sigma (\bar{r}, E) \int_{4\pi} d\Omega \psi (\bar{r}, E, \hat{\Omega})}{\int_{4\pi} d\Omega \psi_g (\bar{r}, \hat{\Omega})},
\]

(2-68)

\[
\nu \sigma_{f g} (\bar{r}) = \frac{\int_{E_g}^{E_{g+1}} dE \nu \sigma_f (\bar{r}, E) \int_{4\pi} d\Omega \psi (\bar{r}, E, \hat{\Omega})}{\int_{4\pi} d\Omega \psi_g (\bar{r}, \hat{\Omega})},
\]

(2-69)

and

\[
\sigma_{g' \to g} (\bar{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \frac{\int_{E_g}^{E_{g+1}} dE \int_{E_{g-1}}^{E_g} dE' \sigma_s (\bar{r}, E', E, \hat{\Omega} \cdot \hat{\Omega}') \int_{4\pi} d\Omega \psi (\bar{r}, E, \hat{\Omega}')}{\int_{4\pi} d\Omega \psi_g (\bar{r}, \hat{\Omega})},
\]

(2-70)

and finally, the fission spectrum is defined as
\[ \chi_g = \int_{Eg}^{Eg-1} dE \chi(E). \]  

(2-71)

**Particle Streaming and Scattering in 3-D**

The most common numerical solvers utilize the discrete ordinates method to represent the phase space in a Cartesian coordinates system. The necessary trigonometric information for this representation is shown in Figure 2-1.

![Figure 2-1. 3-D Cartesian space-angle coordinate system](image)

The streaming operator of EQ. (2-1) is then written in Cartesian coordinates as

\[ \mathbf{\vec{\Omega}} \cdot \nabla = \mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} + \xi \frac{\partial}{\partial z}, \]  

(2-72)

where

\[ \mu = \mathbf{\hat{\Omega}} \cdot \mathbf{\hat{e}}_x = \cos \theta, \]  

(2-73)

\[ \eta = \mathbf{\hat{\Omega}} \cdot \mathbf{\hat{e}}_y = \sqrt{1 - \mu^2 \cos \phi} \]  

(2-74)

and

\[ \xi = \mathbf{\hat{\Omega}} \cdot \mathbf{\hat{e}}_z = \sqrt{1 - \mu^2 \sin \phi}. \]  

(2-75)

Utilizing this form of the streaming term, and expanding the scattering term in EQ. (2-1) using a set of truncated spherical harmonics, the Legendre expanded multi-group form of the transport
equation in 3-D Cartesian coordinates is given in EQ. (2-76). For brevity, the derivation is
omitted (Sjoden, 1997).

\[
\begin{align*}
\left( \mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} + \xi \frac{\partial}{\partial z} \right) \psi_g(x, y, z, \mu, \varphi) + \sigma_g(x, y, z) \psi_g(x, y, z, \mu, \varphi) \\
= \sum_{g'=1}^{G} \sum_{l=0}^{L} (2l + 1) \sigma_{s,g\rightarrow g',l}(x, y, z) \left\{ P_l(\mu) \phi_{g',l}(x, y, z) \\
+ 2 \sum_{k=1}^{l} \frac{(l - k)!}{(l + k)!} P^k_l(\mu) \cdot \left[ \phi^k_{c,g',l}(x, y, z) \cos(k\varphi) + \phi^k_{s,g',l}(x, y, z) \sin(k\varphi) \right] \right\} \\
+ \chi_g \sum_{g'=1}^{G} \nu \sigma_{fg'}(x, y, z) \phi_{g',0}(x, y, z)
\end{align*}
\]  

(2-76)

where,

- \( \mu = x \) direction cosine
- \( \eta = y \) direction cosine
- \( \xi = z \) direction cosine
- \( \varphi = \arctan \left( \frac{\xi}{\eta} \right) \), azimuthal angle
- \( \psi_g = \text{angular flux of group } g \)
- \( \sigma_g = \text{total macroscopic cross section of group } g \)
- \( \sigma_{s,g\rightarrow g',l} = \text{Legendre moment of the macroscopic differential scattering cross section from group } g' \text{ to } g \)
- \( P_l(\mu) = \text{Legendre polynomial} \)
- \( \phi_{g',l} = \text{Legendre flux moment of group } g' \)
- \( P^k_l(\mu) = \text{Associated Legendre polynomial} \)
- \( \phi^k_{c,g',l} = \text{Cosine Legendre flux moment of group } g' \)
- \( \phi^k_{s,g',l} = \text{Sine Legendre flux moment of group } g' \)
- \( \chi_g = \text{fission spectrum of group } g \)
- \( \nu \sigma_{fg'} = \text{fission generation cross section of group } g' \)

Finally, the flux moments are defined as

\[
\begin{align*}
\phi_{g',l}(x, y, z) &= \int_{-1}^{1} \frac{d\mu'}{2} P_l(\mu') \int_{0}^{2\pi} \frac{d\varphi'}{2\pi} \psi_g(x, y, z, \mu', \varphi') \\
\phi^k_{c,g',l}(x, y, z) &= \int_{-1}^{1} \frac{d\mu'}{2} P^k_l(\mu') \int_{0}^{2\pi} \frac{d\varphi'}{2\pi} \cos(k\varphi) \psi_g(x, y, z, \mu', \varphi') \\
\phi^k_{s,g',l}(x, y, z) &= \int_{-1}^{1} \frac{d\mu'}{2} P^k_l(\mu') \int_{0}^{2\pi} \frac{d\varphi'}{2\pi} \sin(k\varphi) \psi_g(x, y, z, \mu', \varphi')
\end{align*}
\]  

(2-77) 
(2-78) 
(2-79)
Angular Discretization via Numerical Quadrature

Numerical quadrature is often utilized in mathematics as a powerful numerical integration technique (Atkinson, 1988). In the discrete ordinates method, the transport equation is solved for a finite set of directions, \( \Omega_m = (\mu_m, \eta_m, \xi_m) \), \( m = 1, 2, \ldots, M \). Each angle has a weight associated with it. This collection of angles and weights replace angular integration with summation. A good quadrature set for discrete ordinates methods preserves the moments of the angular flux.

These directions are located on a unit sphere such that the sum of the squares of the unit directions is equal to unity for any direction as

\[
\Omega_n^2 = \mu_n^2 + \eta_n^2 + \xi_n^2 = 1.
\]

The most common quadrature set utilized with the discrete ordinates method is the level-symmetric quadrature (Carlson and Lee, 1961). The total number of directions in 3-D for level symmetric \( S_N \) quadrature is \( N(N+2) \).

The level-symmetric set is produced based on preservation of the moments of direction cosines and physical symmetry (Lewis and Miller, 1993). Other quadrature sets are utilized above order \( S_{20} \) since some of the weights of the level-symmetric quadrature become negative (Lathrop and Carlson, 1965). Still yet, other quadrature sets may be used for biasing toward a particular direction or directions in which ordinates are split utilizing techniques such as ordinates splitting (OS) (Longoni, 2004; Longoni and Haghighat, 2001) and regional angular refinement (RAR) (Longoni, 2004; Longoni and Haghighat, 2002).

Discretization of the Spatial Domain

In order to solve for the angular flux throughout the geometry of the problem, the spatial domain is partitioned into discrete spatial meshes. In Cartesian geometry, these meshes will correspond to the \( x, y \) and \( z \) variable for which the transport equation has been written.
Commonly, the equation is recast in cylindrical or spherical coordinates, but is not shown here.

If EQ. (2-76) is written without energy dependence, combining source terms (including scattering), and incorporating the angular discretization, the abbreviated result shown in EQ. (2-81) is obtained where \( r \) represents the spatial domain \((x,y,z)\).

\[
\left[ \left( \mu_m \frac{\partial}{\partial x} + \eta_m \frac{\partial}{\partial y} + \xi_m \frac{\partial}{\partial z} \right) + \sigma(r) \right] \psi_m(r) = Q_m(r) \quad \text{where} \ m = 1,2, \ldots, M \quad (2-81)
\]

Note that the \( Q_m(r) \) term can be represented by either the scattering source plus fission source (eigenvalue problem), or the scattering source plus fixed source since these terms don’t explicitly depend on the angular flux. Integrating EQ. (2-81) over a cell volume \( \Delta x_i \Delta y_j \Delta z_k = V_{i,j,k} \) and simplifying terms yields

\[
\begin{align*}
\frac{\mu_m}{\Delta x_i} (\psi_{m,i+1/2,j,k} - \psi_{m,i-1/2,j,k}) + \frac{\eta_m}{\Delta y_j} (\psi_{m,i,j+1/2,k} - \psi_{m,i,j-1/2,k}) \\
+ \frac{\xi_m}{\Delta z_k} (\psi_{m,i,j,k+1/2} - \psi_{m,i,j,k-1/2}) + \sigma_{i,j,k} \psi_{m,i,j,k} = Q_{m,i,j,k} \\
\end{align*}
\quad (2-82)
\]

where,

\[
\begin{align*}
\psi_{m,i\pm1/2,j,k} &= \frac{1}{\Delta y_j \Delta z_k} \int_j d\psi_m(x_{i\pm1/2},y,z) \quad (2-83) \\
\psi_{m,i,j\pm1/2,k} &= \frac{1}{\Delta x_i \Delta z_k} \int_i d\psi_m(x,y_{j\pm1/2},z) \quad (2-84) \\
\psi_{m,i,j,k\pm1/2} &= \frac{1}{\Delta x_i \Delta y_j} \int_i d\psi_m(x,y,z_{i\pm1/2}) \quad (2-85) \\
\psi_{m,i,j,k} &= \frac{1}{\Delta x_i \Delta y_j \Delta z_k} \int_i d\psi_m(x,y,z) \quad (2-86) \\
Q_{m,i,j,k} &= \frac{1}{\Delta x_i \Delta y_j \Delta z_k} \int_i d\psi_m(x,y,z) \quad (2-87)
\end{align*}
\]

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Source Iteration Scheme

The source iteration scheme proceeds by assuming the source term for the first iteration, or is updated from the utilization of previous results for each subsequent iteration. With \( Q_{m,i,j,k} \) assumed constant, EQ. (2-82) can be utilized to solve for the angular flux \( \psi_m(\vec{r}) \), for group \( g \), and then the flux moments can be backed out from EQ. (2-77), EQ. (2-78) and EQ. (2-79). These newly calculated values can then be used to update the source for the next iteration. This process is repeated (iterated) until the zeroth flux moment is acceptably converged. Note that one typically starts with the fastest energy group and convergence proceeds from higher groups to lower and the group iteration is only performed once (no upscattering) since for no upscattering the scattering source of the current group only depends on the converged higher groups. For upscattering, an outer iteration scheme is necessary, while for eigenvalue problems another outer loop is necessary since the fission source and \( k_{\text{eff}} \) need to be updated between the outer iterations and a convergence criterion for \( k_{\text{eff}} \) utilized for this outer iteration.

Differencing Scheme

One final step is necessary to solve the LBE. Note that the streaming term in EQ. (2-82) contains seven unknowns, the incoming and outgoing cell fluxes and the average cell flux. Recall that the average cell flux can be obtained from (2-86), but it is done so using “sweeps” for every fine mesh for a given direction, and repeated for all directions. Utilizing the sweep methodology provides the fluxes through the fine mesh boundary conditions at the interface. To obtain the other three unknowns, a differencing scheme is assumed to represent the angular flux dependence in the spatial mesh. Many differencing schemes are available from simple linear assumptions to advanced differencing algorithms like the Exponential Directional Weighted (EDW), Direction Theta Weighted (DTW) and Exponential Directional Iterative (EDI) schemes.
With the aid of the differencing schemes, the system is now fully determined and can be solved.

**Computer Codes Utilized**

This work in this dissertation builds on the theory and algorithms discussed throughout this chapter. To that end, several well established computer codes which utilize the theory and algorithms discussed have been drawn upon for this work. These codes are discussed here. In addition, a 1-Dimensional Monte Carlo eigenvalue code was developed and its basic features described here. New methodologies added to the code are detailed in the chapter(s) pertinent to the features developed.

Used extensively in this work concerning source convergence diagnostic analysis with Monte Carlo eigenvalue problems is the KENO.V.a code. The KENO.V.a code is not used as standalone software and is part of an analytical sequence inside of the Standardized Computer Analyses for Licensing Evaluation (SCALE) version 5.0 code package.

SCALE is a modular code system that was originally developed by Oak Ridge National Laboratory. The SCALE system utilizes well-established computer codes and methods within standard analysis sequences that (1) provide an input format designed for the occasional user and/or novice, (2) automate the data processing and coupling between modules, and (3) provide accurate and reliable results. System development has been directed at problem-dependent cross-section processing and analysis of criticality safety, shielding, depletion/decay, and reactor physics problems (SCALE, 2005).

KENO V.a is a three-dimensional (3-D), multigroup, Monte Carlo criticality transport program. It is run through the use of the Criticality Safety Analysis Sequence 25 (CSAS25) analytical sequence. This sequence links KENO.V.a to cross section processing codes in order to
obtain an automated procedure for running the 3-D Monte Carlo transport problem with problem dependent cross sections.

Used sparingly in this work is the well known Monte Carlo N-Particle (MCNP) version 5 code. MCNP is a general-purpose Monte Carlo N–Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first-degree and second-degree surfaces and fourth-degree elliptical tori. Pointwise cross-section data are used (X-5 Monte Carlo Team, 2003).

The PENTRAN code is utilized in this work for the determination of an initialized source distribution for Monte Carlo analysis as well as for obtaining importance data for use with importance sampling techniques. The PENTRAN code is a 3-D Discrete Ordinates code with full phase space decomposition providing parallel processing capability in energy, space and angle. Some advanced features of PENTRAN include:

- Parallel I/O
- Parallel Memory
- Space, Angle, & Energy Decomposition
- Adaptive Differencing strategy
- Taylor Projection Mesh Coupling
- Rebalance and Alternating Direction Sweeping
- Flux Moment Preconditioning
- Advanced Quadrature with Refinement Options
- Input/Output processing codes (PENMSHXP, PENDATA).

Lastly, a 1-Dimensional multigroup Monte Carlo code (1Dcrit) was written in FORTRAN90/95 with both a traditional solution algorithm and a modified solution algorithm (discussed in Chapter 6). Implicit capture is always utilized, in conjunction with Russian Roulette. The standard solution algorithm computes $k_{\text{eff}}$ utilizing a standard collision estimator.
The number of fission neutrons is kept near the initial user input particles per generation utilizing normalization with the current $k_{\text{eff}}$ estimate and an error component which reduces the likelihood of too few particles. Scattering currently treated is isotropic only. The particle weight is normalized such that the sum of banked particle weights is equal to initial particles input as is utilized in the KENO.V.a code. 1Dcrit is utilized for testing of new methodologies for source acceleration and fission matrix implementation. Although only 1-D with isotropic scattering, the same behavior associated with difficult problems in terms of slow and poor convergence can be adapted to one dimension with isotropic scattering. Note that while a Monte Carlo code may be 1-D, particle movement is still treated as if it were in three dimensions, with tracking only in one dimension.

The fission matrix is adapted in a separate version of the 1Dcrit. This version includes the option to utilize importance sampling with and without a new source iteration scheme as well as traditional fission matrix acceleration methods. Two starting source options are available and are either random sampling in all fissionable material or a source read as user input. Source convergence diagnostics developed in chapter 3 and 4 for use with the KENO.V.a code have also been incorporated into 1Dcrit.

More advanced features will be described in the next chapter and subsequent chapters as needed. Since the solution algorithm memory structure was adapted differently for the fission matrix algorithm and the fission matrix algorithm with new source iteration methodology, much of the code logic for these solutions is similar, yet different. Each “version” has between ~4000 and ~5000 source lines, with another ~1000 lines added for the parallel implementation discussed in Chapter 7. Several processing utilizes were developed for formatting PENTRAN
output into a format usable by 1Dcrit. These utilities are a combination of shell scripts and FORTRAN codes.
CHAPTER 3
SOURCE CONVERGENCE DIAGNOSTIC METHODOLOGY

Source convergence diagnostics currently available and under development were listed in Chapter 1. Strengths and weaknesses were identified and the point was made that there is no perfect diagnostic tool. With that in mind, the LDA approach was discussed as a promising diagnostic tool; however, its application appears to have fallen short. In the spirit of this work, a new diagnostic methodology called the generalized KPSS test for stationarity detection in Monte Carlo eigenvalue problems is developed here.

Since the generation to generation source may be, and often is correlated, a converged source may not behave as white noise. Source diagnostics aim at diagnosing source stationarity. Stationarity will only guarantee a well defined mean and variance (correlation may still be present), but does not guarantee convergence to the fundamental mode. This cannot be stressed enough. Nevertheless, a stationary source can be used as one indicator that a particular solution can be accurately obtained. This Chapter will discuss information theoretic diagnostics utilized for comparison to the KPSS methodology, and then utilization of the source Center of Mass (COM) series and the theory and implementation of the Generalized KPSS test for stationarity detection in Monte Carlo eigenvalue problems. Before going on to the discussion of the different diagnostics, a word about high dominance ratio problems is given.

The Dominance Ratio and Source Convergence

The dominance ratio is defined as the ratio between the first and second eigenvalue which can be shown to be $DR = \frac{k_1}{k_0} \leq 1$, where $k_0$ is $k_{\text{eff}}$ and $k_1$ is the second eigenvalue. It can be shown at iteration $n$ that

$$k_{\text{eff}}^{(n+1)} \approx k_o \left[ 1 + C_2 \frac{\alpha_1}{\alpha_0} \left( \frac{k_1}{k_0} \right)^n \left( \frac{k_1}{k_0} - 1 \right) \right]$$

(3-1)

and
\[ \psi^{(n+1)} \approx C_1 \left[ \frac{a_1}{a_0} \left( \frac{k_1}{k_0} \right)^{n+1} \left( \frac{k_1}{k_0} - 1 \right) \bar{s}_1 \right], \]  

(3-2)

where \( \psi^{(0)} = \sum_{i=0}^{\infty} a_i \bar{s}_i \), \( a_i = \int dV \psi^{(0)} \bar{s}_i \), \( C_1 \) and \( C_2 \) are constants and \( \bar{s}_0 \) and \( \bar{s}_1 \) are the first (source vector) and second eigenvector. EQ. (3-1) shows that the error associated with the neutron flux convergence dies off as \( (k_1/k_0)^{n+1} \), while EQ. (3-2) shows that \( k_{\text{eff}} \) converges faster for high dominance ratio problems since \( (k_1/k_0 - 1) \) tends to vanish. This means that many difficult source convergence problems will be problems with high dominance ratios. Not only this, but the high DR will then cause high correlation in the source distribution for which bias in tally and tally confidence can result.

**Review of Information Theory, Stationarity and Undersampling Tests**

Three complimentary source stationarity and undersampling diagnostics have been proposed recently (Ueki, 2005). These diagnostics rely on information theoretic concepts in their derivation (Cover and Thomas, 1991). The diagnostics require a source meshing scheme. Only a brief discussion of the criteria are given here;

The Shannon and relative entropy of the Monte Carlo source distribution are given in EQ. (3-3) and (3-4) respectively.

\[ H(S^B) = - \sum_{i=1}^{B} S^B(i) \log_2 (S^B(i)) \]  

(3-3)

\[ D(S^B \parallel T^B) = \sum_{i=1}^{B} S^B(i) \log_2 \frac{S^B(i)}{T^B(i)} \]  

(3-4)

where

\( B \) is the number of spatial bins,

\( i \) is the bin number

\( S^B(i) \) is the source density for the \( i^{th} \) source bin, and
\( T^B(i) \) is the average source density for the \( i^{th} \) source bin over the second half of the active cycles.

Shannon Entropy can be utilized to characterize the state of a random variable (ie, how well a pdf, in this case a source distribution, is known), while the relative entropy can provide a measure between the states of two random variables. These concepts are the basic concepts utilized in the information theoretic diagnostics. Based on this theory and extensions thereof, Ueki has derived the following three criteria (Ueki, 2005):

**Criterion One**

The first criterion deals with the with Shannon and relative entropies for the instantaneously decodable code. Utilizing these concepts, and the Kraft inequality, the following inequality holds (Ueki, 2005):

\[
\min \ H(S^B) \leq \ \text{instantaneously decodable} \ (L(S^B)) \leq H(S^B) + 1
\]

where \( L(S^B) \) is the descriptive length of the particles born under \( S^B \). Since the true \( S^B \) is not known, however, the following inequality can also be derived.

\[
H(S^B) + D(S^B || T^B) \leq L_{T^B}(S^B) \leq H(S^B) + D(S^B || T^B) + 1
\]

where \( L_{T^B}(S^B) \) is the descriptive code length (for an instantaneously decodable code) of particles born according to \( T^B \), while characterizing them with the \( S^B \) distribution (Cover and Thomas, 1991; Ueki, 2005; Ueki and Brown, 2003). What this inequality represents is that the relative entropy between \( S^B \) and \( T^B \), namely \( D(S^B || T^B) \), is the penalty for utilizing \( T^B \) as the true source distribution. Comparing EQ. (3-5) and EQ. (3-6), the penalty \( D(S^B || T^B) \) is negligible if the fluctuation of \( H(S^B) \) is larger than \( D(S^B || T^B) \). In other words, since the relative entropy is a measure of the difference between the density functions \( S^B \) and \( T^B \) and is negligible compared to the fluctuation of the entropy of \( S^B \) itself, then \( S^B \) is deemed stationary.
In previous work by Ueki and Brown (Ueki and Brown, 2003), the stationarity of the 
source distribution is diagnosed in a posterior manner by checking whether or not \( D(S^B || T^B) \) 
crosses its mean level determined from the second half of the active cycles before the first active 
generation. This scheme is utilized in the released version of the MCNP5 code system (X-5 
Monte Carlo Team, 2003). To improve upon this scheme and ensure that \( D(S^B || T^B) \) is 
negligible EQ. (3-6), Ueki proposed the following inequality:

\[
msq(D) \leq cmsq(H),
\]

where

\( msq \) is the mean square posterior relative entropy and

\( cmsq \) the centered mean square Shannon Entropy,

which are defined in EQ. (3-8) and EQ. (3-9) respectively.

\[
msq(D) = \frac{2}{M} \sum_{j=\left(\frac{M}{2}\right)+1}^{M} D(S^B || T^B)^2
\]

(3-8)

\[
cmsq(D) = \frac{2}{M - 2} \sum_{j=\left(\frac{M}{2}\right)+1}^{M} \left( H(S^B_j) - \bar{H} \right)^2,
\]

(3-9)

where

\( M \) is the number of active cycles,

\( j \) is the generation number,

\( B \) is as before, and

\[
\bar{H} = \frac{2}{M} \sum_{j=\left(\frac{M}{2}\right)+1}^{M} H(S^B_j)
\]

(3-10)
due to the fact that $D(S^B||T^B)$ is convex as a function of $S^B$ and assumes a minimum value of zero when $S^B = T^B$, while $H(S_j^B)$ is concave and is maximum when $S^B$ is uniform. This should hold for all but when $T^B$ is uniform (or very close) (Ueki, 2005).

**Criterion Two**

Criterion two relies on the large sample property based on the asymptotic equipartition property (Cover and Thomas, 1991) (AEP) in relation to thermodynamic equilibrium, and also the method of type for its derivation (Cover and Thomas, 1991). The results of which are shown in EQ. (3-11).

$$\text{abs} \left[ D(S^B||T^B) - \left( H(T^B) - H(S_j^B) \right) \right] \leq \varepsilon \quad \text{(Through active cycles)} \quad (3-11)$$

The AEP is a fundamental concept of the typical set, relating to the method of type and implies that though many series of results may be produced by a random process, there is a high probability that the one realized is from a loosely-defined set of outcomes with roughly the same chance of being realized. This criterion assumes independence of source bins which is often not the case, however it is a zeroth-order method for dealing with an equilibrium property of large neutron population. Note that $\varepsilon$ has been currently set to 0.1 (Ueki, 2005).

**Criterion Three**

The third criterion is a direct result of the concavity of Shannon Entropy (Cover and Thomas, 1991; Ueki, 2005) and is written as

$$H(T^B) \leq \bar{H}, \quad (3-12)$$

where an acceptable difference is defined and written as

$$H(T^B) - \bar{H} < \eta \quad \text{for } \eta = 0.1. \quad (3-13)$$
Source Center of Mass

In order to diagnose stationarity with the KPSS stationarity test, a single scalar variable must be obtained which will be indicative of the source behavior, namely the source COM series (Wenner and Haghighat, 2007). The source COM is a natural parameter to consider when dealing with source convergence and is given by

\[
|\vec{R}_g| = \frac{1}{M} \sum_{i=1}^{npg} m_i \sqrt{x_i^2 + y_i^2 + z_i^2} \quad \text{over active gen's } g = 1, G, \tag{3-14}
\]

where,

\( G = \) is the number of active generations,
\( npg = \) the number of particles per generation,
\( g = \) the current generation number,
\( m = \) the neutron mass,
\( i = \) the source particle number and
\( x, y \) and \( z \) are the magnitude of the components of the vector extending from the geometric center of the model to the \( i^{th} \) neutron

Intuitively, one would expect the source COM for each Monte-Carlo generation for a converged problem to fluctuate in a stationary manner about the true COM. One can look at the individual direction \((x_g, y_g, z_g)\) components, and/or use \(\vec{R}_g\) as defined in EQ. (3-14). In this work all of the data is utilized. Since correlation is often present, as with other parameters in Monte Carlo source convergence identification, purely random behavior cannot be tested for. Standard statistical tests do not directly apply. This difficulty of applicability of standard statistical tests applies to the COM and any related parameters such as higher moments of the COM. Nevertheless, higher moments still give some ideas about the symmetry and how peaked the
source COM series is and may provide some physical insight. These parameters were some of the first attempts at better characterizing the variability of a sample in statistics.

**Higher Moments of the Center of Mass**

Moments in the statistical sense are usually central moments. The first central moment then should by definition be zero, and the second moment the numerator of the standard sample variance formulation. The general formulation for the $k^{th}$ central moment of a random variable $X$ about a mean $\mu$ is then given by

$$\mu = E[(X - E[X])^k] = \int_{-\infty}^{\infty} (x - \mu)^k f(x) \, dx.$$  \hspace{1cm} (3-15)

Although this variance estimate is most likely biased for any difficult convergence problem, it still is a measure of the variability in the sample and may provide some useful qualitative analysis if nothing else. The same can be said for higher moments, which should also stabilize and themselves could be theoretically tested for stationary behavior. The next two higher moments are called the skewness and kurtosis.

**Skewness**

The skewness of a probability distribution is a measure of the asymmetry of the distribution and is related to the third central moment about the mean. Skewness can be estimated with EQ. (3-16).

$$skewness = \frac{\sum_{i=1}^{N}(X - \bar{X})^3}{(N - 1)s^3},$$  \hspace{1cm} (3-16)

where $s$ is the sample standard deviation. The expected value of skewness for a sample from a normal distribution is zero as well as for any symmetric distribution. Negative values indicate negative skewed asymmetry in the tails of the data, and positive skewness indicates positive skewed asymmetry in the tails of the data. As a result, the skewness can tell about how symmetric the data is and a change in skewness over time (or generation) should be indicative of
a change in the amount of symmetry. This series then should settle on some stationary result even if correlated and can itself be tested for stationarity of skewness if desired.

Kurtosis

The kurtosis of a probability distribution is a measure of the peakedness of the distribution and is related to the 4th central moment about the mean. Kurtosis can be estimated with Eq. (3-17).

\[
kurtosis = \frac{\sum_{i=1}^{N}(X - \bar{X})^4}{(N - 1)s^4} - 3
\]  

(3-17)

Higher kurtosis means more of the variance is due to infrequent extreme deviations, as opposed to frequent modestly-sized deviations. The more positive the kurtosis, the more peaked is the distribution, while the more negative, the more flat. Here, the kurtosis can give insight about the variance of the COM and whether outliers may contribute significantly to the sample variance. Indeed, since correlation is present, the kurtosis estimator will be biased, however insight is still gained into the variance of the COM and how peaked or flat the source distribution is, and it should also be stationary upon convergence.

Generalized KPSS Test for Stationarity Detection in Monte Carlo Eigenvalue Problems

A formal test procedure is developed here based on analysis of residuals of regression of a scalar series. To investigate the stationarity of the source COM series, a statistical model is utilized given by

\[
y_t = \alpha + \beta t + d \sum_{i=1}^{t} u_i + \epsilon_t, \quad t = 1, ..., T,
\]  

(3-18)

where \(\mu_i\) and \(\epsilon_i\) are both covariance stationary and short term memory (future values related to recent past values only) with mean zero and \(d \in \{0, 1\}\) (Hobin et al., 2004). \(T\) is the total number of terms in the series. Each term represents a different characteristic of the series. The first two
terms together represent the linear behavior in the model, while the third term corresponds to a random walk and the fourth term is a stationary error component. This model differs slightly from the model proposed by Kwiatkowski, et al, for the original KPSS methodology (Kwiatkowski et al., 1992).

The procedure continues by assuming that the source COM follows this statistical model. Different hypotheses are then formed from assumptions concerning the different terms of the model. These hypotheses are given by the following linear regressions of the COM:

\[ H_\tau : y_t = a + bt + e_t \]  \hspace{1cm} (3-19)
\[ H_\mu : y_t = a + e_t \]  \hspace{1cm} (3-20)
\[ H_0 : y_t = e_t \]  \hspace{1cm} (3-21)

where,

- \( H_\tau \) is the null hypothesis of trend stationarity,
- \( H_\mu \) is the null hypothesis of level stationarity and
- \( H_0 \) is the null hypothesis of zero mean stationarity (Hobin et al., 2004).

These null hypotheses correspond to the restrictions \( d=0, \beta=0 \) and \( d=\beta=\alpha=0 \) in EQ. (3-18) and are summarized in Table 3-1.

<table>
<thead>
<tr>
<th>Hypothesis</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_\tau )</td>
<td>Trend Stationarity ( d = 0 )</td>
</tr>
<tr>
<td>( H_\mu )</td>
<td>Level Stationarity ( d = \beta = 0 )</td>
</tr>
<tr>
<td>( H_0 )</td>
<td>Zero Mean Stationarity ( d = \beta = \alpha = 0 )</td>
</tr>
</tbody>
</table>

In order to test whether these regressions follow the test model of EQ. (3-18) with the selected restriction, the following test statistic is given by
\[ w = T^{-2} \sum_{t=1}^{T} S_t^2 / \sigma_{\varepsilon}^2, \quad (3-22) \]

which can be estimated by Eq. (3-23).

\[ \hat{w} = T^{-2} \sum_{t=1}^{T} S_t^2 / \hat{\sigma}^2 \quad (3-23) \]

\( \hat{\sigma}^2 \) is an estimator to \( \sigma_{\varepsilon}^2 \) where \( \sigma_{\varepsilon}^2 \) is known as the “long run variance” (Hobin et al., 2004), \( S_t = \sum_{i=1}^{T} e_i \) are partial sums of the residuals of a linear regression of Eq. (3-14) and \( e_i \)'s are the residuals \( (\bar{y} - y_i) \) for all active generations \( T \).

This methodology is applied to the COM series and its components, applying the test for level stationarity, in which Eq. (3-20) is utilized for \( H_\mu \) since it is postulated that the source COM series should have constant mean. This test statistic is proven to converge to a known distribution under the different hypotheses, for which the KPSS significance test is based.

In general, a test statistic is a function of the sample data on which a conclusion to reject or fail the null hypothesis can be determined. The significance level of a statistical test is the probability of Type I error. Type I error is the error of rejecting the null hypothesis when it is true (false positive). Typically this type of error can be set since the distribution of the null hypothesis is known. For example, if normality is being tested, a significance level of 5% will mean that 5% of the test statistics computed which are from a normal distribution will be identified as not normal. The Type II error is the error of failing to reject the null hypothesis when it is false (false negative). The lower the Type II error, the better the test is at identifying a true alternative hypothesis (higher power). The only way to guarantee zero Type I and Type II error would be to work from the entire population and not just a sample (Peck and Devore, 2005). This is often impractical or impossible. Typically an accepted significance is chosen, and then the power is evaluated and hopefully sufficient for samples from known distributions.
**Significance Testing Procedure**

If the COM series regression can be represented by the model represented by Eq. (3-18), with \( d=\beta=0 \), then the partial sums of the residuals of the regression are shown to converge to the second level Brownian Bridge \( V^2(r) \). As a result, this implies that

\[
H_\mu: w_\mu \rightarrow \int_0^1 V^2(r)dr,
\]

(3-24)

where \( V(r) \) is a first level Brownian Bridge. Upper tail critical values for 10%, 5%, 2.5% and 1% significance levels are 0.348, 0.460, 0.580 and 0.754 respectively. These significance levels set the accepted Type I error. A summary of significance levels for all of the hypotheses are given in Table 3-2. Monte Carlo simulations of a first order autoregressive process, a first order moving average process, and a series with a deterministic component and a simple random walk show desirable statistical size and power properties (Hobin et al., 2004).

<table>
<thead>
<tr>
<th>Level</th>
<th>10%</th>
<th>5%</th>
<th>2.5%</th>
<th>1%</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_\tau )</td>
<td>0.119</td>
<td>0.148</td>
<td>0.178</td>
<td>0.219</td>
</tr>
<tr>
<td>( H_\mu )</td>
<td>0.348</td>
<td>0.460</td>
<td>0.580</td>
<td>0.754</td>
</tr>
<tr>
<td>( H_\omega )</td>
<td>1.195</td>
<td>1.656</td>
<td>2.114</td>
<td>2.759</td>
</tr>
</tbody>
</table>

The standard KPSS test is oversized (rejects the null hypothesis of stationarity too often when it’s true) for highly autoregressive processes because it employs a semiparametric heteroskedasticity and autocorrelation consistent covariance estimator (HAC) of the long run variance of the process with an important positive finite sample bias. A sequence of random variables is heteroskedastic if the random variables have different variances. The generalized form of the KPSS test suggests a more automatic form selection of the long run variance that reduces size distortion without suffering from inconsistency (Hobin et al., 2004).
**Long Run Variance Estimation**

Studies have shown that the accuracy of inferences made using the \( w \) test statistic crucially depends on the actual choice of estimator for the long run variance (Heidelberger and Welch, 1983; Hobin et al., 2004; Schruben, 1982). The estimators employed frequently are heteroskedasticity and autocorrelation consistent (HAC) and are of the form given by EQ. (3-25), EQ. (3-26) and EQ. (3-27).

\[
\hat{\sigma}^2 = \hat{\gamma}_0 + 2 \sum_{j=1}^{T-1} k_m(j) \hat{\gamma}_j \quad (3-25)
\]

\[
\hat{\gamma}_j = T^{-1} \sum_{t=j+1}^{T} e_t e_{t-1} \quad (3-26)
\]

\[
k_m(j) = \frac{25}{12\pi^2(j/m)^2} \left[ \frac{\sin(6\pi(j/m)/5)}{6\pi(j/m)/5} - \cos(6\pi(j/m)/5) \right] \quad (3-27)
\]

\( \hat{\gamma}_j \) is used as an estimate of the \( j \)-th order autocovariance of \( e_t \), and \( k_m(j) \) is a kernel function depending on a bandwidth parameter \( m \) (Hobin et al., 2004). Several kernels are available and the original KPSS work utilizes the Bartlett kernel, while the generalized test proposed utilizes the Quadratic Spectral kernel since the Quadratic Spectral kernel was shown to be superior to the Bartlett kernel (Andrews, 1991; Newey and West, 1994). In the LDA approach, which is very similar in nature to the KPSS testing procedure, an estimate of the long run variance is also necessary. Estimation of this parameter was and still is an active area of research (Hobin et al., 2004; Newey and West, 1994; Schruben, 1982).

Lastly, a bandwidth, \( m \), must be chosen. Two such bandwidth choice options are reviewed in Hobijn et al., a deterministic method of the original KPSS test and a data dependant procedure explored by Andrews and developed further by Newey and West (Andrews, 1991; Hobin et al., 2004; Newey and West, 1994). This procedure still depends on an *a priori* non-
stochastic bandwidth parameter \( \eta_T \), but it has been shown that \( \sigma^2 \) depends much less on this parameter than the directly deterministic one chosen (Hobin et al., 2004; Newey and West, 1994). The bandwidth parameter \( m_T \) is then chosen by the following procedure.

1. \( n_T = o(T^{2/5}) \)
2. \( \hat{s}^{(0)}_0 = \hat{\gamma}_0 + 2 \sum_{i=1}^{n} \hat{\gamma}_i \)
3. \( \hat{s}^{(j)} = 2 \sum_{i=1}^{n} i \hat{\gamma}_i \)
4. \( \hat{\gamma} = 1.3221 \left( \left[ \frac{s^{(2)}}{s^{(0)}} \right] \right)^{1/5} \)
5. \( \hat{m}_T = \min \{ T, \hat{\gamma} T^{1/5} \} \)

In this dissertation, \( T \) is the total active generations, as defined previously. Note that as in Hobijn, \( n_T = \text{integer}[4((T/100)^2/25)] \) is utilized for step five.
CHAPTER 4
IMPLEMENTATION AND TESTING OF STATIONARITY DIAGNOSTICS

Implementation of the Information Theory Methodology

In order to evaluate the ability of the KPSS methodology to diagnose stationarity, it has been chosen to look at results not of the KPSS test alone, but also with results of another method for comparison. The Information Theory (Entropy) approach was chosen for comparison due to its fairly developed nature at the time this work was undertaken. As reviewed earlier in Chapter 1, the sandwich approach is not useful enough and the LDA approach is basically a less developed version of the KPSS test. The Intergeneration Correlation Length method should also provide a good comparison.

As a result, the information theory diagnostics have been implemented into the KENOV.a code. These diagnostics require a source meshing scheme and in KENOV.a it has been coded into the logic of the already present fission matrix methodology to utilize already existing coding to provide the meshing required. Two different available meshing strategies were made available to the user. In both strategies, the entropy approach is utilized only if a KENO matrix \( k_{eff} \) calculation is run, then the bin structure chosen is that of the matrix \( k_{eff} \) calculation. The two different strategies correspond to source bins created from the “matrix by array” or “matrix by unit” KENOV.a input option. If “matrix by array” is chosen, the source bin structure is the array structure for the matrix \( k_{eff} \) calculation, otherwise it is a bin structure by unit for a “matrix by unit” calculation. Consult the SCALE5 manual for more detailed information about matrix \( k_{eff} \) calculations (SCALE, 2005).

An output table is given corresponding to entropy test criterion 1 and 2, giving the generation number, entropy, relative entropy and the left hand side of the inequality in EQ. (3-11). A second table gives \( msq \) and \( cmsq \) from entropy criterion 1 for different numbers of
skipped cycles (corresponding with more skipped cycles than input) for informative purposes. Following this table is a summary table identifying the final result of each entropy test criterion.

**Implementation of the COM**

Determination of the source COM and all associated components has been implemented into the KENOVA code. Output currently consists of a data table by generation for \(x_g, y_g, z_g\) and the \(\vec{R}_g\) series. Note also that the skewness and kurtosis of the entire COM series is calculated for qualitative analysis.

**Implementation of the KPSS Methodology**

The generalized KPSS test statistic has been implemented into the KENOVA code and this test is automatically performed for \(\vec{R}_g\) and its components, \(x_g, y_g\) and \(z_g\). Output of KENOVA has been modified such that the \(\hat{\nu}\) statistic is given for \(\vec{R}_g\) and its components. This analysis is done without the need for any source meshing.

During this study a procedure was developed for which the KPSS test was performed not only on the COM series, but also on its components utilizing a combined approach so that if any two of these failed at the 5% significance level, or any single series failing at the 1% significance level it is concluded that the source is not stationary. This procedure was necessary as original results confirmed the test being slightly oversized (yielding a higher type I error rate in many situations) for problems with a high dominance ratio and strong autocorrelation in which the source behaves like an autoregressive process. Note that this was not observed in other problems, for which tests for independence and normality of the COM could be used alternatively to the KPSS test. If the COM series is independent and drawn from a random normal distribution, the source should be stationary (but if not, this does not mean the source is not stationary).
Final Table Output Additions in KENO.V.A

The final output table has been modified in KENO.V.A to reflect the results of the stationarity tests. Any failure results in a printed message indicating as such. Also, the number of meshes utilized for the entropy tests is listed here.

Implementations into 1Dcrit

Implementations into 1Dcrit of all of the previously discussed methodologies have also been performed. Output is the same format as with the KENO.V.A implementations (except dimension spatially). The meshing structure for the source entropy analysis is different, however, and not written into the logic of the fission matrix methodology. Instead, a virtual mesh structure is provided via user input.

Benchmark Problems Introduction and Analysis

Several Benchmark problems are analyzed in this section where the efficacy of the KPSS methodology is compared to that of the informatics approach. Many of these problems are problems with known source convergence issues. They range from simple geometric configurations to a large spent fuel storage facility and cover both undersampling and loosely coupled scenarios as well as high DR’s.

Stationarity Benchmark Problem 1

The first problem is a simple benchmark problem which is expected to have no source convergence issues (given standard acceptable code inputs). This problem is sample problem 1 from the SCALE 5 KENO.V.A manual. It is a critical 2 x 2 x 2 Array of uranium cylinders (SCALE, 2005; Thomas, 1973) (in void) and is shown schematically with pertinent material and geometric data in Figure 4-1.
Benchmark Problem 1 Analysis

Benchmark problem 1, a critical 2 x 2 x 2 array of uranium metal cylinders is analyzed here. Fifty replications (i.e. same case with different seeds) of 250 total generations with 1000 particles per generation and 50 skipped generations were undertaken. Six of the 50 replications are flagged with the KPSS testing procedure, while none are flagged as potential problems with the entropy diagnostics.

Fifty more replications were then performed with 20000 particles per generation, twenty times the original particles per generation. Knowing that the source intensity per cylinder should be equivalent from symmetry, this equates to 2500 source particles per cylinder, whereas each cylinder is 1117.37 cm$^3$ which implies if the source were evenly distributed there would be just over two neutrons per cubic centimeter. Even with this large number of source particles, eight replications are flagged as possible KPSS failures with none for the entropy diagnostics. A summary of these results is given in Table 4-1, while for completeness, the $k_{\text{eff}}$ values obtained are given in Figure 4-2 for all benchmark problem 1 cases.
Table 4-1. Problem 1 stationarity diagnostic summary

<table>
<thead>
<tr>
<th>History per Generation</th>
<th>Number Pass</th>
</tr>
</thead>
<tbody>
<tr>
<td>KPSS</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>44</td>
</tr>
<tr>
<td>20000</td>
<td>42</td>
</tr>
<tr>
<td>Entropy Test 1</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>*</td>
</tr>
<tr>
<td>20000</td>
<td>*</td>
</tr>
<tr>
<td>Entropy Test 2</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>50</td>
</tr>
<tr>
<td>20000</td>
<td>50</td>
</tr>
<tr>
<td>Entropy Test 3</td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>50</td>
</tr>
<tr>
<td>20000</td>
<td>50</td>
</tr>
</tbody>
</table>

*Test not applicable for a uniform source such as this problem

These results led to several questions. Are the KPSS failures TYPE I error? Could the source series really be not properly converged? If so, what is the cause of this non-convergence? In order to narrow down the answers, the results needed to be looked at more closely.

Figure 4-2. Problem 1 $k_{\text{eff}}$ results (first 50 values represent 2500 histories per generation, last 50 values represent 20000 histories per generation)
In Figure 4-3, the source fraction for the 1st and 5th cylinders are shown, divided by their own average source value beyond the 50 skipped generations for one of the failed replications (replication 1) of benchmark problem 1 with 1000 histories per generation.

Figure 4-3 shows that the source fractions depart significantly from their averages during the simulation and show some strong trends. Figure 4-4 is a similar figure for one of the failed replications (replication 9) of the 20000 histories per generation replications.
Figure 4-4. Benchmark problem 1 source analysis showing the average source in source fraction in cylinders 6 and 8 normalized to their average beyond 50 skipped cycles for replication 9 (failed replication) with 20000 histories per generation.

From Figure 4-4, similar behavior is observed as with Figure 4-3, with source fractions significantly departing from their average behavior and some very strong trending. There is a significant reduction in the overall magnitude of oscillation, however. This is the subtlety of the KPSS test that must be pointed out. Its aim is to determine a nonstationary series, however even if the departure from stationary is insignificant on a physical level, it may still be statistically relevant. To illustrate this point, a purely Gaussian white noise series of with theoretical mean 1.0 and theoretical standard deviation of 0.1 was sampled for 500 data points. This series was modified to include very small deterministic trend with slope $m = 0.0001$. A plot of the pure Gaussian and trend modified Gaussian is shown in Figure 4-5.
Figure 4-5 shows that to the eye, the series are nearly identical, yet if these series are scrutinized with the Generalized KPSS test for level stationarity, the test statistic values for the Gaussian white noise series is 0.131 and for the modified series is 0.5145. The first case easily passes the significance testing criteria, yet the second fails at 5% and nearly 2.5% significance with only a very small trend. This is expected, yet if this same series were the $k_{eff}$ series, it would look “ok” to the eye. Notwithstanding, if the overall scale of the series were mapped to a much smaller change, something much smaller than normal $k_{eff}$ deviations about its average, say with a Gaussian white noise series with mean 1.0 and standard deviation 0.0001, with a linear deterministic trend of $m = 0.0000001$, the expected result of the KPSS test would be identical to that before even though the physical significance of changes so small in the eigenvalue should be
inconsequential. Figure 4-6 illustrates this graphically, for which the same $\hat{\varphi}$ value as before for the case with a deterministic trend was obtained.

Figure 4-6 shows clearly that although the scale has changed dramatically, the result of the KPSS testing is the same since the same trend exists on a different scale. This will apply no matter how small a scale is obtained and is because the relative change of the series to the standard deviation is constant so the deterministic trend is significant when compared to the variance. In practice, this may result in KPSS tests identifying a nonstationary behavior where the physical differences are not significant. In this case, the analyst must observe the data and make a decision as to the reason for the KPSS failure. It should also be noted that even for those simulations where the series is stationary, the error estimates may not be correct when strong
correlation is present as stationarity only guarantees a well established mean and variance, not that the variance can be calculated as if there were no correlation present.

This analysis shows that although the KPSS methodology may indicate nonstationary behavior, this may or may not imply a true nonstationary issue in practicality. Certainly, given the significance testing procedure, Type I error will be present; however, some of these nonstationary series may not be physically nonstationary enough to warrant any alarm. Looking back to the nonstationary diagnoses associated with Figure 4-3 and Figure 4-4, it appears that these series may indeed be nonstationary; however the physical source data shows only a minimal issue which may not be much of a real problem. Another cause of the diagnoses can be that for an autocorrelated series, trending can occur for which a longer sample will be necessary in order to get a representative sample of the population. Not having a large enough sample may result in high TYPE I error. The key thing is that the methodologies implemented provide the user with all information regarding the source behavior with the KPSS results and the ability to plot the COM and its components along with the skewness and kurtosis values of the source COM. In addition, through the entropy diagnostic implementation, the meshed source distribution is available to look at when any issues may arise as well as the entropy and relative entropy series. It should be noted that the KPSS test does have difficulties diagnosing series with strong alternating autocorrelation exhibiting seasonality (periodic fluctuations) (Hobin et al., 2004).

**Stationarity Benchmark Problem 2**

The second benchmark problem is broken up into several variations all based on the OECD/NEA source convergence benchmark 4 problem, array of interacting spheres. The problem can be characterized by its loose coupling among source regions, and in its original form, the most reactive region may even lose its source distribution when simulated with
standard Monte Carlo codes. In this dissertation, both a simplified model with an array of 3 x 3 x 1 highly enriched uranium metal spheres and a full geometry of 5 x 5 x 1 spheres are investigated with and without vacuum boundary conditions (Wenner and Haghighat, 2008). Note that the true OECD/NEA benchmark 4 is the variation with 5 x 5 x 1 spheres, with vacuum boundaries. In the simplified (3 x 3 x 1) model, all spheres are of radius 10 cm, while in the full problem all spheres are of radius 8.71 cm except the central sphere, which is 10 cm. The simplified problem can be seen schematically in Figure 4-7 and the full problem in Figure 4-8, while the material compositions are listed in Table 4-2.

Figure 4-7. Schematic of the simplified benchmark 2 problem
Two cases of modified benchmark 2 are considered: i) Case 1 with vacuum boundary condition; ii) Case 2 with reflective boundary condition. For these cases, 50 replications are performed with a uniform initial source guess, 250 source generations, 5000 neutrons per generation and 50 skipped generations. Table 4-3 gives the overall comparison of the two cases for 50 replications for the generalized KPSS test, entropy tests, and their combination.
Table 4-3. Comparison of the number of replications with correct predictions for the entropy tests and Generalized KPSS test

<table>
<thead>
<tr>
<th>Test Result (Stationarity)</th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Entropy test 1</td>
<td>14</td>
<td>0*</td>
</tr>
<tr>
<td>Entropy test 2</td>
<td>39</td>
<td>50</td>
</tr>
<tr>
<td>Entropy test 3</td>
<td>0</td>
<td>50</td>
</tr>
<tr>
<td>Generalized KPSS</td>
<td>46</td>
<td>46</td>
</tr>
<tr>
<td><strong>Combined</strong></td>
<td>49</td>
<td>46</td>
</tr>
</tbody>
</table>

*Not applicable for a flat source distribution

The combined result given in Table 4-3 is achieved by applying a nonstationary diagnosis whenever either diagnostic approach fails. To illustrate just how significant an error can be made with the entropy diagnostics, $\tilde{R}_g$ is plotted in Figure 4-9 for replication one for both cases.

Replication one of case 1 passed all the stationarity diagnostics.

Figure 4-9. COM series plot for replication 1 for case 1 (vacuum boundary condition) and case 2 (reflective boundary condition) of modified version of benchmark 2

Figure 4-9 shows that for case 1, the departure from stationarity is extreme. This can
easily be proven since both cases are symmetric and the expected distance of the average source from the geometric center of the model should be zero in both cases. This nicely agrees with case 2, however case 1 is not only varying in a strange manner, it has significantly departed from zero indicating that the source behavior is not stationary, and is clearly not settled.

As an aside, a single comparative MCNP5 (X-5 Monte Carlo Team, 2003) calculation with the same input parameters was made for both cases. MCNP5 results recommend at least 44 skipped generations for case 1; however, a tally of the fission source indicates that the source has not converged to a symmetric distribution as expected. This implies that the entropy stationarity diagnostics have failed. Note that the current released version of MCNP5 utilizes a more basic test than the entropy tests given here. Upon completion of the problem, MCNP will compute the average value of entropy for the last half of the active generations as well as the sample standard deviation of the entropy and report the first generation found where the entropy falls within one standard deviation of its average for the last half of the generations, recommending at least that many generations be skipped.

**Analysis of misdiagnosed case 1 replication**

For case 1, the combined test has one false positive which is not correct. This false positive corresponds to replication 21. To look into this result, individual COM component behavior is shown associated with the source as the $x_g, y_g, z_g$ and $\bar{R}_g$ series. Note that 50 cycles were skipped and the testing procedure disregards these generations.
Visual inspection of Figure 4-10 indicates that the replication appears to be nonstationary, however a visual inspection is not always correct or easy to make. It may be that if enough cycles were undertaken, the source may indeed be stationary with a high degree of autocorrelation. The $\hat{\omega}$ values for the $x_g$, $y_g$, $z_g$ and $R_g$ series are 0.492, 0.232, 0.202 and 0.209 respectively. Comparing with the values in Table 3-2, the $x_g$ series fails the KPSS test at 5% significance, but the chosen nonstationary diagnoses in this work is for two series to fail at 5% significance or 1 series at 1% significance. A warning is still given. Data tables are available for plotting the source data and the $\hat{\omega}$ values are printed, and if any series fails at 5% a warning is given. The reasons why the KPSS test may not be accurate here are many. First, the statistical
nature of the test suggests that some Type I error will be made, yet the data here suggests this case should “easily” fail visually. Accordingly, it has been shown that series with alternating correlation exhibiting seasonality can be difficult to identify nonstationary behavior with this approach (Hobin et al., 2004). In addition, utilizing only 200 active generations may not be enough to provide the diagnosis definitively. In fact, the series in question may be stationary indeed, yet have a very high autocorrelation. Significant tally bias will still be evident.

Analysis of a misdiagnosed case 2 replication

For case 2, the combined test predicted four false positives. The behavior of the source COM gives an insight into the overall source variation. As a result, source data for one of the four false positives is shown in Figure 4-11.

Figure 4-11. $x_g, y_g, z_g$ and $COM$ series plot for replication 29 for case 1 (vacuum boundary condition). A) $x$ series, B) $y$ series, C) $z$ series, D) $COM$ series
Figure 4-11 shows that the source is not fluctuating too unreasonably, although at some points some small trending is evident through otherwise fairly random behavior. A strength of the KPSS methodology is in identifying such trends. The \( \hat{\mu} \) values for the \( x_g, y_g, z_g \) and \( \overrightarrow{R}_g \) series are 0.162, 0.639, 0.334 and 0.529. This implies that the \( y_g \) and COM series fail to the KPSS test.

This analysis does show that replication 29 may be acceptable, but it would be the call of the analyst to check for further problems. Having this source information on hand visually allows the analyst to check any source issues that may arise and then a judgment can be made whether the diagnosis of nonstationary behavior is serious or not.

**Full 5 X 5 array of spheres analysis**

Two cases of full benchmark 2 are considered just as in the modified case: i) Case 1 with vacuum boundary condition; ii) Case 2 with reflective boundary condition. For these cases, fifty replications are performed with a uniform initial source guess, 250 source generations, 15000 neutrons per generation and 50 skipped generations. More source particles per generation are utilized since the system is significantly larger, in fact 15000 may not be enough. Table 4-4 gives the overall comparison of the two cases for 50 replications for the generalized KPSS test, entropy tests, and their combination. In this benchmark, the central sphere is larger than the rest, causing a very large percentage of the source population to reside in the central sphere.

<table>
<thead>
<tr>
<th>Test Result (Stationarity)</th>
<th>Case 1 Stationary Diagnoses</th>
<th>Case 2 Stationary Diagnoses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Entropy test 1</td>
<td>50</td>
<td>1*</td>
</tr>
<tr>
<td>Entropy test 2</td>
<td>0</td>
<td>50</td>
</tr>
<tr>
<td>Entropy test 3</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Generalized KPSS</td>
<td>31</td>
<td>44</td>
</tr>
</tbody>
</table>

*Not applicable for a flat source distribution*
Up to this point, it has been evident that the most reliable Information Theory based diagnostic is entropy test 2. It is then important to look at the source behavior for a replication with a discrepancy in diagnosis for Case 1 (vacuum BC) for the full benchmark problem 2. As a result, Figure 4-12 shows a plot of the source parameters \((x_g, y_g, z_g)\) and COM series for one of these replications (replication 1).

![Figure 4-12](image.png)

Figure 4-12. \(x_g, y_g, z_g\) and COM series plot for replication 1 for case 1 of the full benchmark 2 problem (vacuum boundary condition)

Figure 4-12 confirms that the full benchmark 2 problem physics is significantly different. Here, due to the central sphere influence, the source population \(\vec{R}_g\) (COM) never reaches 1.5 cm from the center of the problem, however, some strong seasonal behavior is seen. This behavior does pose some problems for the KPSS methodology when the autocorrelation coefficient would
continuously alternate sign. Nevertheless, a look at the $\hat{w}$ values for the $x_g$, $y_g$, $z_g$ and $\vec{R}_g$ (COM) series (0.411, 0.068, 0.414 and 0.174, respectively) show that although a failure is not given, the $\hat{w}$ values are close to a failure at 5% significance. Also note that entropy test 2 is performed for every active generation, and only 21 generations failed the test. It appears that this simulation is near a converged state, but undersampling is still distorting the source behavior.

Figure 4-13 shows the $x_g$, $y_g$, $z_g$ and $\vec{R}_g$ (COM) series for replication 5 of the full benchmark 2 problem for case 2 (reflective boundary conditions). This replication was identified as possibly nonstationary with the KPSS methodology.

Figure 4-13. $x_g$, $y_g$, $z_g$ and COM series plot for replication 5 for case 2 (reflective boundary condition). A) $x$ series, B) $y$ series, C) $z$ series, D) COM series
Figure 4-13 shows that for the most part, the data support no major problem. The series that failed the KPSS test are the $x_g$ and $z_g$ series. The $x_g$ series appears visually to have some small trend in the first and second half but it appears to be insignificant overall as the overall variability is quite small. The $z_g$ series has a maximum variability of less than 0.25 cm and is not really very important in these simulations since the lattice of spheres does not extend in the $z$ direction, therefore the possibility for a problem with the $z_g$ series is unlikely. Statistically, the KPSS test can be correctly identifying issues that are hard to see visibly from undersampling, or the issues may be physically insignificant. Note that an autocorrelation analysis may also shed more light on whether a source convergence issues is present.

**Stationarity Benchmark Problem 3**

The third benchmark problem utilized is a real world type problem and is also OECD/NEA Source Convergence Benchmark 1: Checkerboard Storage of Assemblies. The model comprises a 24 x 3 array LWR fuel storage rack with fuel assemblies stored in alternate locations. The fuel assemblies are ~5.0% enriched by weight and are located within fully water flooded steel storage racks surrounded by a close-fitting full concrete reflection on three sides with water on the remaining side and water on the top and bottom. The fuel assemblies are formed from a 15 x 15 lattice of Zr-clad UO$_2$ (Blomquist and Nouri, 2002). The geometry is given in detail in Figure 4-14, while material specification is tabulated in Table 4-5. This problem has been studied extensively and it is known that the most reactive source region is the upper left assembly in Figure 4-14 (assembly 49) due to the superior reflection near that area. For clarity, a numbering system has been utilized in Figure 4-14 for the 24 x 3 lattice starting at 1 at the bottom left. This makes the three leftmost lattice regions numbered as 1, 25 and 49, starting with the bottom and moving to the top.
Figure 4-14. Schematic of the benchmark 3 problem

All Dimensions in cm

15 x 15 lattice – water moderated, centrally located
Pitch 1.4
Fuel radius 0.44

Water Channels have same exterior dimensions as fuel channels

Cut view through the assemblies closest to the water reflected side
Table 4-5. Material properties for benchmark problem 3, checkerboard storage of assemblies
material data (atoms/barn cm)

<table>
<thead>
<tr>
<th></th>
<th>Fuel</th>
<th>Concrete</th>
</tr>
</thead>
<tbody>
<tr>
<td>U238</td>
<td>2.2380E-02</td>
<td>H</td>
</tr>
<tr>
<td>O</td>
<td>4.6054E-02</td>
<td>C</td>
</tr>
<tr>
<td>U235</td>
<td>8.2213E-04</td>
<td>Si</td>
</tr>
<tr>
<td>Water</td>
<td></td>
<td>Ca</td>
</tr>
<tr>
<td>H</td>
<td>6.6706E-02</td>
<td>O</td>
</tr>
<tr>
<td>O</td>
<td>3.3353E-02</td>
<td>Iron</td>
</tr>
<tr>
<td>Zirconium</td>
<td></td>
<td>Fe</td>
</tr>
<tr>
<td>Zr</td>
<td>4.2910E-02</td>
<td></td>
</tr>
</tbody>
</table>

After extensive analysis in “Source Convergence in Criticality Safety Analyses, Phase I:
Results for Four Test Problems” (Blomquist et al., 2006), it was suggested that with 5000
histories per generation, that at least 700 cycles are needed to reach a fully converged source.

In order to investigate this, 50 replications of the problem were simulated with 10000 total
cycles, 10000 histories per generation, and 1000 skipped cycles. From the results of these
simulations, the KPSS test indicates that the source may not be converged for all 50 cases.
Interestingly, this is also true of the entropy tests as implemented (note that this wouldn’t be the
case using the entropy diagnostic currently utilized in the MCNP code), as the second of the
three entropy tests fails for all cases, while test 1 and 3 pass for all 50 cases. Figure 4-15 shows
$\bar{R}_g$ for replication 1 with 10000 histories per generation. From Figure 4-15 it is apparent that
skipping 700 cycles is not adequate as the source is still “settling”. It appears that skipping 2000
cycles is more appropriate.
Since it appears that skipping 2000 cycles will definitely be adequate, 50 replications were performed with 2000 skipped generations, 10000 histories per generation and 5000 total generations to save calculation time as simulation time can be quite lengthy for 50 replications with such large numbers of particles per generation and total generations. Results of these calculations yield 50 stationarity failures exactly as before. Undersampling is suspected to be at the heart of the failures as there is no doubt with the diagnostic results that the source is not converged properly.

Two more calculations were performed then with increasing numbers of histories per generation, the first with 100000 histories per generation with 5000 skipped and 5000 active generations. Five thousand generations were skipped to be absolutely certain that an adequate number of cycles were skipped and the skipped cycles are not adversely affecting convergence.
The second calculation is a very extreme trial, and has 1 million histories per generation with 2000 skipped generations and 10000 total generations.

Even with 100000 histories per generation, the KPSS test and entropy test 2 still failed, while the entropy test 2 only failed 277 cycles out of a total of 5000 possible cycles. Figure 4-16 shows $\tilde{R}_g$ (COM) series for replication 1 with 10000 histories per generation, and the $\tilde{R}_g$ (COM) series for the single replication of 100000 histories per generation. Clearly with 5000 skipped cycles for the 100000 histories per generation case, not skipping enough cycles is ruled out.

Figure 4-16. Benchmark problem 2 COM plot for replication 1 with 10000 histories per generation and the single replication case of 100000 histories per generation
To investigate further the undersampling behavior, Figure 4-17 shows the source fraction for assembly numbers 23 (farthest from the most reactive assembly in the bottom row), 21, 19, 17, 15, 13, 11 and 9.

![Figure 4-17. Source fraction plot of problem 3 for assemblies 9, 11, 13, 15, 17, 19, 21 and 23 with 100000 histories per generation](image)

From Figure 4-17 several things can be seen. Most striking is the fact that all of the assemblies with the exception of assembly 9 have a significant amount of cycles for which there is no source neutrons in that assembly, with several of the assemblies lacking source for nearly the entire calculation. This is due to their large distance from the most reactive area.

Also it can be seen that the source fraction in many assemblies oscillates due to some periodic influx of source from other assemblies. Clearly undersampling is still occurring in these assemblies (and others not shown) due to most of the relative source strength being located in
just a few assemblies. Stratified source sampling may improve this problem, as well as some of
the other techniques previously mentioned in chapter 1; however the problem most likely cannot
be eliminated since there are just not enough particles to properly describe the source.

In the case with 1 million histories per generation, this time the entropy tests passed and no
indication of nonstationary behavior is given, while interestingly the KPSS test still fails. A
summary of the stationarity results for problem 2 are given in Table 4-6.

Table 4-6. Problem 2 stationarity diagnostic summary

<table>
<thead>
<tr>
<th>Case</th>
<th>Number Pass</th>
<th></th>
<th></th>
<th></th>
<th>Total Rep's</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>KPSS</td>
<td>Entropy Test 1</td>
<td>Entropy Test 2</td>
<td>Entropy Test 3</td>
<td></td>
</tr>
<tr>
<td>1000 Skip</td>
<td>0</td>
<td>50</td>
<td>0</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>10000 Hist/Gen.</td>
<td>0</td>
<td>50</td>
<td>0</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>2000 Skip</td>
<td>0</td>
<td>50</td>
<td>0</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>10000 Hist/Gen.</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5000 Skip</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>100000 Hist/Gen.</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2000 Skip</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1000000 Hist/Gen.</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Figure 4-18 shows the results of assembly source fractions 9, 11, 13 and 15. Recall that
these assemblies were also included in Figure 4-17 with 100000 histories per generation, ten
times less than the data used to generate Figure 4-18. The trend of reduced source per source
mesh continues with higher assembly numbers as they get increasingly farther from the most
reactive source elements.
Figure 4-18. Source fraction plot of benchmark problem 3 with 1 million histories per generation. A) Assembly 9, B) Assembly 11, C) Assembly 13, D) Assembly 15
Clearly, from Figure 4-18, looking at the source fraction for different assemblies, (9, 11, 13 and 15) what is happening becomes evident. Although now assembly 9 has a “fairly” stable source fraction as does assembly 11, assembly 13 has many significant fluctuations while assembly 15 has even more fluctuations and many generations without any source. It is safe to say that assemblies 17, 19, 21 and 23 are progressively worse. Although the addition of more particles stabilized more assembly locations, there are still many which aren’t and undersampling is still an issue. These assemblies may have a negligible impact on the final $k_{eff}$, but localized tallies in these regions will be erroneous. $k_{eff}$ for this case was $0.8870735 \pm 0.0000089$. A comprehensive plot of the $k_{eff}$ values obtained for benchmark problem 3 for all replications and is shown in Figure 4-19.

Figure 4-19. Problem 2 $k_{eff}$ results for all benchmark problem 2 cases
From Figure 4-19, it is clearly seen that the $k_{\text{eff}}$ value from the 1 million histories per generation case is statistically different than several of the other replications at 10000 histories per generation, yet the results are not far off.

**Conclusions of Stationarity Analyses**

A new stationarity diagnostic for use with Monte Carlo eigenvalue problems known as the generalized KPSS test for stationarity detection in Monte Carlo eigenvalue problems test for stationarity has been developed. It has been compared to information theory based diagnostics for several benchmark problems. The first problem is a simple critical 2 x 2 x 2 lattice of uranium cylinders. Results of these simulations suggest that the KPSS test is comparable to the entropy testing procedure, and appears in some cases to improve diagnostic capability.

Next, comparisons are done for the OECD/NEA Source Convergence Benchmark 4: Array of interacting Spheres. Several variations are also simulated considering only 9 spheres and using reflective boundary conditions. Again, results of these simulations showed the KPSS test to be comparable and at times better than the information theory based diagnostics.

Lastly, comparisons are made for the so called OECD/NEA Source Convergence Benchmark 1: Checkerboard Storage of Assemblies Model. The model comprises a 24x3 array LWR fuel storage rack with fuel assemblies stored in alternate locations. Results of simulations have shown that past researchers may have underestimated the total number of skipped cycles required for the “warm up” period. Beyond this, both the KPSS test and entropy test 2 have shown that even for up to 100000 histories per generation that the source behavior differs from a stationary one.

Through thorough analysis of the actual source distribution per generation, it was shown that undersampling is the key issue. Finally, a case with a single replication of 1 million histories per generation was undertaken, with 2000 skipped and 10000 total cycles. The KPSS
test still correctly identifies nonstationary behavior while the entropy tests do not. Thorough analysis of the source distribution itself shows undersampling is yet still an issue, although to a lesser extent as before. Since the use of the generalized KPSS test is done on the $\bar{R}_g$ (COM) series, this parameter is highly sensitive to the source distribution and is a very good indicator for or against source stationarity for many problems.

As expected, there is no foolproof diagnostic method. As shown here, comparing the effectiveness of the KPSS methodology to that of the implemented information theory diagnostics, it is clear that entropy test 2 and the KPSS test are the most robust by far, however neither is perfect. Therefore, it is a recommendation that a complementary approach incorporating all of these testing procedures is to be used. These tests need not be exclusive. Other tests are mentioned in Chapter 1, and have not been studied extensively here, but having more tests available should only increase reliability. Having these diagnostic tools available, an analyst has an abundance of information available to make a determination if a particular simulation should be scrutinized more carefully. Note that currently only the experimental version of KENO.V.a and the 1Dcrit code include the test procedures utilized here (both KPSS and Information Theoretic diagnostics).

Lastly, note that a misdiagnosis of stationarity may only result in minimal error to the $k_{\text{eff}}$, but may still be significant. Moreover, all localized tally information will be significantly less reliable. Since the KPSS test can be applied to any time series, it may be useful to apply it locally to individual source regions to ensure each region has a stationary source distribution or perhaps the user can be given the flexibility to test a particular source region.
CHAPTER 5
DEVELOPMENT AND IMPLEMENTATION OF NEW FISSION SOURCE
ACCELERATION METHODOLOGIES

This chapter reviews and introduces methodologies that are devised to accelerate the solution of Monte Carlo eigenvalue problems. The methodologies reviewed are not exhaustive, but are necessary for the work involved in this dissertation. Fission matrix methods are discussed as well as methods based on importance sampling such as the extension of the Consistent Adjoint Driven Importance Sampling (CADIS) methodology to eigenvalue problems.

**Extension of CADIS Methodology to Eigenvalue Problems**

The CADIS methodology was developed and implemented by Wagner and Haghighat (Wagner and Haghighat, 1998). The goal of the CADIS methodology is to apply the concept of importance sampling in a consistent manner for use in a Monte Carlo algorithm. It accomplishes this goal by utilizing importance sampling concepts to provide source biasing, and also to apply transport biasing through the weight-window technique. The major points are reviewed here.

**Review of the CADIS Methodology**

The review of the CADIS methodology starts with the essential concept of integration via Monte Carlo methods and how importance sampling can increase the integration efficiency. After that, source and transport biasing procedures are derived utilizing these concepts.

**Integration by Monte Carlo**

Utilizing the definition of expected values, it is easy to see how integrals can be estimated from the Monte Carlo method. Suppose the integral of a function \( g(x) \) is desired over a range of \([a,b]\) as

\[
I(g(x)) = \int_{a}^{b} g(x)dx. \quad (5-1)
\]

Recall from EQ. (2-30), repeated here, that the definition of the expected value of \( g(X) \) is
\[ E[g(X)] = \int_a^b g(x)p(x)\,dx. \]  

(5-2)

Then, given the random variable \( X \) drawn from \( p(x) \), it is written

\[ G_N = \frac{1}{N} \sum_{i=1}^{N} g(X_i). \]  

(5-3)

Utilizing expectation values, it is shown that

\[ E[G_N] = E\left[ \frac{1}{N} \sum_{i=1}^{N} g(X_i) \right] \]  

(5-4)

\[ E[G_N] = \frac{1}{N} \sum_{i=1}^{N} E[g(X_i)] = \frac{1}{N} N E[g(X)] \]  

(5-5)

\[ E[G_N] = E[g(X)] \]  

(5-6)

\[ E[G_N] = \int_a^b g(x)p(x)\,dx. \]  

(5-7)

Since the integral sought is \( I(g(x)) = \int_a^b g(x)\,dx \), \( p(x) \) is chosen to be a constant \( A \) such that

\[ \int_a^b A \,dx = 1, \]  

(5-8)

then,

\[ A = \frac{1}{b - a}, \]  

(5-9)

and substituting into EQ. (5-7) yields

\[ E[G_N] = \frac{1}{b - a} \int_a^b g(x)\,dx = \frac{1}{b - a} I(g(x)). \]  

(5-10)

Rearranging yields

\[ (b - a) E[G_N] = I(g(x)) = (b - a) \frac{1}{N} \sum_{i=1}^{N} g(X_i). \]  

(5-11)
The results of the previous derivations yield an estimator for the integral of a function $g(x)$. It can be shown that the convergence of this estimator to the actual integral is $O(\sqrt{n})$ and converges due to the law of large numbers.

This is the typical brute force method of integration for Monte Carlo methods, and can be extended to multi-dimensions. Recall the $X_i$’s are sampled from a uniform distribution ($p(x)$ was chosen to be constant). Also, this is for a chosen flat $p(x)$ over the range of the problem $[a,b]$, yet typically random numbers are generated over the range $[0,1]$. If desired, a suitable mapping can be done to recast the integral over the range of $[0, 1]$, in which case $p(x)=1$, and $(b-a)=1$. If one wishes to increase accuracy and speed up the convergence of $E[G_N]$ to the desired integral, it is possible to utilize the concept of importance sampling.

**Importance sampling**

Importance sampling is choosing a “good” distribution from which to simulate one's random variables. By multiplying the integrand by 1 ($h(x)/h(x)$), the integral is unchanged, but the sampling distribution can be modified to yield an expectation of a quantity that varies less than the original integrand over the region of integration. Recall again that

$$E[g(X)] = \int_a^b g(x)p(x)\,dx. \quad (5-12)$$

Multiplying by $(h(x)/h(x))$ results in

$$E[g^*(X)] = \int_a^b g^*(x)h(x)\,dx = E[g(x)], \quad (5-13)$$

since

$$g^*(x) = \frac{g(x)p(x)}{h(x)}. \quad (5-14)$$
The two integrals are identical, implying identical expectation values; however the sampling distribution has been modified. Given the random variable $X$ drawn from $h(x)$, the final integral is determined using the estimator

$$
(b - a)G_N = (b - a) \frac{1}{N} \sum_{i=1}^{N} g^*(X_i).
$$

(5-15)

It turns out that the closer $h(x)$ is to $g(x)$ in proportion (must be a pdf), the smaller the variance, with the result of zero variance for $\alpha h(x) = g(x)p(x)$, where $\alpha$ is a constant. This can be seen by substituting for $h(x)$ in $g^*(x)$ as follows:

$$
E[g^*(X)] = E[g(X)] = \int_{a}^{b} \frac{g(x)p(x)}{g(x)p(x)} h(x) dx.
$$

(5-16)

Rearranging yields

$$
E[g(X)] = \int_{a}^{b} \alpha h(x) dx = \alpha.
$$

(5-17)

Utilizing the original expectation, this shows that

$$
\alpha = \int_{a}^{b} g(x)p(x) dx.
$$

(5-18)

This implies that to have a zero variance solution, the original integral involving $g(x)$ is computable and there would be no need for Monte Carlo integration. The usefulness of this is such that the closer the chosen sampling pdf $h(x)$ is to the integrand, the lower the variance and faster the calculation of the integral will be.

**Source biasing**

Recall that if a detector cross-section is utilized for the adjoint source then the detector response can be written as

$$
R = \langle \psi^\dagger(\hat{r}, \hat{\Omega}, E) Q(r, E) \rangle.
$$

(5-19)

Utilizing importance sampling the detector response can then be written as
\[ R = \left\langle \frac{\psi^\dagger(\bar{r}, \bar{\Omega}, E) Q(r, E)}{\hat{Q}(r, E)} \right\rangle \hat{Q}(r, E), \]  \hspace{1cm} (5-20) 

Where \( \hat{Q}(r, E) > 0 \) and \( \langle \hat{Q}(r, E) \rangle = 1 \). According to the previous section a zero variance solution will be arrived at if

\[ \hat{Q}(r, E) = \frac{\psi^\dagger(\bar{r}, \bar{\Omega}, E) Q(r, E)}{R}. \] \hspace{1cm} (5-21) 

Utilizing the following equation to conserve the total number of particles, the biased source distribution from EQ. (5-21) can be applied during a Monte Carlo simulation as

\[ w(\bar{r}, \bar{\Omega}, E) \hat{Q}(r, E) = w_o(\bar{r}, \bar{\Omega}, E) Q(r, E). \] \hspace{1cm} (5-22) 

Substituting EQ. (5-21) into EQ. (5-22), given that \( w_o = 1 \), yields

\[ w(\bar{r}, \bar{\Omega}, E) = \frac{R}{\psi^\dagger(\bar{r}, \bar{\Omega}, E) 0}. \] \hspace{1cm} (5-23) 

Of course, since the true values of \( R \) and \( \psi^\dagger(\bar{r}, \bar{\Omega}, E) \) are not known, their ratio is obtained approximately (often via deterministic methods). The better the approximation is, the more effective the source biasing.

**Transport biasing**

Again, it is assumed that the adjoint source is set to a detector cross-section of interest.

Neglecting the external source, the transport equation can be written in integral form, similar to EQ. (2-14), rewritten again here as \( \psi(\bar{r}, E, \hat{\Omega}) = \int_{\bar{r}}^{r} dr' \int_{4\pi} \int_{0}^{\infty} dE' d\omega' G(\bar{r}' \to \bar{r}, \bar{\omega}' \to \hat{\Omega}, E' \to E) * \frac{\chi(E)}{k4\pi} \int_{4\pi} d\omega' \int_{0}^{\infty} dE' v(E') \sigma_f(E') \psi(\bar{r}', E', \bar{\omega}'). \)

\[ \psi(\bar{r}, E, \hat{\Omega}) = \int_{\bar{r}}^{r} dr' \int_{4\pi} d\omega' \int_{0}^{\infty} dE' K(\bar{r}' \to \bar{r}, \bar{\omega}' \to \hat{\Omega}, E' \to E) \psi(\bar{r}', E', \hat{\omega}'). \] \hspace{1cm} (5-24) 

where \( K(\bar{r}' \to \bar{r}, \bar{\omega}' \to \hat{\Omega}, E' \to E) dr dE d\Omega \) is the expected number of particles emerging at \( \bar{r} \) within \( dr \), \( E \) within \( dE \), with direction \( \hat{\Omega} \) about \( d\Omega \) due to an event in \( dr' dE' d\Omega' \). Multiplying this equation by \( \frac{\psi^\dagger(\bar{r}, \bar{\Omega}, E)}{R} \), and replacing \( dr dE d\Omega \) with \( dP \) for simplicity, EQ. (5-24) becomes
\[ \tilde{\psi}(P) = \frac{\int_{P'} dP' K(P' \rightarrow P) \psi(P')\psi^\dagger(P)}{R}, \] 
\hspace{2cm} (5-25)

where

\[ \tilde{\psi}(P) = \frac{\psi^\dagger(P)\psi(P)}{R}. \] 
\hspace{2cm} (5-26)

Multiplying by \( \frac{\psi^\dagger(P')}{\psi^\dagger(P')} \) results in

\[ \tilde{\psi}(P) = \frac{\int_{P'} dP' K(P' \rightarrow P) \psi(P')\psi^\dagger(P') \frac{\psi^\dagger(P)}{\psi^\dagger(P')}}{R}, \] 
\hspace{2cm} (5-27)

which is reduced to

\[ \tilde{\psi}(P) = \int_{P'} dP' K(P' \rightarrow P) \tilde{\psi}(P') \frac{\psi^\dagger(P)}{\psi^\dagger(P')}, \] 
\hspace{2cm} (5-28)

or

\[ \tilde{\psi}(P) = \int_{P'} dP' \tilde{K}(P' \rightarrow P) \tilde{\psi}(P'), \] 
\hspace{2cm} (5-29)

where

\[ \tilde{K}(P' \rightarrow P) = K(P' \rightarrow P) \left[ \frac{\psi^\dagger(P')}{\psi^\dagger(P)} \right]. \] 
\hspace{2cm} (5-30)

Practically speaking, \( K(P' \rightarrow P) \) is not known. As a result, particle transport is performed in an analog manner but when an event occurs in \( P' \) (changing energy, position or direction), particles emerging from this event are biased according to \( \frac{\psi^\dagger(P')}{\psi^\dagger(P')} \). This will then increase the number of particles in higher importance areas and lower the number of particles in lower importance regions. In order to account for this change in particle population, particle weight must be adjusted for particle conservation according to EQ. (5-31).

\[ w(P) = w_o(P') \left[ \frac{\psi^\dagger(P')}{\psi^\dagger(P)} \right] \] 
\hspace{2cm} (5-31)
This methodology is utilized within the framework of the weight-window technique and is known as Consistent Adjoint Driven Importance Sampling (CADIS). All importance function data is obtained via simplified deterministic models.

At this point a note about zero-variance schemes is prescient. It is possible instead of utilizing the weight-window technique to use a biased transport kernel such that during the transport and collision of particles, the free flight and collision probabilities are modified directly, resulting in a non-analog game whereby weights are then modified accordingly (as in the weight-window technique). This requires the direct computation of the kernels.

**Extension of CADIS methodology to eigenvalue problems**

Theoretically, an extension of the CADIS algorithm to eigenvalue problems hinges directly on the choice of the adjoint source. In a shielding problem, the adjoint source is chosen as the detector cross-section in the region of interest. It is then straightforward to utilize the neutron production, specifically $\nu\sigma_f$ as the adjoint source. Importance obtained will be relative to fission neutron production in the system.

**Adjoint source**

In order to obtain importance to neutron production, the adjoint source in equation (2-8), rewritten here as $H^+\psi^+(\vec{r},\vec{\Omega},E) = Q^+_{\text{ext}}(\vec{r},\vec{\Omega},E)$, is set to

$$Q^+_{\text{ext}}(\vec{r},\vec{\Omega},E) = \nu\sigma_f.$$  \hfill (5-32)

It is also important to note that importance obtained from EQ. (2-8) is different from the importance that would be obtained from the adjoint eigenvalue equation. Importance from the eigenvalue equation would take into account production from a neutron including all its progeny, while from EQ. (2-8) will only include importance of a neutron to direct production of next generation neutrons. Given the generation to generation process of the Monte Carlo calculation,
this is adequate since neutron importance can be utilized to reduce variance in the next
generation neutron source.

Other considerations

An added difficulty with the extension of CADIS to eigenvalue problems, called here
Eigenvalue CADIS (E-CADIS), is the fact that since the fission cross section is non-zero in all
fissionable material, importance obtained is to that of ALL source regions. Efficiency may be
severely affected since source particles are born in fissionable material which are distributed
throughout the model, and the need for extreme biasing to a region of interest is drastically
reduced.

Next, since the source is unknown in an eigenvalue problem, source biasing as applied in
shielding problems is not applicable. Normalization of the weight-window generated values is
more difficult. Several different choices are possible. The simplest choice is to normalize the
most important particles to the center of (or somewhere within) the weight-window. This is most
likely not the best approach since another region may have less importance but more overall
source. To improve this method one should utilize the fractional importance and start source
particles with the most estimated contributed response (to production) inside the weight-window.
Another possibility is starting all particles within the weight-window. This is accomplished by
renormalizing the weight-window values for every source region and energy group combination.

Some of these source weight-window initialization strategies concerning the lower weight
normalization would result in some particles being started outside of the weight-window. If this
is the case, a procedure can be utilized to adjust source particle weight via splitting or Russian
Roulette before the particles are even transported for the first time in order to bring them within
the weight-window bounds.
With that said, transport biasing can still be performed in the same manner as was done for shielding problems. Alternatively, it is possible to derive a zero-variance formulation extended to the eigenvalue problem utilizing the theory just discussed. In fact, if the integral form of the Boltzmann equation for the collision densities (as opposed to the flux) is written, a separate collision kernel and transport kernel can be obtained. Instead of utilizing the weight-window technique, these kernels can be biased directly (as can the transport kernel already discussed) with a corresponding modification of particle weight for conservation. The ideas are formulated with much rigor, and have been reviewed and tested. (Dufek, 2009; Lux and Koblinger, 1991). Utilizing a separated collision and transport kernel was beneficial because it was shown that biasing the transport kernel had a negative impact (slowed down the calculation) while biasing the collision kernel saw speedup of up to 70% in some test cases (Dufek, 2009).

**Modified source-detector algorithm**

To overcome the issue of source neutrons being born in important regions, the eigenvalue problem can be projected as a series of fixed source problems by decomposing the spatial domain via a new source iteration scheme. The difference between the standard solution algorithm and the modified algorithm is how the particles are transported. In the modified algorithm, the spatial domain is segmented as in the fission Matrix algorithm (Kadotani et al., 1991; Morton, 1956). Each source region is then methodically transported to each other source region, one at a time, ignoring the contribution to fission from every other region. This process is repeated for each source region and the $k_{\text{eff}}$ is calculated from a combination of all the separate calculations within the generation. This method is referred to as Modified Eigenvalue CADIS (ME-CADIS). To illustrate, consider a 1-D, mono-energetic, two region problem shown in Figure 5.1.
Figure 5-1. Source discretization with source transfer procedure for 2-region ME-CADIS problem

Transport of particles proceeds as follows:

1) Source particles born in region A are transported, utilizing an importance function specifically generated to minimize variance of particle transport to region A.
   a) Any fission that occurs in the region of interest, region A, is tallied and next generation neutrons are banked from this fission process.
   b) Any fission occurring outside the region (region A) of interest is not tallied, nor are any source particles stored for use in the next generation.

2) Source particles born in region A are transported, utilizing an importance function specifically generated to minimize variance of particle transport to region B.
   a) Any fission that occurs in the region of interest, region A, is tallied and next generation neutrons are banked from this fission process.
   b) Any fission occurring outside the region of interest (region A) is not tallied, nor are any source particles stored for use in the next generation.

3) Repeat Steps 1 and 2 for region B.

In this case, twice the amount of particle tracking is done which obviously increases computation time if no biasing is performed. Although twice the number of histories has been simulated, only half are simulated in the Monte Carlo sense since the contribution to each region
was obtained using the same source particles, and only the contribution to the region of interest obtained. The number of theoretically simulated histories is given by

\[ H_{th} = NPG \times N_{reg} \]  

where \( NPG \) is the number of particles per generation, and \( N_{reg} \) is the number of regions. Given algorithm equality elsewhere, this algorithm would be a factor of \( N_{reg} \) slower.

The division of the source to separate regions and calculating the contribution from each region to every other is similar to simulating multiple fixed-source calculations within each generation. In order to obtain region specific importance data, \( N_{reg} \) approximate importance calculations must be performed deterministically such that for each calculation the adjoint source is set to be sensitive to fission in only one source region. Transport biasing through the CADIS approach can be utilized for each Monte Carlo segmented source region reducing the penalty of more simulated particles. For simulations with undersampling issues or loose coupling, this methodology aims to help stabilize source population in regions with little to no source (within reason). If the flux gradient is too large, however, the method may not be effective enough to mitigate undersampling.

**Fission Matrix Methods**

In the fission matrix acceleration methods, the fission matrix elements from equation (2-20), repeated here, are utilized to provide an approximate solution for the fundamental mode eigenvector.

\[
(A_i)_{i,j} = \frac{\int_{V_i} \int_{V_j} d\bar{r} d\bar{r}' a(\bar{r}' \rightarrow \bar{r}) S_0(\bar{r}')}{\int_{V_j} d\bar{r}' S_0(\bar{r}')} 
\]

(5-34)
Standard Fission Matrix Method Review

Recall from chapter 2 that \((\mathbb{A})_{i,j}\) is approximated as \((\mathbb{A})_{i,j} = \frac{(\mathbb{B})_{i,j}}{(\mathbb{C})_{j}}\), and that if the matrix elements of \((\mathbb{A})_{i,j}\) are zeroed after every generation, the result is the cycle-wise fission matrix. Alternatively, if the elements of \((\mathbb{A})_{i,j}\) are kept over all desired generations, the cumulative fission matrix is obtained. Once obtained, the fundamental mode eigenvalue \((k_{\text{eff}})\) and eigenvector \(((s_i)_j)\) are solved for numerically. Fission source acceleration methods assume that the source distribution represented by \((s_i)_j\) converges faster than the fission source in the standard Monte Carlo eigenvalue calculations. \((s_i)_j\) is then used to correct the fission source during the simulation. Various methodologies have been proposed for doing this, with the most common approach modifying the particle weights in source regions given by

\[ w^*(n) = \frac{(s_{fm}^{(n)})_j}{(s_{mc}^{(n)})_j} w^{(n)}_i, \text{ for all } i,j, \]  

(5-35)

where,

- \(w\) = particle weight  
- \(i\) = particle number  
- \(n\) = generation number  
- \(j\) = source mesh (from fission matrix)  
- \(fm\) \sim fission matrix  
- \(mc\) \sim Monte Carlo.

All attempts at using the cycle-wise fission matrix computed by Monte Carlo have met with limited success due to the problematic convergence (often statistical noise) of \((s_i)_j\) (Dufek, 2007; Urbatsch, 1995). Using the cumulative fission matrix can also be problematic if generations with unconverged source were to be included. In addition, noise may be reduced but not eliminated when utilizing the cumulative fission matrix (Dufek, 2007; Dufek, 2009; Urbatsch, 1995). The success that has been achieved has been the reduction in skipped cycles.
necessary since \((s_i)_j\) does converge close to the true solution faster than the traditional power iteration algorithm.

**Combined Fission Matrix Acceleration with CADIS**

Utilizing fission matrix acceleration methods while applying E-CADIS/ME-CADIS can be utilized. This methodology takes advantage of the reduced variation in the fission matrix elements when utilizing the CADIS methodologies and is nothing more than a simultaneous use of both methods. Several variations of biasing are possible including weighted percentages of the fission matrix eigenvector (source) with the standard Monte Carlo source.

**Implementation into 1Dcrit**

All of the methodologies discussed in this chapter have been implemented into the 1Dcrit code. No new input information is necessary in the main input file, however a secondary input file (bias.dat) containing the importance is needed for the E-CADIS or ME-CADIS algorithms. This file contains the number of energy groups and spatial bin structure and importance information for each region and group combination. The E-CADIS and ME-CADIS execution are actually separately compiled codes due to the memory restructuring required in the modified iteration scheme for ME-CADIS.

To benchmark the new source iteration structure utilized in the ME-CADIS algorithm, a simple 3 region, 2 energy group problem with 2 fissile regions of the same material sandwiching a non-fissile region was simulated as shown in Figure 5-2. The first region is 20 cm thick, the second region is 10 cm thick and the third region is 15 cm thick. Vacuum boundary conditions were considered. To benchmark 1Dcrit, reference calculations were performed with the PENTRAN code and the MCNP5 code in multigroup mode. 1Dcrit was utilized with standard and modified (ME-CADIS) solution algorithms. Note that all simulations with PENTRAN utilize the DTW differencing scheme.
For the Monte Carlo analysis, 10000 particles per generation were utilized with 20 skipped cycles and 200 total cycles. Material properties are given for the 2 group cross sections in Table 5-1, while results of a comparative simulation for $k_{eff}$ are given in Table 5-2.

### Table 5-1. Material properties for algorithm test problem

<table>
<thead>
<tr>
<th>Material</th>
<th>Group</th>
<th>$\Sigma_a$ (cm$^{-1}$)</th>
<th>$\nu\Sigma_f$ (cm$^{-1}$)</th>
<th>$\Sigma_t$ (cm$^{-1}$)</th>
<th>$\chi$</th>
<th>$\Sigma_s$ (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.025</td>
<td>0.025</td>
<td>0.045</td>
<td>0.70</td>
<td>0.005</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0.030</td>
<td>0.050</td>
<td>0.060</td>
<td>0.30</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0.020</td>
<td>0.000</td>
<td>0.040</td>
<td>0.00</td>
<td>0.000</td>
</tr>
</tbody>
</table>

### Table 5-2. Comparison of $k_{eff}$ predicted by different codes for algorithm test problem

<table>
<thead>
<tr>
<th>Code/Algorithm</th>
<th>$k_{eff}$</th>
<th>Std. Dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP/Multigroup</td>
<td>1.17932</td>
<td>0.00085</td>
</tr>
<tr>
<td>PENTRAN (DTW)</td>
<td>1.17905*</td>
<td>n/a</td>
</tr>
<tr>
<td>1-D/Standard</td>
<td>1.17921</td>
<td>0.00048</td>
</tr>
<tr>
<td>1-D/Modified (ME-CADIS)</td>
<td>1.17959</td>
<td>0.00055</td>
</tr>
</tbody>
</table>

*Based on a convergence criterion of $1 \times 10^{-5}$

Table 5-2 shows that all of the algorithms essentially achieve the same result for $k_{eff}$. To further support this claim, the average source distribution over the active cycles is 0.593 for region 1 and 0.412 for region 3 for the standard source algorithm, while it is 0.592 for region one and 0.413 for region three for the ME-CADIS algorithm. This provides confidence that the modified source iteration scheme and the traditional scheme are both consistent. More information about the input necessary to run 1Dcrit is given in appendix A.
CHAPTER 6
TESTING OF NEW SOURCE ACCELERATION METHODOLOGIES

The selected methodologies detailed in chapter 5 are tested in this chapter. The E-CADIS and ME-CADIS techniques are evaluated for their effectiveness, and their combinations with the fission matrix acceleration method are examined. In order to benefit from E-CADIS/ME-CADIS, approximate adjoint flux (importance) is required. This importance is obtained utilizing the PENTRAN code. Shell scripts combined with FORTRAN processing codes have been written to semi-automate the process of running PENTRAN and 1Dcrit for a single problem.

**PENTRAN Importance Calculations**

To obtain E-CADIS and ME-CADIS approximate importance information for the test problems, the PENTRAN code is utilized. For the E-CADIS approach, recall that the adjoint source in EQ. (2-11), repeater here as \( \langle \psi \dagger Q \rangle = \langle \psi Q \dagger \rangle \), is set to the “detector” cross section, which when adapted to the eigenvalue problem, is represented by EQ. (5-32). Note that the resulting importance relating to the adjoint source defined by EQ. (5-32) is then a global importance to production from all fissile source regions.

For the ME-CADIS approach, a separate PENTRAN calculation is performed for each discretized source region \((i)\) such that the adjoint source of EQ. (5-32) is modified to be \( Q \dagger_{\text{ext}} (\tilde{\Omega}, E)_i = (v \sigma_f)_i \). Each resulting importance function is then the importance to production for only the region for which the adjoint source was defined. This provides the ability to optimize region to region transfers as discussed in Chapter 5.

Note that the importance utilized is both space and energy dependent as a separate importance is obtained for every energy group and is utilized separately inside the weight-window framework. Note also that since the goal of the work in this dissertation is to determine whether or not the E-CADIS/ME-CADIS approaches are viable, the importance is calculated
with high fidelity to ensure little effect should be seen relating to a poorly determined importance function. Nevertheless, a well defined importance distribution on too fine a mesh can result in poor performance due to the need of locating particles within the weight-window (in both space and energy in 1Dcrit) becoming too time consuming. Note also that the total source magnitude in PENTRAN utilized for the importance cases is \( \sum (\nu \sigma) \), for all I source regions utilized in the particular importance calculation, with the energy spectrum (serg in PENTRAN) normalized to 1.0.

**Source Acceleration Test Problems**

Test problem 1 is a simple 3 energy group (Fast, epi-thermal, thermal) 3 source region problem without upscatter. As shown in Figure 6-1, this problem has 19 distinct geometry regions, with 4 different materials.

![Figure 6-1. Schematic of test source acceleration test problem 1](image)

Test problem 1 was devised to specifically test the effectiveness of the CADIS-like methodologies since fissile material is separated by large moderator regions whereby importance should vary significantly. Relevant geometry and material information is located in Table 6-1.

Boundary conditions are an albedo of 0.5 on the left and 1.0 on the right.

**Table 6-1. Material component radii for test problem 1 and 2**

<table>
<thead>
<tr>
<th>Region</th>
<th>Radius</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel ((3%_0 \text{ UO}_2))</td>
<td>0.3922</td>
<td>\text{UO}_2 \sim 3%_0</td>
</tr>
<tr>
<td>Gap (He)</td>
<td>0.40005</td>
<td>He</td>
</tr>
<tr>
<td>Clad (Zr)</td>
<td>0.4572</td>
<td>Zr</td>
</tr>
</tbody>
</table>
The second problem is a 3 group (same as previous), 3 region slab problem shown in Figure 6-2. The first (left) region is a 20 cm slab of fuel, the center region is a 35 cm slab of moderator and the 3rd region is a 20 cm fuel slab.

![Figure 6-2. Geometry for test problem 2](image)

The material compositions again follow those given in Table 6-1. This problem illustrates larger source regions separated by a large moderating material. Vacuum boundaries are set on both sides.

**E-CADIS Test Problem Results**

The E-CADIS implementation in 1Dcrit was optimized by testing several implementation options (as well as weight-window normalizations). On average, the most efficient results are achieved based on the following considerations:

1. On-the-fly weight-window normalization to the average relative response
2. Use of source weight biasing before any free flight (all generations)
3. Biasing only on collision and boundary crossing (biasing on mfp too computationally expensive)

For the first item (1), since it is easy to estimate the response of a source population to production utilizing the fission matrix, an on-the-fly relative response is utilized to adjust the
weight-window boundary so that for a given energy group and spatial source region the response utilized to normalize the weight window is the average response from that region and group combination, not the total response. The second item (2) refers to a form of Russian Roulette and splitting. Since the contribution of each source region/group to the total detector response can be estimated, this ratio is used to split or coalesce the starting source particles and set the starting weights within the windows set from step 1. This is done before the particles start their normal history. Every particle in a particular weight-window mesh is modified at once accordingly (and effectively split or coalesced). For the third item, due to the time constraint required by calling the weight-window and checking particle location every mfp or any factor thereof (greater or less than a mfp), weight-window checking is only performed during a boundary crossing. This is essentially the same conclusion as seen in the literature (Dufek, 2009; Lux and Koblinger, 1991) that the direct biasing of the collision kernel is too expensive. All data given in this and subsequent chapters utilize these options unless otherwise stated.

A PENTRAN importance simulation pertaining to test problem 1 was performed to initialize weight-window parameters via the importance obtained from the simulation. The importance was also used to obtain approximate response to neutron production for initialization of generation 1 in 1Dcrit. Neutron importance for this simulation is shown in Figure 6-3. 115 equally spaced meshes were utilized with an S₈ quadrature. Additionally, P₃ cross sections were utilized.
Figure 6-3 shows that the neutron importance is fairly flat near the fuel material for energy group 1 and 2 (in which particles are born) and peaked for the thermal energy group, i.e., group 3. Near the boundaries importance declines significantly, with a lower value on the left due to the different boundary conditions on the ends.

Ten replications of benchmark problem 1 were simulated for both the standard algorithm with no CADIS biasing and the E-CADIS algorithm. All simulations were performed with 3000 particles per generation, 3350 generations with 350 skipped generations and a $k_{\text{eff}}$ guess of 1.0. The results of these ten replications are given in Table 6-2.
From Table 6-2, it can be seen that the final average values are within statistics at one σ confidence. The average speedup over the cases was just over 1.06 as defined by EQ. (2-58).

Repeated here as speedup = \frac{FOM_2}{FOM_1}. This is a modest speed gain as should be expected after observing the obtained importance obtained from PENTRAN since a flatter importance should correlate with a reduced E-CADIS speedup. While each problem is unique and significantly different speedup may be obtained for other problems, this problem illustrates well why eigenvalue problems are difficult problems for acceleration methods predicated on importance sampling since particles are born in fissionable material, where they are often most important (energy spectrum complicates the matter some).

While these results for \( k_{eff} \) may be accurate, as \( k_{eff} \) convergence is much simpler than the source convergence in high DR problems, it is prudent to analyze the source distribution. If any other information from the simulation is desired the source must be properly converged, as tally confidence estimates will be unbiased only if the source appears random. Shown in Figure 6-4 is the source COM for replication 1 for both the standard algorithm and the E-CADIS algorithm.
Figure 6-4 shows that the source appears for the most part to be well behaved and the source convergence diagnostics indicate as such. To confirm the source behavior being converged, a Shapiro-Wilk normality test yields a p-value of ~0.32 and ~0.86 for the standard and E-CADIS cases respectively. If the p-value is less than the chosen significance level (typically from 1% to 10%), then the null hypothesis is rejected (i.e. one concludes the data are not from a normally distributed population). If the p-value is greater than the chosen significance level, then one does not reject the null hypothesis that the data came from a normally distributed population. The test suggests no reason to reject the hypothesis of normally distributed data at all typical significance levels.
Next, ten replications of benchmark problem 2 were simulated for both the standard algorithm with no CADIS biasing and the E-CADIS algorithm. Importance obtained via PENTRAN for this problem is shown in Figure 6-5.

Figure 6-5. Problem 2 (2 source region) global importance to production (plotted at deterministic mesh center)

PENTRAN simulation parameters were as follows:

- 118 equally spaced meshes
- $S_8$ level symmetric quadrature
- $P_3$ cross sections.

All simulations were performed with 5000 particles per generation, 5350 generations with 350 skipped generations and a $k_{eff}$ guess of 1. Given in Table 6-3 are the $k_{eff}$ values for all replications along with the standard error.
Data from Table 6-3 indicates that results are consistent statistically as in test problem 1. Average speedup for this problem was 1.18, showing better performance, yet still a modest gain of 18%. Again, the source distribution is analyzed. This time stationarity diagnostics are not favorable for a converged source distribution. For the standard MC algorithm replications, the entropy tests all pass, but the KPSS test shows ten failures. Shown in Figure 6-6 is the source COM for replication 1 for both the standard algorithm and the E-CADIS results.

<table>
<thead>
<tr>
<th>Replication</th>
<th>Standard Algorithm $k_{eff}$</th>
<th>Standard Algorithm Standard Error</th>
<th>E-CADIS $k_{eff}$</th>
<th>E-CADIS Standard Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.165342E-1</td>
<td>1.543E-4</td>
<td>7.165885E-1</td>
<td>1.492E-4</td>
</tr>
<tr>
<td>2</td>
<td>7.163229E-1</td>
<td>1.507E-4</td>
<td>7.160510E-1</td>
<td>1.488E-4</td>
</tr>
<tr>
<td>3</td>
<td>7.162166E-1</td>
<td>1.506E-4</td>
<td>7.163476E-1</td>
<td>1.496E-4</td>
</tr>
<tr>
<td>4</td>
<td>7.161542E-1</td>
<td>1.517E-4</td>
<td>7.161822E-1</td>
<td>1.505E-4</td>
</tr>
<tr>
<td>5</td>
<td>7.159475E-1</td>
<td>1.571E-4</td>
<td>7.160875E-1</td>
<td>1.506E-4</td>
</tr>
<tr>
<td>6</td>
<td>7.165154E-1</td>
<td>1.546E-4</td>
<td>7.162615E-1</td>
<td>1.504E-4</td>
</tr>
<tr>
<td>7</td>
<td>7.162641E-1</td>
<td>1.533E-4</td>
<td>7.163767E-1</td>
<td>1.526E-4</td>
</tr>
<tr>
<td>8</td>
<td>7.161802E-1</td>
<td>1.538E-4</td>
<td>7.161852E-1</td>
<td>1.500E-4</td>
</tr>
<tr>
<td>9</td>
<td>7.163624E-1</td>
<td>1.531E-4</td>
<td>7.163218E-1</td>
<td>1.511E-4</td>
</tr>
<tr>
<td>10</td>
<td>7.161230E-1</td>
<td>1.546E-4</td>
<td>7.160740E-1</td>
<td>1.508E-4</td>
</tr>
</tbody>
</table>
It is visibly apparent that the source has typical behavior indicative of a high DR problem.

At the very least, very strong fission source autocorrelation is observed as can be seen visually with the strong localized trending seen for both the standard and the E-CADIS results. This indicates that the source is strongly correlated with and without E-CADIS, and for this particular replication, the correlation appears very similar between the E-CADIS and standard algorithm. To see this further and rule out undersampling, the source fractions for the left and right source slabs are plotted in Figure 6-7 for replication 1 with E-CADIS.
Figure 6-7 shows that the lowest source fraction is roughly 30%, which is about 1500 particles, which should rule out undersampling. These findings indicate that any localized tally information from this simulation will have biased confidence estimates. A better solution procedure is needed for the high DR problems.

**ME-CADIS Test Problem Results**

Similarly to the E-CADIS technique, the ME-CADIS technique in 1Dcrit was optimized by testing several implementation options (including weight-window normalizations). This time a clear choice of the best path forward is not as obvious. The original intention of ME-CADIS was to provide a “source-detector” relationship as in the original CADIS methodology. The difficulty with this approach is that while the source detector relationship is made, much time may be spent on reducing variance in low probability transfers. In other words, variance is
reduced for less probable region to region transfers, yet these transfers contribute less than the most important transfers to the final $k_{eff}$ (and eigenvector).

This procedure may not be very effective in reducing $k_{eff}$ variance since the contribution is not a large percentage of the final result; however since they still contribute a significant amount to the final result, the overall accuracy of the simulation may be improved if the lower probability transfers are causing a bias as in a loosely coupled system.

Alternatively, one can proceed by trying to optimize run time utilizing a source biasing scheme whereby estimated response from a source region and energy group combination utilizing EQ. (5-23) sets the weight-window boundaries, thereby reducing the need to simulate particles which contribute minimally to the current objective. This then reduces the amount of sampling for the unimportant “source-detector” configurations, nullifying the original intent of decreasing variance for these configurations. All detailed testing of ME-CADIS presented here then utilizes a weight-window normalization scheme such that all source particles are normalized to start within the weight-window.

To begin the ME-CADIS testing, ten replications of test problem 1 were simulated for both the standard algorithm with no CADIS biasing and the selected ME-CADIS algorithm. Region-wise importance is obtained via PENTRAN and is shown in Figure 6-8. The same PENTRAN meshing, quadrature and cross section Legendre order are utilized as with E-CADIS, however recall multiple importance calculations are performed for each distinct source region.
From figure 6-8, it can be seen that region to region transfers are fairly improbable for all groups and that a transfer from group 3 region 2 to region 3 is most likely to occur. All replications were performed with 3000 particles per generation, 3350 generations with 350 skipped generations and a $k_{eff}$ guess of 1.0. Given in Table 6-4 are the $k_{eff}$ values for all replications. Additionally in Table 6-4 are the standard error and total average information with standard error.
Table 6-4. $k_{\text{eff}}$ Data for benchmark Problem 1 comparing ME-CADIS to the standard algorithm

<table>
<thead>
<tr>
<th>Replication</th>
<th>Standard Algorithm $k_{\text{eff}}$</th>
<th>Standard Algorithm Standard Error</th>
<th>ME-CADIS $k_{\text{eff}}$</th>
<th>ME-CADIS Standard Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.080380E-1</td>
<td>2.565E-4</td>
<td>8.082874E-1</td>
<td>2.739E-4</td>
</tr>
<tr>
<td>2</td>
<td>8.081437E-1</td>
<td>2.552E-4</td>
<td>8.082515E-1</td>
<td>2.690E-4</td>
</tr>
<tr>
<td>3</td>
<td>8.083118E-1</td>
<td>2.623E-4</td>
<td>8.081293E-1</td>
<td>2.748E-4</td>
</tr>
<tr>
<td>4</td>
<td>8.082848E-1</td>
<td>2.600E-4</td>
<td>8.085346E-1</td>
<td>2.752E-4</td>
</tr>
<tr>
<td>5</td>
<td>8.077993E-1</td>
<td>2.543E-4</td>
<td>8.081553E-1</td>
<td>2.703E-4</td>
</tr>
<tr>
<td>6</td>
<td>8.081518E-1</td>
<td>2.605E-4</td>
<td>8.082704E-1</td>
<td>2.614E-4</td>
</tr>
<tr>
<td>7</td>
<td>8.085063E-1</td>
<td>2.567E-4</td>
<td>8.080805E-1</td>
<td>2.724E-4</td>
</tr>
<tr>
<td>8</td>
<td>8.079978E-1</td>
<td>2.583E-4</td>
<td>8.077524E-1</td>
<td>2.778E-4</td>
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<tr>
<td>9</td>
<td>8.079605E-1</td>
<td>2.593E-4</td>
<td>8.081826E-1</td>
<td>2.747E-4</td>
</tr>
<tr>
<td>10</td>
<td>8.081535E-1</td>
<td>2.638E-4</td>
<td>8.079795E-1</td>
<td>2.707E-4</td>
</tr>
<tr>
<td>Average</td>
<td>8.081348E-1</td>
<td>8.181E-5</td>
<td>8.081624E-1</td>
<td>8.602E-5</td>
</tr>
</tbody>
</table>

Data in Table 6-4 show that results are within statistics. Average speedup was significantly negative (-4.5). Overall error achieved for $k_{\text{eff}}$ is comparable favoring the standard methodology meaning a slightly more precise calculation of the eigenvalue is obtained per particle simulated. This can be due to the fact that the particular weight-window normalization and window width chosen is not optimal for this problem. The chosen scheme should reduce variance in lower value (representing less probability) fission matrix elements, however. To investigate whether this implementation of ME-CADIS can be useful for more precise fission matrix element determination, the fission matrix elements are compared when using E-CADIS vs. ME-CADIS. Given in Table 6-5 are the final average fission matrix elements corresponding with each element of the 3 X 3 fission matrix determined from the 3 source region problem, and their associated relative error.

Table 6-5. Fission matrix elements and standard error for benchmark problem 1

<table>
<thead>
<tr>
<th>Type</th>
<th>$A_{11}$</th>
<th>$A_{12}$</th>
<th>$A_{13}$</th>
<th>$A_{21}$</th>
<th>$A_{22}$</th>
<th>$A_{23}$</th>
<th>$A_{31}$</th>
<th>$A_{32}$</th>
<th>$A_{33}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-CADIS</td>
<td>0.591</td>
<td>0.140</td>
<td>0.0154</td>
<td>0.14</td>
<td>0.589</td>
<td>0.142</td>
<td>0.0156</td>
<td>0.144</td>
<td>0.625</td>
</tr>
<tr>
<td>E-CADIS Rel. Error (%)</td>
<td>4.35</td>
<td>8.53</td>
<td>30.12</td>
<td>9.74</td>
<td>3.17</td>
<td>9.12</td>
<td>32.05</td>
<td>8.26</td>
<td>3.68</td>
</tr>
<tr>
<td>ME-CADIS</td>
<td>0.590</td>
<td>0.140</td>
<td>0.0154</td>
<td>0.141</td>
<td>.590</td>
<td>0.142</td>
<td>0.0157</td>
<td>0.144</td>
<td>0.625</td>
</tr>
<tr>
<td>ME-CADIS Rel. Error (%)</td>
<td>4.34</td>
<td>5.99</td>
<td>12.59</td>
<td>7.25</td>
<td>3.64</td>
<td>6.51</td>
<td>14.27</td>
<td>5.96</td>
<td>3.73</td>
</tr>
</tbody>
</table>
From Table 6-5, it can be seen that the standard deviation of the off diagonal (concerning the fission matrix) elements generated by the ME-CADIS algorithm are consistently lower than those generated by the E-CADIS algorithm. This shows that the fission matrix elements describing coupling between regions is calculated with less variance. This has little impact on the calculated eigenvalue yet may significantly impact the eigenvector accuracy. The same analysis was repeated for ten times less particles per generation, with the final results showing similar behavior. Lower probability transfers had greater than 90% relative error while for the ME-CADIS algorithm they were between 35% and 45%.

Ten replications of benchmark problem 2 were then simulated for both the standard algorithm with no CADIS biasing and the ME-CADIS algorithm. Region-wise importance obtained via PENTRAN is shown in Figure 6-9 on a log scale. PENTRAN quadrature, cross section Legendre order and mesh size are the same as with the E-CADIS replications.

![Figure 6-9. Benchmark problem 2 (2 source region) global importance to production (plotted at deterministic mesh center)](image)
From Figure 6-9, it is easy to see that coupling between regions is minimal. Given in Table 6-6 are the $k_{\text{eff}}$ values for all replications along with the standard error.

Table 6-6. $k_{\text{eff}}$ data for benchmark problem 2 comparing ME-CADIS to the standard algorithm

<table>
<thead>
<tr>
<th>Replication</th>
<th>Standard Algorithm $k_{\text{eff}}$</th>
<th>Standard Algorithm Standard Error</th>
<th>ME-CADIS $k_{\text{eff}}$</th>
<th>ME-CADIS Standard Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.165342E-1</td>
<td>1.543E-4</td>
<td>7.161984E-1</td>
<td>1.180E-4</td>
</tr>
<tr>
<td>2</td>
<td>7.163229E-1</td>
<td>1.507E-4</td>
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</tr>
<tr>
<td>3</td>
<td>7.162166E-1</td>
<td>1.507E-4</td>
<td>7.162365E-1</td>
<td>1.177E-4</td>
</tr>
<tr>
<td>4</td>
<td>7.161542E-1</td>
<td>1.517E-4</td>
<td>7.160200E-1</td>
<td>1.194E-4</td>
</tr>
<tr>
<td>5</td>
<td>7.159475E-1</td>
<td>1.571E-4</td>
<td>7.160991E-1</td>
<td>1.165E-4</td>
</tr>
<tr>
<td>6</td>
<td>7.165154E-1</td>
<td>1.546E-4</td>
<td>7.163848E-1</td>
<td>1.178E-4</td>
</tr>
<tr>
<td>7</td>
<td>7.162641E-1</td>
<td>1.533E-4</td>
<td>7.166461E-1</td>
<td>1.203E-4</td>
</tr>
<tr>
<td>8</td>
<td>7.161802E-1</td>
<td>1.538E-4</td>
<td>7.162801E-1</td>
<td>1.196E-4</td>
</tr>
<tr>
<td>9</td>
<td>7.163624E-1</td>
<td>1.531E-4</td>
<td>7.162927E-1</td>
<td>1.200E-4</td>
</tr>
<tr>
<td>10</td>
<td>7.161230E-1</td>
<td>1.546E-4</td>
<td>7.164100E-1</td>
<td>1.154E-4</td>
</tr>
</tbody>
</table>

Average speedup was significantly negative (-16.1). Overall error achieved for $k_{\text{eff}}$ for this set of replications favors the ME-CADIS methodology meaning a more precise calculation of the eigenvalue is obtained per particle via ME-CADIS, however each particle takes a significant time longer to simulate. Table 6-7 gives the fission matrix elements corresponding to a 2 X 2 fission matrix determined from the two source region problem.

Table 6-7. Fission matrix elements and standard error for benchmark problem 2

<table>
<thead>
<tr>
<th>Type</th>
<th>Fission Matrix Element ID</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$A_{11}$</td>
</tr>
<tr>
<td>E-CADIS</td>
<td>7.132E-01</td>
</tr>
<tr>
<td>E-CADIS Rel. Error</td>
<td>1.59%</td>
</tr>
<tr>
<td>ME-CADIS</td>
<td>7.126E-01</td>
</tr>
<tr>
<td>ME-CADIS Rel. Error</td>
<td>1.65%</td>
</tr>
</tbody>
</table>

While the ME-CADIS methodology may provide an increase in the accuracy of calculation of fission matrix elements, the effort required to achieve this gain may or may not be worthwhile, depending on the problem, and the goal of the simulation. Surely ME-CADIS does provide a mechanism for sampling less probable region to region transfers which may be important to obtain an unbiased solution for some problems.
Note that as in the E-CADIS technique, the ME-CADIS simulations also failed the KPSS diagnostic. Although the fission matrix elements were calculated with less variance, it seems that this was not enough to yield a converged source. Shown in Figure 6-10 is the fission matrix element $A_{12}$ for both E-CADIS and ME-CADIS.

![Figure 6-10](image)

Figure 6-10. Benchmark problem 2 fission matrix element $A_{12}$ for both E-CADIS and ME-CADIS

Figure 6-10 shows visually the reduction in the variance of the $A_{12}$ fission matrix element. Figure 6-10 also shows that while this problem has exhibited strong source correlation indicative of high DR problems, it appears that the fission matrix element $A_{12}$ does not appear correlated. An autocorrelation plot of the $A_{12}$ fission matrix element for the E-CADIS approach is given in Figure 6-11.
Figure 6-11 confirms that the $A_{12}$ fission matrix element for the E-CADIS approach is independent due to the very small lag 1 autocorrelation (as well as higher lags). Other fission matrix coefficients should also be investigated and will be studied in more detail in chapter 7. An autocorrelation plot of the $A_{12}$ fission matrix element for the ME-CADIS technique is given in Figure 6-12.
Similarly to the E-CADIS technique, Figure 6-12 confirms that the $A_{12}$ fission matrix element for the ME-CADIS approach is independent due to the very small lag 1 autocorrelation (as well as higher lags). A Shapiro-Wilk normality test indicates the data may not come from a normal distribution. This means that the fission matrix elements are independent but not normal.

Since the fission matrix elements are not correlated, it should be possible to utilize the fission matrix method to obtain reliable estimates to all derived parameters associated from the converged fission matrix eigenvector (source) for high DR problems. Chapter 7 investigates this finding in much more detail and utilizes it in conjunction with a recently proposed “fission matrix based Monte Carlo calculation” (FMBMC) (Dufek, 2009).
E-CADIS/ME-CADIS Final Remarks

Testing of different options (source biasing schemes with and without updated response normalization) was done for the same two benchmark problems. For benchmark problem 1 (3 source regions), ten replications were simulated for the standard algorithm and each of the different implemented ME-CADIS variations. The best performance in terms of speedup was between 2 and 3 times slower than the standard method. For test problem 2 (2 source regions), achieving nearly the same FOM as the standard calculation was obtained, but still lower. This is the reason for the chosen ME-CADIS weight-window implementation since the use of ME-CADIS for acceleration in the traditional sense is ineffective as discussed earlier. However, by applying ME-CADIS to normalize all starting particles to be within the weight-window for each source location/energy region to each detector location/energy region (effectively meaning each “source-detector” relationship), all transfers will be nearly as accurate as possible for the given configuration. This may allow a more precise and accurate simulation of fission matrix elements since those elements whose probability is lower yet still important will be determined much more accurately. The final result may be a more robust and reliable solution. If speedup is desired and a biased result is unlikely, then E-CADIS should be chosen, while if bias is a concern, ME-CADIS is the better choice.

While the ME-CADIS algorithm was chosen to obtain the best possible accuracy, normalizing the weight window to include all starting particles will result in weight windows with extremely low values when particles are starting in a low local importance region. More studies should be done to obtain a more efficient methodology which can still take into account the significant importance increase between source and detector location such as the use of a lower weight hard limit, or a moderate increase in starting weight window values. This will result in a less accurate result, yet the speed gain may prove extraordinary.
**Fission Matrix Biasing Method with E-CADIS/ME-CADIS**

In the essence of brevity, only some remarks are given for the combination of E-CADIS/ME-CADIS techniques with traditional fission matrix biasing. While the source variations were reduced significantly to the point of the source appearing much more random, stationarity and autocorrelation tests confirmed that the source is not converged, while bias was observed in the final $k_{eff}$ and source. Several variants of biasing were also attempted utilizing weighted percentages of the fission matrix eigenvector (source) with the standard Monte Carlo source, to no avail. Lastly, source correlation was reduced but not eliminated and it appears that utilizing the fission matrix acceleration methods as a source feedback mechanism alone is not adequate for solving high DR and other difficult source convergence problems, yet should be more thoroughly examined for other problems.
CHAPTER 7
DEVELOPMENT OF FMBMC FOR HIGH DOMINANCE RATIO PROBLEMS

Fission Matrix Based Monte Carlo Method

The benchmark problem 2 results in Chapter 6 indicated poor source convergence (at the very least high DR behavior). In high DR problems, the source distribution will be highly correlated with itself resulting in non-random source behavior. This chapter investigates a fission matrix based approach for high DR problems.

Recently, a complete fission matrix based Monte Carlo calculation was proposed (Dufek, 2007; Dufek, 2009; Dufek and Gudowski, 2009). In this approach, only the result of a final converged fission matrix over all generations is utilized to calculate all desired information. It is shown that the spatial dependence of the calculated fission matrix elements is only an artifact of discretization of the original eigenvalue equation.

In the limit of “very small” meshes, the source distribution should be irrelevant in the calculation of the fission matrix elements, in which case no skipped cycles are necessary and all particles can contribute to the final result. In fact, the traditional power method solution procedure isn’t required and particles can be sampled randomly throughout the phase space if desired. Practically speaking, however, the mesh size required may make this approach intractable. Instead, this chapter will investigate the use of an initialized source distribution and coarser meshing to the level of information desired, and apply this methodology to high DR problems. Since from Chapter 6, the fission matrix element autocorrelation appeared insignificant statistically speaking, coarser meshing may be adequate and the source dependence may be weak with fission matrix mesh size. This issue will be examined here.
Test Problems for High Dominance Ratio Problems

Three test problems are studied in this chapter. The first test problem is a simple monoenergetic single slab problem with vacuum boundaries and is in a slightly supercritical configuration. It was chosen since it has been studied before and it was determined to have a dominance ratio of ~0.991 (Urbatsch, 1995). The reference $k_{eff}$ for this problem was given as 1.02082. Geometry and material properties are shown in Figure 7-1.

![Figure 7-1. Geometry and material data for test problem 1](image)

\[ \Sigma_t = 1.0 \quad \Sigma_s = 0.7, \quad \nu \Sigma_t = 0.3071 \]
\[ \text{DR} \sim 0.991 \]

The second test problem is a simple infinitely long single fuel pincell. This problem is very similar in the physical sense to test problem 1 (1-D slab representation). A problem of this type was studied extensively recently due to the observation of odd source behavior typical of high DR problems as the simulated length of the pincell increases (Dumonteil and Courau, 2008; L’Abbate et al., 2007). Utilizing reflective boundaries on the ends of a pincell, if all source material is identical, a completely flat source distribution along the length of the fuel pin is expected.

Contrary to the expectation, however, as the simulated length (top and bottom boundaries) is increased, usual convergence behavior breaks down (Dumonteil and Courau, 2008; L’Abbate et al., 2007). The simulated model utilizes homogenized one-group cross sections with $\Sigma_t=1.13,$
The concept of the dominance ratio may not apply in this case due to the fact that there is only one solution and it is a flat source solution, meaning the DR does not exist. If one considers 1 group diffusion theory, however, a formulation for the DR can be obtained for a 1-D slab with vacuum boundaries. If the length of the slab approaches infinity, the DR tends to 1.0 asymptotically, regardless of the material properties (although the details of this asymptotic behavior do change), yet if reflective boundaries are applied, again the DR is not meaningful. This problem is analyzed due to the behavior observed only and its possible mitigation with FMBMC.

The third and last test problem for the FMBMC method is test problem 2 from Chapter 6. This problem has 3 energy groups and 3 geometric regions with the center region a moderating material, and two identical source regions on either side.

**Fission Matrix Based Monte Carlo Method (FMBMC) Solution Procedure**

As discussed earlier, the 1Dcrit code includes the fission matrix algorithm. The fission matrix is calculated every generation and a cumulative fission matrix is calculated. In addition to the fission matrix method, a source initialization option is available utilizing the converged flux from a converged PENTRAN eigenvalue solution. Deterministic importance is also optionally obtained for use with ME-CADIS/E-CADIS while utilizing the FMBMC implementation if desired. Processing codes were written to convert the PENTRAN eigenvalue calculation output to a source particle distribution for 1Dcrit to read as source input for the first generation and also to convert PENTRAN importance distributions to a format usable by 1Dcrit. These different options are illustrated in Figure 7-2.
The final results of the FMBMC method are obtained by numerically solving for the first eigenvalue and eigenvector corresponding to the final resulting fission matrix within 1Dcrit for the cumulative fission matrix utilizing the power method. The power method utilized in 1Dcrit may not be the most efficient, but was used for simplicity. The second eigenvalue and eigenvector are also calculated including an estimation of the DR for the discretized fission matrix. Note that the dominance ratio estimated for the discretized matrix will differ from the true DR of the problem. Figure 7-3 shows this procedure within the framework of 1Dcrit at the end of a source generation.
Confidence Estimation with FMBMC

Although it is easy to calculate the resulting $k_{eff}$ and source eigenvector from the final converged fission matrix, determination of the final confidence on these values is not as straightforward. The variance of each fission matrix element is stored in $1D_{crit}$; however, rigorous propagation of the error in the calculated eigenvalue and eigenvector of the numerical solver cannot currently be calculated (Dufek and Gudowski, 2009). Instead, the use of the plus and minus fission matrix was proposed as bounding values, where the plus fission matrix corresponds to adding the variance estimate to each fission matrix element for the entire fission matrix, and the same but subtracting for the minus fission matrix. The plus and minus fission matrix in equation form can be expressed by,
\((\mathbb{A})_{ij}^+ = (\mathbb{A})_{ij} + s_{\mathbb{A}_{ij}}, \quad (\mathbb{A})_{ij}^- = (\mathbb{A})_{ij} - s_{\mathbb{A}_{ij}} \ \forall \ i, j. \quad (7-1)\)

The resultant eigenvalues and eigenvectors for the plus and minus fission matrix then form a very conservative confidence bound. In “Fission Matrix Based Monte Carlo Calculations”, (Dufek and Gudowski, 2009), Dufek rigorously derives a formulation for the variance of the fission matrix elements. In this work, however, an estimate of the fission matrix element variance is obtained by tabulating the generation-to-generation sample variance for the cumulative fission matrix. Note this is only accurate if the fission matrix element distributions are independent.

Although a rigorously derived confidence bound cannot currently be obtained, an alternate confidence estimation procedure can be devised since the process itself can be simulated utilizing the sample mean and sample standard deviation of the fission matrix elements.

In this procedure, each fission matrix element is sampled utilizing the average and standard deviation of each element, assuming that the elements are independent and normally distributed. The resulting eigenvalue and eigenvector are calculated for the fission matrix generated from the sampling procedure. This procedure is repeated 10000 times. If the distribution being sampled is not very skewed, a Monte Carlo iterated confidence interval can be derived with the ends of the interval following a Beta Type I distribution (Buckland, 1984).

As a benchmark calculation, in an example where sampling was undertaken from a symmetric distribution with known mean and variance, approximate 1-\(\sigma\) and 2-\(\sigma\) confidence intervals were found to actually be 67.2\% to 69\% and 94.6\% to 95.4\% with 95\% probability for a random sample of 10000 trials. This procedure is utilized throughout the remainder of this dissertation and is referred to as the Monte Carlo iterated confidence interval.
FMBMC Test Problem Results

Test problem 1 analysis

Importance related to neutron production was calculated with PENTRAN for test problem 1. $P_3$ cross sections were utilized with $S_8$ level symmetric quadrature with a spatial discretization of 60 equally spaced meshes. The resulting importance to production is shown in Figure 7-4.

From Figure 7-4, it is apparent that the importance to production for this problem is very flat, except near the problem boundary. With this in mind, E-CADIS will most likely be ineffective at increasing speedup with nearly all particles being of the same importance. The FMBMC method was performed with E-CADIS for a 5 fission source region (12 cm source mesh) and 12 fission matrix region (5 cm source mesh) case. In total, ten replications of test problem 1 were simulated for the standard algorithm and E-CADIS concurrently with 1, 5 and 12
fission matrix source regions. Note that E-CADIS and FMBMC results are obtained within the same simulation, however E-CADIS weight-window meshing is dependent of the input mesh structure from the weight-window information obtained from PENTRAN and is independent of the fission matrix meshing. 50000 histories per generation were chosen for all simulations for the following reasons:

- simulation time per history is low
- avoid undersampling
- facilitate comparison with the known $k_{eff}$ (Urbatsch, 1995).

Additionally, a total of 350 skipped generations with 5350 total generations, a uniform randomly sampled source, and a $k_{eff}$ guess of 1.0 were chosen. $k_{eff}$ results are given in Table 7-1 for the standard algorithm and E-CADIS with 1 source region.

Table 7-1. $k_{eff}$ Comparison for FMBMC test problem 1 with the standard and E-CADIS algorithm with 1 source region

<table>
<thead>
<tr>
<th>Rep</th>
<th>Std. Alg. $k_{eff}$</th>
<th>Std. Alg. Std. Error</th>
<th>E-CADIS $k_{eff}$</th>
<th>E-CADIS Std. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0207053</td>
<td>2.75E-5</td>
<td>1.0206392</td>
<td>3.36E-5</td>
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<td>2.69E-5</td>
<td>1.0206894</td>
<td>3.33E-5</td>
</tr>
<tr>
<td>9</td>
<td>1.0207144</td>
<td>2.72E-5</td>
<td>1.0206841</td>
<td>3.35E-5</td>
</tr>
<tr>
<td>10</td>
<td>1.0207258</td>
<td>2.69E-5</td>
<td>1.0206472</td>
<td>3.32E-5</td>
</tr>
</tbody>
</table>

*1 region E-CADIS

Data in table 7-1 show that the standard algorithm and E-CADIS (1 source region) are consistent. Table 7-2 gives $k_{eff}$ results for E-CADIS with 1 source region, E-CADIS with 5 source regions and E-CADIS with 12 source regions.
Data in table 7-2 shows that different E-CADIS results with differing numbers of fission matrix regions are indeed comparable as expected. The error value indicates similar performance in which case FOM analysis will be a better indicator of performance. Table 7-3 gives \( k_{\text{eff}} \) results for E-CADIS with 5 source regions and the FMBMC method with 5 source regions for both the conservative and Monte Carlo based confidence intervals.

<table>
<thead>
<tr>
<th>Rep</th>
<th>E-CADIS ( k_{\text{eff}} ) 5 reg</th>
<th>E-CADIS ( k_{\text{eff}} ) 5 reg</th>
<th>FMBMC ( k_{\text{eff}} ) (5 reg)</th>
<th>5 reg err (+, cons)</th>
<th>5 reg err (-, cons)</th>
<th>5 reg err (+, MC)</th>
<th>5 reg err (-, MC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0206392 3.36E-5</td>
<td>1.0207330 3.28E-5</td>
<td>1.0207007 3.35E-5</td>
<td>1.3379E-4</td>
<td>1.3463E-4</td>
<td>4.012E-5</td>
<td>4.021E-5</td>
</tr>
<tr>
<td>7</td>
<td>1.0206784 3.35E-5</td>
<td>1.0207022 3.36E-5</td>
<td>1.0206937 3.34E-5</td>
<td>1.3437E-4</td>
<td>3.992E-5</td>
<td>4.034E-5</td>
<td>4.034E-5</td>
</tr>
</tbody>
</table>

Data in Table 7-3 shows that the \( k_{\text{eff}} \)'s resulting from the FMBMC method are in fact consistent with the E-CADIS results (the standard methodology as well). More interesting,
however, is the magnitude of the resulting confidence intervals with the FMBMC method for both the conservative and Monte Carlo based confidence intervals. Clearly the Monte Carlo based interval is far superior. Table 7-4 gives $k_{eff}$ results for E-CADIS with 12 source regions and the FMBMC method with 12 source regions for both the conservative and Monte Carlo based confidence intervals.

Table 7-4. $k_{eff}$ comparison for FMBMC test problem 1 with the E-CADIS algorithm (12 fission matrix regions) and the FMBMC algorithm with 12 fission matrix regions (conservative and MC confidence intervals)

<table>
<thead>
<tr>
<th>Rep</th>
<th>E-CADIS $k_{eff}$</th>
<th>E-CADIS Std. Error</th>
<th>FMBMC $k_{eff}$ (5 reg)</th>
<th>12 reg err (+, cons)</th>
<th>12 reg err (-,cons)</th>
<th>12 reg err (+, MC)</th>
<th>12 reg err (-,MC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0207007</td>
<td>3.35E-5</td>
<td>1.0207133</td>
<td>2.4131E-4</td>
<td>2.4141E-4</td>
<td>4.257E-5</td>
<td>4.246E-5</td>
</tr>
<tr>
<td>2</td>
<td>1.0207600</td>
<td>3.39E-5</td>
<td>1.0207519</td>
<td>2.4227E-4</td>
<td>2.4236E-4</td>
<td>4.250E-5</td>
<td>4.303E-5</td>
</tr>
<tr>
<td>3</td>
<td>1.0206580</td>
<td>3.43E-5</td>
<td>1.0206534</td>
<td>2.4232E-4</td>
<td>2.4241E-4</td>
<td>4.299E-5</td>
<td>4.282E-5</td>
</tr>
<tr>
<td>4</td>
<td>1.0206943</td>
<td>3.38E-5</td>
<td>1.0206976</td>
<td>2.4270E-4</td>
<td>2.4279E-4</td>
<td>4.262E-5</td>
<td>4.341E-5</td>
</tr>
<tr>
<td>7</td>
<td>1.0206937</td>
<td>3.34E-5</td>
<td>1.0206955</td>
<td>2.4193E-4</td>
<td>2.4201E-4</td>
<td>4.316E-5</td>
<td>4.306E-5</td>
</tr>
<tr>
<td>8</td>
<td>1.0206899</td>
<td>3.42E-5</td>
<td>1.0207061</td>
<td>2.4124E-4</td>
<td>2.4133E-4</td>
<td>4.213E-5</td>
<td>4.338E-5</td>
</tr>
<tr>
<td>9</td>
<td>1.0207499</td>
<td>3.30E-5</td>
<td>1.0207564</td>
<td>2.4099E-4</td>
<td>2.4107E-4</td>
<td>4.226E-5</td>
<td>4.311E-5</td>
</tr>
<tr>
<td>10</td>
<td>1.0206978</td>
<td>3.44E-5</td>
<td>1.0207105</td>
<td>2.4227E-4</td>
<td>2.4236E-4</td>
<td>4.186E-5</td>
<td>4.248E-5</td>
</tr>
</tbody>
</table>

*12 region E-CADIS

Data in Table 7-4 shows that the $k_{eff}$’s resulting from the FMBMC method are again consistent with the E-CADIS results (the standard methodology as well). Again the Monte Carlo generated confidence interval is far superior to the conservative; however the increase from 5 to 12 source regions did have an impact on the interval width (increased). Also, note that the $k_{eff}$ results obtained from both PENTRAN and 1Dcrit were consistent, yet slightly lower than the 1.02082 reference value. PENTRAN results yielded a $k_{eff}$ of 1.020691, more consistent with the results shown in this work.

If the standard and FMBMC method are comparable in eigenvalue determination, the motivation to utilize the FMBMC must come from elsewhere. Table 7-5 gives the final average results for speedup analysis for FMBMC test problem 1. To calculate speedup for FMBMC, the
error interval is divided by two and utilized as the relative error in equation (2-57). All speedup is calculated relative to the completely separate code without E-CADIS. Note that the standard algorithm may be biased.

Table 7-5. Speedup (relative to the standard algorithm) for FMBMC test problem 1 with the E-CADIS and FMBMC algorithm with 1, 5 and 12 fission matrix regions

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>1 region</th>
<th>5 region</th>
<th>12 region</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-CADIS</td>
<td>0.48</td>
<td>0.40</td>
<td>0.34</td>
</tr>
<tr>
<td>FMBMC (Cons.)</td>
<td>0*</td>
<td>0.025</td>
<td>0.008</td>
</tr>
<tr>
<td>FMBMC (MC)</td>
<td>0*</td>
<td>0.27</td>
<td>0.21</td>
</tr>
</tbody>
</table>

*Not Determined for 1 source region

Data in Table 7-5 demonstrates several things. First, if accurate, the standard algorithm is more effective for this problem than when E-CADIS with FMBMC is utilized. This is not unexpected due to the almost constant importance and any overhead associated with the E-CADIS algorithm will become evident as the time is wasted, yet 0.48 seems to be too low. Investigating the cause of this difference in speedup resulted in two findings. First, particle information bank variables were allocated to values unnecessarily large and their use within the framework of 1Dcrit caused unnecessary calculation. Second, weight window width is slightly different than in the standard algorithm causing some differences. Improving the memory management and adjusting the weight window values for this problem result in speedup between 0.9 and 1.0, which is more sensible given there will still be expected overhead due to weight window location searches being performed at each collision. Note that all the results in this dissertation are with the unimproved memory management.

Continuing analysis of data in Table 7-5, the Monte-Carlo based confidence interval is significantly more efficient than the conservative plus and minus fission matrix based interval. Comparing the relative speedup of the Monte-Carlo based confidence interval with the E-CADIS
results give a ratio of about 0.6 to 0.7. Table 7-6 gives the final average results for speedup analysis for FMBMC test problem 1.

Table 7-6. Source convergence diagnostic results for FMBMC test problem 1 with the E-CADIS and FMBMC algorithm with 1, 5 and 12 fission matrix regions

<table>
<thead>
<tr>
<th>Src. Conv. Diag.</th>
<th>1 region</th>
<th>5 region</th>
<th>12 region</th>
</tr>
</thead>
<tbody>
<tr>
<td>KPSS (Fail)</td>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>Entropy Test 1 (Fail)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Entropy Test 2 (Fail)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Entropy Test 3 (Fail)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Data from Table 7-6 indicates, through the KPSS diagnostic, that the source has not converged. To show the source behavior and poor convergence of this problem, COM behavior is shown in Figure 7-5 for replication 5 (chosen at random) with E-CADIS with 5 fission matrix regions.

Figure 7-5. Replication 5 FMBMC COM behavior
Figure 7-5 clearly shows the source is not behaving as a typical converged stochastic source. To investigate the FMBMC effectiveness, the mesh based source fraction convergence obtained for the same replication (12 cm meshes) is shown in Figure 7-6 for the first source mesh.

![Figure 7-6. FMBMC test problem two replication one source mesh one convergence](image)

From Figure 7-6 it can be seen that although there is significant initial variation, the source fractions begin to converge relatively quickly. Note that until the skipped generations are finished, the cumulative fission matrix is not utilized, which results in more random behavior at the beginning of the simulation. A zoomed view of source region 3 is also shown in Figure 7-6 for the second half of the simulation, for clarity. From generation 3500 to the simulation end, a maximum total change of 0.05% is observed. The final converged fission matrix source fractions for all replications are given in Table 7-7.
Table 7-7. FMBMC test problem 1 FMBC final converged source fractions for the 5 source region case

<table>
<thead>
<tr>
<th>Replication</th>
<th>Mesh 1</th>
<th>Mesh 2</th>
<th>Mesh 3</th>
<th>Mesh 4</th>
<th>Mesh 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1020</td>
<td>0.2484</td>
<td>0.3038</td>
<td>0.2459</td>
<td>0.0998</td>
</tr>
<tr>
<td>2</td>
<td>0.1038</td>
<td>0.2502</td>
<td>0.3018</td>
<td>0.2441</td>
<td>0.1001</td>
</tr>
<tr>
<td>3</td>
<td>0.1037</td>
<td>0.2503</td>
<td>0.3032</td>
<td>0.2438</td>
<td>0.0991</td>
</tr>
<tr>
<td>4</td>
<td>0.1007</td>
<td>0.2456</td>
<td>0.3031</td>
<td>0.2486</td>
<td>0.1020</td>
</tr>
<tr>
<td>5</td>
<td>0.1035</td>
<td>0.2495</td>
<td>0.3022</td>
<td>0.2446</td>
<td>0.1001</td>
</tr>
<tr>
<td>6</td>
<td>0.1026</td>
<td>0.2490</td>
<td>0.3025</td>
<td>0.2450</td>
<td>0.1009</td>
</tr>
<tr>
<td>7</td>
<td>0.1031</td>
<td>0.2492</td>
<td>0.3023</td>
<td>0.2449</td>
<td>0.1006</td>
</tr>
<tr>
<td>8</td>
<td>0.1003</td>
<td>0.2459</td>
<td>0.3036</td>
<td>0.2482</td>
<td>0.1021</td>
</tr>
<tr>
<td>9</td>
<td>0.1011</td>
<td>0.2462</td>
<td>0.3024</td>
<td>0.2486</td>
<td>0.1019</td>
</tr>
<tr>
<td>10</td>
<td>0.1001</td>
<td>0.2453</td>
<td>0.3030</td>
<td>0.2492</td>
<td>0.1023</td>
</tr>
</tbody>
</table>

Data in Table 7-7 shows the consistency to which the FMBMC final converged source fractions are obtained. Maximum variations are on the order of 0.5% for any source mesh.

Final combined source fractions with combined standard deviation over the replications is given in Table 7-8

Table 7-8. FMBMC test problem 1 combined converged sources with associated combined standard deviation

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0209E-1</td>
<td>7.26E-5</td>
<td>1.02270E-1</td>
<td>3.32E-05</td>
</tr>
<tr>
<td>2</td>
<td>2.47953E-1</td>
<td>1.03E-4</td>
<td>2.48083E-1</td>
<td>4.79E-05</td>
</tr>
<tr>
<td>3</td>
<td>3.02792E-1</td>
<td>5.94E-5</td>
<td>3.02654E-1</td>
<td>3.68E-05</td>
</tr>
<tr>
<td>4</td>
<td>2.46275E-1</td>
<td>1.03E-4</td>
<td>2.46114E-1</td>
<td>4.77E-05</td>
</tr>
<tr>
<td>5</td>
<td>1.00890E-1</td>
<td>7.29E-5</td>
<td>1.00880E-1</td>
<td>3.34E-05</td>
</tr>
</tbody>
</table>

Table 7-8 shows that while the source is calculated with high precision, the symmetric values are not within statistics. This indicates that the standard method and the FMBMC method are biased, indicating that most likely the fission matrix elements are correlated with this mesh structure. Table 7-9 shows a comparison of meshes 1 and 3 for the final converged source for the standard algorithm (avg source in mesh) and FMBMC.
Data in Table 7-9 indicates that for this problem, the final converged sources for 5 cm meshes are similar for both the standard and FMBMC methods. This may lead one to believe that the mesh based source may be acceptable utilizing the standard method. While this may be true, a confidence estimate on the source fractions should not be reliable with the standard method due to source autocorrelation or with the FMBMC method if fission matrix elements are not independent. Data for the 12 mesh case (5 cm meshes) source fractions are presented in Table 7-10 for cases with source meshes 1, 6 and 12.

<table>
<thead>
<tr>
<th>Replication</th>
<th>Standard</th>
<th>FMBMC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mesh 1</td>
<td>Mesh 6</td>
</tr>
<tr>
<td>1</td>
<td>0.0206</td>
<td>0.0513</td>
</tr>
<tr>
<td>2</td>
<td>0.0208</td>
<td>0.0521</td>
</tr>
<tr>
<td>3</td>
<td>0.0209</td>
<td>0.0525</td>
</tr>
<tr>
<td>4</td>
<td>0.0211</td>
<td>0.0527</td>
</tr>
<tr>
<td>5</td>
<td>0.0209</td>
<td>0.0523</td>
</tr>
<tr>
<td>6</td>
<td>0.0208</td>
<td>0.0522</td>
</tr>
<tr>
<td>7</td>
<td>0.0203</td>
<td>0.0508</td>
</tr>
<tr>
<td>8</td>
<td>0.0208</td>
<td>0.0521</td>
</tr>
<tr>
<td>9</td>
<td>0.0201</td>
<td>0.0505</td>
</tr>
<tr>
<td>10</td>
<td>0.0211</td>
<td>0.0526</td>
</tr>
</tbody>
</table>
Data in Table 7-10 suggests that for all cases of source meshes, the standard methodology source fractions and FMBMC source fractions appear fairly consistent with each other. Looking back at Figure 7-5, it can be seen that although the source oscillates with significant trending for all cases, the overall magnitude is only moderately large and for the replication shown, much of the variation averages out over the replication. While this is true, autocorrelation in the source should have an effect on the standard deviation accuracy for confidence estimates.

Since the E-CADIS and FMBMC results are obtained utilizing the same simulation, the source distributions obtained between these results are now analyzed for the following cases shown in Table 7.11. The E-CADIS methodology in these cases represents the accuracy of the “standard” methodology since it has already been shown that fission matrix element variation can be reduced with E-CADIS, however the source distribution itself comparing to the standard method is similar.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>5</td>
<td>350</td>
<td>50k</td>
<td>5350</td>
</tr>
<tr>
<td>11-20</td>
<td>12</td>
<td>350</td>
<td>50k</td>
<td>5350</td>
</tr>
<tr>
<td>21-30</td>
<td>12</td>
<td>350</td>
<td>100k</td>
<td>5350</td>
</tr>
<tr>
<td>31-40</td>
<td>24</td>
<td>350</td>
<td>100k</td>
<td>5350</td>
</tr>
<tr>
<td>41-50</td>
<td>24</td>
<td>350</td>
<td>100k</td>
<td>20350</td>
</tr>
</tbody>
</table>

Although the purpose of this methodology is to provide accurate localized data, $k_{eff}$ is shown for comparison for all cases in Figure 7-7. Note that several of these cases are the same replications already analyzed.
Figure 7-7 shows that the $k_{\text{eff}}$ values are fairly consistent. At one $\sigma$, both the E-CADIS method and the FMBMC method yield similar results, yet the error bars for the FMBMC method are slightly wider. This could be in part due to the effect of the high dominance ratio and some small correlation in $k_{\text{eff}}$ may be present biasing the standard $k_{\text{eff}}$ confidence. To continue the analysis where the source is concerned, the source distributions for cases 1, 11, and 31 are shown in Figure 7-8.
Figure 7-8 shows visually that the results appear symmetric and therefore some measure of accuracy is expected. Other replications yield similar results.

Contrasting this result, however, is the fact that the KPSS source convergence diagnostic indicates possible source convergence difficulty in 44 of the 50 replications. Recall also the source behavior seen in Figure 7-5, which is representative of all cases. In order to observe the impact of the source behavior on the tallied results, source mesh 1 is plotted for both the E-CADIS and FMBMC method for all cases. Cases 1 through 10 are shown in Figure 7-9.
Cases 1-10 represent the coarsest source meshing with 12 cm source meshes. Figure 7-9 shows that the final obtained source fraction from mesh 1 for the ten replications are inconsistent even for 2 sigma (\(\sigma\)). While the overall variation in the data is small, the calculated uncertainty for both the E-CADIS and FMBMC method are completely erroneous. Note that without such detailed analysis, current methodologies would not indicate that any problem exists, and with the small uncertainties obtained, it would be easy to improperly accept the solution as accurately converged. Cases 11-20 are shown in Figure 7-10.
Cases 11-20 represent an increase of 5 to 12 source meshes compared to cases 1-10. Figure 7-10 shows that the final obtained source fraction from mesh 1 for the ten cases are again inconsistent for several cases even at $2\sigma$. There appears to be an improvement in the calculation of the uncertainty with the FMBMC methodology as can be seen by the wider intervals obtained. Cases 21-30 are shown in Figure 7-11.
Cases 21-30 represent an increase of particle per generation compared to cases 11-20.

Figure 7-11 shows that the final obtained source fraction from mesh 1 for the ten replications are again inconsistent for the E-CADIS method, yet consistency has improved even more for the FMBMC results, yet results still appear inconsistent at 1 $\sigma$. It appears that the changing source meshing is having a significant impact, however, on the FMBMC final results. Cases 31-40 are shown in Figure 7-12.
Figure 7-12. Mesh 1 source fraction for cases 31-40

Cases 31-40 represent an increase in the number of fission matrix meshes to 24. Figure 7-12 shows that the final obtained source fraction from mesh 1 for the ten replications are again inconsistent for the E-CADIS method, yet the FMBMC results now appear acceptable. This is a very significant finding. To reduce the size of the error bars for the FMBMC results further, cases 41-50 are shown in Figure 7-13 for an increased total active generations from 5000 to 20000.
Figure 7-13 shows that the final obtained source fraction from mesh 1 for the ten replications are still inconsistent for the standard method. The FMBMC results still appear acceptable for all of the FMBMC cases, however, as was seen in 7-12. Again, this is a very significant finding. Since independence of the fission matrix elements is required in order to accurately calculate the eigenvalue and eigenvector, the autocorrelation element of the $A_{12}$ element is shown for case 1, 11, 21, 31 and 41 in Figure 7-14.
Figure 7-14 illustrates the effect of source discretization and density on the $A_{12}$ fission matrix element. Elements one off of the diagonal often have the highest correlation, which is why this element was chosen for illustration. As mesh size is decreased, the correlation is reduced. Note that for case 11 and 21, the same size fission matrix is utilized with different particles per generation, yet the fission matrix autocorrelation is not changed significantly. Cases 31 and 41 indicate that increasing the number of generations has little effect on the autocorrelation.

Recall that in order to form accurate confidence intervals the elements need to be uncorrelated, and their average values must be able to be represented by a normal distribution. With such large sample sizes, however, normality tests are often unreliable as they identify insignificant deviations from the normal distribution. This is because with a large sample size,
normality tests have enough data at hand to identify very small deviations from normality. Even if the element being sampled is drawn from a normal distribution, the sample itself may at times appear slightly non-normal.

Fortunately, for large sample sizes, so long as the fission matrix correlation is small, the CLT should apply and the fission matrix elements average values should tend toward a normal distribution and be accurately quantified. A Shapiro-Wilk Normality test was utilized, however, for each element, and is even more informative for smaller sample sizes.

Using the final converged fission matrix, it is possible to estimate the fraction of the final $k_{\text{eff}}$ obtained from non-independent fission matrix elements (at a chosen significance). If the lag 1 autocorrelation is too high (as compared to a standard normal curve with the same mean and standard deviation), the element is considered correlated and its’ contribution to the final $k_{\text{eff}}$ is estimated by $A_{i,j} \times S$ ($S$—fractional source). A similar contribution from non-normal fission matrix elements can be calculated (at a chosen significance) utilizing the Shapiro-Wilk (or another) normality test.

For case 1, it was determined that all of the fission matrix elements but one were not independent. This corresponded to an approximate 100% contribution from correlated elements. Similarly the $k_{\text{eff}}$ for non-normal meshes was determined to be ~13%. Note that if the fission matrix element series is correlated, the normality test for that mesh is not valid. Comparatively, for case 41, the approximate non-independent percentage was 17% while the non-normal percentage was 26%.

**Test problem 2 analysis**

Ten replications of test problem 2 were simulated. A total of 350 skipped generations with 5350 total generations, a uniform random source, and a $k_{\text{eff}}$ guess of 1.0 were chosen. For test problem two, the E-CADIS algorithm was utilized with constant importance (as in the standard
methodology, where all particles are of equal importance). Both the 10 cm and 100 cm reflected pincell were initially simulated with 5 source zones (meshes, 2 cm and 20 cm respectively).

Figure 7-15. FMBMC test problem 2 $k_{\text{eff}}$ summary (5 source meshes)

Figure 7-15 shows results of $k_{\text{eff}}$ for all cases across the 10 replications. Error bars are purposely omitted since their inclusion inhibits the ability to distinguish between simulations. Standard error is between approximately 4e-5 and 6e-5 for all simulations except for the conservative FMBMC intervals which are much wider (standard error~2.6e-4). From Figure 7-15 it is observed that all $k_{\text{eff}}$ values appear relatively consistent as most would be within one standard deviation, and all within two standard deviations. As in FMBMC problem 1, no indication of high DR behavior is observed with $k_{\text{eff}}$ analysis alone. Note that for the E-CADIS/FMBMC final resulting $k_{\text{eff}}$ values (10 cm and 100 cm) for the same replication, the FMBMC method appears slightly higher (<1e-5) on average.
Table 7-12 gives the final average results for speedup analysis for the FMBMC test problem two, along with KPSS and entropy source convergence information. Speedup for the FMBMC cases are calculated as before relative to the standard methodology.

Table 7-12. Speedup data for FMBMC test problem 2 with the E-CADIS and FMBMC algorithm (10 cm and 100 cm model length)

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>10 cm</th>
<th>100 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-CADIS</td>
<td>0.59</td>
<td>.57</td>
</tr>
<tr>
<td>FMBMC (Cons.)</td>
<td>0.024</td>
<td>0.041</td>
</tr>
<tr>
<td>FMBMC (MC)</td>
<td>0.44</td>
<td>0.43</td>
</tr>
</tbody>
</table>

* all speedup is relative to the 10 cm standard case

Data from Table 7-12 indicates that the differences between the 10 cm and 100 cm cases concerning speedup are marginal if not inconsequential, with the exception of the conservative confidence interval case, which is much lower. Table 7-12 also shows that the standard method is superior to the E-CADIS method modified to mimic the standard method. To investigate this source of discrepancy, the fission matrix was turned off and the same simulations performed with only E-CADIS. Similar speedup was obtained indicating that the algorithm is not as efficient without importance data and the FMBMC method provides minimal impact. There is no limitation on the FMBMC being included into the standard algorithm in which case this loss in efficiency would be avoided. Table 7-13 gives the final average results for speedup analysis for the FMBMC test problem two.

Table 7-13. Source convergence diagnostic results for FMBMC test problem 2 with the E-CADIS and FMBMC algorithm (10 cm and 100 cm model length)

<table>
<thead>
<tr>
<th>Src. Conv. Diag.</th>
<th>10 cm</th>
<th>100 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>KPSS (Fail)</td>
<td>2</td>
<td>10</td>
</tr>
<tr>
<td>Entropy Test 1 (Fail)</td>
<td>Not valid</td>
<td>Not valid</td>
</tr>
<tr>
<td>Entropy Test 2 (Fail)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Entropy Test 3 (Fail)</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
KPSS failures in Table 7-12 for the 100 cm replications show that the simulated physics may be in a different regime than that of the 10 cm replications. A COM plot for replication 1 for both the 10 cm and 100 cm case is shown in Figure 7-16 with the 10 cm COM renormalized by multiplying by a factor of 10 to show both data series on the same figure.

![Figure 7-16. FMBMC benchmark problem 2 replication 1 COM for the 10 cm (renormalized for plot) and 100 cm cases](image)

Figure 7-16 shows that the 10 cm replication COM behaves more randomly than the 100 cm replication. This should be evident since during the course of the simulation, the source migrates more to the upper half of the fuel rod, and often significantly so, final source fractions obtained from the standard methodology will be biased. While mathematically the DR may not have true meaning for this problem, it is the simulated length that appears to be related to the
source convergence behavior. To investigate the FMBMC effectiveness, the mesh based source fraction for replication 1, mesh 1 of the 100 cm pincell is shown in Figure 7-17.

Figure 7-17 shows that the mesh 1 FMBMC source fraction appears not yet converged. In fact, it appears that the fission matrix element dependence on the source may be stronger than is acceptable for an accurate determination by the FMBMC for this mesh size and the analysis of correlation of fission matrix elements should shed some light on the overall source behavior and will be investigated. The final converged fission matrix source fractions for all replications are given in Table 7-14.
Table 7-14. FMBMC test problem 2 final converged source fraction for source mesh 1, 3 and 5 for both the 10 cm and 100 cm pincells

<table>
<thead>
<tr>
<th>Replication</th>
<th>10 cm</th>
<th>100 cm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mesh 1</td>
<td>Mesh 3</td>
</tr>
<tr>
<td>1</td>
<td>0.2000</td>
<td>0.2001</td>
</tr>
<tr>
<td>2</td>
<td>0.2001</td>
<td>0.2001</td>
</tr>
<tr>
<td>3</td>
<td>0.1999</td>
<td>0.1999</td>
</tr>
<tr>
<td>4</td>
<td>0.2001</td>
<td>0.2000</td>
</tr>
<tr>
<td>5</td>
<td>0.1999</td>
<td>0.2000</td>
</tr>
<tr>
<td>6</td>
<td>0.2001</td>
<td>0.2000</td>
</tr>
<tr>
<td>7</td>
<td>0.2001</td>
<td>0.2001</td>
</tr>
<tr>
<td>8</td>
<td>0.2001</td>
<td>0.2000</td>
</tr>
<tr>
<td>9</td>
<td>0.2001</td>
<td>0.2001</td>
</tr>
<tr>
<td>10</td>
<td>0.1999</td>
<td>0.1999</td>
</tr>
</tbody>
</table>

Data from Table 7-14 indicates that the 10 cm FMBMC case is well converged to the expected 20% source per source mesh. The 100 cm FMBMC case while not as well converged, fluctuates around the true average. Longer simulation time should tighten convergence without any biasing if the fission matrix elements are not correlated. A comparison of the final converged source for meshes 1, 3 and 5 for the standard algorithm and the FMBMC source for the 100 cm pincell is given in Table 7-15.

Table 7-15. FMBMC test problem 2 final converged source fraction comparison for source mesh 1, 3 and 5 for the standard algorithm and FMBMC (5 total source meshes) for the 100 cm pincell

<table>
<thead>
<tr>
<th>Replication</th>
<th>Standard</th>
<th>FMBMC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mesh 1</td>
<td>Mesh 3</td>
</tr>
<tr>
<td>1</td>
<td>0.1647</td>
<td>0.1772</td>
</tr>
<tr>
<td>2</td>
<td>0.1938</td>
<td>0.1946</td>
</tr>
<tr>
<td>3</td>
<td>0.2196</td>
<td>0.2096</td>
</tr>
<tr>
<td>4</td>
<td>0.2201</td>
<td>0.2190</td>
</tr>
<tr>
<td>5</td>
<td>0.1838</td>
<td>0.1948</td>
</tr>
<tr>
<td>6</td>
<td>0.1933</td>
<td>0.1923</td>
</tr>
<tr>
<td>7</td>
<td>0.1857</td>
<td>0.1915</td>
</tr>
<tr>
<td>8</td>
<td>0.1994</td>
<td>0.1979</td>
</tr>
<tr>
<td>9</td>
<td>0.2080</td>
<td>0.2014</td>
</tr>
<tr>
<td>10</td>
<td>0.1959</td>
<td>0.1998</td>
</tr>
</tbody>
</table>

Data in Table 7-15 indicates similar behavior for final converged source fractions for both the standard method and FMBMC. Neither the FMBMC nor the standard methodology should
be considered converged. Figures 7-16 and 7-17 confirm this as the source for the standard methodology is fluctuating wildly, while for the FMBMC source appears somewhat unstable.

To investigate dependency in the fission matrix source, an autocorrelation plot for fission matrix element $A_{12}$ is shown in Figure 7-18.

![Autocorrelation plot](image)

Figure 7-18. FMBMC test problem 2 replication 1 $A_{12}$ fission matrix element autocorrelation plot

Figure 7-18 shows that the $A_{12}$ fission matrix element autocorrelation for this case is moderately high at lag 1 and decreases slowly with increasing lag. In order to investigate the cause of the correlation, which is present in varying degrees in other matrix elements as well, the effect of source meshing and particle population per generation was investigated. Table 7-16 gives the different subcases investigated, delineated by input.
Table 7-16. FMBMC test problem 2 subcase input parameters (E-CADIS no importance)

<table>
<thead>
<tr>
<th>Subcase</th>
<th>Fission Matrix Meshes</th>
<th>Replications</th>
<th>Skipped Generations</th>
<th>Histories per Generation</th>
<th>Total Generations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1*</td>
<td>5</td>
<td>10</td>
<td>350</td>
<td>50000</td>
<td>5350</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>1</td>
<td>350</td>
<td>500000</td>
<td>5350</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
<td>10</td>
<td>350</td>
<td>500000</td>
<td>5350</td>
</tr>
<tr>
<td>4</td>
<td>20</td>
<td>1</td>
<td>350</td>
<td>500000</td>
<td>5350</td>
</tr>
<tr>
<td>5</td>
<td>50</td>
<td>1</td>
<td>350</td>
<td>50000</td>
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<tr>
<td>6</td>
<td>50</td>
<td>1</td>
<td>350</td>
<td>500000</td>
<td>5350</td>
</tr>
<tr>
<td>7</td>
<td>100</td>
<td>1</td>
<td>350</td>
<td>500000</td>
<td>5350</td>
</tr>
<tr>
<td>8</td>
<td>100</td>
<td>1</td>
<td>350</td>
<td>500000</td>
<td>5350</td>
</tr>
</tbody>
</table>

*This subcase is the original case replications.

In subcase 2, an increase of particles per generation by a factor of 10 was utilized. This was done since in the 100 cm case, the pincell is 10 times larger by volume and the source density should be equivalent to the original 10 cm subcase. Final source fractions for subcase 2, replication 1 with no biasing (the standard method was not run since the E-CADIS method without biasing behaves the same as the standard method concerning source convergence) corresponding to source meshes 1 through 5 were 0.1996, 0.1994, 0.2005, 0.2013 and 0.1994. The corresponding results for the FMBMC method were 0.1996, 0.1996, 0.2008, 0.2011 and 0.1989. By simply comparing this data with the expected result, both methods appear much better converged. A COM plot of subcase 2 is shown in Figure 7-19. Additionally, to look at the cumulative behavior of the FMBMC source, the FMBMC mesh based source fraction for subcase 1, mesh 1 is shown in Figure 7-20.
Figure 7-19. FMBMC test problem 2 standard algorithm COM for subcase 2, replication 1

Figure 7-20. FMBMC test problem 2 subcase 2 replication 1 mesh 1 source fraction evolution
While it appears that an increase in particles per generation did dampen the level of fluctuation, more so for the FMBMC methodology than the standard methodology, correlation is still evident in the COM shown in figure 7-19. Figure 7-20 shows that the mesh 1 FMBMC based source fraction over time accuracy increases slowly with total simulated particles, yet still appears somewhat erratic. More generations may be necessary to see long term fluctuations if present. To investigate autocorrelation in the FMBMC method for subcase 2, an autocorrelation plot of fission matrix element $A_{12}$ is shown in figure 7-21.

![Autocorrelation Plot](image)

**Figure 7-21.** FMBMC test problem 2 replication 1 subcase 2 $A_{12}$ fission matrix element autocorrelation plot

Figure 7-21 shows that although increasing particles per generation reduces overall variations, significant correlation is still evident and in fact for this element actually increased. Note that fission matrix element $A_{13}$ has insignificant autocorrelation while $A_{11}$ has significant
but reduced autocorrelation. To further investigate this issue, subcases 3 and 4 with 20 fission
matrix meshes are examined. Each source mesh will be expected to contain 5% of the overall
source. Figure 7-22 shows a COM plot for subcase 4.

Figure 7-22. FMBMC test problem 2 standard algorithm COM for subcase 4, replication 1

Figure 7-22 shows that the source behavior seen in Figure 7-19 is the same type of source
behavior seen for this subcase, which is a strong source correlation. Figure 7-23 shows the
source fraction behavior for mesh 1, subcase 4.
Figure 7-23 shows that the mesh 1 source fraction indicates increasing accuracy with particles simulated. This is to be expected as the number of terms utilized to calculate the fission matrix elements increases by generation. Figure 7-24 gives the final source fractions for both the standard and FMBMC method for subcase 3 (replication 1) and subcase 4.
Figure 7-24 shows that both subcases 3 and 4 source fractions exhibit similar behavior when compared to subcases 1 and 2 respectively. Subcase 4 results show an improvement over subcase 3 as expected. A conclusion drawn here is that increasing particles per generation yields less variation as expected due to more simulated particles. The difficulty is that for a problem with a high DR, convergence, assuming no undersampling and adequate skipped cycles, may still not be apparent due to the high source autocorrelation. Figure 7-25 shows an autocorrelation plot of element $A_{12}$ for subcase 4.
Figure 7-25 shows that the autocorrelation of fission matrix element $A_{12}$ has reduced significantly to under 0.2 at lag 1. Better convergence is indicated with the increased mesh size but constant particles per generation and total generations. This supports the fact that as mesh size reduces, the fission matrix elements should be independent of the source distribution, but it also shows that the fission matrix dependence on mesh size for larger meshes may be able to be quantified in terms of fission matrix element autocorrelation. Continued analysis of subcases 5 and 6 for 50 source meshes shows more of the same trend as was seen for 20 meshes. A source fraction plot is shown in Figure 7-26.
Figure 7-26. FMBMC test problem 2 subcase 5 and 6 source fractions

Figure 7-26 shows subcase 6 varies less about the expected source fraction of 0.0200. An autocorrelation plot for fission matrix element $A_{12}$ is shown in Figure 7-27.

Figure 7-27. FMBMC test problem 2 subcase 6 $A_{12}$ fission matrix element autocorrelation plot
Clearly, subcase 6 with more source particles outperforms subcase 5 as expected while the significant autocorrelation is reduced even more as seen from the autocorrelation plot in Figure 7-27. This indicates that at 50 meshes, confidence estimates derived from the final converged fission matrix should be more accurate using the procedure described earlier in this chapter. Still of interest is the fact that reducing mesh size also appears to increase the accuracy of the standard methodology.

Normality of fission matrix elements $A_{11}, A_{12}, A_{13}$ and $A_{14}$ were tested with the Cramer-von Mises (CVM) and Kolmogorov-Smirnov (KS) normality tests. The Shapiro Wilk normality test was not utilized since it the CVM and KS tests have more desirable properties at large sample sizes (5000 in this case), yet as noted before, such large sample sizes are problematic in general concerning normality tests. Elements $A_{11}, A_{12}$ passed both tests at the 10 percent significance level, while the $A_{13}$ element failed the CVM test and the $A_{14}$ element failed both.

This implies that utilizing more source particles impacts the distribution of the fission matrix elements not only in their autocorrelation, but increases their convergence to a normal distribution. It appears that the lower the fission matrix element value (representing probability of fission from cell $j$ to cell $i$), the more source particles that are necessary per generation to allow the element to converge to a normal distribution. Fission matrix element $A_{16}$ for subcase 6 is the first element which contains a significant number of zero values, representing zero probability of neutrons being generated from that fission matrix transfer during the generation in which the zero value occurred. Continuing to farther off diagonal fission matrix elements, the fraction of zero values are increased until all zeroes are observed.

Subcases 7 and 8 have a further increase in fission matrix meshes to 100. This means an expected 1% of the source will be in each source mesh. Similar behavior was observed for these
subcases as was observed for subcases 5 and 6. Note that with increasing mesh density, fewer particles will contribute to the average value achieved, yet an increase in reliability is seen. This is most likely a result of the loss of dependence of the source distribution on the fission matrix elements. Consequently, however, as the grid density increases further, more particles simulated (per generation) are necessary. More analysis of this problem will follow in the development of diagnostics to evaluate the FMBMC method mesh density and particle population size. Fission matrix element independence and normality is investigated more thoroughly.

**Test problem 3 analysis**

FMBMC test problem 3 is the same as E-CADIS/ME-CADIS test problem 2. A detailed $k_{\text{eff}}$, source convergence, and fission matrix element analysis for the standard, E-CADIS and ME-CADIS algorithm was given in Chapter 6. Subcases utilizing 10, 20, 40 and 80 equally spaced fission matrix meshes were simulated to provide a similar analysis as was done for test problem 1 and 2. Utilizing these cases it was determined that for this problem, no significant correlation was present in any fission matrix elements. Although correlation is insignificant for all subcases, it appears that the simulations may be suffering from undersampling within each generation. This conclusion was drawn due to a large number of the fission matrix elements often resulting in zero values for a significant percentage of generations, yet nonzero for most when the mesh grid density increases (more, smaller meshes). To test whether this is the case, particle population was increased for all subcases beyond 20 meshes and fission matrix elements remain uncorrelated with better sampling as expected. Note that since the importance sharply decreases near the problem boundary, the poorest sampled region corresponds to the regions nearest to the boundaries. Although the final converged source distribution is unknown, symmetry is expected.
To compare the standard and FMBMC method, source fractions are given in Table 7-17 for the subcase with 10 fission matrix meshes and 5000 particle per generation for the standard and FMBMC method for mesh 1, 2 and 3.

Table 7-17. FMBMC Test Problem 3 Final Converged Source for Source Meshes 1-3

<table>
<thead>
<tr>
<th>Replication</th>
<th>Standard Mesh 1</th>
<th>Standard Mesh 2</th>
<th>Standard Mesh 3</th>
<th>FMBMC Mesh 1</th>
<th>FMBMC Mesh 2</th>
<th>FMBMC Mesh 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0312</td>
<td>0.0623</td>
<td>0.0889</td>
<td>0.0315</td>
<td>0.0629</td>
<td>0.0898</td>
</tr>
<tr>
<td>2</td>
<td>0.0304</td>
<td>0.0607</td>
<td>0.0862</td>
<td>0.0284</td>
<td>0.0565</td>
<td>0.0805</td>
</tr>
<tr>
<td>3</td>
<td>0.0296</td>
<td>0.0591</td>
<td>0.0841</td>
<td>0.0294</td>
<td>0.0587</td>
<td>0.0837</td>
</tr>
<tr>
<td>4</td>
<td>0.0288</td>
<td>0.0574</td>
<td>0.0819</td>
<td>0.0292</td>
<td>0.0581</td>
<td>0.0829</td>
</tr>
<tr>
<td>5</td>
<td>0.0296</td>
<td>0.0591</td>
<td>0.0842</td>
<td>0.0285</td>
<td>0.0571</td>
<td>0.0816</td>
</tr>
<tr>
<td>6</td>
<td>0.0296</td>
<td>0.0590</td>
<td>0.0841</td>
<td>0.0302</td>
<td>0.0602</td>
<td>0.0858</td>
</tr>
<tr>
<td>7</td>
<td>0.0305</td>
<td>0.0608</td>
<td>0.0864</td>
<td>0.0304</td>
<td>0.0607</td>
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</tr>
<tr>
<td>8</td>
<td>0.0294</td>
<td>0.0587</td>
<td>0.0834</td>
<td>0.0295</td>
<td>0.0589</td>
<td>0.0838</td>
</tr>
<tr>
<td>9</td>
<td>0.0296</td>
<td>0.0592</td>
<td>0.0845</td>
<td>0.0304</td>
<td>0.0607</td>
<td>0.0865</td>
</tr>
<tr>
<td>10</td>
<td>0.0293</td>
<td>0.0584</td>
<td>0.0833</td>
<td>0.0281</td>
<td>0.0562</td>
<td>0.0799</td>
</tr>
</tbody>
</table>

Table 7-17 shows similar final source fractions are obtained for both the standard and FMBMC source even when sampling may be poor. Note that it was also observed that although symmetric values are similar, they are not even close to being within statistics.

Since symmetry is expected, another simple metric utilized for accuracy of the final result can be the difference between symmetric meshes (as well as consistency of a particular mesh across replications as in test problem 1). In the 40 fission matrix mesh subcase, a maximum of 1.73% difference was observed between any two reflected meshes for replication 1, which again shows the increasing accuracy when fission matrix density is increased.

FMBMC test problem 3 results indicate that although the standard method had trouble with source correlation, only a minimal amount of fission matrix meshes was required to provide an accurate solution and provide results within statistics. Essentially, the same behavior as in problem 1 is observed and therefore detailed analysis is not presented here for brevity.
Cycle-wise Fission Matrix Analysis

While the cycle-wise fission matrix is not utilized in this work, it was implemented into the 1Dcrit code. During the course of the analysis of the FMBMC method, it was observed that for some problems the cycle-wise fission matrix produced significantly biased results. A note is being made here since the reason for this bias should be made clear. The cause is due to the fluctuation in fission matrix elements having a non-uniform effect on the outcome and is the same reason the plus and minus fission matrix do not yield a symmetric confidence interval, yet utilizing the final converged fission matrix results in a much more accurate result since the elements are much closer to their true value and individual element variation has less of an overall effect.

Effect of Initialized Source Distribution

1Dcrit allows for the utilization of an initialized source distribution as discussed. Two major factors affect the effectiveness of an initialized source distribution for the FMBMC method. The first is the only moderate dependence of the source on the fission matrix elements, which decreases with fission matrix mesh size. This is not just an additional benefit, but a requirement if the FMBMC method is going to yield accurate results. As a result, the dependence on the source distribution to yield uncorrelated fission matrix elements is vastly reduced for the FMBMC method. The second is the fact that for high dominance ratio problems, the actual generation-to-generation Monte Carlo source distribution is highly irregular if tallied, resulting in a source which is not “converged” in the normal sense. This does not altogether eliminate the effect of an initialized source; but its impact is reduced. In large high dominance ratio problems where the initial source must migrate to a particularly reactive region, and if source particles are not started in the highly reactive region, or are started in limited amount, it may take many generations for the source to gather to the highly reactive problem phase space.
For the analysis of this problem, the result may be skewed from poor sampling. An initialized source will remedy this problem. For this fact, an initialized source can still be very beneficial and is very beneficial for all other problems. Note that undersampling effects may still materialize and must be accounted for.

**Automatic Independence Method with Minimum Sampling (AIMS)**

Since it is critical that independence of the fission matrix elements is maintained, an automatic procedure would be desirable to test for fission matrix element independence internally. In order to achieve this goal, FMBMC test problem two was reevaluated with another set of cases. These cases are not as lengthy (total generations) as 1000 active generations appears adequate to provide necessary information. A more systematic analysis concerning fission matrix convergence is performed. Cases simulated are shown in Table 7-18.

<table>
<thead>
<tr>
<th>Case</th>
<th>Meshes</th>
<th>Skip</th>
<th>Total</th>
<th>Histories per Generation</th>
<th>Expected Particles per Source Mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>50</td>
<td>1050</td>
<td>20 million</td>
<td>200000</td>
</tr>
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<td>1050</td>
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<td>20000</td>
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<tr>
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<td>50</td>
<td>1050</td>
<td>200000</td>
<td>2000</td>
</tr>
<tr>
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<td>1050</td>
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<td>200000</td>
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<td>50</td>
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<td>20000</td>
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<tr>
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<td>1050</td>
<td>100000</td>
<td>2000</td>
</tr>
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<td>20 million</td>
<td>1 million</td>
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<td>20</td>
<td>50</td>
<td>1050</td>
<td>4 million</td>
<td>200000</td>
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<td>5</td>
<td>50</td>
<td>1050</td>
<td>5 million</td>
<td>1 million</td>
</tr>
<tr>
<td>4a</td>
<td>5</td>
<td>50</td>
<td>1050</td>
<td>1 million</td>
<td>200000</td>
</tr>
<tr>
<td>4b</td>
<td>5</td>
<td>50</td>
<td>1050</td>
<td>100000</td>
<td>20000</td>
</tr>
<tr>
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</tr>
</tbody>
</table>

In a posterior manner, each simulation was evaluated utilizing two major criteria. These criteria are the expected contribution to the final $k_{eff}$ from non-independent fission matrix elements, and the expected contribution to the final $k_{eff}$ from non-normally distributed fission.
matrix elements. Non-independence is determined by calculating the lag 1 autocorrelation for every fission matrix element, flagging any mesh whose correlation was greater than the max lag autocorrelation (0.058) that would be obtained from a randomly distributed uncorrelated normal random variable with 1000 values, with a 95% confidence. Non-normally distributed elements are determined using a Shapiro-Wilk normality test at 0.05 significance. These two metrics should give an indication of the dependence on mesh size and particle population to a final converged result. Results of the cases concerning these metrics are given in Table 7-19.

Table 7-19. FMBMC test problem 2 AIMMS cases input

<table>
<thead>
<tr>
<th>Case</th>
<th>Meshes</th>
<th>Histories per Generation</th>
<th>Expected Particles per Source Mesh</th>
<th>Non-Independent %</th>
<th>Non-Normal %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>20 million</td>
<td>200000</td>
<td>7.29</td>
<td>14.10</td>
</tr>
<tr>
<td>1a</td>
<td>100</td>
<td>2 million</td>
<td>200000</td>
<td>6.08</td>
<td>65.69</td>
</tr>
<tr>
<td>1b</td>
<td>100</td>
<td>200000</td>
<td>2000</td>
<td>18.16</td>
<td>100.00</td>
</tr>
<tr>
<td>2</td>
<td>50</td>
<td>10 million</td>
<td>200000</td>
<td>7.75</td>
<td>7.92</td>
</tr>
<tr>
<td>2a</td>
<td>50</td>
<td>1 million</td>
<td>200000</td>
<td>11.19</td>
<td>35.22</td>
</tr>
<tr>
<td>2b</td>
<td>50</td>
<td>100000</td>
<td>2000</td>
<td>18.49</td>
<td>95.76</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
<td>20 million</td>
<td>1 million</td>
<td>22.04</td>
<td>5.42</td>
</tr>
<tr>
<td>3a</td>
<td>20</td>
<td>4 million</td>
<td>200000</td>
<td>22.32</td>
<td>7.48</td>
</tr>
<tr>
<td>3b</td>
<td>20</td>
<td>400000</td>
<td>200000</td>
<td>46.81</td>
<td>18.74</td>
</tr>
<tr>
<td>3c</td>
<td>20</td>
<td>400000</td>
<td>2000</td>
<td>29.59</td>
<td>79.04</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>5 million</td>
<td>1 million</td>
<td>22.77</td>
<td>0.47</td>
</tr>
<tr>
<td>4a</td>
<td>5</td>
<td>1 million</td>
<td>200000</td>
<td>41.01</td>
<td>19.77</td>
</tr>
<tr>
<td>4b</td>
<td>5</td>
<td>100000</td>
<td>200000</td>
<td>41.29</td>
<td>2.85</td>
</tr>
<tr>
<td>4c</td>
<td>5</td>
<td>10000</td>
<td>2000</td>
<td>3.91</td>
<td>59.50</td>
</tr>
<tr>
<td>4d</td>
<td>5</td>
<td>50 million</td>
<td>10 million</td>
<td>22.94</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>200</td>
<td>10 million</td>
<td>50000</td>
<td>7.47</td>
<td>65.40</td>
</tr>
</tbody>
</table>

In general, Table 7-19 shows that as particle population for a set meshing structure increases, the non-independent fission matrix contribution tends to decrease. This is seen for all cases except cases 1, 3b, 4c and 4d. Case 4d has nearly the same non-independent percentage as case 4 (an increase in particle density from case 4 to 4d) in which this behavior is nothing out of the ordinary. For the other cases, within each set of cases with the same meshing (same case number, different letter or no letter), the behavior is complex.
With low particle density, a “false” sense of independence may be observed if source meshes are appearing to be independent of each other due to undersampling (lack of coupling with neighbors). As this density increases, eventually transfers between meshes which were not well sampled will be better sampled, resulting in a better estimate of the non-independence fraction, unless the mesh size is small enough to negate the source spatial dependence. Further increases in particle density should see undersampling reduce to the point that the meshes should not have undersampling. At this point the non-independent percentage should stabilize if the fission matrix mesh size is not small enough, or reduce to an inconsequential percentage if the mesh density is large enough.

For cases 4c and 3b, a large increase in non-independent percentage is seen as the phase space is better sampled and stabilizes to about 22 percent as particle density increases. Case 4c is particularly interesting as a false sense of independence is observed. This is due to the fact that with only 2000 source particles for 20 cm meshes, the off diagonal fission matrix elements are minimally contributing, whereas their true contribution if sampled properly is higher. A check for the total contribution to $k_{eff}$ from the diagonal elements can be utilized to check for undersampling.

For case 1, only a small increase in non-independence is observed with the decreasing non-normal percentage. Note also that these are statistically based metrics cased on 95% confidences, meaning there will be some expected fission matrix elements there will be mislabeled as both non-independent and non-normal, and vice versa.

Note that the non-normal percentage reduces as particle density is increased with constant mesh size for all cases except those with 5 source meshes. This is due to the aforementioned undersampling seen with 5 source meshes. Also note that although it is desired to obtain
normally distributed fission matrix elements in principle, as long as the fission matrix elements
are independent and well sampled, the CLT can be applied to obtain proper confidence estimates
of the fission matrix elements. The non-normal metric is important, however, to aid in the
understanding of the problem behavior.

Further analysis with a single processor was limited due to memory limitations. Case 1 is
at a maximum particle density since 1Dcrit was structured as a learning tool and therefore stores
most information for the entire calculation. When increasing mesh density and particle
population to these levels, the memory requirements necessary precluded further study. Note
that with parallel processing these cases could be further studied as the overall memory required
is shared among processors, yet due to different initial seeds, an extra level of randomness will
be obtained from parallel processing (adding two separately generated autocorrelated series for
the same element). In order to utilize the metrics previously, a procedure was developed to
incorporate their usage “on-the-fly”. A schematic of the procedure is shown in Figure 7-28 and
is known as the Automatic Independence Method and Minimum Sampling testing method
(AIMS).
Figure 7-28. AIMS flowchart
In words, the procedure is as follows: A sample of the total solution must be utilized to make a decision on whether the simulation is acceptable. It was determined that 100 active generations of data would be utilized for statistics related testing. For the first metric, 100 active generations is utilized to calculate the lag 1 autocorrelation for which the max lag autocorrelation that would be obtained from a randomly distributed uncorrelated normal random variable is approximately 0.2.

The second metric is the same as before, utilizing the Shapiro-Wilk normality test on each fission matrix element series. Initially each tolerance is set to 10%. When metric 1 fails, the fission matrix density is doubled for the first failure. For successive failures of metric 1, particle population is increased until there is less than a 5% relative decrease in the fractional contribution from non-independent fission matrix elements, in which case the fission matrix density is again doubled. When only metric 2 fails, particle density is doubled. Two other criteria were added, one which determines the contribution from the principal diagonal fission matrix elements. If this is greater than 66%, the fission matrix mesh size is automatically doubled even if metric 1 and 2 pass, since this indicates that the fission matrix meshes are too large and may lead to a false convergence. The other is that the minimum mesh size is 1 mfp.

Note that doubling meshing requires reallocation of many variables, and this is done internally in 1Dcrit. Also, doubling of the particle source requires the same type of problem for variable allocation since bank sizes and other variable storage requirements are functions of the particle population per generation. This reallocation is handled internally as well by 1dcrit. Another difficulty occurs with increasing particle density, namely where the extra particles come from. In this case (doubling), each particle location is used twice, with half weight to conserve the total particle weight. In other words, if \( N \) particles are initially required, total starting source
particle weight for the generation is \( N \), yet when doubling the source population, a total weight of \( 2N \) is necessary to describe the total neutron source weight. At the beginning of a generation, all particles are loaded with the same weight, in this case each particle weight is essentially doubled and the particle split in two. No change is done to the source distribution, yet the particle density is increased.

The AIMS technique was tested with benchmark problem 2 in both the 10 cm and 100 cm configuration with 5 equally spaced fission matrix meshes as the initial meshing structure. Other input parameters are as follows: 50 skipped generations, 2000 and 20000 particles per generation for the 10cm and 100 cm cases respectively, 1050 total generations and a \( k_{eff} \) guess of 1.0.

The 10 cm case required a change to 10 fission matrix meshes and 25600 particles per generation before passing all criteria. The 100 cm case required a change to 40 fission matrix meshes and 256000 particles per generation. The AIMS methodology shows promising potential, and must be more thoroughly investigated. Note that for the 10 cm case, an upgrade to 10 meshes should not be necessary. While AIMS appears to guide the solution toward a path with independent and normally distributed fission matrix elements, it is not necessary for the elements to be truly no-normal if they are independent and well sampled. Future studies should focus on increasing AIMS efficiency in choosing the most effective particle population and mesh size.

**Extension to Parallel Computing Environment**

Although the fission matrix method differs from the standard methodology, final results are still dependent on tracking of independent particles, thereby making the FMBMC method with or without AIMS extremely suitable for implementation on a parallel computing environment. To show its viability, an algorithm was developed without the use of advanced
message passing with MPI or PVM. Instead, a driver code was written to start independent
simulations through rsh or ssh, without any change in the input file. The driver code requires as
input only the number of processors to request, and a file containing the host names for the other
processors (currently hardwired for convenience).

Independent simulations are started, and when complete, final results are combined
statistically and summarized into a final output file. Parallel implementation of the AIMS
algorithm is slightly more complicated, since there is no guarantee the same fission matrix mesh
structure will result from each independent calculation and was not yet implemented. One
strategy for parallel implementation of the AIMS methodology would be that one calculation can
serve as the master calculation whereby all other simulations are not started until the mesh size
and particle density of the master is set. Subsequently, the slave simulations are started and
locked to the same fission matrix and particle density. This has been left for future development.

Testing with the parallel processing was performed with FMBMC benchmark problem 2.
For this testing, the following input parameters were utilized: 350 skipped generations, initial
randomly sampled source, 5350 totally generations (5000 active), 50 equally spaced fission
matrix meshes and 500000 particles per generation. 350 skipped generations were utilized to
show their impact on parallel performance.
Speedup obtained for 3 and 5 processors was observed to be 2.57 and 3.71, respectively. Since 350 skipped cycles were utilized, each processor is also performing 350 skipped cycles, and a penalty in parallel speedup is taken due to this. If an initialized source is being utilized (which for this problem is the case by default), skipped cycles are unnecessary (or minimally necessary). The estimated extra time spent on skipped cycles for each parallel case was calculated and removed from the total time to approximate the ideal speedup case without the loss of speedup from skipped cycles. The adjusted ideal speedups for these cases were 2.91 and 4.68 for the 3- and 5-processor cases, respectively, as shown in Figure 7-29.

![Parallel speedup with FMBMC for 3 and 5 processors](image)

Figure 7-29. Parallel speedup with FMBMC for 3 and 5 processors

Note that in the 5 processor case, the individual processor times were 2230 seconds, 2147 seconds, 2152 seconds, 2150 and 2148 seconds, with a total time (with processing of results) of 2235 seconds. This means 4 of the 5 processors were finished 78 seconds before the slowest. If the slowest processor had finished at 2152 seconds (second slowest) 5 processor adjusted speedup would have been 4.85.
CHAPTER 8
CONCLUSIONS AND FUTURE WORK

Conclusions

This work has introduced new methodologies concerning Monte Carlo eigenvalue problems. First, a new stationarity detection methodology called the KPSS test for stationarity has been developed for use in Monte Carlo eigenvalue problems. This methodology contains the following features:

• Use of the particle population center-of-mass as a single metric for describing overall source movement (also a good stand alone visual diagnostic)

• No need for meshing structure as needed in other tests such as the information theoretic tests

• Utilizes an adapted form of the KPSS statistical stationarity test

The methodology was incorporated into the KENOV.a code in the SCALE 5 package. Also added to the KENOV.a code were three information theoretic (Shannon Entropy) based diagnostics for stationarity/undersampling detection. Important features of this implementation are:

• No new user inputs required (User must turn on the fission matrix option)

• COM determined and printed for the system as an output table

• Posterior KPSS test automatically implemented into the KENOV.a code

• Meshing structure for information theoretic diagnostics automatically generated by use of the fission matrix option

• Final output table provides summary of stationarity diagnostic results

In addition to the stationarity detection methods, a new solution algorithm was developed to utilize multiple importance functions with a modified CADIS methodology. Features of this solution algorithm include:
• Application of multiple importance calculations to provide importance for reduced variance for particular region to region transfers

• Reuse of source particles to calculate more exactly the source transfer probability from region to region

• Coupling with well known fission matrix variance reduction methods (both utilized at the same time)

Furthermore, a new variation of a fission matrix based solution algorithm was developed for use with high dominance ratio problems. Traditional algorithm tally estimators will be biased for high dominance ratio problems. This methodology should reduce and possibly eliminate this bias and has the following features:

• Solution based on final converged fission matrix only

• Posterior evaluation based on two metrics
  • the fraction of the $k_{eff}$ obtained from non-independent fission matrix elements
  • the fraction of the $k_{eff}$ obtained from non-normal fission matrix elements

• On the fly particle population change and fission matrix mesh increase beta version based on the evaluation of the previous 2 metrics during the simulation (Automatic Independence method and Minimum Sampling testing – AIMS)

• Confidence estimates based on Monte Carlo iterated confidence approach

Moreover, the new solution algorithm and the FMBMC approach were tested in a 1-dimensional multigroup Monte Carlo eigenvalue code developed for this purpose. The code was written in FORTRAN90/95 and has both a traditional power iteration and fission matrix solver. The traditional CADIS approach was incorporated as well as the modified solution algorithm. Traditional fission matrix biasing is included as an option for source biasing. A version of the code contains the AIMS algorithm as well as the posterior diagnostic test.

Processing codes were developed to format PENTRAN deterministic Sn calculation output into a starting source distribution, as well as utilize importance information for the CADIS
methodologies tested. It was determined that the FMBMC approach with or without AIMS is a viable solution approach to obtain unbiased eigenvalue (multiplication factor) and eigenvector (discretized source), whereby the standard approach will yield biased confidence estimates. The algorithm was extended in parallel with high efficiency.

Testing of the KPSS diagnostic test on both simple and difficult source convergence benchmark problems showed its ability to identify source convergence problems where other tests fail. While false positives are observed, the test is fairly capable of source non-stationarity diagnosis. For high DR problems, both the KPSS and entropy tests have some difficulty. The KPSS test appears to identify more false positive tests when there is strong source correlation. In cases of false positive identification, the source COM, entropy and relative entropy series are available to visually inspect as well as the skewness and kurtosis of the source COM distribution.

Variance reduction methods tested with 1Dcrit included the two extensions of the CADIS methodology to eigenvalue problems. A straightforward extension, E-CADIS, utilized the neutron production cross section as adjoint source globally. Modest speedup up to about 20 percent was obtained for the sample problems. This algorithm was not optimized to the fullest extent and some overhead in implementation is most likely unnecessary for which speedup can be increased.

The modified source algorithm developed was used in conjunction with region-wise importance calculations. This methodology was called ME-CADIS, where importance sampling is utilized to reduce variance in lower probability source regions thereby increasing coupling in loosely coupled source regions. Off diagonal fission matrix elements standard deviation was significantly reduced with the utilization of ME-CADIS versus E-CADIS, at the expense of computer time.
The modified FMBMC method was successfully applied to high dominance ratio problems where it was shown that the proper choice of particle density and source mesh size can eliminate any autocorrelation in the fission matrix elements, facilitating the usage of the Monte Carlo generated confidence estimates for the source eigenvalue and eigenvector developed for use with the fission matrix algorithm.

**Future Work**

There are many pursuits that can be undertaken to continue this work. Concerning the stationarity diagnostics, other versions of the KPSS test have become available as the work was being done and can be evaluated. The robustness of this test can be evaluated with further testing and analysis. The COM visual diagnostic can be made into a visual plot to view the source movement throughout the simulation. Continuing with the source diagnostic area, the lag 1 autocorrelation coefficient can be used as an indicator of independence. Although independence is not guaranteed by uncorrelatedness, it appears a strong indicator for Monte Carlo eigenvalue problems. The source COM can be tested for autocorrelation, and if present, other stationarity diagnostics (such as the information theoretic and KPSS) diagnostics can attempt to diagnose whether stationarity has been achieved.

Monte Carlo solutions algorithm with ME-CADIS should be effective for solving loosely coupled problems for which the ME-CADIS algorithm should be extended to 3-D and a detailed analysis of problems of this type in the way of benchmark studies should be undertaken. Improvements can be made to ME-CADIS to mitigate the effect of extremely low weights being utilized due to very low value weight windows that may result from particles starting in locally “unimportant” regions that actually reach the detector.

The modified solution algorithm with the modified-CADIS approach, although slower than the traditional approach for many problems, will provide strong coupling between loosely
coupled regions. Problems of this nature should be studied with this approach to assess this methods effectiveness concerning loosely coupled systems.

The particular fission matrix based Monte Carlo (FMBMC) approach developed here should be implemented in a full 3-D Monte Carlo code with implicit parallel capability for analysis of high dominance ratio problems. The Monte Carlo Iterated Confidence approach can be improved with the utilization of a bootstrapping methodology which corrects the method for skewed sampling distributions.

Another simple possibility for the reduction in skip generation time necessary for problems with slow convergence can be through the use of increasing particle population on the fly. It was noticed during the testing of the particle doubling feature of 1Dcrit that the source converges loosely to the final result in approximately the same number of generations regardless of the source population size. If this is the case, a smaller number of particle per generation can be initially started, and increased after a period of time.
APPENDIX A
1DCRIT INPUT DESCRIPTION

Appendix A contains the input required for 1Dcrit in the form of a user guide, for all
versions. 1Dcrit is evoked at the command prompt with two arguments. Argument 1 is the input
file name and argument 2 is the output file name. The output file name is overwritten if it
already exists.

Standard Input File Format

The standard input file is composed of all the data needed to run 1Dcrit without any
CADIS biasing. Input is required in a particular order, and a new input variable should start on a
new line, however, the data within each variable can be freely formatted. Also, the slash “/”
character serves a line input terminator. Anything after a slash on a line is considered a
comment. The following cards describe the input

1. Replication – This is an integer number describing the total number of replications of the
   same problem to be run. 1Dcrit has built in seeds for repeatability.
2. Regions or Seed Identifier – This is an integer giving the total regions in the problem
   unless it is alternatively the keyword “yes”. If the keyword yes is here, the next line
   (card 2a) should contain a random user defined seed instead of materials. All other input
   proceeds linearly as below regardless.
3. Materials – This is an integer giving the total number of materials used in the problem
4. Groups – This is an integer giving the number of energy groups used in the problem
5. Legendre Order – This currently should always be set to 0 for isotropic scattering and
   was utilized if 1Dcrit were to be adapted to higher order Legendre scattering
6. Position Bounds – This is an array of double precision data of length “regions +1” giving the position bounds for each region starting with the most negative and increasing from most negative to most positive.

7. Material ID’s – This is an array of integers of length “regions” indicating the material associated with each region, starting from region 1 (most negative) to region “regions”, the most positive.

8. Group Energy Boundaries – An array containing the energy group boundaries is here, however the energy group boundaries themselves are not utilized in the code and are currently placeholders only.

9. Cross Sections – Card 9 contains the cross section information. Each line reads “abs, nusigfis, sigmaT, Chi, Sigmas”, where sigmas is the up and downscatter matrix in the following format (5 group example):
   - sigs1→1 sigs1→2 sigs1→3 sigs1→4 sigs1→5
   - sigs2→1 sigs2→2 sigs2→3 sigs2→4 sigs2→5
   - sigs3→1 sigs3→2 sigs3→3 sigs3→4 sigs3→5
   - sigs4→1 sigs4→2 sigs4→3 sigs4→4 sigs4→5
   - sigs5→1 sigs5→2 sigs5→3 sigs5→4 sigs5→5

10. Parameters – Card 10 contains the initialization parameters: nskip, Particles per generation, total generations, k-guess, in that order.

11. Source Input Flag – Card 11 is a source input flag, where a 0 indicates random sampling of the source in all fissionable regions for the first generation, and a 1 indicates reading the source from a file names 1dcrit.src.

12. Boundary Conditions – Card 12 contains the left and right albedo conditions and can be any number.

13. Source Meshes – Card 13 is an integer identifying the number of source meshes utilized in the virtual mesh for the information theoretic source convergence diagnostics.
14. Source Mesh Boundaries – Card 14 is the final card and contains an array of double precision data of length “source meshes +1” giving the position bounds for each virtual mesh source region starting with the most negative and increasing from most negative to most positive.

**Standard Input File Example**

An example input file is given below:

```
/replications
10
/regions
19
/materials
4
/groups
3
/legendre order/
0
/position bounds/
-25.88969994
-13.71699995
-13.65984997
-13.65199995
-12.86759996
-12.85974994
-12.80259997
-0.457199991
-0.400050014
-0.392199993
0.392199993
0.400050014
0.457199991
12.80259997
12.85974994
12.86759996
13.65199995
13.65984997
13.71699995
25.88969994
/mat id's
4 3 2 1 2 3 4 3 2 1 2 3 4 3 2 1 2 3 4
/group energy boundaries/
20 1.01 6.25e-07 0
```
1Dcrit.src Input File Structure

The file 1dcrit.src is necessary for a user input source. This file has minimal amount of data and should contain on each line the energy group of the particle and the location. 1Dcrit will then determine which region the particle resides.

Bias.dat Input File Structure

When utilizing E-CADIS or ME-CADIS, importance information is necessary and is stored in a file names “bias.dat”. this file has the following format:

1. Number of importance regions – the first line should contain the number of importance regions (meshes)
2. **Biasing Position Bounds** – This is an array of double precision data of length “number of importance regions +1” giving the position bounds for each importance region starting with the most negative and increasing from most negative to most positive.

3. **Energy Groups** – Card 3 contains the number of energy groups.

4. **Energy Group Boundaries** – Card 4 contains the energy group boundaries (not utilized, but necessary placeholder).

5. **Importance data** – Importance data is input for each region, for each group. First data for group 1 for each mesh, then proceeding to group 2 for each mesh, and so on until all groups are input.

**Seedwrapper Parallel Driver Information**

Parallel execution of 1Dcrit was only implemented utilizing the versions containing the fission matrix algorithm. Execution is performed through a separate FORTRAN driver code which initializes the independent runs and collects data upon exit. The same input file structure is utilized for 1Dcrit as above except the seed is read in as an option for card 2 and 2a. First the keyword “yes” is looked for and if found, a user defined seed is read, if not the calculation will fail for parallel execution. The driver code (seedwrapper) has the following command line arguments:

1. Number of processors
2. File name containing seed for each processor, one per line
3. Input file name
4. Hosts file containing location of other processors (currently not necessary since this was hardwired internally because all parallel analysis was done on a single cluster)
Final output is hardcoded to the file output.out for the standard output file and combined.out for the fission matrix combined output data.
LIST OF REFERENCES


BIOGRAPHICAL SKETCH

Michael Todd Wenner was born on 1978 in Wilkes-Barre, Pennsylvania. He grew up in St. Johns, Pennsylvania, the youngest of four children in a blended family. Michael graduated from Hazleton Area High School in 1996 and enrolled at the Pennsylvania state University. Four years later in May, 2000, Michael graduated as the College of Engineering Nuclear engineering Student Marshall and continued his education at Penn State, receiving his master’s degree in August of 2003.

Before graduation, Michael had already enrolled at the University of Florida, and had finished his studies at Penn State while at the University of Florida, where he continued his education via enrollment in their PhD program. While at the University of Florida, Michael was able to intern at Oak Ridge National Laboratory, in Oak Ridge, TN, in 2005. He also served as a consultant for NUCSAFE, INC in Oak Ridge TN and was an instructor for reactor physics related Power Plant Operator continued education training classes at the Crystal River Nuclear Training Center in 2007. He also served as a co-instructor for an undergraduate class during the Spring 2009 semester.

Michael left the University of Florida on a full time basis in the Spring of 2010 and moved to western Pennsylvania with Jennifer Fiddner and took a position at Westinghouse Electric Company. Michael currently works in their Research and Technology Unit.