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Development of New Monte Carlo Methods in Reactor Physics

Criticality, Non-Linear Steady-State and Burnup Problems

JAN DUFEK

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KTH
School of Engineering Sciences
SE-106 91 Stockholm
SWEDEN

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Abstract

The Monte Carlo method is, practically, the only approach capable of giving detail insight into complex neutron transport problems. In reactor physics, the method has been used mainly for determining the k_{eff} in criticality calculations. In the last decade, the continuously growing computer performance has allowed to apply the Monte Carlo method also on simple burnup simulations of nuclear systems. Nevertheless, due to its extensive computational demands the Monte Carlo method is still not used as commonly as deterministic methods.

One of the reasons for the large computational demands of Monte Carlo criticality calculations is the necessity to carry out a number of inactive cycles to converge the fission source. This thesis presents a new concept of fission matrix based Monte Carlo criticality calculations where inactive cycles are not required. It is shown that the fission matrix is not sensitive to the errors in the fission source, and can be thus calculated by a Monte Carlo calculation without inactive cycles. All required results, including k_{eff}, are then derived via the final fission matrix. The confidence interval for the estimated k_{eff} can be conservatively derived from the variance in the fission matrix. This was confirmed by numerical test calculations of Whitesides's "k_{eff} of the world problem" model where other Monte Carlo methods fail to estimate the confidence interval correctly unless a large number of inactive cycles is simulated.

Another problem is that the existing Monte Carlo criticality codes are not well shaped for parallel computations; they cannot fully utilise the processing power of modern multi-processor computers and computer clusters. This thesis presents a new parallel computing scheme for Monte Carlo criticality calculations based on the fission matrix. The fission matrix is combined over a number of independent parallel simulations, and the final results are derived by means of the fission matrix. This scheme allows for a practically ideal parallel scaling since no communication among the parallel simulations is required, and no inactive cycles need to be simulated.

When the Monte Carlo criticality calculations are sufficiently fast, they will be more commonly applied on complex reactor physics problems, like non-linear steady-state calculations and fuel cycle calculations. This thesis develops an efficient method that introduces thermal-hydraulic and other feedbacks into the numerical model of a power reactor, allowing to carry out a non-linear Monte Carlo analysis of the reactor with steady-state core conditions. The thesis also shows that the major existing Monte Carlo burnup codes use unstable algorithms for coupling the neutronic and burnup calculations; therefore, they cannot be used for fuel cycle calculations. Nevertheless, stable coupling algorithms are known and can be implemented into the future Monte Carlo burnup codes.

List of Papers

Included Papers

The following papers constitute the thesis:

I. Dufek, J. and Gudowski, W., "Stability and convergence problems of the Monte Carlo fission matrix acceleration methods," *Ann. Nucl. Energy*, submitted for publication, 2008.

II. Dufek, J. and Gudowski, W., "Fission matrix based Monte Carlo criticality calculations," *Ann. Nucl. Energy*, accepted for publication, 2009.

III. Dufek, J. and Gudowski, W., "An efficient parallel computing scheme for Monte Carlo criticality calculations," *Ann. Nucl. Energy*, accepted for publication, 2009.

IV. Dufek, J. and Gudowski, W., "Stochastic Approximation for Monte Carlo Calculation of Steady-State Conditions in Thermal Reactors," *Nucl. Sci. Eng.*, Vol. 152, 2006, pp. 274.

V. Dufek, J. and Hoogenboom, E., "Numerical Stability of Existing Monte Carlo Burnup Codes in Cycle Calculations of Critical Reactors," *Nucl. Sci. Eng.*, accepted for publication, 2009.

Author's Contribution

The author has devised the new methods presented in the included papers, accomplished the numerical calculations, and written the text.

Papers not Included

The following papers are not included in the thesis:

i. Dufek, J. and Gudowski, W., "Managing the Xenon Oscillations in Monte Carlo Burn-up Calculations of Thermal Reactors," In *Proc. XII Meeting on Reactor Physics Calculations in the Nordic Countries*, Halden, Norway, May 17-18, 2005.

ii. Dufek, J., "Accelerated Monte Carlo Eigenvalue Calculations," In *Proc. XIII Meeting on Reactor Physics Calculations in the Nordic Countries*, Västerås, Sweden, March 29-30, 2007.

iii. Dufek, J., "Analysis of Coupling Schemes of the Major Monte Carlo Burnup Codes," In *Proc. XIV Meeting on Reactor Physics Calculations in the Nordic Countries*, Roskilde, Denmark, May 18-19, 2009.

iv. Dufek, J. and Gudowski, W., "Analysis and Improvement of the Fission Matrix Method for Source Convergence Acceleration in Monte Carlo Eigenvalue Calculations," Tech. rep., 2006, NURESIM work package no. T1.1.2., Milestone no. 4c

v. Dufek, J. and Gudowski, W., "Accelerated Stochastic Approximation of Steady-State Core Conditions," Tech. rep., 2007, NURESIM work package no. T1.1.2., Milestone no. 4d

vi. Dufek, J., "Analysis of Efficient Monte Carlo Reactor Cycle Calculations (Theoretical and Feasibility Study)," Tech. rep., 2007, NURESIM work package no. T1.1.2., Milestone No. 4e

vii. Dufek, J., "Performance of the Superhistory Powering Method," Tech. rep., 2008, NURESIM work package no. T1.1.2., Milestone No. 4h

viii. Dufek, J., Arzhanov, V., and Gudowski, W., "Nuclear Spent Fuel Management Scenarios," Swedish Nuclear Fuel and Waste Management Co, Box 5864, June 2006, SKB R-06-61.

ix. Ålander, A., Dufek, J., and Gudowski, W., "From Once-Through Nuclear Fuel Cycle to Accelerator-Driven Transmutation," *Nuclear Instruments and Methods in Physics Research A*, Vol. 562, 2006, pp. 630–633.

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Stockholm, May 2009

Jan Dufek

Contents

To the Free World

Chapter 1

Introduction

> Progress cannot be organised.
>
> *Ludwig Von Mises (1881-1973)*

The Monte Carlo method approximates solutions to mathematical problems via statistical sampling experiments on a computer. The method is commonly applied to problems with some probabilistic structure; but it is not limited to these problems. The main advantage is that, no matter how complicate the problem is, the absolute error in the estimated solution can decrease as $n^{-1/2}$ through collecting n random observations. On the contrary, other (deterministic) methods that perform n-point evaluations in d-dimensional space can converge as $n^{-1/d}$ at best [2]. The Monte Carlo method can thus solve very complicate problems more efficiently than the deterministic methods.

1.1 Brief History

Origins of statistical sampling methods can be traced back to the seventeenth and eighteenth century when mathematicians started to form the probability theory. Nineteenth-century statisticians realised that the mean of a continuous random variable took the form of an integral, and statistical sampling methods could be used to approximate the integral solution in a non-probabilistic problem. In the early twentieth century, mathematicians noticed that solutions to stochastic problems often corresponded to solutions of partial differential equations, and, so the stochastic problems could be solved by difference equation methods. It became apparent later that, conversely, the partial differential and integral equations had analogs in stochastic processes, and statistical sampling methods could be used to approximate solutions of these equations. Yet, the statistical sampling methods were of little use in the pre-electronic computing era.

The statistical sampling methods became useful with the advent of electronic computers. The first ambitious statistical sampling experiments, simulating the

neutron transport in fissile materials, were suggested by Stanislaw Ulam and John von Neumann after the World War II, and accomplished on the very first electronic computer, the ENIAC (the Electronic Numerical Integrator and Computer). At that time, the method was assigned a new attractive name, "the Monte Carlo method", by Nicholas Metropolis [3]. The Monte Carlo method was also further developed and popularised by Enrico Fermi, Robert Richtmyer, and others.

In particular, Stanislaw Ulam and John von Neumann realised that the standard Monte Carlo method could be modified to generate the solution to the original problem with a reduced variance at the same computational cost. The modified methods, known as the variance reduction techniques, became essential for any efficient application of the Monte Carlo method. The availability of the variance reduction techniques distinguishes the Monte Carlo method from the simple sampling experiments that preceded it historically. In fact, the notion "Monte Carlo methods" is commonly used as a synonym for the variance reduction techniques.

Today, the Monte Carlo methods are successfully applied to many problems in mathematics, physics, chemistry, environmental modelling, financial engineering, and many other fields. In reactor physics, the Monte Carlo method is recognised as the only feasible approach capable of providing detail insight into complex neutron transport problems.

1.2 Thesis Overview

The author has focused on development of methods for three relating problems in Monte Carlo reactor physics: efficient Monte Carlo criticality calculations, effective non-linear steady-state Monte Carlo calculations, and reliable and numerically stable Monte Carlo burnup calculations.

Author's work is presented exclusively in the included papers. Paper I demonstrates and explains a dubious convergence of the fission matrix acceleration methods that have been suggested for accelerating the convergence of the Monte Carlo fission source in criticality calculations. A new method, based on the fission matrix, is suggested for criticality calculations in Paper II; the method allows to cancel the inactive cycles, and thus solves the problem of the slow convergence of the fission source in Monte Carlo criticality calculations. Paper III introduces a new parallel-computing scheme for Monte Carlo criticality calculations. This scheme, based on the method described in Paper II, is expected to be very efficient on computers with a large number of processors. Paper IV describes an efficient iteration of steady-state core conditions by the Monte Carlo approach; this method is useful for effective Monte Carlo analyses of running power reactors. Finally, Paper V reviews coupling schemes in existing Monte Carlo burnup codes, and demonstrates their numerical instability in fuel cycle calculations; the paper recommends implementing the stable coupling schemes from accomplished deterministic burnup codes into the future Monte Carlo burnup codes. Papers I-V are briefly summarised in Chapter 5.

Chapters 2-4 introduce the known methods, phenomena, equations and quantities that the reader of the included papers should be informed about; these chapters are introductory and do not describe author's work. Specifically, Chapter 2 briefly presents the Monte Carlo methods in general; Chapter 3 describes some elements of the reactor physics that are relevant to the convergence of the Monte Carlo fission source in criticality calculations; and Chapter 4 introduces the steady-state and burnup problems.

Chapter 2

Introduction to Monte Carlo Methods

> The 50-50-90 rule:
> Anytime you have a 50-50 chance of getting something right, there's a 90% probability you'll get it wrong.
>
> *Andy Rooney (1919 -)*

This chapter describes the elementary algorithms needed to perform statistical sampling experiments, and introduces the basic Monte Carlo methods.

2.1 Random Variables

A random variable X is a function that can take on either a finite number of values $x_i \in R$ (discrete random variable), each with a certain associated probability $f_X(x_i) = P(X = x_i)$, or an infinite number of values x (continuous random variable) whose probabilities are described by a probability density function (pdf) $f_X(x)$,

$$\int_{-\infty}^{\infty} f_X(x)\mathrm{d}x = 1.$$

The probability that a continuous random variable X gives a value smaller or equal a certain x is given by the cumulative distribution function (cdf)

$$F_X(x) \equiv P(X \leq x) = \int_{-\infty}^{x} f_X(\xi)\mathrm{d}\xi.$$

The distribution function is defined for discrete random variables as

$$F_X(x) = \sum_{x_i \leq x} P(X = x_i).$$

Each random variable X has an expectation value $\mathrm{E}[X]$ that is the mean of all possible values x weighted according to their probability. The expectation value of a continuous random variable is

$$\mathrm{E}[X] = \int_{-\infty}^{\infty} x f_X(x) \mathrm{d}x;$$

similarly, the expectation value of a discrete random variable is

$$\mathrm{E}[X] = \sum_i x_i f_X(x_i).$$

It is often important to quantify how the random values are spread about the expectation value. A common measure of the spread is the variance $\mathrm{Var}[X]$, i.e. the expected quadratic deviation from the expectation value,

$$\mathrm{Var}[X] = \mathrm{E}[(X - \mathrm{E}[X])^2]. \tag{2.1}$$

It follows from Eq. (2.1) that

$$\begin{aligned} \mathrm{Var}[X] &= \mathrm{E}[X^2 - 2X\mathrm{E}[X] + (\mathrm{E}[X])^2] \\ &= \mathrm{E}[X^2] - 2(\mathrm{E}[X])^2 + (\mathrm{E}[X])^2 \\ &= \mathrm{E}[X^2] - (\mathrm{E}[X])^2. \end{aligned} \tag{2.2}$$

It is convenient to measure the spread with the same unit as that of the expectation value; therefore, the standard deviation σ_X has been introduced,

$$\sigma_X = \sqrt{\mathrm{Var}[X]}.$$

Sometimes, several random variables need to be combined. It is then useful to know how the respective random variables relate to each other. This can be quantified by the covariance $\mathrm{Cov}[X, Y]$ of two random variables X and Y,

$$\mathrm{Cov}[X, Y] = \mathrm{E}[(X - \mathrm{E}[X])(Y - \mathrm{E}[Y])]. \tag{2.3}$$

It follows from Eq. (2.3) that

$$\begin{aligned} \mathrm{Cov}[X, Y] &= \mathrm{E}\left[XY - Y\mathrm{E}[X] - X\mathrm{E}[Y] + \mathrm{E}[X]\mathrm{E}[Y]\right] \\ &= \mathrm{E}[XY] - \mathrm{E}[X]\mathrm{E}[Y]. \end{aligned} \tag{2.4}$$

Since the covariance is an absolute measure of the relation between two random variables it is sometimes useful to use the correlation coefficient

$$\rho_{X,Y} = \frac{\mathrm{Cov}[X, Y]}{\sqrt{\mathrm{Var}[X]\mathrm{Var}[Y]}}.$$

The correlation coefficient is always in the interval $[-1, 1]$. When $\rho_{X,Y} > 0$ then X and Y are positively correlated, i.e. it is likely that both X and Y give large

(or small) values at the same time. When $\rho_{X,Y} < 0$ then X and Y are negatively correlated, i.e. it is likely that X gives a small value when Y gives a large value and vice versa. If $\rho_{X,Y} = 0$ then X and Y are uncorrelated.

Uncorrelated random variables, however, still may be dependent on each other. For instance [4], let $X = Y^2$ with Y being uniformly distributed between -1 and 1; then $\rho_{X,Y} = 0$, although X is dependent on Y. Two random variables X and Y are independent if for each x and y holds that

$$f_{X,Y}(x, y) = f_X(x) f_Y(y),$$

where $f_{X,Y}(x, y)$ is the probability that $(X, Y) = (x, y)$. Nevertheless, if two random variables are independent then they are also uncorrelated.

2.2 Generators of Pseudorandom Numbers

A random variable can be sampled e.g. via the *inverse transform method* (see Sec. 2.3) using random numbers generated from a uniform distribution between 0 and 1, $\mathscr{U}(0, 1)$. The most convenient and reliable way of generating the random numbers for simulations is via deterministic algorithms - pseudorandom number generators. In fact, the numbers produced by pseudorandom number generators are not random; the same sequence of numbers will be generated on the same conditions. Nevertheless, numbers generated by good generators should appear to be statistically independent, not correlated; the sequence of generated numbers should be indistinguishable from a real random sequence.

The most widely used generators are the *linear congruential generators* (LCGs) [2, 5, 6]. Integer numbers, x_n, are generated by the recurrence

$$x_n = (a x_{n-1} + c) \bmod m, \tag{2.5}$$

where $m > 0$, $a > 0$, and c are integers called the modulus, the multiplier, and the additive constant, respectively. The "mod m" is the operation of taking the least nonnegative residue modulo m. In order to produce values u_n in the interval [0, 1], one can divide x_n by m,

$$u_n = x_n / m.$$

In general, the maximal period length for LCGs is m. If $c = 0$ (*multiplicative linear congruential generator*) then the maximal period length cannot exceed $m - 1$ as $x_n = 0$ must be avoided. Common values of m are $m = 2^{31} - 1$ and $m = 2^{32}$. These values, however, appear to be too small for the requirements of today's simulations.

The following example illustrates generating several numbers via the LCG with $m = 2^{31} - 1 = 2147483647$, $c = 0$, and $a = 16807$ (originally suggested in [7]). For

the initial seed $x_0 = 987654321$ one gets

$$\begin{aligned} x_1 &= 16807 \times 987654321 \bmod m = 1605065384, \\ u_1 &= 1605065384/m = 0.7474168133, \\ x_2 &= 16807 \times 1605065384 \bmod m = 1791818921, \\ u_2 &= 1791818921/m = 0.8343807058, \\ x_3 &= 16807 \times 1791818921 \bmod m = 937423366, \\ u_3 &= 937423366/m = 0.4365217716, \end{aligned}$$

and so on. To correctly evaluate the products of the integer numbers, the described generator must operate with 8 byte integer numbers (at least).

Many random number generators used for simulation are based on linear recurrences of the general form [8]

$$x_n = (a_1 x_{n-1} + \ldots + a_k x_{n-k}) \bmod m, \tag{2.6}$$

where k is a positive integer, and the coefficients $a_1, \ldots, a_k$ are integers in

$$\{1 - m, \ldots, m - 1\}$$

with $a_k \neq 0$. The output is again $u_n = x_n/m$. The generator (2.6), called a *multiple recursive generator* (MRG), corresponds to LCG for k = 1.

There are other, more advanced, generators, e.g. the *nonlinear generators* [9, 10].

2.3 Generating Samples

Sample values of a random variable X may be generated by several various methods, depending on the properties of F_X. All methods, however, produce samples x from F_X by transforming the random variable U described by pdf $\mathscr{U}(0, 1)$.

The *inverse transform method* [11] provides the most direct way of generating samples from $F_X(x)$ on the interval $[a, b]$; it uses the inverted form of $F_X(x)$,

$$F_X^{-1}(u) = \inf\{x \in [a, b] : F_X(x) \geq u, 0 \leq u \leq 1\}.$$

A random sample x of X can be obtained easily as

$$x = F_X^{-1}(u),$$

where u is randomly sampled from pdf $\mathscr{U}(0, 1)$.

Although F_X^{-1} exists for any random variable X, it may not be in a form suitable for efficient computation. In such a case, the *acceptance-rejection method* [12] can be more efficient. This technique generates samples from any pdf $f_X(x)$ using another pdf $h(x)$ for that holds that

$$f_X(x) \leq h(x)c,$$

where

$$c = \sup_x [f_X(x)/h(x)].$$

The value of c is ≥ 1. The algorithm generates two random numbers: x from pdf $h(x)$, and u from pdf $\mathscr{U}(0,1)$; if

$$u \cdot c \cdot h(x) < f_X(x), \tag{2.7}$$

then x is accepted. If Eq. (2.7) is not satisfied then x is rejected, and the algorithm must start from the beginning. It can be proved that the accepted samples have pdf $f_X(x)$. The proportion of proposed samples which are accepted is

$$\frac{\int_{-\infty}^{\infty} f_X(x)\mathrm{d}x}{\int_{-\infty}^{\infty} c \cdot h(x)\mathrm{d}x} = \frac{1}{c}.$$

Thus, to ensure a good efficiency, c should be close to unity. This can be satisfied only when $h(x)$ is chosen close to $f_X(x)$. Yet, it must be possible to generate the samples from $h(x)$ easily using the inverse transform method.

2.4 Sampling Methods

During Monte Carlo simulations, random variables with unknown pdf's, that are difficult to calculate deterministically to a required precision (e.g., neutron collision densities in a fissile system), are studied via sampling the random variables with known pdf's (e.g., particle transport kernels). Sec. 2.4.1 describes the basic Monte Carlo method, the *simple sampling*.

Often, some information about the solution is known or easily available. Methods, commonly referred to as the variance reduction techniques, can use this information to increase the accuracy of the Monte Carlo calculations. The basic variance reduction techniques are introduced in Sections 2.4.2 - 2.4.5. Nevertheless, reducing the variance does not necessarily implies an improvement of the computational efficiency as the method may be computationally demanding. The efficiency of a calculation may be expressed by the figure-of-merit (FOM),

$$\mathrm{FOM} = \frac{1}{\sigma^2 t}, \tag{2.8}$$

where t is the total computational time, and σ is the relative standard deviation of a calculated quantity.

2.4.1 Simple Sampling

In its simplest form, a Monte Carlo calculation samples an unknown random variable Y using a numerical model (function) g,

$$Y = g(X), \tag{2.9}$$

where X is an input random variable described by a known cdf F_X. The objective is to estimate the expectation value and variance of Y, and the variance of the estimated expectation value of Y. The Monte Carlo calculation becomes useful if the required results (e.g. the expectation value of Y) cannot be computed easily due to a very complex function g.

After sampling n values, y_1, y_2, ..., y_n , of Y, the expectation value of Y can be estimated by the mean value of y_1, y_2, ..., y_n,

$$m_Y = \frac{1}{n}\sum_{i=1}^{n} y_i. \tag{2.10}$$

The mean value m_Y is also a random variable. According to the central limit theorem [13], m_Y is normally distributed with a mean $\mathrm{E}[Y]$,

$$\mathrm{E}[m_Y] = \mathrm{E}[Y].$$

The variance of m_Y, which estimates the precision of the computed m_Y, equals

$$\begin{aligned}
\mathrm{Var}[m_Y] &= \mathrm{E}[(m_Y - \mathrm{E}[Y])^2] \\
&= \mathrm{E}\left[\left(\frac{\sum y_i}{n} - \mathrm{E}[Y]\right)^2\right] \\
&= \mathrm{E}\left[\left(\frac{\sum (y_i - \mathrm{E}[Y])}{n}\right)^2\right] \\
&= \mathrm{E}\left[\frac{(\sum \xi_i)^2}{n^2}\right] \\
&= \frac{\mathrm{E}(\sum \xi_i)^2}{n^2} \\
&= \frac{1}{n^2}\left[\sum \mathrm{E}[\xi_i^2] + 2\sum \mathrm{E}[\xi_i\xi_{i+1}] + 2\sum \mathrm{E}[\xi_i\xi_{i+2}] + \ldots\right],
\end{aligned} \tag{2.11}$$

where

$$\xi_i \equiv y_i - \mathrm{E}[Y].$$

If ξ_i are statistically independent then the cross products $\mathrm{E}[\xi_i\xi_{i+1}]$, $\mathrm{E}[\xi_i\xi_{i+2}]$, etc. in Eq. (2.11) equal zeros, and

$$\begin{aligned}
\mathrm{Var}[m_Y] &= \frac{\sum \mathrm{E}[\xi_i^2]}{n^2} \\
&= \frac{n\mathrm{E}[\xi_i^2]}{n^2} \\
&= \frac{\mathrm{Var}[Y]}{n}.
\end{aligned} \tag{2.12}$$

Nevertheless, Var[Y] in Eq. (2.12) is not known, and must be estimated by

$$\begin{aligned} s_Y^2 &= \frac{1}{n}\sum_{i=1}^{n}(y_i - m_Y)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n} y_i^2 - m_Y^2, \end{aligned} \tag{2.13}$$

i.e., the variance of m_Y is approximated by

$$s_{m_Y}^2 = \frac{s_Y^2}{n}. \tag{2.14}$$

In order to estimate E[Y] by Eq. (2.10) and Var[m_Y] by Eq. (2.13), only the values of $\sum y_i^2$ and $\sum y_i$ need to be updated after collecting a new sample of Y.

It is important to realise that even when Var[m_Y] is estimated very small by Eq. (2.13), the actual error in m_Y may be surprisingly large; the real error in m_Y is not known. It is a common misunderstanding to assume that collecting more samples will always result in a smaller error in the computed value of m_Y. In reality, the error in m_Y may become larger when more samples are collected.

It is common to enumerate a confidence interval $(m_Y - \delta, m_Y + \delta)$ that includes the correct value of E[Y] with some probability P. Assuming that m_Y is normally distributed with the expectation value E[Y], the pdf of m_Y can be written as

$$f_{m_Y} = \frac{1}{\sigma_{m_Y}\sqrt{2\pi}} \exp\left(-\frac{(m_Y - \mathrm{E}[Y])^2}{2\sigma_{m_Y}^2}\right),$$

where $\sigma_{m_Y} = \sqrt{\mathrm{Var}[m_Y]}$ is the standard deviation of m_Y.

The value E[Y] is then present inside the interval $[m_Y - \delta, m_Y + \delta]$ (and so the value m_Y is present inside the interval $[\mathrm{E}[Y] - \delta, \mathrm{E}[Y] + \delta]$) with probability

$$\begin{aligned} P &= \int_{\mathrm{E}[Y]-\delta}^{\mathrm{E}[Y]+\delta} \frac{1}{\sigma_{m_Y}\sqrt{2\pi}} \exp\left(-\frac{(y - \mathrm{E}[Y])^2}{2\sigma_{m_Y}^2}\right)\mathrm{d}y \\ &= \frac{2}{\sigma_{m_Y}\sqrt{2\pi}} \int_{\mathrm{E}[Y]}^{\mathrm{E}[Y]+\delta} \exp\left(-\frac{(y - \mathrm{E}[Y])^2}{2\sigma_{m_Y}^2}\right)\mathrm{d}y \\ &= \frac{2}{\sigma_{m_Y}\sqrt{2\pi}} \int_{0}^{\delta} \exp\left(-\frac{y^2}{2\sigma_{m_Y}^2}\right)\mathrm{d}y \\ &= \mathrm{erf}\left(\frac{\delta}{\sigma_{m_Y}\sqrt{2}}\right), \end{aligned} \tag{2.15}$$

where erf(x) is the Gauss error function. Since σ_{m_Y} in Eq. (2.15) is not known, it must be approximated by s_{m_Y}. The probability P given by Eq. (2.15) is enumerated for several δ/σ_{m_Y} in Table 2.1.

Table 2.1: Probability level P for various confidence intervals [14].

P	δ/σ_{m_Y}
0.6826895	1
0.9544997	2
0.9973002	3
0.9999366	4
0.9999994	5

2.4.2 Control Variates

In some cases, the numerical model $g(X)$ from Eq. (2.9) with an unknown expectation value $\mathrm{E}[Y] \equiv \mathrm{E}[g(X)]$ may be approximated by a simpler model (*control variate*, see e.g. [15])

$$Z = g^*(X)$$

with a known expectation value $\mathrm{E}[Z]$. The mean value of Y can be then computed as

$$m_Y = m_{(Y-Z)} + \mathrm{E}[Z]$$

by sampling the difference between the random variables Y and Z, and computing the mean value of the difference. The variance of m_Y is equal to the variance of $m_{(Y-Z)}$,

$$\begin{aligned}\mathrm{Var}[m_Y] =& \mathrm{Var}[m_{(Y-Z)}] \\ =& \frac{\mathrm{Var}[Y-Z]}{n} \\ =& \frac{\mathrm{Var}[Y]+\mathrm{Var}[Z]-2\mathrm{Cov}[Y,Z]}{n}.\end{aligned}$$

Therefore, if the control variate Z is strongly positively correlated to Y, it is then possible that

$$2\mathrm{Cov}[Y,Z] > \mathrm{Var}[Z], \tag{2.16}$$

in which case $\mathrm{Var}[m_Y]$ will be decreased. Evaluating the function $g^*(X)$ must, however, not slow down the calculation, otherwise, the efficiency of the technique may not be improved over the efficiency of simple sampling.

2.4.3 Correlated Sampling

Often, a difference between two very similar models g_1 and g_2 needs to be studied,

$$\begin{aligned}Y_1 &= g_1(X), \\ Y_2 &= g_2(X).\end{aligned}$$

Commonly, g_2 is a slightly modified model g_1. Since the difference

$$\mathrm{E}[Y_1] - \mathrm{E}[Y_2]$$

may be very small, the simple sampling would need to calculate $\mathrm{E}[Y_1]$ and $\mathrm{E}[Y_2]$ to a very good accuracy, which could require a large computational time. *Correlated sampling* can efficiently resolve this problem by studying the random variable

$$\begin{aligned} Z &= Y_1 - Y_2 \\ &= (g_1 - g_2)(X). \end{aligned}$$

Variance of Z is

$$\mathrm{Var}[Z] = \mathrm{Var}[Y_1] + \mathrm{Var}[Y_2] - 2\mathrm{Cov}[Y_1, Y_2].$$

Thus, if Y_1 and Y_2 are strongly positively correlated to each other, which is likely when g_1 and g_2 are very similar, then simple sampling of Z is more efficient than sampling Y_1 and Y_2 separately using independent input random variable X. While correlated sampling can efficiently improve the estimate of $\mathrm{E}[Y_1 - Y_2]$, it does not affect the accuracy of the estimates of $\mathrm{E}[Y_1]$ and $\mathrm{E}[Y_2]$.

2.4.4 Stratified Sampling

Depending on the numerical model

$$Y = g(X),$$

simple sampling the random variable X from f_X may not be the most efficient way of estimating $\mathrm{E}[Y]$. It may happen that $g(x)$ is very large for some values x with a very small $f_X(x)$. If these important values of X are not sampled, the value of $\mathrm{E}[Y]$ would not be estimated well. It is then appropriate to separate an interval with important values of X, and analyse it separately. This is the idea of the *stratified sampling*. The value interval for X is divided into several strata (groups), and each stratum is analysed separately. In order to divide the values of X into strata some knowledge about f_Y is needed.

Let X be divided into L strata X_i, $i = 1, \ldots, L$. Since f_X is known, the probability ω_i that x sampled from f_X falls into X_i can be precisely calculated. Dividing X into strata X_i causes Y be also divided into corresponding strata Y_i; i.e., samples x from X_i will generate samples $y = g(x)$ from Y_i. It can be shown that

$$\mathrm{E}[Y] = \sum_{i=1}^{L} \omega_i \, \mathrm{E}[Y_i],$$

and

$$\mathrm{Var}[m_Y] = \sum_{i=1}^{L} \omega_i^2 \, \frac{\mathrm{Var}[Y_i]}{n_i}, \tag{2.17}$$

where n_i is the total number of samples x in X_i. Since $\mathrm{E}[Y_i]$ is not known for any i, the expectation value must be estimated by

$$m_Y = \sum_{i=1}^{L} \omega_i \, m_{Y_i}.$$

If strata have been designed well then it is likely that $\mathrm{Var}[m_Y]$ given by Eq. (2.17) is smaller than $\mathrm{Var}[m_Y]$ resulting from simple sampling. On the other hand, a poor stratification will result in an increased variance.

The variance given by Eq. (2.17) is minimised if the samples are distributed in strata according to the *Neyman allocation* [16]

$$n_i = n\frac{\omega_i\sigma_{Y_i}}{\sum_{j=1}^{L}\omega_j\sigma_{Y_j}}, \tag{2.18}$$

where σ_{Y_i} is the standard deviation of Y_i. Nevertheless, Eq. (2.18) cannot be used for distributing samples at the beginning of the calculation since σ_{Y_i} are not known for any i. Therefore, the simulation is commonly divided into batches; the strata in the first batch may contain equal number of samples. In the following batches, σ_{Y_i} can be estimated for all i, and samples can be distributed more efficiently. Nevertheless, there is a risk of estimating σ_{Y_i} incorrectly in the first batch, which could result in a wrong distribution of the following batches. This would increase the variance of $\mathrm{E}[Y]$.

2.4.5 Importance Sampling

Importance sampling (e.g. [17]) is similar to the stratified sampling in the sense that values of X that have larger impact on $\mathrm{E}[Y]$ are preferred. This is achieved by sampling X not from f_X, but from another pdf f_Z (the importance function). This must be compensated by multiplying the sampled values of Y by a correction factor

$$\frac{f_X(x)}{f_Z(x)}.$$

Let the random variable Z be defined as

$$Z = g(x)\frac{f_X(x)}{f_Z(x)}.$$

If x is sampled from f_Z then the expectation value $\mathrm{E}[Z]$ equals $\mathrm{E}[Y]$,

$$\begin{aligned}\mathrm{E}[Z] &= \int_x g(x)\frac{f_X(x)}{f_Z(x)}f_Z(x)\mathrm{d}x \\ &= \int_x g(x)f_X(x)\mathrm{d}x \\ &= \mathrm{E}[Y].\end{aligned}$$

The variance of Z is

$$\begin{aligned}\mathrm{Var}[Z] &= \mathrm{E}[Z^2] - \mathrm{E}[Z] \\ &= \int_x g^2(x)\frac{f_X^2(x)}{f_Z(x)}\mathrm{d}x - \mathrm{E}[Y].\end{aligned} \tag{2.19}$$

Thus, if the importance function is chosen such that

$$f_Z(x) = \frac{g(x) f_X(x)}{\mathrm{E}[Y]} \tag{2.20}$$

then, according to Eq. (2.19),

$$\mathrm{Var}[Z] = 0.$$

In this case, only one sample would be sufficient to obtain the precise value of $\mathrm{E}[Y]$ (with a zero variance). Therefore, this method is sometimes called the *zero-variance scheme*.

Computing the precise importance function $f_Z(x)$ according to Eq. (2.20) is computationally equivalent to enumerating the value of $\mathrm{E}[Y]$. Therefore, in practice, the importance function must be derived using numerical models much simpler than $g(x)$, so the zero variance is never obtained. Nevertheless, a certain variance reduction can be achieved if the importance function is designed sufficiently well. The efficiency, however, may not be improved proportionally to the variance since the correction factors must be computed for each sample, which may be computationally expensive. Again, there is a risk that this technique will increase the variance if the importance function is not optimal.

Chapter 3

Criticality Problems

How much easier it is to be critical than to be correct.

Benjamin Disraeli (1804 - 1881)

This chapter describes the general neutron transport equation, its relation to the eigenvalue equation, and the Monte Carlo solution of the eigenvalue equation. Existing techniques designed to improve the convergence of the Monte Carlo fission source are introduced.

3.1 The Transport Equation

The transport theory aims at determining the distribution of particles in a system, accounting for the motion of particles and their interaction with the medium. In order to determine the particle density $N(\mathbf{r}, t)$, that would be sufficient for most applications, the particle velocity $\mathbf{v}$ must also be considered as there is no equation that could adequately describe $N(\mathbf{r}, t)$ [18]. The distribution of particles is then described by a particle phase space density function $n(\mathbf{r}, \mathbf{v}, t)$;

$$n(\mathbf{r}, \mathbf{v}, t)\, \mathrm{d}^3 r\, \mathrm{d}^3 v \tag{3.1}$$

equals the expected number of particles in $\mathrm{d}^3 r$ about $\mathbf{r}$ with velocity in $\mathrm{d}^3 v$ about $\mathbf{v}$ at time t. If $n(\mathbf{r}, \mathbf{v}, t)$ is known then the particle density can be obtained as

$$N(\mathbf{r}, t) = \int \mathrm{d}^3 v\; n(\mathbf{r}, \mathbf{v}, t).$$

The particle velocity vector $\mathbf{v}$ is usually decomposed into the unit vector in the direction of motion, $\mathbf{\Omega} = \mathbf{v}/\|\mathbf{v}\|$, and the particle kinetic energy, $E = mv^2/2$. The particle phase space density is then defined so that

$$n(\mathbf{r}, E, \mathbf{\Omega}, t)\, \mathrm{d}^3 r\, \mathrm{d}E\, \mathrm{d}\mathbf{\Omega} \tag{3.2}$$

equals the expected number of particles in d^3r about $\mathbf{r}$ with kinetic energy E in $\mathrm{d}E$ moving about direction $\mathbf{\Omega}$ in solid angle $\mathrm{d}\mathbf{\Omega}$. Equating (3.1) to (3.2) shows that the particle phase space density can be transformed between various sets of variables as

$$n(\mathbf{r}, E, \mathbf{\Omega}, t) = \frac{v}{m} n(\mathbf{r}, \mathbf{v}, t)$$

since

$$\begin{aligned} \mathrm{d}\mathbf{\Omega} &= \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\varphi, \\ \mathrm{d}^3 v &= v^2 \mathrm{d}v \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\varphi, \\ \mathrm{d}E &= mv \, \mathrm{d}v, \end{aligned}$$

where (θ, φ) are the spherical coordinates. Similarly,

$$\begin{aligned} n(\mathbf{r}, v, \mathbf{\Omega}, t) &= v^2 n(\mathbf{r}, \mathbf{v}, t), \\ n(\mathbf{r}, E, \mathbf{\Omega}, t) &= \frac{1}{mv} n(\mathbf{r}, v, \Omega, t). \end{aligned}$$

Sometimes, $n(\mathbf{r}, E, \mathbf{\Omega}, t)$ is referred to as the angular density to distinguish it from the total particle density $N(\mathbf{r}, t)$.

The general form of the transport equation can be derived by equating the substantial derivative describing the time rate of change of the local particle density along the particle trajectory to the change in the local density due to collisions $(\partial n/\partial t)_{\mathrm{coll}}$ and sources $q(\mathbf{r}, \mathbf{v}, t)$,

$$\frac{\mathrm{d}n(\mathbf{r}, \mathbf{v}, t)}{\mathrm{d}t} = \left(\frac{\partial n}{\partial t} \right)_{\mathrm{coll}} + q(\mathbf{r}, \mathbf{v}, t). \tag{3.3}$$

Since

$$\begin{aligned} \frac{\mathrm{d}n}{\mathrm{d}t} &= \frac{\partial n}{\partial t} + \frac{\partial \mathbf{r}}{\partial t} \frac{\partial n}{\partial \mathbf{r}} + \frac{\partial \mathbf{v}}{\partial t} \frac{\partial n}{\partial \mathbf{v}} \\ &= \frac{\partial n}{\partial t} + \mathbf{v} \nabla n + \frac{\mathbf{F}}{m} \frac{\partial n}{\partial \mathbf{v}}, \end{aligned}$$

where $\operatorname{grad} n = \nabla n = \partial n / \partial \mathbf{r}$, the transport equation takes the form

$$\frac{\partial n}{\partial t} + \mathbf{v} \nabla n + \frac{\mathbf{F}}{m} \frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\partial n}{\partial t} \right)_{\mathrm{coll}} + q. \tag{3.4}$$

In order to specify the collision term $(\partial n/\partial t)_{\mathrm{coll}}$, several following quantities need to be defined:

- $\Sigma(\mathbf{r}, \mathbf{v})$ is the mean number of particle interactions per unit distance travelled by particle of velocity $\mathbf{v}$ at position $\mathbf{r}$, and is referred to as the *macroscopic cross section*. The inverse of $\Sigma(\mathbf{r}, \mathbf{v})$ corresponds to the *mean free path* (mfp). $\Sigma(\mathbf{r}, \mathbf{v})$ can be decomposed as

$$\Sigma(\mathbf{r}, \mathbf{v}) = N_B(\mathbf{r}) \sigma(\mathbf{r}, \mathbf{v}),$$

where $N_B(\mathbf{r})$ is the number density of the medium. σ is referred to as the *microscopic cross section*.

- $f(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ is the *scattering probability function* that describes the probability distribution of velocities of the secondary particle (i.e. the collided particle, not necessarily the same particle as before the collision). Exactly,

$$f(\mathbf{r}, \mathbf{v}' \to \mathbf{v})\mathrm{d}^3 v$$

is the probability that a secondary particle induced by an incident particle with velocity $\mathbf{v}'$ at position $\mathbf{r}$ will be emitted with velocity $\mathbf{v}$ in $\mathrm{d}^3 v$.

- $c(\mathbf{r}, \mathbf{v})$ is the mean number of secondary particles emitted in a collision event experienced by an incident particle with velocity $\mathbf{v}$ at position $\mathbf{r}$. In non-absorbing and non-multiplying medium, $c = 1$.

- $\Sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$, the *collision kernel*, is defined as

$$\Sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) = \Sigma(\mathbf{r}, \mathbf{v}')c(\mathbf{r}, \mathbf{v}')f(\mathbf{r}, \mathbf{v}' \to \mathbf{v}),$$

and equals the mean number of secondary particles of velocity $\mathbf{v}$ produced per unit distance travelled by an incident particle of velocity $\mathbf{v}'$ at position $\mathbf{r}$.

The frequency of collision events experienced by a particle of velocity $\mathbf{v}$ is then given by

$$v\Sigma(\mathbf{r}, \mathbf{v}),$$

and the rate at which the reactions occur in a unit volume equals

$$v\Sigma(\mathbf{r}, \mathbf{v})n(\mathbf{r}, \mathbf{v}, t).$$

The collision term $(\partial n/\partial t)_{\mathrm{coll}}$ can be thus written as

$$\left(\frac{\partial n}{\partial t}\right)_{\mathrm{coll}} = \int \mathrm{d}^3 v'\, v' \Sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) - v\Sigma(\mathbf{r}, \mathbf{v})n(\mathbf{r}, \mathbf{v}, t).$$

So, the general transport equation takes the form

$$\frac{\partial n}{\partial t} + \mathbf{v}\nabla n + \frac{\mathbf{F}}{m}\frac{\partial n}{\partial \mathbf{v}} + v\Sigma n = \int \mathrm{d}^3 v'\, v' \Sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) + q. \tag{3.5}$$

The term $\frac{\mathbf{F}}{m}\frac{\partial n}{\partial \mathbf{v}}$ in Eq. (3.5) can be neglected in the theory of neutron transport. Moreover, the neutron transport equation is commonly written in terms of the angular flux

$$\phi(\mathbf{r}, \mathbf{v}, t) \equiv vn(\mathbf{r}, \mathbf{v}, t)$$

as

$$\frac{1}{v}\frac{\partial \phi}{\partial t} + \mathbf{\Omega}\nabla\phi + \Sigma\phi = \int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega'\ \Sigma(\mathbf{r}, E' \to E, \Omega' \to \Omega)\phi(\mathbf{r}, E', \Omega', t) + q. \tag{3.6}$$

Considering only the neutron transport in a medium without an external source of neutrons ($q = 0$), $\Sigma(\mathbf{r}, \mathbf{v})$ and $\Sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ are known and independent of $n(\mathbf{r}, \mathbf{v}, t)$; therefore, Eq. (3.6) is linear, which means that if $\phi_1(\mathbf{r}, E, \Omega, t)$ and $\phi_2(\mathbf{r}, E, \Omega, t)$ are solutions of Eq. (3.6) then any linear combination of ϕ_1 and ϕ_2 is also a solution of Eq. (3.6).

The transport equation must be completed with the initial and boundary conditions. The initial angular flux $\phi_0(\mathbf{r}, E, \Omega)$ describes $\phi(\mathbf{r}, E, \Omega, t)$ for $t = 0$ for all $\mathbf{r}$ and $\mathbf{v}$, while the common boundary conditions usually include either the free surface (neutrons can only escape through the surface) or reflecting boundary (neutrons are reflected by the boundary) or interfaces (continuity of $\phi(\mathbf{r}, E, \Omega, t)$ is demanded across interfaces).

The collision kernel $\Sigma(\mathbf{r}, E' \to E, \Omega' \to \Omega)$ in Eq. (3.6) is commonly separated into two parts; a part

$$\Sigma_{\mathrm{f}}(\mathbf{r}, E' \to E, \Omega' \to \Omega)$$

that describes the fission events and a part

$$\Sigma_{\mathrm{sc}}(\mathbf{r}, E' \to E, \Omega' \to \Omega)$$

that describes all scattering events including $(\mathrm{n}, 2\mathrm{n})$, $(\mathrm{n}, 3\mathrm{n})$, capture and other reactions. Since the fission neutrons are emitted isotropically, the corresponding scattering probability function can be written as

$$f_{\mathrm{f}}(\mathbf{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) = \frac{1}{4\pi}\chi(\mathbf{r}, E' \to E),$$

where $\chi(\mathbf{r}, E' \to E)$ is the normalised energy spectrum of fission neutrons that is dependent of the fissile material; usually, it is possible to assume that χ is not dependent on E',

$$\chi(\mathbf{r}, E' \to E) = \chi(\mathbf{r}, E),$$

and can be approximated e.g. for $^{235}\mathrm{U}$ as [19]

$$\chi(\mathbf{r}, E) = \sqrt{\frac{2}{\pi \mathrm{e}}}\mathrm{e}^{-E}\sinh\sqrt{2E}.$$

The mean number of secondary (fission) neutrons emitted in a fission event induced by a neutron with energy E at position $\mathbf{r}$ is usually denoted as $\nu(\mathbf{r}, E)$; thus, $\Sigma_{\mathrm{f}}(\mathbf{r}, E' \to E, \Omega' \to \Omega)$ can be written as

$$\Sigma_{\mathrm{f}}(\mathbf{r}, E' \to E, \Omega' \to \Omega) = \Sigma_{\mathrm{f}}(\mathbf{r}, E')\frac{\chi(\mathbf{r}, E)}{4\pi}\nu(\mathbf{r}, E').$$

The transport equation with the separated collision kernels is then written as

$$\begin{aligned}\frac{1}{v}\frac{\partial\phi}{\partial t} + \boldsymbol{\Omega}\nabla\phi + \Sigma\phi = &\int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega'\ \Sigma_{\mathrm{sc}}(\mathbf{r}, E' \to E, \Omega' \to \Omega)\phi(\mathbf{r}, E', \Omega', t) \\ &+ \frac{\chi(\mathbf{r}, E)}{4\pi}\int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega'\ \Sigma_{\mathrm{f}}(\mathbf{r}, E')\nu(\mathbf{r}, E')\phi(\mathbf{r}, E', \Omega', t) + q.\end{aligned} \tag{3.7}$$

3.2 The Eigenvalue Equation

In general, the transport equation Eq. (3.7) yields a time-dependent neutron flux. A solution that is not dependent on time can only be achieved in sub-critical systems with external sources of neutrons (that are not in the scope of this thesis), or in critical systems (fixed systems providing a constant power with no external source of neutrons). In reality, however, there are no systems that are exactly critical; the reactors must be controlled continuously by small movements of control rods to maintain the required total power. Similarly, the numerical models of critical reactors are also never exactly critical; Eq. (3.7) would give a solution strongly dependent on time when applied on any system without an external source of neutrons. Yet, computing the equilibrium solutions for fissile systems is of a large importance to the reactor physics. The only way to achieve an equilibrium solution is to force the numerical model to become exactly critical. This is usually done by changing the value of $\nu(\mathbf{r}, E)$ in Eq. (3.7) to

$$\frac{\nu(\mathbf{r}, E)}{k}$$

with the value of k such that the solution is not dependent on time, i.e. $\partial\phi/\partial t = 0$ in Eq. (3.7). This changes Eq. (3.7) into

$$\begin{aligned} \mathbf{\Omega}\nabla\phi + \Sigma\phi = &\int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega' \; \Sigma_{\mathrm{sc}}(\mathbf{r}, E' \to E, \Omega' \to \Omega)\phi(\mathbf{r}, E', \Omega') \\ &+ \frac{1}{k}\frac{\chi(\mathbf{r}, E)}{4\pi} \int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega' \; \Sigma_{\mathrm{f}}(\mathbf{r}, E')\nu(\mathbf{r}, E')\phi(\mathbf{r}, E', \Omega'), \end{aligned} \tag{3.8}$$

where the external source of neutrons q is set to zero as Eq. (3.8) is designed for systems without the external source of neutrons. As shown below, Eq. (3.8) is an eigenvalue equation; it has many eigenvalues k_i and corresponding eigenfunctions ϕ_i. It should be, however, understood, that Eq. (3.8) has physical meaning only when $k = 1$, which means practically never. Nevertheless, the equation can be used to approximate the equilibrium neutron flux in systems that are almost critical, or to quantify how far from criticality the system actually is (by studying the value of k).

Using the following operators

$$S\phi = \mathbf{\Omega}\nabla\phi,$$

$$A\phi = \Sigma\phi,$$

$$S_{\mathrm{c}}\phi = \int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega' \; \Sigma_{\mathrm{sc}}(\mathbf{r}, E' \to E, \Omega' \to \Omega)\phi(\mathbf{r}, E', \Omega'),$$

$$F\phi = \frac{\chi(\mathbf{r}, E)}{4\pi} \int_0^\infty \mathrm{d}E' \int_{4\pi} \mathrm{d}\Omega' \; \Sigma_{\mathrm{f}}(\mathbf{r}, E')\nu(\mathbf{r}, E')\phi(\mathbf{r}, E', \Omega'),$$

Eq. (3.8) can be rewritten into the form

$$(S + A - S_{\mathrm{c}})\phi = \frac{1}{k} F\phi,$$

or

$$k\phi = L\phi, \tag{3.9}$$

where

$$L \equiv (S + A - S_{\mathrm{c}})^{-1} F,$$

where $(\cdot)^{-1}$ denotes an operator inverted to the operator inside the brackets. The k-eigenvalue spectrum of Eq. (3.9) may consist of infinite numbers of complex k-eigenvalues; the eigenvalues may be ordered so that $k_0 > |k_1| > |k_2| > \ldots$, where k_0 is always real. Nevertheless, only one eigenfunction ϕ_0 corresponding to the fundamental mode (largest) eigenvalue k_0 can be non-negative in the whole system, and has thus a physical meaning. The largest eigenvalue k_0 is denoted as k_{eff}.

Systems with $k_{\mathrm{eff}} < 1$ are subcritical, and cannot maintain the fission chain reaction (in reality); while systems with $k_{\mathrm{eff}} > 1$ are supercritical, and the power released during the fission chain reaction grows exponentially with time (in reality, as long as the macroscopic cross sections are constant in time).

The neutron flux $\phi(\mathbf{r}, E, \Omega)$ closely relates to the distribution of fission neutrons $s(\mathbf{r}, E)$ in the system; it is also possible to write the eigenvalue equation for $s(\mathbf{r}, E)$,

$$ks = Hs, \tag{3.10}$$

where the operator H applied on $s(\mathbf{r}, E)$ gives the next generation fission source. H is defined as

$$Hs \equiv \int_0^\infty \mathrm{d}E' \int_V \mathrm{d}^3 r'\, h(\mathbf{r}', E' \to \mathbf{r}, E) s(\mathbf{r}', E'), \tag{3.11}$$

where $h(\mathbf{r}', E' \to \mathbf{r}, E)\,\mathrm{d}E\,\mathrm{d}^3 r$ is an expected number of first generation fission neutrons produced in the volume element $\mathrm{d}^3 r$ at $\mathbf{r}$, in the energy element $\mathrm{d}E$ at E, resulting from a fission neutron born at $\mathbf{r}'$ with an energy E'. The angular dependence is not considered since fission neutrons are emitted isotropically. Solving Eq. (3.10) is equivalent to solving Eq. (3.9), and ϕ_0 and s_0 can be computed simultaneously.

3.3 Monte Carlo Solution of the Eigenvalue Equation

Let the eigenfunctions s_j and eigenvalues k_j of H (from Eq. (3.10)) be ordered so that $k_0 > |k_1| > |k_2| > \dots$. The fundamental mode source $s_0(\mathbf{r}, E)$ is usually computed by the power iteration

$$s_0^{(n)} = \frac{H s_0^{(n-1)}}{k_0^{(n)}}, \qquad n = 1, 2, \dots, \tag{3.12}$$

where $s_0^{(0)}$ is an initial nonzero guess, and $k_0^{(n)}$ (i.e. $k_{\text{eff}}^{(n)}$) may be computed, e.g., as

$$k_0^{(n)} = \frac{\int_0^\infty \mathrm{d}E \int_V \mathrm{d}^3 r \, H s_0^{(n-1)}(\mathbf{r}, E)}{\int_0^\infty \mathrm{d}E \int_V \mathrm{d}^3 r \, s_0^{(n-1)}(\mathbf{r}, E)}.$$

Any real function in the domain of H can be expressed as a weighted sum of the eigenfunctions s_i of H; therefore

$$\exists \gamma_i, \ i = 0, 1, \dots, \ s^{(0)} = \sum_i \gamma_i s_i. \tag{3.13}$$

Equations (3.12) and (3.13) yield

$$\begin{aligned} s^{(n)} &= H^n \sum_i \gamma_i s_i \\ &= \sum_i \gamma_i H^n s_i \\ &= \sum_i \gamma_i k_i^n s_i. \end{aligned} \tag{3.14}$$

If (3.14) is multiplied by k_0^n then

$$\frac{s^{(n)}}{k_0^n} = \gamma_0 s_0 + \left(\frac{k_1}{k_0}\right)^n \gamma_1 s_1 + \left(\frac{k_2}{k_0}\right)^n \gamma_2 s_2 + \dots$$

Since $1 > |k_1/k_0| > |k_2/k_0| > \dots$, $s^{(n)}$ converges to s_0 as $O\left((k_1/k_0)^n\right)$. The convergence rate of the power iteration is therefore governed by the dominance ratio k_1/k_0 [20]. Thus, the fission source converges slowly in systems with dominance ratios close to unity.

The power iteration is adapted in all Monte Carlo codes that support the criticality calculations. This is done by simulating successive neutron generations; each generation (cycle) contains a certain number, m, of neutrons. The neutron transport is simulated with the use of known pdf's of various random variables (e.g., the distance between collisions, the type of isotope and reaction at the collision site, the number of new fission neutrons, scattering angles, etc.). The fission source is thus

defined only in m sites in the system. The new fission neutrons sampled during the neutron transport are added into the so-called delay bank. At the end of each cycle, the delay bank is converted into the fission source for the subsequent cycle.

The neutron transport is usually not simulated analogously to the real transport. A better efficiency can be achieved in non-analogue simulations where each fission neutron is assigned a statistical weight that is multiplied at each collision by the factor

$$\frac{\Sigma_s}{\Sigma_t}.$$

A neutron is terminated when its statistical weight drops below a certain limit value. At each collision c of a neutron history h, $b_{h,c}$ fission neutrons with unit statistical weights are added into $\mathscr{S}^{(n)}$,

$$b_{h,c} \xleftarrow{\text{integer}} \frac{f_{h,c}}{k_{\text{eff}}^{(n-1)}},$$

where $f_{h,c}$ is the expected number of first generation fission neutrons, and $f_{h,c}/k_{\text{eff}}^{(n-1)}$ is randomly rounded to a neighbouring integer. The value of $f_{h,c}$ can be computed as

$$f_{h,c} = w_{h,c} \frac{\sum_q a_q \bar{\nu}_q \sigma_{f\,q}}{\sum_q a_q \sigma_{tot\,q}}\bigg|_{h,c},$$

where q is summed over all nuclides of the material, a_q is the atomic fraction of the q^{th} nuclide, $w_{h,c}$ is the statistical weight of the neutron h entering the collision c, and $\bar{\nu}_q$ is the average number of neutrons produced per fission by the q^{th} nuclide at the incident neutron energy. The actual number of neutrons in $\mathscr{S}^{(n)}$ may differ from m at the end of cycle n; therefore, the statistical weights of neutrons in $\mathscr{S}^{(n)}$ are normalised so that their total statistical weight equals m.

The value of k_{eff} can be sampled in each history h by the collision estimator as

$$k_{\text{eff}\,h} = \frac{\sum_c f_{h,c}}{w_{h,0}},$$

where $w_{h,0}$ is the initial statistical weight of neutron h (and also the statistical weight of $k_{\text{eff}\,h}$). Thus, the value of k_{eff} can be estimated in cycle n by

$$\begin{aligned} k_{\text{eff}}^{(n)} &= \frac{\sum_h w_{h,0} k_{\text{eff}\,h}}{\sum_h w_{h,0}} \\ &= \frac{\sum_{h,c} f_{h,c}}{m}, \quad \text{history } h \in \text{cycle } n, \end{aligned}$$

where index h is summed over all neutron histories in cycle n, and c is summed over all collisions in history h.

A number of inactive cycles must be performed to achieve the convergence of the fission source. The quantities of interest, like k_{eff}, neutron flux, reaction rates, etc., must be combined over a number of active cycles with a converged fission source.

3.4 Convergence of the Fission Source

Random sampling introduces statistical errors of the order $O(1/\sqrt{m})$ into the Monte Carlo source in each cycle. Although these errors decay in the subsequent cycles, the net error propagation over cycles causes the expected source $E(s^{(n)})$ to converge to a biased stationary distribution $s_{0,m}$ rather than to s_0. The difference between s_0 and $s_{0,m}$ is of the order $O(1/m)$ [21]. It has been shown [22] that the expected distribution of the Monte Carlo fission source $E(s^{(n)})$ convergences to $s_{0,m}$ in the order $O\left((k_1/k_0)^n\right)$. Typically, the spatial distribution of a biased source is flatter than the distribution of the fundamental mode source. Figure 3.1 shows an example of the biased source (for several values of m) in a slab reactor.[1]

The biased fission source causes a bias in the k_{eff} estimator of the order $O(1/m)$. The biased k_{eff} is usually smaller than the correct one. This is caused partially by an increased neutron leakage from the system, and partially by the reduced concentration of the fission source in most reactive places due to the flatter source. Figure 3.2 shows an example of the bias in k_{eff} in a slab reactor. The absolute value of the bias in the fission source depends on the system properties. It has also been shown that the standard method of computing the confidence limits is not valid for iterated-source calculations due to correlation of the fission source between the subsequent cycles [24–28].

The Monte Carlo fission source is defined only in a limited number of positions (sites). This creates problems as the initial Monte Carlo fission source might not be sampled in certain, possibly very important (most reactive), parts of the system. This problem appears to be severe especially in criticality safety calculations of loosely-coupled multi-component systems. If the fission neutrons are not present in important components then these components become "invisible" in the system, and the source convergence is not governed by the dominance ratio of the whole system; instead it is governed by the dominance ratio of a system consisting of the components with the fission source sampled in. Such dominance ratio may be very close to unity, resulting in a slow convergence, although the real dominance ratio may be small. While the fission source is not sampled in the important components the k_{eff} estimate may be largely underestimated. This problem is known as the "k_{eff} of the world problem" [29]. A reliable diagnostics of the source convergence appears to be very problematic [30–42].

Choosing the batch size m affects the efficiency of the criticality calculation. It is required, especially in systems with dominance ratios close to unity, to iterate the fission source in many cycles (> 1000), which may require a small m (since the computational time is proportional to nm for a one-processor calculation). On the other hand a small m implies a large bias in the fission source and k_{eff}. Thus, m should not be very small, but also not very large. This problem is demonstrated in Figure 3.3 where the error in the cumulative fission source is measured in two

[1] Numerical calculations in this section have been accomplished by a proprietary Monte Carlo code written by the author; the code is based on algorithms of the COHORT-II code [23].

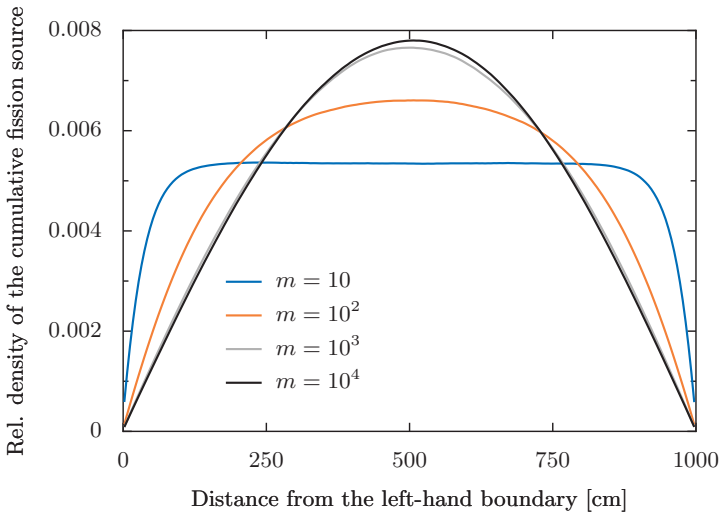

Figure 3.1: An example of the spatial distribution of the Monte Carlo fission source in a slab reactor. Parameters - total number of neutron histories in active cycles: 3×10^9, the slab thickness: 1000 cm, material properties: ^{235}U 0.14 g/cm^3, ^{238}U 1.0 g/cm^3, Cnat 2.0 g/cm^3, cross section library: JEFF 3.1.

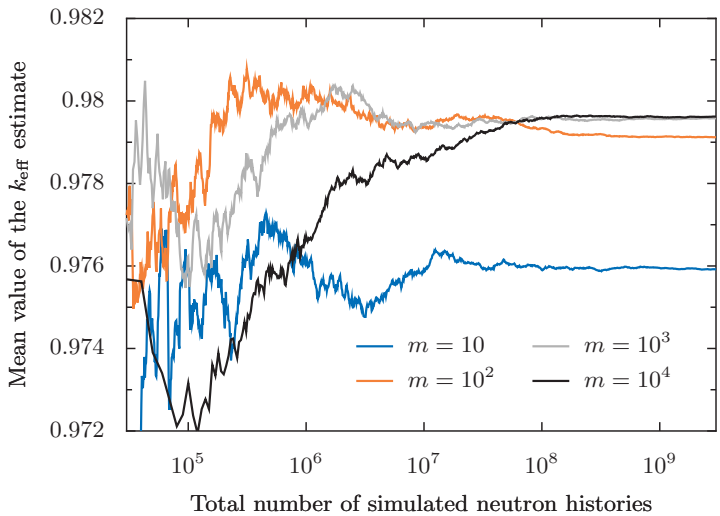

Figure 3.2: The k_{eff} estimate combined over the active cycles of the Monte Carlo calculation specified in the caption of Figure 3.1.

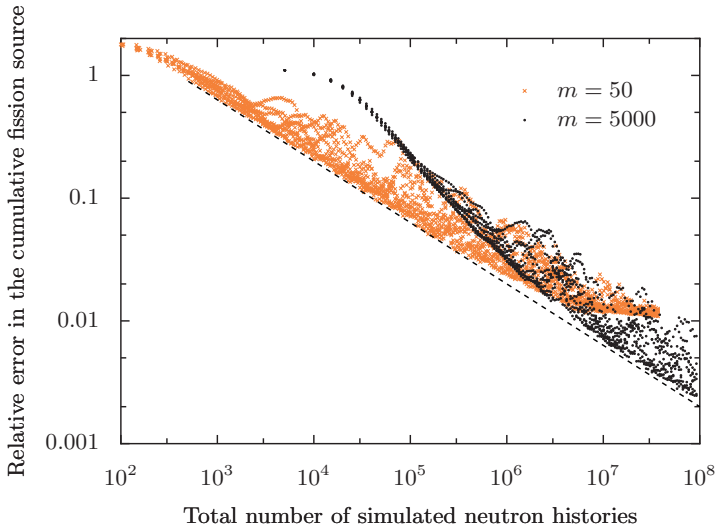

Figure 3.3: An example of the convergence of the cumulative fission source in a Monte Carlo eigenvalue calculation with the neutron batch size of 50 and 5000 neutrons, respectively. Each calculation was repeated 10×. This example was taken from Paper vii.

sets of test calculations; the first set uses the batch size of 50 neutrons, the second set uses the batch size of 5000 neutrons. The cumulative fission source (i.e., the fission source combined over the active cycles) is convenient for this demonstration since its random noise decays in the order $O(1/\sqrt{mn})$. Convergence of the Monte Carlo fission source is otherwise difficult to demonstrate due to its constant noise $O(1/\sqrt{m})$.

In general, the optimal batch size depends on the error in the initial fission source, the dominance ratio of the system and other properties of the system, and the target number of simulated histories.

3.5 Improving the Convergence of the Fission Source

Improving the convergence of the Monte Carlo fission source is commonly done by dividing the inactive cycles into several stages; the batch size is increased in each subsequent stage, which allows to perform a large number of cycles, and decrease the source bias gradually [43]. This section describes several other methods that have been proposed to improve the convergence of the fission source.

3.5.1 The Superhistory Powering

Brissenden and Garlick [21] have shown that the bias in the fission source and k_{eff} is caused by normalising the neutron batch size at the end of each cycle. They have suggested the *superhistory powering method* to reduce the bias by simulating l neutron generations in each cycle. According to the authors, l-values up to 10 are easy to cope with. The number of fission neutrons may grow or decay over the generations within a single cycle. Only the neutron batch generated in the last generation of each cycle is normalised.

We have tested the superhistory powering method in Paper vii, and observed that the method could considerably decrease the bias in the fission source at no extra computational cost. Nevertheless, this method could not accelerate the convergence of the fission source. Similar conclusions have been made by Blomquist and Gelbard [44].

3.5.2 The Fission Matrix Acceleration Methods

The *fission matrix acceleration methods* approximate H in Eq. (3.10) by a fission matrix $\mathbb{H}$, and modify the delay bank using the fundamental mode eigenvector $\mathbf{h}$ of $\mathbb{H}$. A number, d, of space zones must be introduced over the system in order to calculate the fission matrix. The $(i,j)^{\text{th}}$ element of $\mathbb{H}$ represents the probability that a fission neutron born in zone j (Z_j) causes the subsequent birth of a fission neutron in zone i,

$$\mathbb{H}[i,j] = \frac{\int_0^\infty \mathrm{d}E \mathrm{d}E' \int_{Z_i} \mathrm{d}^3 r \int_{Z_j} \mathrm{d}^3 r' f(\mathbf{r}', E' \rightarrow \mathbf{r}, E) s_0(\mathbf{r}', E')}{\int_0^\infty \mathrm{d}E' \int_{Z_j} \mathrm{d}^3 r' \, s_0(\mathbf{r}', E')},$$

where $f(\mathbf{r}', E' \rightarrow \mathbf{r}, E)\, \mathrm{d}E\, \mathrm{d}^3 r$ is an expected number of first generation fission neutrons produced in the volume element $\mathrm{d}^3 r$ at $\mathbf{r}$, in the energy element $\mathrm{d}E$ at E, resulting from a fission neutron born at $\mathbf{r}'$ with an energy E'. The angular dependence is not considered since fission neutrons are emitted isotropically.

The value of $\mathbb{H}[i,j]$ can be approximated during the n^{th} cycle of a Monte Carlo criticality calculation as

$$\mathbb{H}^{*(n)}[i,j] = \mathbb{F}^{*(n)}[i,j] / \mathbf{s}^{(n-1)}[j], \tag{3.15}$$

where $\mathbb{F}^{*(n)}[i,j]$ is the total expected number of fission neutrons from all collisions in zone i produced by neutrons from $\mathscr{S}^{(n-1)}$ originated from zone j, and $\mathbf{s}^{(n-1)}[j]$ is the sum of statistical weights of neutrons from $\mathscr{S}^{(n-1)}$ in zone j. The fission matrix computed by Eq. (3.15) is referred to as the *cycle fission matrix* $\mathbb{H}^{*(n)}$. It is possible to combine the fission matrix over all simulated cycles; such matrix is then referred to as the *cumulative fission matrix* $\mathbb{H}^{(n)}$,

$$\mathbb{H}^{(n)}[i,j] = \mathbb{F}^{(n)}[i,j] / \mathbf{t}^{(n-1)}[j], \quad \forall i,j,$$

where

$$\mathbb{F}^{(n)}[i,j] = \sum_{l=1}^{n} \mathbb{F}^{*(l)}[i,j],$$
$$\mathbf{t}^{(n-1)}[j] = \sum_{l=1}^{n} \mathbf{s}^{(l-1)}[j].$$

The fundamental mode eigenvector of $\mathbb{H}^{(n)}$ ($\mathbb{H}^{*(n)}$) is denoted as $\mathbf{h}^{(n)}$ ($\mathbf{h}^{*(n)}$).

The existing fission matrix methods [45–49] assume that $\mathbf{h}^{(n)}$ (or $\mathbf{h}^{*(n)}$) converges faster than the fission source in standard Monte Carlo calculations, which can be utilised for accelerating the convergence of the fission source. The fission matrix methods correct the fission bank using $\mathbf{h}^{(n)}$ (or $\mathbf{h}^{*(n)}$) in various ways. For instance, Kadotani, et al. [46] proposed to set the number of the fission neutrons in zone i to $\mathbf{h}^{(n)}[i]$, where $||\mathbf{h}^{(n)}||_1 = m$. Similarly, Kitada, et al. [48] suggested to normalise the total statistical weight of the fission neutrons in zone i to $\mathbf{h}^{(n)}[i]$. This method was tested on a large core, and an acceleration of the source convergence was achieved with a batch of 10000 neutrons during 50 inactive cycles. Urbatsch [47] proposed an additive correction to the fission source using both the direct and adjoint fundamental mode eigenvectors of the cumulative fission matrix. The high frequency noise in the additive correction was to be filtered, and the correction had to be scaled down by a damping factor to enhance stability. An acceleration of the source convergence with a batch of 5000 neutrons was achieved during inactive cycles on several tested systems.

Yet, the success of existing fission matrix methods has been limited due to stability problems and a dubious convergence of the fundamental mode eigenvector of the fission matrix; therefore, these methods have not been considered reliable. The fission matrix, however, represents valuable information about the system [50]. Therefore, some Monte Carlo codes [51, 52] calculate the fission matrix, although the matrix is not used for the acceleration of the source convergence.

3.5.3 The Stratified Source Sampling

The stratified sampling technique described in Sec. 2.4.4 cannot be applied directly on sampling the fission source since the pdf of the fundamental mode fission source is not known. Yet, this technique inspired the existing Monte Carlo *stratified source sampling* method [53–55] that addresses the convergence problems of the Monte Carlo fission source in weakly-coupled multi-component systems.

At the end of each cycle, the expected statistical weight $W_i^{(n)}$ of the fission source is computed in the i^{th} component as

$$W_i^{(n)} = \frac{m \int_{V_i} Hs^{(n-1)} \, \mathrm{d}^3 r}{\int_V Hs^{(n-1)} \, \mathrm{d}^3 r}, \ \forall i.$$

When $W_i^{(n)}$ falls below a certain low weight cutoff threshold W_{cut} (user specified, e.g. $W_{\text{cut}} = 0.1$), then a fission neutron carrying a unit statistical weight is sampled in the i^{th} component with a probability $p = W_i^{(n)}$; no fission neutron is sampled in this component with a probability $p = 1 - W_i^{(n)}$. If $W_i^{(n)} \geq W_{\text{cut}}$ then an integer number $N_i^{(n)}$ is found as the closest integer to $W_i^{(n)}$; if $N_i^{(n)}$ equals zero then exactly one fission neutron carrying the statistical weight $W_i^{(n)}$ is sampled in the i^{th} component. If $N_i^{(n)}$ is positive then $N_i^{(n)}$ fission neutrons each carrying the statistical weight $W_i^{(n)}/N_i^{(n)}$ is simulated in i^{th} component.

The Monte Carlo stratified source sampling method was shown to be effective in several numerical tests [54, 56]. The method decreases the probability that fission neutrons disappear, by chance, from some important component. The risk of losing the fission neutrons from an important component can also be lowered by increasing the neutron batch size m.

3.5.4 The Zero-Variance Scheme

The *zero-variance scheme* [57] has been also adapted [58, 59] for Monte Carlo criticality calculations. The method biases the scattering angles and distances between neutron collisions so that neutrons get scattered into more important places, which is compensated by correcting the statistical weights of simulated neutrons. Although the method was designed to lower the variance of the computed k_{eff}, biasing the neutron transport can improve the convergence of the fission source.

First, we introduce the zero-variance scheme for reactor shielding calculations here because the zero-variance scheme for criticality calculations is based on it. Reactor shielding calculations seek for a response R of a small detector in a large multiplying system. Most of the sampled neutron histories do not cross the small detector, and thus are of no use. The zero-variance scheme tries to sample only those neutron histories that contribute to the detector response. This is done by changing the neutron transition and scattering probability distributions (transport kernels) so that the neutrons tend towards the detector.

The detector response R can be formally written as

$$R = \int \eta_\chi(\mathbf{P})\chi(\mathbf{P})\,\mathrm{d}\mathbf{P} = \int \eta_\psi(\mathbf{P})\psi(\mathbf{P})\,\mathrm{d}\mathbf{P},$$

where $\mathbf{P} \equiv (\mathbf{r}, \Omega, E)$, $\chi(\mathbf{P})$ and $\psi(\mathbf{P})$ are the emission and collision density, respectively, and $\eta_\chi(\mathbf{P})$ and $\eta_\psi(\mathbf{P})$ are the detector response functions with respect to $\chi(\mathbf{P})$ and $\psi(\mathbf{P})$, respectively. $\chi(\mathbf{P})$ and $\psi(\mathbf{P})$ are given by the transport equations

$$\chi(\mathbf{P}) = s(\mathbf{P}) + \int K(\mathbf{P}' \to \mathbf{P})\chi(\mathbf{P}')\,\mathrm{d}\mathbf{P}',$$

and

$$\psi(\mathbf{P}) = s(\mathbf{P}) + \int L(\mathbf{P}' \to \mathbf{P})\psi(\mathbf{P}')\,\mathrm{d}\mathbf{P}',$$

where the transport kernels K and L are given as

$$K(\mathbf{P}' \to \mathbf{P}) \equiv T(\mathbf{r}' \to \mathbf{r}, \Omega', E')C(\mathbf{r}, \Omega' \to \Omega, E' \to E),$$

and

$$L(\mathbf{P}' \to \mathbf{P}) \equiv C(\mathbf{r}, \Omega' \to \Omega, E' \to E)T(\mathbf{r}' \to \mathbf{r}, \Omega', E'),$$

respectively. The transition kernel

$$T(\mathbf{r}' \to \mathbf{r}, \Omega', E')\,\mathrm{d}^3 r$$

is the probability that a particle starting a flight path at $\mathbf{r}'$ will have its next collision in $\mathrm{d}^3 r$ at $\mathbf{r}$. The collision kernel

$$C(\mathbf{r}, \Omega' \to \Omega, E' \to E)\,\mathrm{d}\Omega\,\mathrm{d}E$$

is the probability that a particle will exit a collision at $\mathbf{r}'$ with direction Ω in $\mathrm{d}\Omega$ and energy E in $\mathrm{d}E$.

During the neutron transport simulation, the transport kernel $L(\mathbf{P}' \to \mathbf{P})$ can be efficiently biased using the adjoint form of $\psi(\mathbf{P})$ as

$$\bar{L}(\mathbf{P}' \to \mathbf{P}) \equiv L(\mathbf{P}' \to \mathbf{P})\frac{\psi^*(\mathbf{P})}{\psi^*(\mathbf{P}')},$$

which must be compensated by a suitable change of the statistical weight w of the neutron, so that wL is conserved. The adjoint form $\psi^*(\mathbf{P})$ is the solution of the adjoint equation

$$\psi^*(\mathbf{P}) = \eta_\psi + \int L(\mathbf{P} \to \mathbf{P}')\psi^*(\mathbf{P}')\,\mathrm{d}\mathbf{P}'.$$

Similarly, the adjoint form of $\chi(\mathbf{P})$ can be obtained, and used for biasing the transport kernel $K(\mathbf{P}' \to \mathbf{P})$. The efficiency of biasing the neutron transport depends on the precision of the adjoint functions that must be computed in advance.

The zero-variance scheme was adapted for criticality calculations by introducing a large virtual detector (superimposed on the whole system) with a response function

$$\eta_\psi = \nu\frac{\Sigma_f(\mathbf{P})}{\Sigma_t(\mathbf{P})}.$$

Then, the detector response

$$R = \int \frac{\nu\Sigma_{\mathrm{f}}(\mathbf{P})}{\Sigma_{\mathrm{t}}(\mathbf{P})}\psi(\mathbf{P})\,\mathrm{d}\mathbf{P}$$

reflects all new fission neutrons during each cycle, and k_{eff} can be computed as

$$k_{\mathrm{eff}} = \frac{R^{(n)}}{m}.$$

The adjoint functions may be computed, to some precision, by deterministic codes. The efficiency of the zero-variance scheme in criticality calculations depends, similarly as in the shielding calculations, on correctness of the adjoint functions. The existing numerical tests [60] show that the method is more efficient when only the collision kernel is biased since biasing the transition kernel is time consuming.

3.5.5 The Wielandt Method

The *Wielandt method* is a known acceleration technique used in deterministic criticality calculations where it guarantees a rapid and stable convergence. Recently, the method has been adapted for Monte Carlo criticality calculations [61]. This adaptation simulates several neutron generations in each cycle, which makes the method similar to the superhistory powering. In contrast to the superhistory powering method, the neutron population always decays completely within a cycle. Moreover, new fission neutrons for the subsequent cycle are sampled in all neutron histories, i.e. not only in the last generation.

A fission neutron carrying the parent particle weight is emitted within the current cycle from each collision with probability

$$w\frac{\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{t}}}\frac{\nu}{k_{\mathrm{e}}},$$

where k_{e} must be chosen larger than k_{eff}. New fission neutrons are tracked by the same random walk process as other particles; they may produce progenies that are also tracked within the current cycle until their deaths by escape, Russian roulette and so on. If $k_{\mathrm{e}} < k_{\mathrm{eff}}$ then the fission chain will not terminate within the current cycle.

A standard k_{eff} estimator will calculate an apparent eigenvalue, k_{w}. The correct k_{eff} of the system can be obtained as

$$k_{\mathrm{eff}} = \left(\frac{1}{k_{\mathrm{w}}} + \frac{1}{k_{\mathrm{e}}}\right)^{-1}.$$

Fission neutrons for the subsequent cycle are produced in each collision with probability

$$w\frac{\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{t}}}\frac{\nu}{k_{\mathrm{w}}} = w\frac{\Sigma_{\mathrm{f}}}{\Sigma_{\mathrm{t}}}\nu\left(\frac{1}{k_{\mathrm{eff}}} - \frac{1}{k_{\mathrm{e}}}\right).$$

If $k_{\mathrm{e}} > k_{\mathrm{eff}}$ then the expected number of fission neutrons per collision is smaller than in standard Monte Carlo calculations. However, all neutrons tracked within the current cycle (including the new fission neutrons) may produce new fission neutrons for the subsequent cycle; thus, the number of first generation fission neutrons is preserved in each cycle. This causes the fission neutrons to spread more within a cycle.

The existing numerical test calculations [61] show that the Wielandt method decreases the number of cycles necessary to achieve the convergence of the Monte Carlo fission source; however, the reduction of the total number of cycles does not always compensate for the increased computer time per cycle (as more neutron histories need to be followed at each cycle).

Chapter 4

Non-Linear Steady-State and Burnup Problems

> I have yet to see any problem, however complicated, which, when you looked at it in the right way, did not become still more complicated.
>
> *Poul Anderson (1926 - 2001)*

4.1 Non-Linear Steady-State Problems

Criticality calculations assume that the macroscopic cross sections in the eigenvalue equation (3.8) are constant; thus, the criticality calculations solve the fundamental mode neutron flux in static systems. In reality, however, the local coolant density, concentration of ^{135}Xe, fuel temperature, etc. are all dependent on the local neutron flux. Thus, a steady-state solution must describe unknown concentrations of some isotopes (steady-state core conditions) and the corresponding equilibrium distribution of the neutron flux. The eigenvalue equation (3.8) is not sufficient to describe the solution of the steady-state problem, and must be completed with equations for the unknown concentrations of relevant isotopes. Indeed, only a small subset of all isotopes needs to be described by the additional equations as there are many isotopes that do have constant (or almost constant) concentrations. The solution of Eq. (3.8) where the macroscopic cross sections depend on the flux is not linear, so the steady-state solution must be obtained by non-linear methods.

The Monte Carlo method has practically not been used in computing the steady-state core conditions mainly due to extensive computational demands of multiple criticality calculations needed to solve the non-linear problem. Moreover, the strong thermal-hydraulic, Doppler, and ^{135}Xe feedbacks, common mainly in thermal reactors, do not allow for solving the non-linear problem by the common fixed-point method.

4.2 Burnup Problems

Burnup calculations provide isotopic changes in irradiated nuclear fuel, and allow to study neutronic properties of nuclear systems over long time periods, typically, the fuel cycles of power reactors. In general, the time dependent neutron flux is described by the transport equation (3.7). The time dependent macroscopic cross-sections in Eq. (3.7) are, however, not known. The local macroscopic cross-sections in Eq. (3.7) are dependent on the local neutron flux, and must be given by additional equations. The concentration of the fuel isotopes can be described by the burnup equation [62]

$$\frac{d\mathbf{N}(\mathbf{r},t)}{dt} = \mathbb{M}(\phi,T)\mathbf{N}(\mathbf{r},t), \tag{4.1}$$

where

$$\mathbb{M}[\phi(\mathbf{r},E,t),T(\mathbf{r},t)] = \int_0^\infty \phi(\mathbf{r},E,t)\mathbb{X}(T)\mathrm{d}E + \mathbb{D}, \tag{4.2}$$

where $\mathbb{X}(T)$ is a temperature dependant cross-section and yield matrix, and $\mathbb{D}$ is a decay matrix. (In Eq. (4.1), $N_i(\mathbf{r},t)$ is the concentration of isotope i at $\mathbf{r}$ time t.) Eq. (4.1) has a formal solution [62]

$$\mathbf{N}(\mathbf{r},t) = \mathbf{N}(\mathbf{r})|_{t_0} \exp[\mathbb{M}(\phi,T)(t-t_0)] \tag{4.3}$$

for a known neutron flux $\phi(\mathbf{r},E,t)$. Other isotopes, present in e.g. in the coolant, must be described by thermal-hydraulic equations. In general, the movements of control rods should also be well specified to achieve criticality of the system at any time.

Indeed, the numerical solution of the system of equations sketched above (completed with initial and border conditions) requires many simplifications. First of all, the exact criticality of the numerical model can hardly be maintained by adjusting the control rods, that is why Eq. (3.7) is not used in burnup calculations. Instead, the time period is divided into a number of time steps, and the neutron flux in each step is approximated using the eigenvalue equation (3.9). The flux is usually assumed to be constant during a time step; the matrix exponential in Eq. (4.3) can be then enumerated using various algorithms. The simplest algorithm approximates the matrix exponential by several terms of the power series

$$\exp[\mathbb{M}(t-t_0)] = \mathbb{I} + (t-t_0)\mathbb{M} + \frac{(t-t_0)^2\mathbb{M}^2}{2!} + \dots. \tag{4.4}$$

A good solution for typical burnup matrices and time steps, however, requires more sophisticated algorithms [63–65].

Chapter 5

Summary of the Included Papers

> The scientific theory I like best is that the rings of Saturn are composed entirely of lost airline luggage.
>
> *Mark Russell (1932 -)*

5.1 Paper I

The existing Monte Carlo fission matrix acceleration methods, briefly introduced in Sec. 3.5.2, have been shown capable of accelerating the convergence of the Monte Carlo fission source in several test criticality calculations [47, 48]. Nevertheless, authors of these calculations have alerted to possible stability problems. These problems have not been well described and explained in the literature; therefore, we have decided to study this problem.

We have implemented the fission matrix acceleration method [48] into our proprietary Monte Carlo code, and performed a series of test calculations. Performance of the method appeared to be strongly dependent on the neutron batch size and the total number of space zones used for computing the fission matrix. While studying the spatial distribution of the iterated fission source and the fundamental mode eigenvector of the fission matrix we could observe error propagation in the fission matrix due to a feedback between the fission matrix and the fission source. Any error in the fission source is reflected into the fission matrix at each cycle of the Monte Carlo calculation. At the end of each cycle, the errors in the fission matrix are transfered to the fundamental mode eigenvector from where these errors affect the fission source in the next cycle (as the fission source is normalised by the eigenvector).

When the neutron batch size is small with respect to the total number of space zones, then the fission matrix is sampled with large statistical errors during many inactive cycles; these errors are reflected to the fission source. Typically, the fis-

sion source normalised by the eigenvector of a noisy fission matrix behaves very chaotically over the cycles, and the calculation may diverge.

If the neutron batch size is large with respect to the total number of space zones, then the fundamental mode eigenvector of the fission matrix may converge faster than the fission source, and so the convergence of the fission source can be accelerated. Nevertheless, if the space zones are relatively large, then the feedback between the fission matrix and the fission source will slow down the overall convergence rate (and so the acceleration method must be stopped after several cycles). It is thus not surprising that the successful demonstrations of the Monte Carlo fission matrix acceleration methods have been done only with large neutron batch sizes, and the acceleration methods have been applied on several inactive cycles only.

It should be understood that standard Monte Carlo criticality calculations with very large neutron batch sizes converge slowly since each cycle requires a large computational time. Therefore, reducing the neutron batch size can improve the performance of the standard Monte Carlo criticality calculations considerably. We have noticed that the performance of the Monte Carlo calculations "successfully" accelerated by the fission matrix acceleration method has generally not been better than the performance of standard Monte Carlo calculations with optimised neutron batch sizes.

5.2 Paper II

The Monte Carlo fission matrix is a very unique quantity that is worth of sampling in the course of Monte Carlo criticality calculations. Its fundamental mode eigenvalue equals k_{eff}, and the corresponding eigenvector equals a spatially discretised fission source in equilibrium. This paper describes a new concept of "fission matrix based Monte Carlo criticality calculations". It is explained that the Monte Carlo fission matrix can be sampled to a very good precision using inaccurate fission source if the matrix is created using a space mesh with sufficiently small zones. Practically, this means that no inactive cycles need to be performed before calculating the fission matrix. It is moreover possible to zone-wise decompose all random variables, and make them dependent on the fission matrix. This way, no inactive cycles are needed for sampling any of the random variables (like, a detector response, spatial distribution of neutron flux, power, etc.). Space discretization into a large number of zones can produce very large fission matrices; however, such matrices are very sparse, and their eigenvectors can be computed efficiently e.g. by the Arnoldi method [66].

The way of using the fission matrix in the fission matrix based Monte Carlo criticality calculations differs significantly from the way it is used by the Monte Carlo fission matrix acceleration methods. In the fission matrix based Monte Carlo criticality calculations, the fission source is not accelerated - it does not need to since there are no inactive cycles. Moreover, the fission matrix is sampled during all cycles, and all final results are derived using the fission matrix. On the contrary,

the Monte Carlo fission matrix acceleration methods use the fission matrix only during the inactive cycles for modifying the fission source, and the fission matrix is used for no other purpose than biasing the fission source.

The fact that the fission matrix based Monte Carlo criticality calculations do not use the inactive cycles implies that the calculations should, theoretically, provide a conservative (reliable) estimation of error in k_{eff} at any cycle. Conservative error estimations can really be computed if the Monte Carlo calculation samples also variances in the computed fission matrix. Our numerical test calculations of Whitesides' "k-effective of the world" model problem have confirmed this. This makes the fission matrix based Monte Carlo criticality calculations especially attractive for criticality safety calculations where conservative estimations of the error in the computed k_{eff} is required.

5.3 Paper III

Any source convergence acceleration method, described in Chapter 2, will turn out useless if it cannot run efficiently on multi-processor computers. Monte Carlo criticality calculations require an efficient parallel computing scheme to lower the computational time on modern multi-core and multi-processor computers. So far, criticality calculations have been parallelised either by the master/slave scheme (used e.g. in the MCNP5 code [OECD/NEA, 2008a]) or by combining the results from independent parallel simulations (used e.g. in the TRIPOLI-4 code [OECD/NEA, 2008b]). The both schemes have disadvantages that do not allow for the ideal parallel scaling. The master/slave scheme requires vast communication among the processors, which limits the overall efficiency [68]. On the contrary, the independent parallel simulations do not require any communication, but they all converge at the same rate as a single-processor calculation. So the combined computational time wasted in the inactive cycles in all parallel calculations may be enormous.

We present a new parallel computing scheme based on the Monte Carlo fission matrix. In this scheme, parallel criticality calculations (with unique initial seeds in their random number generators) independently sample the Monte Carlo fission matrix; thus, no communication among the processors is needed. At the end of the calculation, the final fission matrix is combined from all parallel calculations. All required results are then derived by means of the final fission matrix. No inactive cycles are needed if the space mesh contains sufficiently small zones.

The efficiency of this scheme outperforms all existing parallel computing schemes since the scheme does not require any communication among the processors, and no inactive cycles are simulated. The scheme allows for a practically ideal parallel scaling.

5.4 Paper IV

In this paper, we have presented an efficient Monte Carlo method of iterative computing the steady-state core conditions and neutron flux in a critical power reactor. The method carries out a series of Monte Carlo criticality and thermal-hydraulic calculations of a power reactor model. At each iteration step, the spatial distribution of neutron flux (power) from the Monte Carlo calculation is combined over all finished iterations, and the resulting flux (power) distribution is used for improving the accuracy of the core conditions (the spatial distribution of the coolant density, strongly absorbing fission products like ^{135}Xe, etc.) in the numerical core model.

Numerical stability of solving this non-linear problem is ensured by a newly developed control of the step size and sample size parameters at each iteration step. At the first iteration step, the Monte Carlo criticality calculation simulates a small number of neutron histories (sample size) as the core conditions are not known to a good precision yet. In each of the following steps, the Monte Carlo criticality calculation simulates more neutron histories (the sample size grows) as the core conditions are computed to a better precision. The final core conditions reflect results from the Monte Carlo criticality calculations from all iteration steps, which makes the calculation very efficient. According to the numerical test calculations, this method reaches the highest possible convergence rate.

5.5 Paper V

A number of new Monte Carlo burnup codes [69–73] have been written during the last decade. Usually, they couple the existing Monte Carlo criticality codes to solvers of the burnup equations. The Monte Carlo burnup codes divide the target time period into a number of time steps; at each step, the neutron flux and the burnup matrix are computed [74] by the Monte Carlo criticality code, and these data is used to compute the fuel burnup.

We have noticed that the existing major Monte Carlo burnup codes are numerically instable in fuel cycle calculations of critical reactors. Large spatial oscillations of the neutron flux (power), ^{135}Xe and fissile materials can be observed over the time steps, which results in uselessness of these codes in the fuel cycle calculations. The reason of this problem is that the affected Monte Carlo burnup codes couple the criticality and burnup calculations by the explicit Euler method or the midpoint method [75]; these methods are known to be only conditionally stable, i.e. stable only for sufficiently short time steps [76]. The maximal length of the time step that ensures a stable calculation depends on the problem being solved. We have shown that even fuel cycle calculations with very short time steps of two days suffer from serious numerical instabilities. The spatial oscillations of neutron flux are not driven by propagation of the statistical errors [77, 78].

On the contrary, the existing deterministic burnup codes couple the criticality and burnup calculations by more stable methods [79]. A common method used in

deterministic burnup codes is the linear flux approximation [80] (the modified Euler method). We have recommended implementation of the linear flux approximation into the future Monte Carlo burnup codes.

It should be understood that in some cases, the affected Monte Carlo burnup codes can provide correct results even with relatively large time steps. For example, the spatial oscillations of the flux may not appear in systems with small dominance ratios. Also, if the total power is small then the saturated density of ^{135}Xe (and other poisons) may be too small to provoke the spatial oscillations of the flux. A fast neutron energy spectrum in fast reactors decreases the effective cross section of ^{135}Xe for neutron capture, which also improves the numerical stability. Many problems assume only one burnable material in the system; in such cases the burnup calculations are always stable since the spatial oscillations in the nuclide field are not possible.

Chapter 6

Conclusions

> Ah! Don't say you agree with me. When people agree with me I always feel that I must be wrong.
>
> *Oscar Wilde (1854 - 1900)*

Monte Carlo calculations of reactor physics problems have been made possible only thanks to the existence of electronic computers. The complexity of the Monte Carlo calculations has been growing with the growing computing power. There is no acceleration method that could have so big impact on the Monte Carlo calculations as the progress in the computer technology. Nevertheless, the architecture of computers changes. No longer the speed of a single processor doubles every two years; instead, more processors are being implemented into a single chip. It is not unreasonable to assume that the near future mainstream computers will have several hundreds of cores. Fast Monte Carlo calculations will be possible only with the full and efficient utilisation of all available processors. Therefore, the future Monte Carlo calculations (criticality, steady-state, and burnup) will have to be heavily parallelised. We have presented new methods that will help to realise this.

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