

**Accelerating the convergence of
Monte Carlo calculations of k_{eff} in
systems with weakly coupled fissile
units**

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SUMMARY

The goal of this research is to assess the developments made recently to improve the Monte Carlo method for the calculation of the k_{eff} in geometries containing different weakly coupled fissile units. The field of application is the nuclear criticality safety.

Four methods presented by different teams have been compared, which have a different approach to the problem. In short the four different methods are:

- **Superhistory powering:** In Monte Carlo simulations for criticality studies the neutron population is often renormalized at every generation in order to keep artificially a stable chain reaction, which gives a negative bias. By renormalizing every L (e.g. 10) generations this problem could be avoided
- **Fission matrix method:** The convergence could be accelerated by use of the eigenvector of the K_{ij} -matrix, customarily called the fission matrix.
- **Importance sampling:** Accelerating the convergence by use of the importance function relative to the spatial distribution of the fission sources.
- **Stratified sampling:** When the neutron population is not important, this can lead to distributions where the number of neutrons in certain volumes is less than one. This method introduces a weight, and makes sure that always at least one neutron will be simulated per volume.

The different methods have first been tested on a one-dimensional model, after which they have been programmed in the Monte Carlo code MORET. Computational tests have been performed with three different geometries.

The results were not always coherent and none of the methods satisfied in all cases. The problem investigated thus still remains, but improvements have been found in certain cases. The effect of the different methods appeared to vary for the different geometries.

PREFACE

This graduation report has been written as a conclusion of the study of Applied Physics at the Delft University of Technology. The research for this report has been performed at the Criticality Studies Department (SEC) of the Institut de Protection et Sureté Nucleaire (IPSN) in Fontenay-aux-Roses in France.

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NOMENCLATURE

D	Diffusion coefficient
E	Energy
g	Generation
h	Width of box
I	Importance function
k_{eff}	Effective multiplication factor
k_{ij}	Element of fission matrix
k_n	Estimate of multiplication factor at iteration n
k_{∞}	Infinite multiplication factor
K	Probability for transition in phase space
l	Track length
L	Size of superhistory
M	Number of neutrons
M_0	Total number of starting neutrons
n	Number of elements
N	Number of fissile volumes
p	Probability density function
P_{nv}	Total weight of neutrons in a volume
P_m	Number of neutrons produced in a superhistory
\vec{r}	Position vector
R	Reflection coefficient
s	(Covered) distance
S	Neutron source
V	Volume
W	Neutron weight
W_{cut}	Cutoff threshold
η	Production factor
ϑ	Random number between 0 and 1
ϕ	Neutron flux
λ	Eigenvalue
μ	Cosine of scattering angle
ν	(Expected) number of produced neutrons
σ	Standard deviation
σ_x	Microscopic crosssection for interaction x
Σ	Macroscopic cross section
χ	Energy spectrum
χ	Outgoing collision density
ψ	Ingoing collision density
$\vec{\Omega}$	Unit direction vector

1. INTRODUCTION

The goal of this study is to assess the developments made recently to improve the Monte Carlo method for the calculation of k_{eff} in geometries containing different weakly coupled fissile units. First the field of application, the nuclear criticality safety, will be presented, then the basis of the Monte Carlo method will be described, followed by the problem of weak coupling.

1.1 Nuclear criticality safety

The present nuclear energy is based on the nuclear fission process. Nuclear reactors are specifically designed to produce energy from fission by controlling the neutron chain reaction, while shielding against the radiation and containing the radioactive products. This, however, is generally not the case for the different operations in the fuel cycle (Appendix A), during which a sustained chain reaction has to be avoided. The produced energy and radiation could be very harmful for the personnel and the equipment. Nuclear criticality safety could therefore be defined as the prevention or termination of inadvertent nuclear chain reactions in non-reactor environments.

To analyze the state of a neutron chain reaction, the most direct way is to look at the balance between the neutron production rate and the rate of neutron loss. This state is described by the effective multiplication factor, denoted as k_{eff} . It is defined as:

$$k_{\text{eff}} = \frac{\text{rate of neutron production}}{\text{rate of neutron loss}} \quad (1.1)$$

where neutron production comprises neutrons born following fission events and neutron loss comprises neutrons absorbed or lost to the system by leakage. This gives us three regions of interest with respect to the multiplication factor:

$$\begin{aligned} k_{\text{eff}} < 1 & \text{ subcritical} \\ k_{\text{eff}} = 1 & \text{ critical} \\ k_{\text{eff}} > 1 & \text{ supercritical} \end{aligned}$$

Subcritical systems (without external source) have zero power or a decreasing power level depending on the initial state of the system. When production and losses exactly balance, k_{eff} is unity and the system is said to be critical. The critical condition is a very delicate balance characterized by a steady power level. Supercritical systems have a growing neutron population and increasing power.

Criticality safety is concerned with preventing both criticality and supercriticality. It seeks to assure that any operation in the nuclear fuel cycle can be realized without a risk of a critical excursion. This means that every measure should be taken to prevent an uncontrolled chain reaction and that intervening solutions have to be defined for the case that it would happen.

The figure in Appendix A, representing the fuel cycle, gives an idea of the range of the fields of investigation that are of concern to criticality safety studies. Although the operations for military purposes should be considered too, the main operations performed upon the fissile material in the civil cycle could be summarized as:

- enrichment
- manufacturing of fuel elements
- reprocessing of spent fuel

- fuel and waste storage
- transportation between the different factories

All these very different operations bring along very different materials, chemical compositions and geometries. Added to this that various moderation conditions are to be treated. This could be translated, from the neutronic point of view, in an enormous variety of energetical spectra and complexities of geometrical modelling. In comparison to the situations of a nuclear reactor the following differences could be found:

- more heterogeneous compositions
- more complicated geometries than the regular pattern of the fuel assemblies in a reactor
- a greater variety of neutron spectra
- the safety margins considered in criticality studies lead to lower accuracy requirements than those for reactor calculations, provided the approximations made are demonstrated to overestimate k_{eff} .

When experimental data are not available to establish critical conditions for a given system, it may be necessary to employ a calculational method. Two approaches can be used. The first one is to calculate the effective multiplication factor of a given configuration. The second one is to look for the critical parameters of the considered materials, e.g. the critical dimensions or compositions. In the situations met in nuclear installations these parameters should not be reached.

The general approach for criticality calculations is to use numerical methods to solve the transport equation. Transport theory is usually applied through discrete ordinates or Monte Carlo formulations. The first method allows to solve the transport equation in its integro-differential form, and is widely used for one- and two-dimensional problems. For more complicated configurations the computing time makes it less competitive, and for these problems the Monte Carlo method seems to be the most adequate method to solve the transport equation.^{[1],[2]}

1.2 Monte Carlo method

Contrary to the method of discrete ordinates the Monte Carlo method does not solve the transport equation with a deterministic numerical procedure, but it is based on the simulation of neutrons in matter. It considers neutrons as individual particles that interact with nuclei on a random basis obeying certain fundamental laws of probability. These laws may be based directly on a physical system, using experimental results, to establish the various probabilities.

The method allows to deduce from numerous simulated histories macroscopic parameters of the system. The unknown parameters can be found by taking the average of the contributions of the simulated neutrons, and the result will be characterized by this value and the standard deviation, that corresponds with the statistical dispersion of the studied population.

A great advantage of the method is that geometries do not have to be approximated and can be represented in either one, two or three dimensions. In contrast to other deterministic methods, increasing the number of dimensions does not greatly influence the dependence of calculation time on the number of points chosen.^[3]

1.3 Problems of weak coupling

The performances of the Monte Carlo method and the ease of its use, allow to calculate more and more complex configurations. Such a configuration will be called weakly coupled when there is little exchange of neutrons between the different fissile parts of the system. In certain cases, a careful evaluation of the course of the calculation for these complex configurations is needed. In the domain of nuclear criticality the use of the actual codes and the reliability of their results have certain limitations. In fact, as was stressed out by Whitesides in a famous article^[4], the calculated k_{eff} becomes erroneous under certain circumstances (often under-estimating the reactivity of the system).

The extreme example would be, according to Whitesides, to compute the ' k_{eff} of the world'. If one attempts to use the Monte Carlo method to calculate the multiplication factor of the world, which contains critical assemblies, the result would most likely be the value for the same system with no critical assemblies present. The cause of the erroneous result is the fact that the volume of the fissile material in the world would be so large relative to the volume of fissile material in the critical assemblies that most commonly used forms of sampling would almost never 'see' the critical assemblies. Hence this would not reflect their existence in the computed k_{eff} .

This example seems far from the concerns of criticality safety. Another example, closer to this field of application, is presented in the same article, in which the difficulty could be observed when using a Monte Carlo program. First it should be specified that the k_{eff} of a system composed of many fissile units will be at least equal to the k_{eff} of the most reactive subsystem, as a separate unit, but with the same moderating and reflecting conditions. Whitesides considers a $9 \times 9 \times 9$ array of plutonium metal spheres with a radius of 4 cm, spaced on 60 cm centers. The array is reflected on all its sides by a thick water reflector. The k_{eff} of this system is computed to be 0.93. If the sphere in the centre unit of the array is replaced by a sphere of plutonium that is exactly critical as a bare unit and the calculation is repeated using the conventional Monte Carlo sampling method, the calculation could still yield a k_{eff} of 0.93, reflecting the same difficulty encountered in the problem of the ' k_{eff} of the world': the simulation ignores the presence of the critical sphere^[4].

To understand the origin of the problem it is useful to recall the principle of the strategy followed by a Monte Carlo calculation. The basic idea is to simulate histories of a representative neutron-population in a system. The k_{eff} determines the evolution of the size of the neutron-population. The procedure for calculation would be simple if the starting source distribution is known. Unfortunately it is at least as hard to estimate this distribution as it is to estimate k_{eff} , and an iterative calculation scheme will therefore be needed. This iterative process should be followed until equilibrium in the source distribution is reached.

The answer to the problem lies in being sure that the source convergence is achieved. The statistical aspects of the Monte Carlo method make this problem of convergence a more delicate one. As where for the deterministic methods the convergence criteria can well be fixed, the statistical dispersion, inherent to the Monte Carlo method, brings along that there are two types of convergence looked for: first the convergence towards equilibrium of the source distribution, and second convergence of the sampling to reach the statistical precision desired. The problem can thus be translated in an unknown parameter which appears in every Monte Carlo code used in criticality safety studies, being the amount of iterative stages needed to settle with a converged source distribution, and which can be eliminated in the estimation of k_{eff} .

1.4 Methods for approaching the problem

The difficulty of convergence mentioned above can be apprehended from different positions. Four* methods that have been proposed by different teams will be briefly presented in this section (in chronological order), and a more elaborate discussion follows in the next chapter. These methods have a different approach to the problem, and their combination remains possible.

- **Superhistory powering:** In Monte Carlo simulations for criticality studies the neutron population is often renormalized at every generation in order to keep artificially a stable chain reaction. Brissenden and Garlick^[5] showed that this leads to a bias on the value found for k_{eff} and proposed a method which renormalizes every L generations (L is of the order of 10).
- **Fission matrix method:** Kadotani c.s.^[6] have proposed a method of accelerating the convergence based on the eigenvector of the K_{ij} -matrix, customarily called the fission matrix. An improvement to this approach has been proposed by Nouri^[2].
- **Importance sampling:** The importance function relative to the spatial distribution of the fission sources is used to accelerate the convergence. The system is divided into zones of uniform importance and the number of produced neutrons depends on the zone where the neutron was born and on the zone where the collision occurred. This method was applied by Nouri^[2].
- **Stratified sampling:** When the neutron population is relatively small, this can lead to distributions where the expected number of neutrons in certain volumes is less than one. The conventional sampling can miss generating sources in these volumes. These will then be ignored (from the point of view of the simulation), if the units are weakly coupled. To avoid this Roussel and Gelbard^[7] proposed a method of stratified sampling, introducing weights. Every fissile zone will always contain at least one neutron, possibly with a weight inferior to one.

1.5 Approach of the research

In order to compare the different methods proposed, the problem has been approached in two stages. First the different methods have been programmed for a simple one-dimensional case, allowing to learn the basic ideas of a Monte Carlo scheme and of the different methods to accelerate the convergence of the source distribution. This way it was avoided to immediately encounter all the difficulties of a Monte Carlo code used for criticality safety studies. After having understood the different aspects arising when using the different methods proposed, these have been built in the code MORET.

The actual comparison has been done with calculations on geometries described in the articles by Kadotani c.s.^[6], Whitesides^[4] and Smith^[8]. In the various calculations the convergency has been studied as a function of the number of generations, the standard deviation, the number of simulated neutrons and the initial source distribution.

The report has been written in the following order. After this introduction the theory of the different methods, as well as the theory of the conventional Monte Carlo sampling method are described. This is being followed by four chapters with the descriptions of the numerical experiments done, the results and their discussion. The report will end with a conclusion and recommendations.

* A fifth method that has been described by Lux and Koblinger^[3], the quota sampling, has been tested, but did not give acceptable results. The method and the results are briefly described in Appendix B.

2. THEORY

MORET^[9] is a code written to calculate the effective multiplication factor, k_{eff} , of an arbitrary multiplying system. As said in the introduction it uses the Monte Carlo method to solve the transport equation. The geometry is treated by decomposing the configuration in volumes of elementary shapes (spheres, cylinders, boxes, half-spaces, etc.) on which can be applied assembly operations (intersection, reunion etc.). The cross-sections used can be taken from its own 16 group library, or from any other external library. These external libraries may be temporary and a result of preliminary calculations performed with a specified assembly code as APOLLO*.

Since in this study we will mostly be interested in the distribution of fission neutrons, the equation representing the neutron density due to fission, which is derived from the transport equation, will be recalled. The derivation can be found in the book by Lux and Koblinger^[3] or in Nouri's thesis^[2].

In formula (1.1) k_{eff} was defined as the ratio of the rate of neutron production over the rate of neutron loss. The definition of the standard estimators of reaction rates used in Monte Carlo codes will therefore briefly be described before treating the simulation in the actual version of MORET and the proposed methods to improve the code.

2.1 Spatial distribution of neutrons emitted by fission

The spatial distribution of the density of neutrons emitted by fission is given by:

$$S(\vec{r}) = \frac{1}{k_{\text{eff}}} \int d\vec{r}' K(\vec{r}' \rightarrow \vec{r}) S(\vec{r}') \quad (2.1)$$

with \vec{r} being the position vector, and K representing the number of next generation fission neutrons produced in \vec{r} by a neutron emitted by fission in \vec{r}' .

2.2 Estimators of reaction rates

Conventionally, the estimators (collision and track length) are introduced for the flux, ϕ . The reaction rates are then deduced by multiplying the flux with the desired cross-sections.

2.2.1 Collision estimator

The density ψ of neutrons entering a collision is given by the product of the total macroscopic cross-section and the flux:

$$\psi = \Sigma_t \phi \quad (2.2)$$

Since the most straightforward quantity available in Monte Carlo simulation is precisely ψ , one can derive an estimation of the flux by tallying the contributions of collisions occurring in a volume V . This estimation is given by:

$$\phi_v = \sum_{\text{collisions in } V} \frac{\psi_i}{\Sigma_t} \quad (2.3)$$

where ψ_i is the number of neutrons entering collisions in V . Any reaction rate can then be deduced in the following way:

* See for example: L , C H and Mathonniere, G. *Apollo 1 - Notice d'utilisation - Version 133*, CEA, Rapport DMT/94-573, SERMA/LENR/1683, 1994

$$R_v^x = \sum_{\text{collisions in } V} \frac{\psi_i}{\Sigma_t} \sigma_x \quad (2.4)$$

with x indicating the kind of reaction.

2.2.2 Track length estimator

The track length estimator does not take into account the actual collisions that are being simulated, but estimates by considering the length of the track of a neutron in a certain volume, and the resulting probability for the neutron to contribute to the reaction rate by covering that path. As the mean free path is equal to $1/\Sigma_t$, the track length estimator can be introduced by replacing $1/\Sigma_t$ in equation (2.4) by the distance traveled by the neutron, l_i . Since the properties of the neutron remain unchanged during the flight, one has to consider the density of neutrons coming out of a collision, χ_i , giving:

$$\phi_v = \sum_{\text{flights in } V} \chi_i l_i \quad (2.5)$$

and

$$R_v^x = \sum_{\text{flights in } V} \chi_i l_i \sigma_x \quad (2.6)$$

2.3 Analog Monte Carlo simulation in MORET

The most straightforward manner to perform a Monte Carlo calculation is simply to simulate numerically the real physical events. In case of neutron transport this means to follow the neutrons in their motions and collisions. Such direct simulations are called *analog* Monte Carlo games^[3]. This section will describe how the analog simulation is implemented in MORET. Before will be presented the essence of a Monte Carlo simulation, which are the sampling techniques that aim to find realisations that follow from a given probability density function (pdf).

2.3.1 Sampling probability distributions

Sampling from probability distributions is based, in all practical cases, on sampling one or more random numbers, ϑ_i , uniformly distributed over the interval (0,1) and on transformations of them. A complete overview of sampling techniques can be found in the book by Lux and Koblinger^[3], limiting the description here to the methods essentially used in MORET.

To choose an event from a discrete distribution lets assume that P_1, P_2, \dots, P_n be the probabilities of the mutually exclusive events E_1, E_2, \dots, E_n and that the probabilities are normalized such that:

$$\sum_{i=1}^n P_i = 1 \quad (2.7)$$

To select one of the events, first a random number ϑ , with uniform probability distribution between 0 and 1, has to be drawn. Then the event E_i is selected when ϑ satisfies the double inequality:

$$P_1 + \dots + P_{i-1} \leq \vartheta < P_1 + \dots + P_i \quad (2.8)$$

To select a value from a continuous distribution the following method can be used when the probability density function, $p(x)$, is known (and the primitive function exists and can be inverted). If the variable x lies in between a and b , a value for x will be determined by the relations:

$$\vartheta = P(x) = \int_a^x p(x)dx \quad (2.9)$$

$$x = P^{-1}(\vartheta) \quad (2.10)$$

with again ϑ being a random number equidistributed over (0,1).

2.3.2 Simulation

A principle which the analog simulation uses is the idea of the neutrons 'living' in generations. All the neutrons of one generation will be followed one at the time from their 'birth' to their 'death', and if new neutrons are produced these will form the next generation, and will be followed in the next stage. Using a time sequence of one generation, the definition of k_{eff} becomes

$$k_{\text{eff}} = \frac{\text{neutrons produced in one generation}}{\text{neutrons lost in the same generation}} \quad (2.11)$$

and in this way an estimate can be found every generation for k_{eff} .

The life of a neutron is a succession of separated events in space: birth, elementary motion, collision, crossing of surfaces, leakage or absorption.

At the birth of a neutron, besides the point of birth in space, \vec{r} , three parameters need to be attributed: its energy, E , its direction of motion, $\vec{\Omega}$, and the probable distance to the next collision, s . These are to be chosen randomly while obeying the laws of probability governed by the physical laws of the system simulated.

Now finding values for the energy, the direction of motion and the probable distance to the next collision can be done in the following way:

- Energy: MORET is a multigroup-code, and the choice of the starting energy is thus reduced to the choice of an energy group. This is being done by drawing a random number ϑ , and comparing it to the cumulative probabilities calculated from the fission spectrum χ .

If $P_1 = \chi_1$, $P_2 = \chi_1 + \chi_2$, ..., $P_j = \sum_{i=1}^j \chi_i$ the energy group j will be chosen when ϑ

satisfies the double inequality:

$$P_{j-1} < \vartheta \leq P_j \quad (2.12)$$

- Direction of motion: The direction of motion $\vec{\Omega}$ can be decomposed with standard spherical coordinates in:

$$\vec{\Omega}_x = \sin\theta \cos\varphi \quad (2.13)$$

$$\vec{\Omega}_y = \sin\theta \sin\varphi \quad (2.14)$$

$$\vec{\Omega}_z = \cos\theta \quad (2.15)$$

in which x, y, z represent the Cartesian axes. To cover the entire space (isotropically), φ must be chosen between 0 and 2π , and $1 \geq \cos\theta \geq -1$ (or θ between 0 and π). The random choice of the vector $\vec{\Omega}$ is done by drawing two random numbers ϑ_1 and ϑ_2 and setting:

$$\varphi = 2\pi\vartheta_1 \quad (2.16)$$

$$\cos\theta = 2\vartheta_2 - 1 \quad (2.17)$$

- Probable distance to next eventual collision: the probability that a neutron covers the distance s without a collision is: $\exp(-\Sigma_t s)$. The probability density function for the neutron such that it does not collide between 0 and s and that it does have collision between s and $s+ds$ is:

$$p(s) = (\exp(-\Sigma_t s))\Sigma_t \quad (2.18)$$

Using (2.5) one finds:

$$\vartheta = \int_0^s \exp(-\Sigma_t s) \Sigma_t ds = 1 - \exp(-\Sigma_t s) \quad (2.19)$$

and:

$$s = -\frac{1}{\Sigma_t} \log(1 - \vartheta) \quad (2.20)$$

The probable distance to be covered can thus be obtained by drawing a random number ϑ (or $1-\vartheta$, which is the same) between 0 and 1, and applying equation (2.20).

These three parameters determine the place and nature of the next event, which may be:

- collision followed by
 - capture
 - fission
 - scattering
- exit of volume and entrance in another volume
- reach of exterior surface followed by
 - leakage
 - reflection

Knowing the direction of the neutron, the distance to the closest surface can be calculated. If the distance is smaller than the probable distance estimated, the neutron will leave the volume, otherwise a collision will take place.

If the neutron leaves the volume and enters a new one, a new probable distance, accounting for the different material environment, is drawn randomly. The direction of motion, however, is kept the same.

If the neutron reaches one of the outer boundaries of the system, depending on the type of boundary conditions, it can be reflected or leak out. To every reflecting surface a reflecting coefficient, R , is associated, being the probability that a neutron, coming in under a certain angle, with a certain energy, will be reflected. If a random number drawn is smaller than R the neutron is reflected and the laws of physics, dependent on the kind of reflection, will be obeyed. Otherwise the neutron leaks out of the system and the pursuit will be abandoned.

The pursuit of the neutron will also be abandoned when in the case of a collision the neutron is captured. If, however, the neutron is considered to be scattered three aspects need to be accounted for: the change of energy, the change of direction and in the case of MORET the possibility of $(n,2n)$ reactions, $(n,3n)$ reactions etc. These last reactions are accounted for by introducing a weight to the neutron, W , which will be increased by:

$$W' = W \cdot \frac{\Sigma_{s,(n,n')} + 2\Sigma_{s,(n,2n)} + 3\Sigma_{s,(n,3n)} + \dots}{\Sigma_{s,(n,n')} + \Sigma_{s,(n,2n)} + \Sigma_{s,(n,3n)} + \dots} \quad (2.21)$$

with $\Sigma_{s,(n,xn)}$ being the cross section for the (n,xn) reactions.

The change in energy is found by using the library containing the cumulative probabilities of transfers from energy group g to energy group g' . In the thermal domain the group g' can represent a higher energy than g (upscattering). The direction is being picked from the probability density function for the cosine of the scattering angle, μ , that uses as much information as the first order Legendre-polynomial approximation, which can be written as:

$$p(\mu)d\mu = \frac{1}{2}(1 + 3\mu\bar{\mu}) \quad (2.22)$$

where $\bar{\mu}$ is the average of the cosine of the scattering angle for each transfer. The approximation can not be directly applied since a part of the probability density function becomes negative when $|\bar{\mu}| > \frac{1}{3}$. This difficulty has been overcome by using the

approximation:

$$p(\mu)d\mu = \delta(\mu - \bar{\mu})d\mu \quad (2.23)$$

which physically means that for each energy transfer all the scattered neutrons have the same cosine of the scattering angle*.

The last option for the neutron is absorption followed by fission. In this case new neutrons are being produced for simulation in the next generation. The coordinates and resulting weight of these neutrons need to be scored. The coordinates need to be kept, because the starting points in the next generation will have to be chosen from the ones where fission has taken place, and the weight is needed to establish how many neutrons will start in each volume.

The problem exists that when k_{eff} is smaller than one, the neutron-population simulated would die out, and in the case of an k_{eff} bigger than one, the population would explode. Therefore to keep a stable situation the produced neutrons will always have to be renormalized (to the total number of starting neutrons, M_0). The source distribution is estimated with the collision estimator.

In MORET all configurations consist of uniform and homogeneous elements, and since neutrons can only be produced in fissile material, the number of starting neutrons, M_v , in a volume v , will be calculated in the following way from the total weight, P_v , of the neutrons in this volume for a generation $g-1$:

$$P_v = \frac{\sum_{\text{positions in } v} \left(\frac{v \Sigma_{f_i}}{\Sigma_{t_i}} W_i \right)}{\sum_{\text{all positions}} \left(\frac{v \Sigma_{f_i}}{\Sigma_{t_i}} W_i \right)} \cdot M_0 \quad (2.24)$$

$$M_v = \begin{cases} \text{INT}(P_v) + 1 & \text{if } (P_v - \text{INT}(P_v)) > \vartheta \\ \text{INT}(P_v) & \text{if } (P_v - \text{INT}(P_v)) < \vartheta \end{cases} \quad (2.25)$$

with ϑ being a random number between 0 and 1, and W representing the weight of the neutrons. This means that the number of neutrons is not really renormalized to M_0 , but that the total weight of the neutrons is renormalized to M_0 . The description of the simulation in MORET has been schematized in figure 2.1**.

2.3.3 Estimation of k_{eff}

As mentioned above, the k_{eff} resulting from the pursuit of one generation is calculated after each stage. This k_{eff} is in fact a track length estimator, as it is being calculated from the distance covered and the cross sections.

* Further developments have recently been introduced that enable to represent the anisotropy in higher order approximations: Nouri, A and LeCocq A, *Anisotropy treatment in criticality multigroup Monte Carlo codes*; International Conference on the Physics of Reactors, PHYSOR '96, Mito-Japan, September 1996

** This has been done in a somewhat simplified way, skipping steps that were less relevant for this study. The complete scheme can be found in the document by Courtois, Moret-Bailey and Poulot^[9].

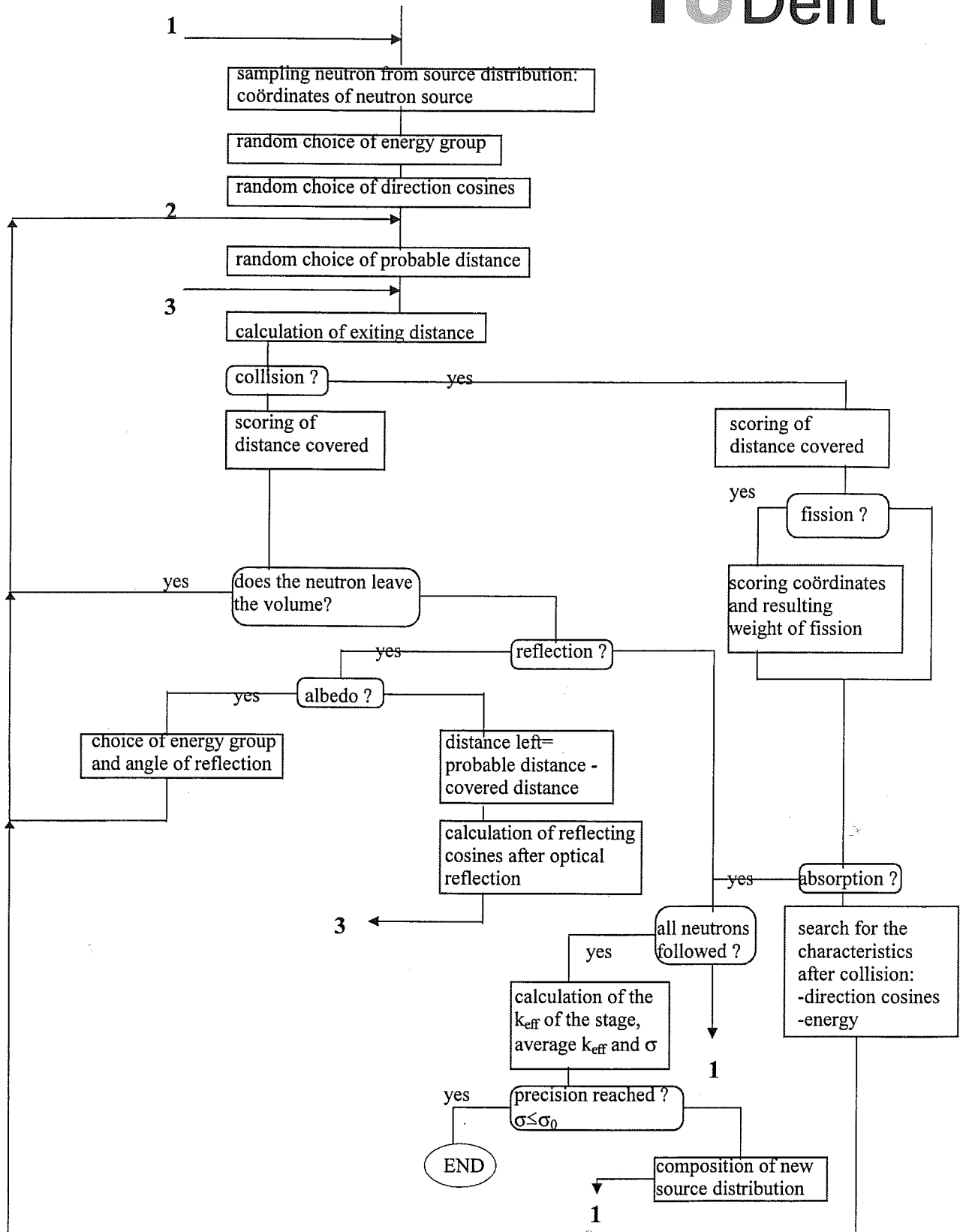


Figure 2.1. Principle of neutronic pursuit in MORET.

The average over the values of all generations will give the final estimate for k_{eff} . To characterize the uncertainty of the average the standard deviation *of the mean*, $s_{\bar{k}}$ will be used, which is defined as:

$$s_{\bar{k}} = \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^n (k_i - \bar{k})^2} \quad (2.26)$$

or written in a more suitable form for computation:

$$s_{\bar{k}} = \sqrt{\frac{1}{n(n-1)} \left[\sum_{i=1}^n k_i^2 - \frac{1}{n} \left(\sum_{i=1}^n k_i \right)^2 \right]} \quad (2.27)$$

with n being the number of generations over which the average is taken, and k_i being the values found for k_{eff} in the different generations.

In the introduction it was mentioned that the calculation of k_{eff} should start when the source distribution has converged. This means that in the calculation of the average and the standard deviation the settling iterations should not be considered. MORET uses three settling iterations (although it also gives an output setting the number of settling iterations at $3+i$, with $0 < i \leq 30$). This seems insufficient since in most cases the source distribution will not have converged that rapidly. Obviously it will depend on the configuration and on the initial source how fast this convergence is reached, but to improve the code it would be useful to have a better estimate of the number of settling iterations. However, the random aspect of the Monte Carlo method makes it not that evident to find the number of generations after which convergence is found.

A method that can be used to get an estimate of the number of generations to skip uses the idea that the removal of settling iterations is done to obtain a minimum variance. Generally when the number of points over which a variance is calculated is diminished, the variance should increase. When, however, the points that are ignored are the points that are far off the average, the variance will decrease.

At the end of a calculation it is fairly easy to calculate the variance over all the generations starting at a generation, g , to the last one. Since the first estimates of k_{eff} have been found with a non-converged source distribution, ignoring them would generally decrease the variance. So when g is increased and the variance still decreases the distribution will not have converged yet. Although the generation g (which might equal 1) at which the lowest variance will be found does not exactly indicate the point of convergence, it does give a good estimate of the number of generations that are advised to skip in the calculation of k_{eff} .

2.4 Superhistory powering

2.4.1 Superhistory powering algorithm

Brissenden and Garlick^[5] identified that, because of the renormalization performed at every generation, the analog simulation is not even-handed. For standard algorithms, iterations with below-average contribution will tend to produce fewer children (and these will also tend to have below-average importance*) and require above-average duplication to make up the next N source neutrons. Conversely an iteration of above-average contribution will tend to produce more children (of above-average importance) and these will require below-average duplication to form the next iteration source. The effect of this is that the source distribution is distorted by

* The importance of a neutron will be discussed in section 2.6. It indicates the contribution of the neutron with regard to the answer searched.

favouring the less important neutrons at the expense of the more important neutrons, thereby biasing the calculated value of k_{eff} . However for many practical criticality applications this k_{eff} bias is likely to be small (or even negligible). Note that all supplementary scored quantities such as fluxes and reaction rates will be similarly affected.

Of more significance is the effect on the calculated standard errors, where Brissenden and Garlick demonstrated that the bias introduced can take non-negligible negative value and hence impact on safety arguments which are based on confidence limits on calculated values of k_{eff} . The main cause of the under-estimation is the positive correlation that exists between iterations in analog simulation, whereas the derivation of the standard error assumes the sample histories in different iterations are independent. A further source of variation comes from the finite size of the neutron population sampled from the source distribution and in some situations this can also be significant.

The analysis of the standard fission source iteration process described above led to the development of the superhistory powering algorithm by Brissenden and Garlick to significantly reduce the biases in the calculation of k_{eff} and its standard error. The superhistory algorithm requires the definition of the unit sample size to be changed.

Each iteration, instead of comprising single generation histories (from birth due to fission to termination by fission, capture or leakage), now comprises multi-generation superhistories, each of which starts from birth due to fission and terminates at the L^{th} generation fission (or capture or leakage as before). A neutron superhistory is therefore the set of histories from a neutron and all its progeny through L fission generations (a typical value of L is 10). Neutrons that undergo fission in the L^{th} generation are saved for use in determining the starting source for the next iteration. The first part of a superhistory is shown in Figure 2.2. Note that all branches of the tree are followed as part of the superhistory up to the L^{th} generation.

In the normal course of events, for a sub-critical system, few superhistories will survive to the L^{th} generation; conversely for a super-critical system they will be too numerous. In order to stabilize the situation, the superhistory powering algorithm modifies the ν -value for fission throughout the system by dividing the actual value by the best current estimate of k_{eff} . This maintains the required approximation to equilibrium without in any way biasing the calculation. Obviously when scoring quantities used to compute k_{eff} this modification to the ν -value needs to be taken into account. As each iteration now comprises say ten generations rather than one (and as the algorithm is effectively simulating a critical system by the ν -value modification), each superhistory iteration is on average about ten times larger than a conventional iteration, and hence fewer iterations are required to achieve a particular statistical precision on k_{eff} . In addition fewer settling iterations are required before scoring commences.^[8]

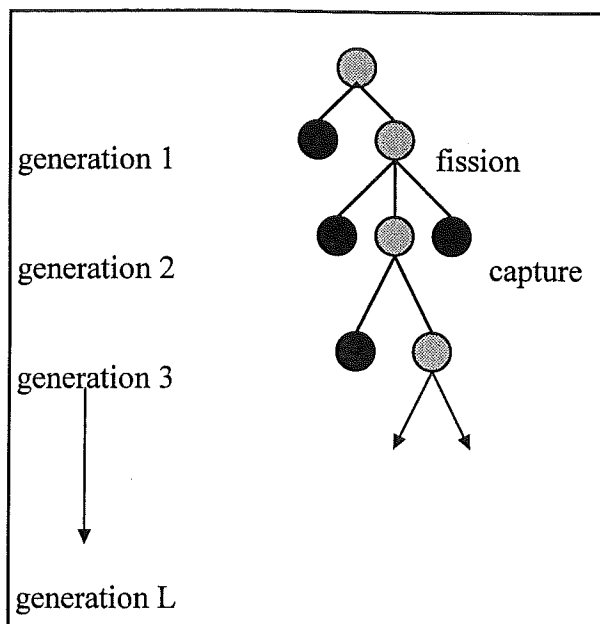


Figure 2.2. Part of a typical superhistory

2.4.2 Superhistory powering in MONK

The superhistory powering algorithm was included in the British code MONK in 1987. When implementing the method in MORET it has been done as in MONK with one (deliberate) exception, which will be described here.

The neutrons tracked by a MONK calculation are handled by the powering algorithm in three stores, as can be seen in figure 2.3:

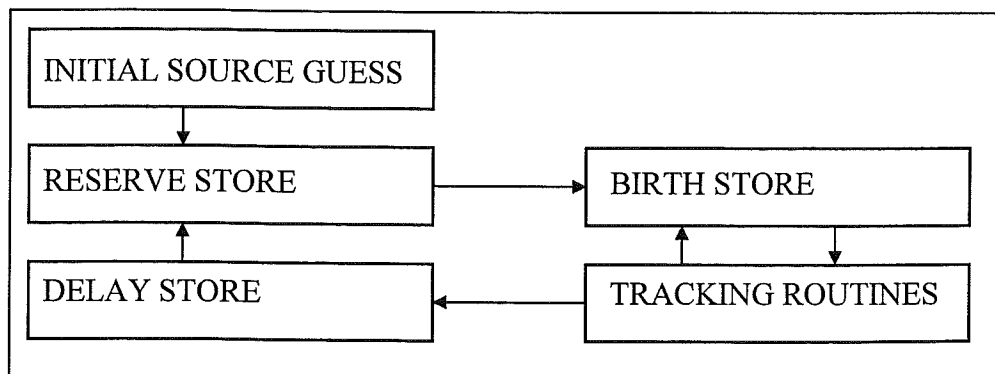


Figure 2.3. Implementation of superhistory powering in MONK

- the birth store, from which the current stage neutrons are selected and held
- the delay store, in which neutrons for use in the next stage are held
- the reserve store, from which neutrons forming the next birth store are selected

The birth store is operated as a stack. A neutron is taken from the top of the stack and tracked. If a fission event occurs, of the emerging M neutrons, $M-1$ are put on top of the stack; the remaining neutron is tracked on. Therefore the birth store also contains the outstanding neutrons forming the current superhistory. When all those have been tracked, the next superhistory starts.

When the L^{th} generation is reached, rather than placing the $M-1$ emergent neutrons on top of the birth store, one neutron of weight v is added to the delay store. This weight is used as a relative probability for selection in the next birth store.

At the end of the stage, the contents of the delay store are added to the end of the reserve store, replacing the same number of the oldest neutrons there. The reserve store contains neutrons from more than one stage, but the neutrons of the last stage will have a weight that is superior to the older ones. The next birth store is then selected by sampling with replacement from the reserve store.^[10]

The use of a reserve store may have advantages when the source distribution has converged. But when it has not, it slows down the convergency, since the old neutrons have a certain probability of being picked again. This effect has been shown using the simple geometry that will be presented in the next chapter. The results of the test performed are presented in Appendix C.

Since the use of a reserve store appeared to be a nuisance, it has been omitted in the implementation of the superhistory powering method in MORET. The birth store is now directly calculated from the delay store.

2.4.3 Calculation of k_{eff} in MONK

In MONK k_{eff} is not calculated as the average of the k_{eff} -values by stage, but as the ratio of the average of the number of produced neutrons by superhistory over the average number of neutrons followed by superhistory. If H_m is the number of tracked neutrons during a superhistory and P_m is the number of neutrons produced during a superhistory, the estimator for k_{eff} would be * :

$$k_{\text{eff}} = \frac{\sum P_m}{\sum H_m} \quad (2.28)$$

and an estimate for the variance of the ratio of correlated random quantities is given by:

$$\sigma_k^2 = \left(\frac{\bar{P}}{\bar{H}} \right)^2 \left[\frac{\sigma_H^2}{\bar{H}^2} + \frac{\sigma_P^2}{\bar{P}^2} - \frac{2\sigma_{PH}}{\bar{P}\bar{H}} \right] \quad (2.29)$$

with σ_{PH}^2 being the covariance of P_m and H_m .

In MORET P_m is the expected number of produced neutrons which has been calculated with the collision estimator.

2.5 Fission matrix method

2.5.1 Fission matrix

In section 2.1 the spatial distribution of neutrons emitted by fission was given by the equation (2.1):

$$S(\vec{r}) = \frac{1}{k_{\text{eff}}} \int d\vec{r}' K(\vec{r}' \rightarrow \vec{r}) S(\vec{r}')$$

with $K(\vec{r}' \rightarrow \vec{r})$ representing the number of neutrons produced in \vec{r} due to a neutron emitted by fission in \vec{r}' .

* Actually MONK uses a more elaborate way to estimate k_{eff} . It uses a linear combination of correlated estimators that has a minimum variance. This can be found in reference 10.

We will consider a system existing of N fissile units (with index i). (The other parts of the system being of non-fissile material.) The integral of the equation (2.1) above will therefore only be taken over the volume of the N fissile units and can be written as the sum of integrals. By integrating both sides of the equation over the volume of unit i, and by setting:

$$S_i = \int_i S(\vec{r}) d\vec{r} \quad (2.30)$$

which represents the number of neutrons emitted in unit i, one gets:

$$S_i = \frac{1}{k_{\text{eff}}} \sum_{j=1}^N \left[\frac{\int_i d\vec{r} \int_j d\vec{r}' K(\vec{r}' \rightarrow \vec{r}) S(\vec{r}')}{S_j} \right] S_j \quad (2.31)$$

The quantity between brackets represents the number of next generation fission neutrons produced in the unit i as result of a neutron emitted by fission in the unit j, and will be denoted as k_{ji} . This gives us a system of discrete equations:

$$\sum_j k_{ji} S_j = k_{\text{eff}} S_i \quad \text{with } i = 1, N \quad (2.32)$$

which can be written as:

$$\begin{pmatrix} k_{11} & k_{21} & \cdots & k_{N1} \\ k_{12} & k_{22} & \cdots & k_{N2} \\ \vdots & \vdots & \ddots & \vdots \\ k_{1N} & k_{2N} & \cdots & k_{NN} \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \\ \vdots \\ S_N \end{pmatrix} = k_{\text{eff}} \begin{pmatrix} S_1 \\ S_2 \\ \vdots \\ S_N \end{pmatrix} \quad (2.33)$$

The eigenvalues of this matrix can be found by solving the characteristic equation:

$$\begin{vmatrix} (k_{11} - \lambda) & k_{21} & \cdots & k_{N1} \\ k_{12} & (k_{22} - \lambda) & \cdots & k_{N2} \\ \vdots & \vdots & \ddots & \vdots \\ k_{1N} & k_{2N} & \cdots & (k_{NN} - \lambda) \end{vmatrix} = 0 \quad (2.34)$$

The largest of the eigenvalues represents the k_{eff} of the system; the eigenvector belonging to this eigenvalue gives the fraction of the neutron-sources in each unit. A proof for the case with two fissile units is presented in Appendix D.

2.5.2 Use of the eigenvector of the fission matrix

In their article Kadotani et al.^[6] proposed to use the eigenvector of the fission matrix to recalibrate the sources. These eigenvectors do not correspond to the correct fission distribution of each divided zone, but since they are the region-integrated fission distribution, they are supposed to be more stable than the fission events calculated by the Monte Carlo method.

Kadotani et al. proposed to calculate the elements of the matrix only by considering the neutrons of the last generation. It could, however, very well be that the number of neutrons of one generation would not be enough to guarantee a precise determination of the terms of the matrix. The uncertainty of these terms could be high and the calculated eigenvector inadequate. Nouri^[2] therefore proposes to calculate the terms of the matrix for generation g using all the simulated histories during the generations 1,2, ... ,g.

Kadotani et al. used the calculated eigenvectors to recalibrate the sources every three generations. Obviously the fission matrix can be used more or less often, and there probably exists an optimum in the relation between time lost in calculating the eigenvector and the time won by accelerated convergence. This optimum could, however, depend on the configuration. In the different calculations in MORET we have recalibrated every ten generations.

2.6 Importance sampling

The basic principle of the method of importance sampling is that the importance of a neutron, with regard to the answer searched, is being accounted for. The form of the importance function, describing this, as well as the numerical value attached to it, will depend on the parameter one wants to estimate. On the other side, for every answer searched, one can define different importance functions depending on the physical parameter that is chosen to characterize the neutron population.

In this case the problem consists of the spatial convergence of the neutrons emitted by fission. It is therefore evident that an importance function will be chosen in relation to this distribution. The function will be defined in a point \bar{r} as the number of neutrons produced in the system by fission induced by the neutrons emitted in \bar{r} .

In order to get an idea of the possibilities of importance sampling a method with zero expected variance will be described. This description comes from Kalos^[11]. From this description a possible method of calculating an importance function and improving the Monte Carlo simulation will be deduced.

2.6.1 Method with zero expected variance

Let's recall once more equation (2.1) representing the spatial distribution of neutrons:

$$S(\bar{r}) = \frac{1}{k_{\text{eff}}} \int d\bar{r}' K(\bar{r}' \rightarrow \bar{r}) S(\bar{r}')$$

with $K(\bar{r}' \rightarrow \bar{r})$ representing the number of neutrons produced in \bar{r} by a neutron emitted by fission in \bar{r}' . The equation, being homogeneous, can be solved iteratively. With (n) representing the number of the generation, it can be written as:

$$S^{(n)}(\bar{r}) = \int d\bar{r}' K(\bar{r}' \rightarrow \bar{r}) S^{(n-1)}(\bar{r}') \quad (2.35)$$

with k_n being an estimate at generation (n) of the multiplication factor, being given by:

$$k_n = \frac{\int d\bar{r} S^{(n)}(\bar{r})}{\int d\bar{r} S^{(n-1)}(\bar{r})} \quad (2.36)$$

Let's introduce the function I, defined positive for every point \bar{r}' , where production of neutrons might be possible, that is:

$$\int d\bar{r} K(\bar{r} \rightarrow \bar{r}') > 0 \quad (2.37)$$

If we replace $S(\bar{r})$ by: $\hat{S}(\bar{r}) = S(\bar{r})I(\bar{r})$, we get:

$$\hat{S}(\bar{r}) = \frac{1}{k_{\text{eff}}} \int d\bar{r}' \hat{K}(\bar{r}' \rightarrow \bar{r}) \hat{S}(\bar{r}') \quad (2.38)$$

with

$$\hat{K}(\bar{r}' \rightarrow \bar{r}) = \frac{I(\bar{r})K(\bar{r}' \rightarrow \bar{r})}{I(\bar{r}')} \quad (2.39)$$

Having transformed K into \hat{K} the equations operate the same on S and \hat{S} , giving:

$$\hat{S}^{(n)}(\bar{r}) = \int d\bar{r}' \hat{K}(\bar{r}' \rightarrow \bar{r}) \hat{S}^{(n-1)}(\bar{r}') \quad (2.40)$$

and for the estimation of k_{eff} at the generation (n):

$$k_n = \frac{\int d\bar{r} \hat{S}^{(n)}(\bar{r})}{\int d\bar{r} \hat{S}^{(n-1)}(\bar{r})} \quad (2.41)$$

If now I would be defined as the solution of the adjoint equation to (2.1):

$$I(\bar{r}) = \frac{1}{k_{\text{eff}}} \int d\bar{r}' I(\bar{r}') K(\bar{r} \rightarrow \bar{r}') \quad (2.42)$$

where $I(\bar{r})$ gives the importance of a neutron at the point \bar{r} , i.e.: the number of next generation fission neutrons produced in the system by a neutron emitted by fission in the point \bar{r} . By using the definition of k_n given in equation (2.41) and the relations (2.39) and (2.40), one finds:

$$\begin{aligned} k_n &= \frac{\int d\bar{r} \hat{S}^{(n)}(\bar{r})}{\int d\bar{r} \hat{S}^{(n-1)}(\bar{r})} \\ &= \frac{\int d\bar{r} \int d\bar{r}' \hat{K}(\bar{r}' \rightarrow \bar{r}) \hat{S}^{(n-1)}(\bar{r}')}{\int d\bar{r} \hat{S}^{(n-1)}(\bar{r})} \\ &= \frac{\int d\bar{r} \int d\bar{r}' \frac{I(\bar{r}) K(\bar{r}' \rightarrow \bar{r})}{I(\bar{r}')} \hat{S}^{(n-1)}(\bar{r}')}{\int d\bar{r} \hat{S}^{(n-1)}(\bar{r})} \\ &= \frac{\int d\bar{r} \left[\int d\bar{r}' I(\bar{r}') K(\bar{r} \rightarrow \bar{r}') \right] \frac{\hat{S}^{(n-1)}(\bar{r}')}{I(\bar{r}')}}{\int d\bar{r} \hat{S}^{(n-1)}(\bar{r})} \end{aligned}$$

According to equation (2.42) the part between brackets is equal to: $k_{\text{eff}} I(\bar{r})$, so this gives:

$$k_n = \frac{\int d\bar{r} k_{\text{eff}} \hat{S}^{(n-1)}(\bar{r})}{\int d\bar{r} \hat{S}^{(n-1)}(\bar{r})} = k_{\text{eff}} \quad (2.43)$$

This last equation means that at every generation the estimate k_n of the multiplication factor leads to the true looked for value of k_{eff} . An importance function defined as in (2.42) therefore leads to zero variance, if the reaction rates in the fraction in equation (2.41) are estimated without statistical fluctuation.

To realize such a calculation with zero expected variance one needs to know from the start the importance function, being the solution of the adjoint equation. Obviously this is at least as hard to find as the source distribution, and it would in fact be a method of solving a problem already solved, which is of no use. However, if one has a function close to I it could accelerate the convergence of the Monte Carlo simulation.

2.6.2 Use of the importance function

As we have seen that the importance function is the solution of the equation adjoint to the equation of the source distribution, we will therefore act as in the case of the fission matrix. The fissile system is divided into N cells, which will be supposed to have a constant importance inside each cell. Equation (2.42) then leads to the system of equations:

$$I_i = \frac{1}{\lambda} \sum_{j=1}^N I_j K(i \rightarrow j) \quad \text{with } i = 1, N \quad (2.44)$$

The importance function is thus given by the eigenvector associated to the highest eigenvalue found for the matrix $[K(i \rightarrow j)]_{i,j=1,N}$, being the adjoint of the fission matrix.^[2]

Just as Kadotani et al., Kalos proposed to calculate the fission matrix by only considering the neutrons of the previous generation. The problem encountered in the previous section will obviously be solved in the same way, and the matrix will be built up using all the generations 1,2, ... ,g-1.

The importance function is then used in the pursuit of the neutrons. Once a neutron enters a fissile volume, v , other than the one it was born in, its weight will be altered in the following way:

$$W' = \frac{I(v)}{I(nvb)} W \quad (2.45)$$

where nvb indicates the number of the volume where the neutron was born.

This means that when regions have very different importances this can lead to enormous differences in the weights of the neutrons. In the extreme case volumes that have not been visited will have importance 0. This is highly undesirable from a computational point of view. This problem can be solved by a smoothening procedure. This has been done by Nouri in his previous research on MORET and the importance sampling^[2], but has been omitted in this research. This problem can also be prevented by putting neutrons in every volume at the start of the calculation. If this is not being done the user should assure himself that every volume will have been visited before the eigenfunction of the adjoint fission matrix is calculated for the first time.

2.7 Stratified sampling

A problem that can be caused by renormalizing the source distribution at every generation and creating a new starting source distribution by sampling randomly is that certain parts of the fissile material could be neglected. If few neutrons are being produced in a volume v , P_v in equation (2.24) could be less than one, which results in the fact that M_v has a finite probability of being zero, and thus no neutron will be simulated in that generation in that volume. In the case of weak coupling it can take many generations before a zone will be visited again.

To avoid this behaviour Roussel and Gelbard^[7] have developed a method in which a weight is associated to every simulated neutron, and where it is assured that every fissile zone will have at least one neutron. To prevent simulating neutrons with a very low weight, and thus preventing to spend much calculation time on neutrons that will barely contribute to the estimate of k_{eff} , a cutoff threshold can be introduced. This cutoff threshold is also a parameter that has to be optimized. This has not been done in this study, nor did Roussel and Gelbard show to have investigated this problem.

The number of neutrons, M_i , that will be simulated in each volume will depend on its production, S_i , in the previous generation, g . The probability density function for each volume is defined similarly as it has been done for the conventional sampling method:

$$p_i^g = \frac{S_i}{\sum_{j=1}^J S_j}$$

but the number of neutrons in each volume will be * :

* NINT returns the nearest integer value

$$\begin{cases} M_i^{g+1} = \text{NINT}(M_0 \cdot p_i^g) & \text{if } M_0 \cdot p_i^g \geq \frac{1}{2} \\ M_i^{g+1} = 1 & \text{if } M_0 \cdot p_i^g < \frac{1}{2} \end{cases} \quad (2.46)$$

with M_0 being the number of starting neutrons as it was in the case of the analog simulation. The weight associated to the neutrons is:

$$W_i^{g+1} = \frac{M_0 \cdot p_i^g}{M_i^{g+1}} \quad (2.47)$$

Obviously the number of followed neutrons will generally be superior to M_0 , but the total weight does equal this value.

As mentioned above a cutoff threshold, W_{cut} , can be introduced to avoid following neutrons with too low weight. Once the value of the cutoff threshold ($W_{\text{cut}} \ll 1$) is chosen and $W_i^{g+1} < W_{\text{cut}}$, 'Russian Roulette' can be played, which means that:

- with a probability W_i^{g+1} , the neutron survives and will be followed with a weight $W_i^{g+1}=1$.
- with a probability $1 - W_i^{g+1}$ the neutron is killed, and will not be followed anymore.

A problem that still remains is the problem of all simulated neutrons that leave the volume without colliding, and thus not creating a potential fission site. Gelbard and Feline^[12] therefore defined the Delta scattering method, which purpose is to create at least one potential fission site in each volume. This is being done by forcing the first collision of each neutron to be in the volume of birth.

This problem can also be avoided by using the track length estimator for the sources, instead of the collision estimator which is generally being used. The stratified sampling method has therefore been implemented in MORET with the track length estimator, and in the version used the cutoff threshold is set to zero.

3. ONE-DIMENSIONAL MODEL

The one-dimensional model has been used to get acquainted with the different methods proposed, and with the idea behind a Monte Carlo program in general. The results found with the model gave a first idea of what was to be expected from the different methods.

3.1 Description of the model

The model used was first described by Roussel^[7] and consists of a one-dimensional system of boxes. All these boxes, except the middle one, have a $\eta=1$. The middle box has a $\eta=1.1$. Neutrons in these boxes have three options: they can be absorbed in the box, with a

probability: $P_a = \frac{\Sigma_a}{\Sigma_a + 2D/h^2}$, or can jump left or right, with a probability:

$P_l = P_r = \frac{D/h^2}{\Sigma_a + 2D/h^2}$, with D being the diffusion coefficient, and h representing the width

of the boxes, which can be varied.

The neutrons cannot leak out of the system and are reflected at the ends. The situation is sketched in Figure 3.1.

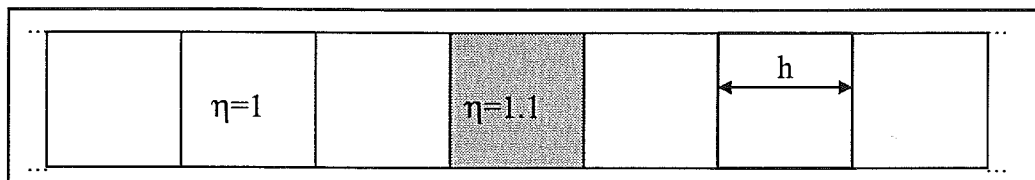


Figure 3.1. One-dimensional model.

In all the test cases the used constants were:

$N_{\text{box}}=41$ (Number of boxes, boxes have index i)

$D=1/3$ cm

$\Sigma_a=0.2$ cm⁻¹

$(\nu\Sigma_f)_i=\Sigma_a$ for $i\neq 21$

$(\nu\Sigma_f)_{21}=0.22$ cm⁻¹ (middle box)

3.2 Calculations

The convergence of the different methods have been tested with this model. This has been done for two different widths of the boxes, $h=10$ cm and $h=100$ cm, having a less and a more weakly coupled system. These simulations have been performed both with 100 and 500 starting neutrons.

For the case of 100 starting neutrons the calculations have been repeated with different random numbers a couple of times to see whether the results were stable. A further calculation has been performed with the analog simulation, to try to find a minimum number of neutrons that is necessary to find good results.

3.3 Results

The convergency-curves found for the calculations with the variations of the width of the boxes, h , and the number of starting neutrons, M_0 , are given in the figures 3.1, 3.2, 3.3 and 3.4.

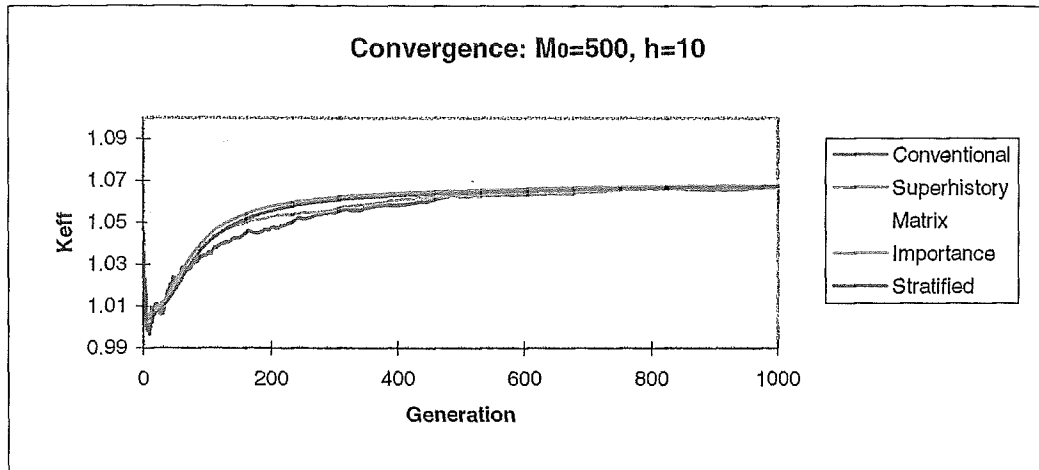


Figure 3.1. Convergence of the different methods for the one-dimensional model, with $M_0=500$, and $h=10$ cm

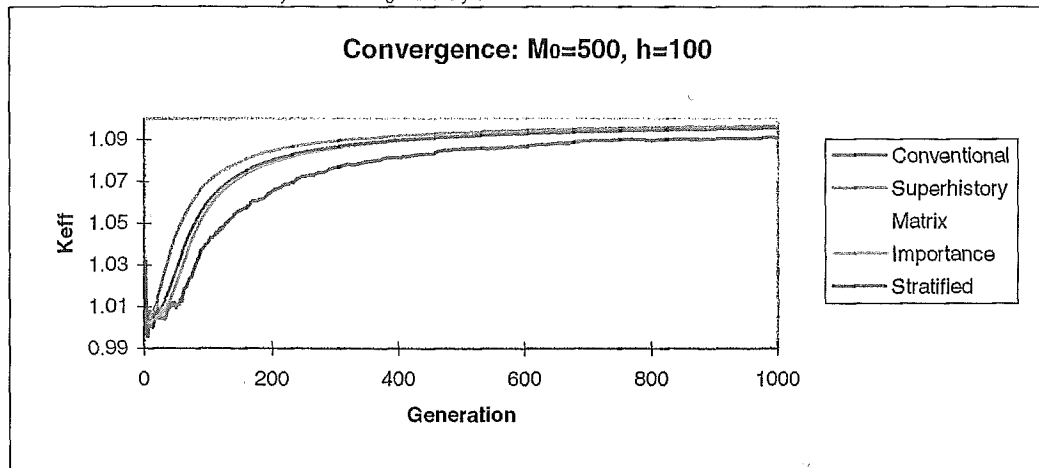


Figure 3.2. Convergence of the different methods for the one-dimensional model, with $M_0=500$, and $h=100$ cm

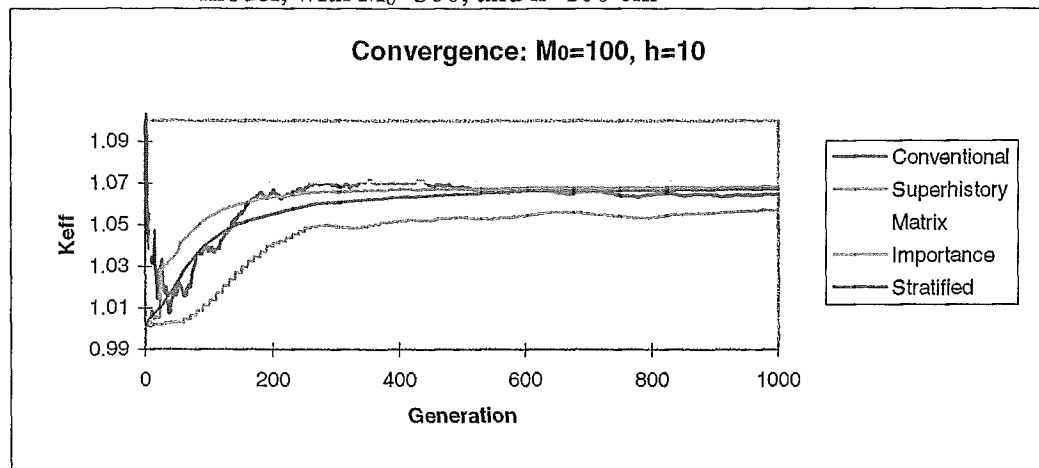


Figure 3.3. Convergence of the different methods for the one-dimensional model, with $M_0=100$, and $h=10$ cm

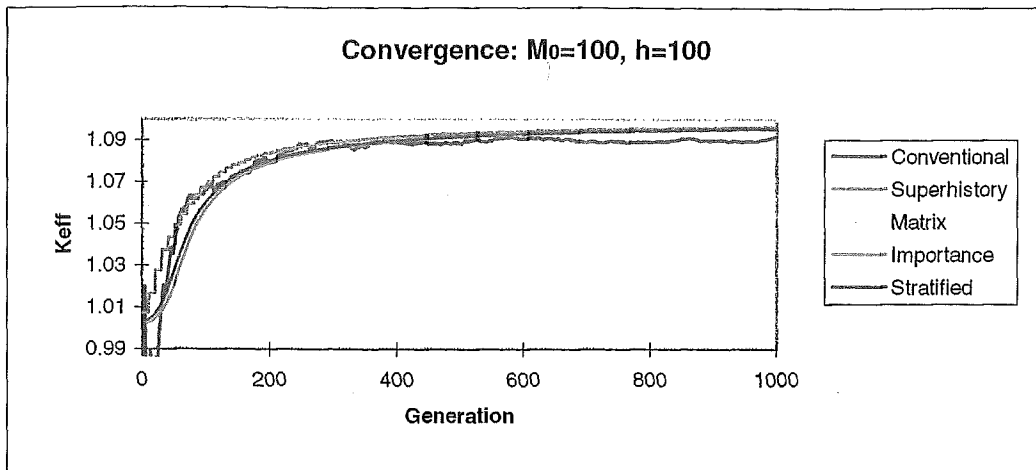


Figure 3.4. Convergence of the different methods for the one-dimensional model, with $M_0=100$, and $h=100$ cm

For the cases with 100 starting neutrons the conventional Monte Carlo method and the superhistory powering appeared not to be stable. When repeating the calculation the simulation converged in many cases to a value for k_{eff} very close to 1, being the k_{eff} of all the boxes, except the central one. The other methods did not show instability, when repeating the calculation ten times with different random numbers.

The calculations done to find a minimum number of neutrons that have to be simulated in order to get a correct result, has mainly become a calculation to test the stability of the conventional sampling. In fact, calculations did not converge to the right answer (source distribution and k_{eff}) in all the repeated calculations. The final result in the calculations performed, with a standard deviation of 150 pcm, were in all cases $k_{eff} \approx 1$ or $k_{eff} \approx 1.1$, having set $h=100$ cm. Figure 3.5 presents the average of k_{eff} taken over ten simulations for each number of starting neutrons. From this graph it is simple to see that when the average is considerably below 1.1, one or more of the simulations have converged to the wrong value.

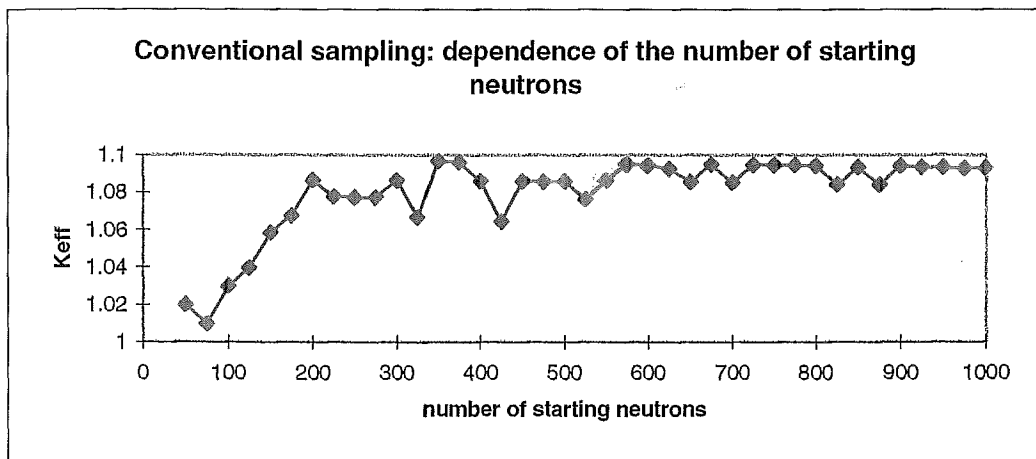


Figure 3.5. The average value found for k_{eff} as a function of the number of simulated neutrons

3.4 Discussion of results

The one-dimensional model has in the first place been used to get acquainted with the different methods. The results showed, however, that when enough neutrons were simulated all the proposed methods did improve the convergence of the Monte Carlo simulation. The best method by far for this case was the fission matrix method, which shows an almost instantaneous convergence to final value found for k_{eff} .

The simulations done with few neutrons, however, showed that the conventional sampling method and the superhistory powering method did not always converge to the correct value, which means that the central box is not visited enough by the simulated neutrons.

It is hard to deduce from the results of the calculations done with variable number of neutrons, a minimum of neutrons required. Even simulations with more than 800 neutrons have converged to the wrong value, but taking less than 200 neutrons seems unadvised. Additional calculations using a converged source distribution at the start showed that the system converged to the right value independent of the number of neutrons chosen.

4. GEOMETRY OF KADOTANI ET AL.

4.1 Geometry

The system is a lattice of 5x5x1 (highly enriched) uranium metal spheres of radius 8.71 cm (critical radius for a bare sphere: $k_{eff}=1.00018$, $\sigma=150$ pcm), with exception of the central sphere, which has a radius of 10 cm (bare sphere in air: $k_{eff}=1.11713$, $\sigma=150$ pcm). The spheres are considered to be in interaction in air with a distance of 20 cm from center to center. There is no reflector. The number densities of atoms for metal uranium are $0.045449 \cdot 10^{24} \text{ cm}^{-3}$ and $0.00256 \cdot 10^{24} \text{ cm}^{-3}$ for ^{235}U and ^{238}U , respectively.

4.2 Results

The convergence of the different methods found for this system with a simulation using 250 neutrons over 500 generations and a uniform source distribution is presented in figure 4.1. The estimates of k_{eff} are given in table 4.1.

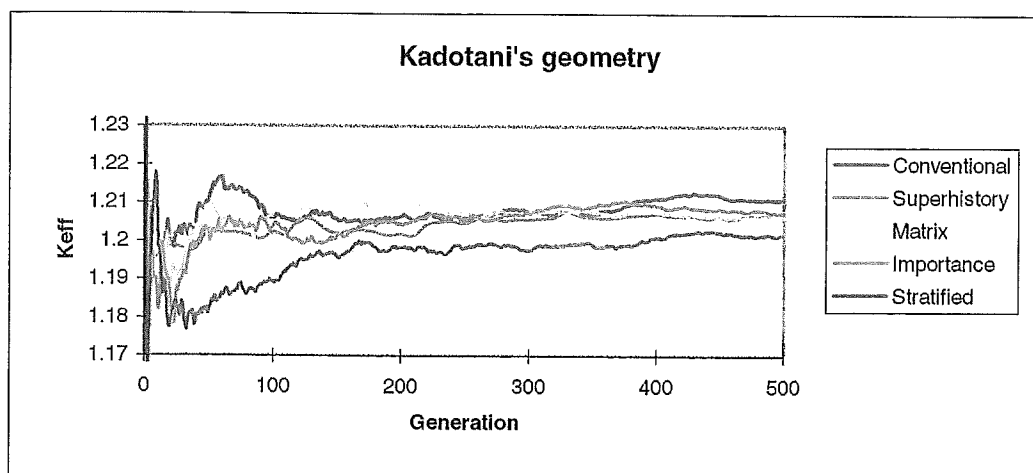


Figure 4.1. Convergence of the different methods in Kadotani's geometry with a uniform initial source distribution

Table 4.1. The estimates of k_{eff} for Kadotani's geometry.

Method	k_{eff}	$\sigma(\text{pcm})$
Conventional	1.20957	233
Superhistory	1.20466	368
Matrix	1.20606	238
Importance	1.20747	239
Stratified	1.20166	246

In order to get an impression of how weakly coupled this system is, and of the distribution of the neutrons, table 4.2 gives the fission matrix, the eigenvalues and the eigenvector corresponding to the largest eigenvalue of the system. Instead of giving a 25 by 25 matrix, however, the outer (16) spheres have been regrouped in group 1, the centre sphere in group 3 and those in between (8) in group 2. The values in the matrix thus represent the number of

Table 4.2. The (reduced) fission matrix, the eigenvalues and the eigenvector corresponding to the largest eigenvalue for Kadotani's geometry.

Fission matrix	Eigenvalues	Eigenvector
$\begin{pmatrix} 1.051 & 0.090 & 0.020 \\ 0.068 & 1.070 & 0.201 \\ 0.002 & 0.050 & 1.101 \end{pmatrix}$	$\begin{pmatrix} 1.063 \\ 0.950 \\ 1.208 \end{pmatrix}$	$\begin{pmatrix} 0.301 \\ 0.473 \\ 0.226 \end{pmatrix}$

Other calculations that have been performed with this geometry, were done with the aim of finding a minimum number of neutrons needed to find good results with the Monte Carlo simulation. All these tests used the analog simulation, supposing that a minimum found would also hold for the other methods, as they are supposed to improve the conventional method. These simulations were also done with a uniform source distribution till a standard deviation of 200 pcm was reached, and the only parameter that was varied was the number of starting neutrons. The results can be found in figure 4.2.

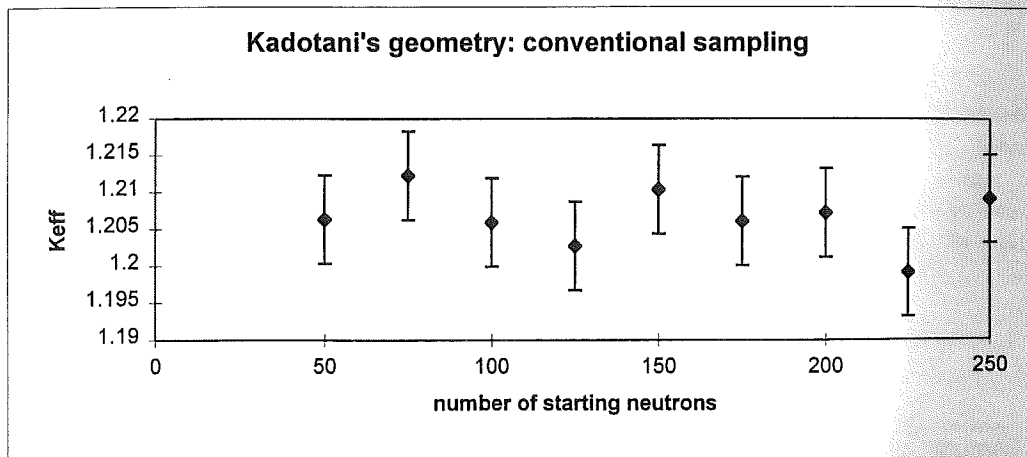


Figure 4.2. Dependence of k_{eff} when varying the number of starting neutrons in calculations with Kadotani's geometry

4.3 Discussion of results

The results found with the different methods are statistically not coherent. The conventional method and the stratified sampling are in conflict. Seen the start of the curves it could appear that if settling iterations were skipped the results would come closer to each other, but this is not the case. Only using these results it is impossible to say which result is wrong or what the reasons are for the differences. When the results of the variable number of neutrons are being looked at, one can see that these results are conflicting too. These calculations have only been done up to 250 neutrons, being the amount used in the comparison of the different methods, and it might be that this does not suffice. More calculations have to be performed with variable number of neutrons to get a better idea of how many neutrons are needed to get good results, and then the different methods should be compared again.

5. WHITESIDES' GEOMETRY

5.1 Geometry

This system, which has also been described in the introduction, exists of a 9x9x9 array of plutonium metal spheres with a radius of 4 cm (bare sphere in air: $k_{\text{eff}}=0.82925$, $\sigma=116$ pcm), spaced on 60 cm centers in air. Again the central sphere is slightly different, and in this case has a radius of 4.9387 cm (bare sphere in air: $k_{\text{eff}}=0.99805$, $\sigma=141$ pcm). The array is reflected on all sides by a thick water reflector. The plutonium considered is pure ^{239}Pu , with a density of $19.84 \text{ g}\cdot\text{cm}^{-3}$.

5.2 Results

5.2.1 Convergence

The calculations have been performed by starting with 15 neutrons in every sphere, and simulating 500 generations. The convergence of the different methods can be found in figure 5.1.

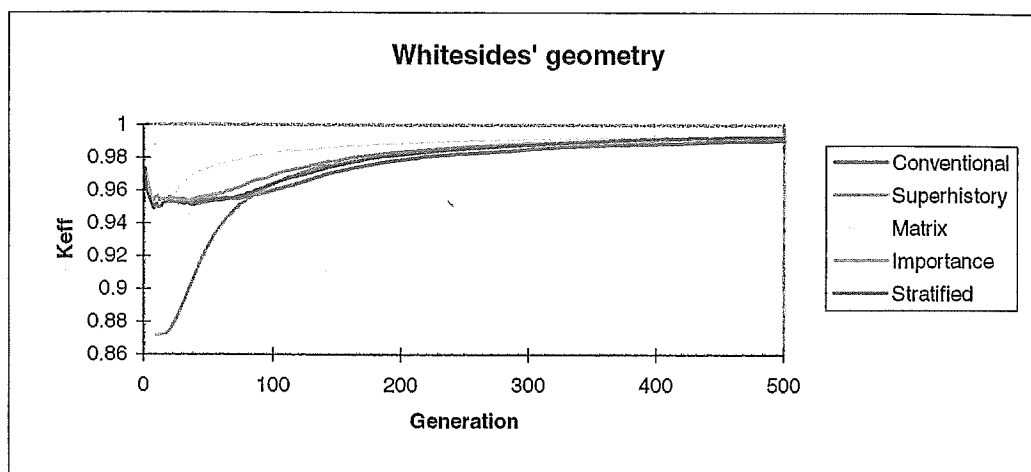


Figure 5.1. Convergence of the different methods in Whitesides' geometry with a uniform source distribution

This representation does give an idea of the rate of convergence, but nothing can be said about the statistical precision of the results using the different methods. We see that after 500 generations the results of the different methods seem to be consistent, but the speed of convergence is quite different. One can also stop the calculation after reaching a desired statistical precision and wonder whether the results are statistically correct (within the confidence interval). In figure 5.2 the k_{eff} is therefore given as a function of the standard deviation.

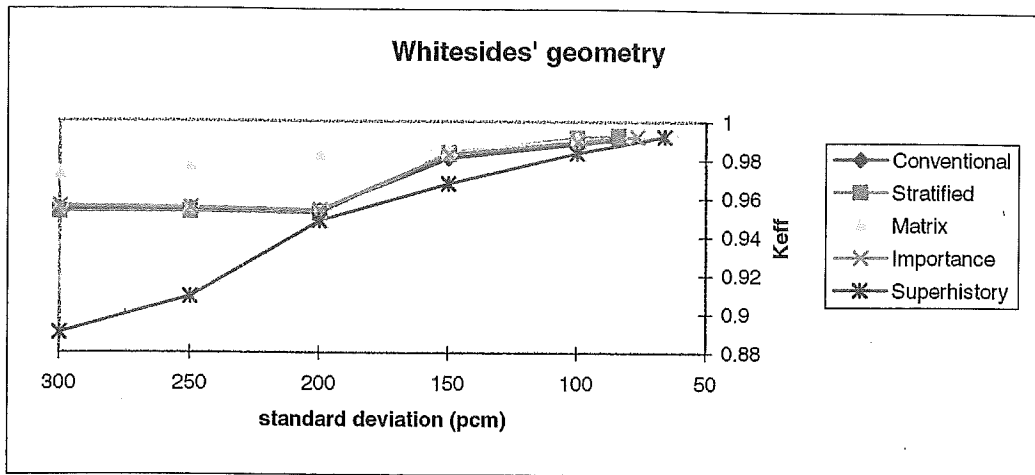


Figure 5.2. k_{eff} as a function of the standard deviation for Whitesides' geometry

5.2.2 Suppressing settling iterations

As was described in chapter two the number of generations to suppress for minimal variance has been calculated for the simulations. This method, though applicable in principle for all methods, was not applied for the calculations with the superhistory powering since the mean and variance are calculated in a different way. The estimate after every superhistory stage does include the contributions of all neutrons, and the data that would have been needed to estimate the number of stages to suppress is no standard output of the calculation. The results are presented in table 5.1 (superhistory powering: $k_{eff}=0.99236$, $\sigma=66$ pcm).

Table 5.1. Values found for k_{eff} and σ with (superscript s) and without suppressing generations for Whitesides' geometry

Whitesides	k_{eff}	σ (pcm)	gen. suppr.	k_{eff}^s	σ^s (pcm)
Conventional	0.99055	85	113	0.99859	54
Matrix	0.99307	62	22	0.99477	50
Importance	0.99240	77	95	0.99815	52
Stratified	0.99270	84	92	0.99966	52

5.2.3 Fission matrix, eigenvalues and eigenvector

Table 5.2 gives the fission matrix, the eigenvalues and the eigenvector corresponding to the largest eigenvalue for the Whitesides' geometry. As in the case of Kadotani's geometry the spheres have been regrouped. This has been done by layer of spheres. The outer spheres (386) are put together in group one, the second layer (218) in group two, the third (98) in group three, the fourth (26) in group four, and the centre sphere in group five. To get an idea of the coupling between two spheres: $k_{ji}=0.00085$, for i representing the centre sphere and j one of its neighbours.

Table 5.2. The (reduced) fission matrix, the eigenvalues and the eigenvector corresponding to the largest eigenvalue for Whitesides' geometry.

Fission matrix	Eigenvalues	Eigenvector
$\begin{pmatrix} 0.821 & 0.018 & 0.011 & 0.012 & 0.010 \\ 0.009 & 0.826 & 0.015 & 0.011 & 0.011 \\ 0.003 & 0.007 & 0.833 & 0.016 & 0.010 \\ 0.001 & 0.002 & 0.004 & 0.818 & 0.012 \\ 0.000 & 0.000 & 0.000 & 0.001 & 0.994 \end{pmatrix}$	$\begin{pmatrix} 0.994 \\ 0.849 \\ 0.823 \\ 0.811 \\ 0.815 \end{pmatrix}$	$\begin{pmatrix} 0.061 \\ 0.063 \\ 0.058 \\ 0.053 \\ 0.765 \end{pmatrix}$

5.3 Discussion of results

5.3.1 Convergence

In contrary to the tests performed on Kadotani's geometry these calculations show that for this geometry the different methods do improve the rate of convergence, at least as a function of the number of generations simulated. The fission matrix method does show a fast convergence, but when k_{eff} is estimated with suppressed generations the result appears not to be coherent with the other methods. Skipping as many generations as was done for the other methods does not really affect the result.

It is also remarkable to see that the superhistory powering starts from very low. This can partly be explained by the fact that in the beginning of the simulation, having a uniform starting source distribution, one can find relatively more neutrons in the outer spheres. When these neutrons leak out of the system, they do not produce any other neutrons that can be followed in the superhistory. This gives less neutrons followed and relatively more of them will be added to the lost neutrons. In table 5.3 the first 10 stages (after the three settling ones) are given, with the number of neutrons followed, and the number and percentage of neutrons that have leaked out during that stage. In the first stages considerably less neutrons have been followed, and the leakage-percentage is higher. After three stages, however, more neutrons are being followed than is being done in the other methods in ten generations, which makes it improbable that leakage would be the only reason for the low results. It would be useful to repeat the calculation with the source distribution as an output. Giving the eigenvector of the reduced fission matrix as output after every stage might give valuable information to find a reason for the slow start of the superhistory powering.

Table 5.3. Number of followed and leaked out neutrons in the first 10 superhistories in the calculation with the Whitesides-geometry

superhistory	followed	leaked	percentage
1	60291	42344	70.2
2	100558	70438	70.0
3	115079	79193	68.8
4	121593	82032	67.4
5	134042	89028	66.4
6	124193	82093	66.1
7	124367	81881	65.8
8	118802	78321	65.9
9	116170	76549	65.9
10	119962	78659	65.6

5.3.2 Suppressing settling iterations

The results show that suppressing three generations is too little. For this geometry it appears to be necessary to skip about a hundred generations. If we recall what was being said in the introduction about a system composed of many fissile units, we can conclude that the system should have a k_{eff} that is at least equal to the k_{eff} of the most reactive subsystem, as a separate unit (with the same moderating and reflecting conditions). The most reactive subsystem is in this case the central sphere with a calculated $k_{\text{eff}}=0.99805$. Except for the fission matrix method the others, from which generations have been skipped, do indeed give an estimate of k_{eff} that is higher. Since the first stages in the superhistory powering appear to give very low estimates of k_{eff} , it is probable that this method too would give a higher result if generations would be skipped.

6. SMITH'S GEOMETRY

6.1 Geometry

This case reflects the main properties of the classic interaction problem, with more than one area of fissile material of differing multiplications with little interaction between the low and the high multiplication areas.^[8] The model comprises four cylinders containing UO_2 /graphite located in the corners of a concrete walled room ($k_{\text{eff}}=0.8682$ ^[8]), with a sphere of highly-enriched uranium located in the centre of the room ($k_{\text{eff}}=1.0376$ ^[8]). A plan view of the model is shown in Figure 6.1.

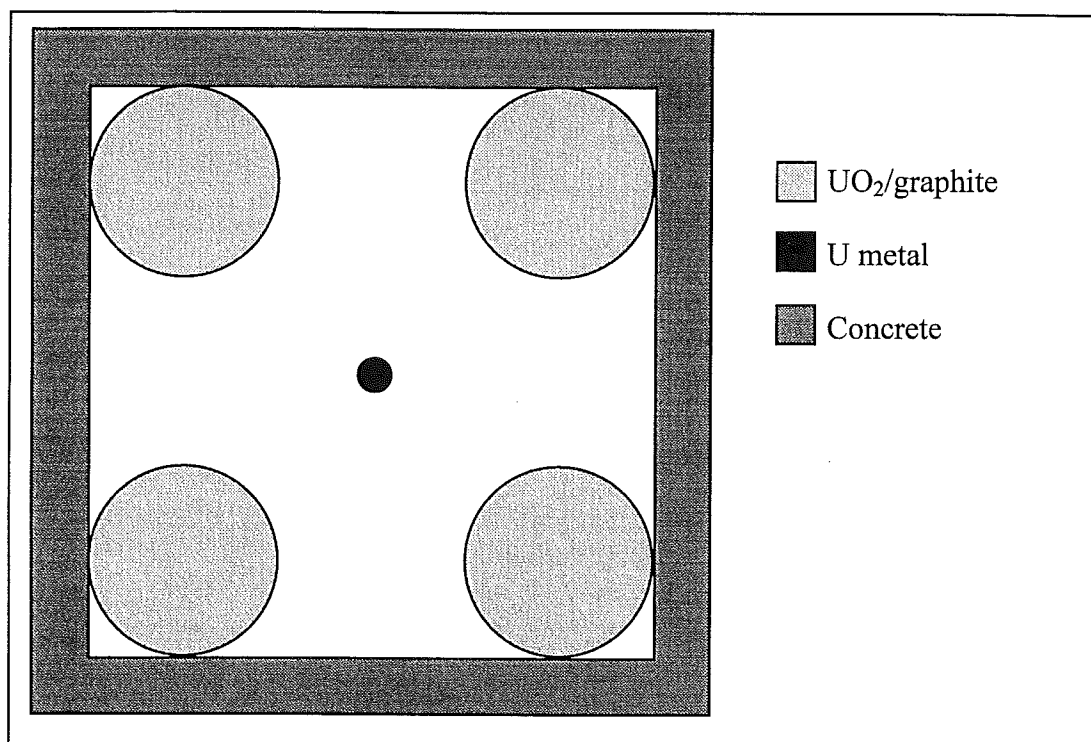


Figure 6.1. Geometry described by Smith

The cylinders have a radius of 50.0 cm and a height of 100.0 cm. The density of their material is $3.3 \text{ g}\cdot\text{cm}^{-3}$, and the weight ratios of the atoms are:

C	0.51643
²³⁵ U	0.04695
²³⁸ U	0.37934
O	0.05728

The sphere has a radius of 9.0 cm, and the density of the uranium is $18.74 \text{ g}\cdot\text{cm}^{-3}$. The atom ratios are:

²³⁴ U	0.000492
²³⁵ U	0.045
²³⁸ U	0.002498

The concrete wall has a thickness of 30.0 cm and the inner face exactly encloses the four cylinders. The concrete has a density of $2.24 \text{ g}\cdot\text{cm}^{-3}$, and the atom ratios are:

H	1.0
O	3.954
Si	1.527

6.2 Calculations

Calculations have been done for the different methods with the following starting distributions:

- uniform source distribution
- all neutrons in the sphere
- all neutrons in one of the cylinders
- neutrons divided over the four cylinders

The simulations have been continued until a standard deviation of 150 pcm was reached, and 1000 starting neutrons were simulated.

A calculation with a variable amount of neutrons has also been performed for this geometry with the conventional sampling method. The starting source distribution for this case has been a distribution deduced from the final converged distribution of the different calculations done before. In this distribution half of the neutrons started from the sphere, and the others were divided over the four cylinders. These calculations have been performed up to a standard deviation of 200 pcm.

6.3 Results

6.3.1 Convergence

In figure 6.2 and 6.3 the convergence of the different methods is given as a function of the generations simulated up to 500 generations, for a uniform source distribution, and a distribution in which all neutrons started in one of the cylinders.

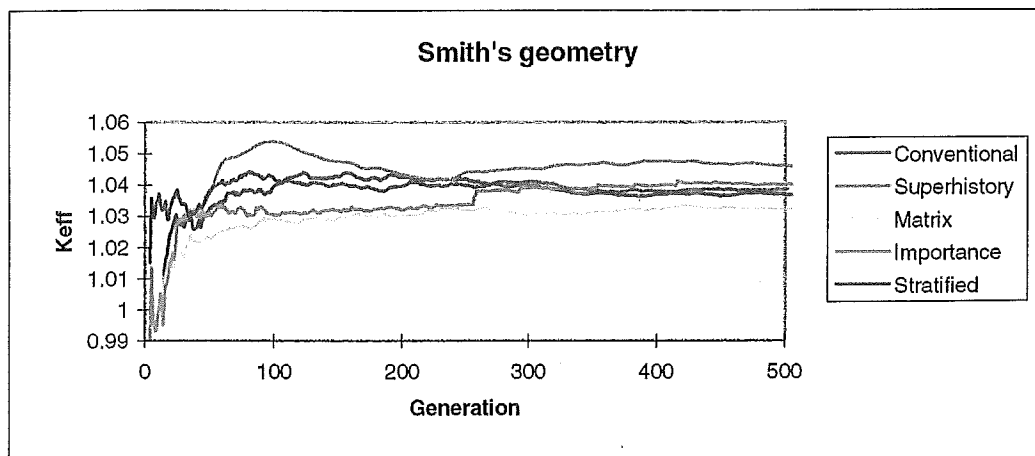


Figure 6.2. Convergence of the different methods in Smith's geometry with a uniform source distribution

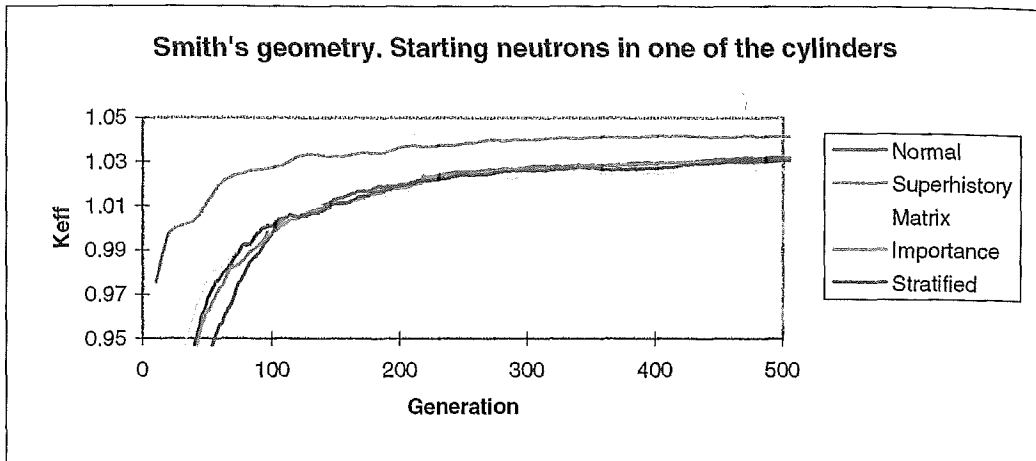


Figure 6.3. Convergence of the different methods in Smith's geometry with all neutrons starting in one of the cylinders

These results can also be presented with k_{eff} as a function of the standard deviation. In the figures 6.4, 6.5, 6.6 and 6.7 the results found with different starting distributions are given.

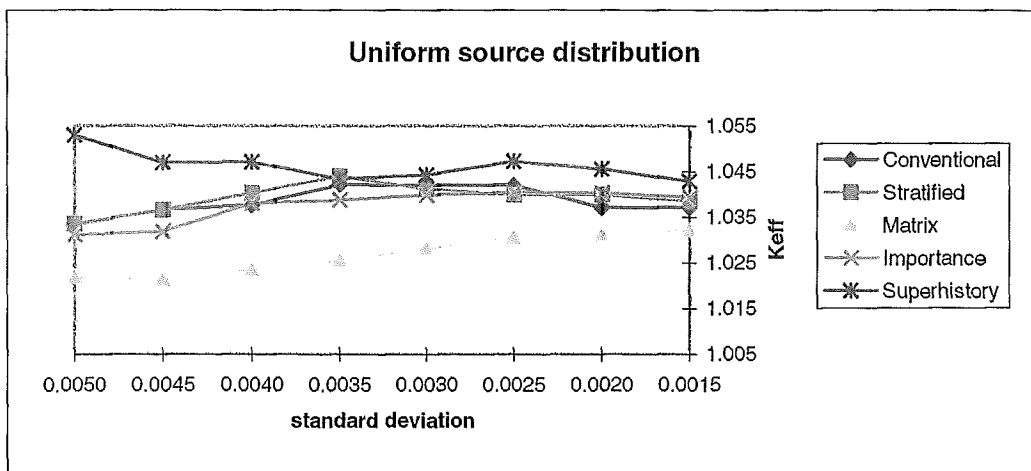


Figure 6.4. k_{eff} as a function of the standard deviation for Smith's geometry and a uniform source distribution

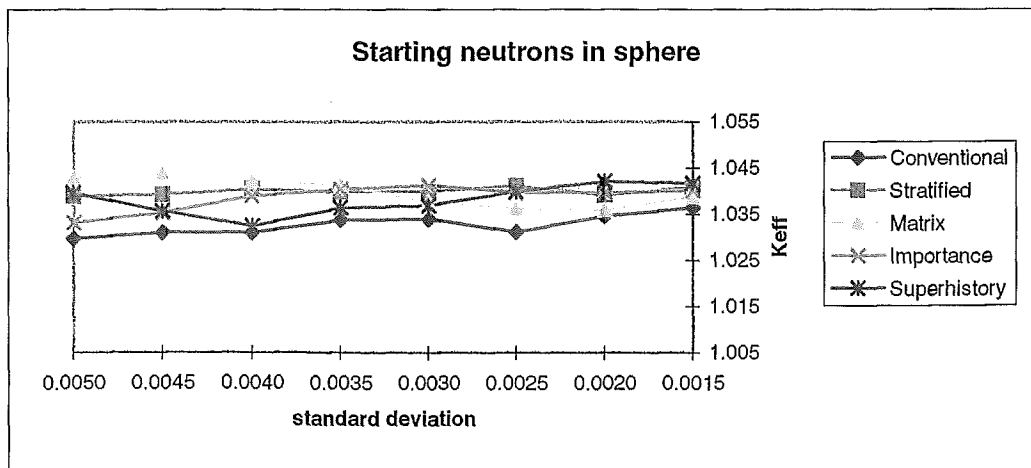


Figure 6.5. k_{eff} as a function of the standard deviation for Smith's geometry and all neutrons starting in the uranium-sphere

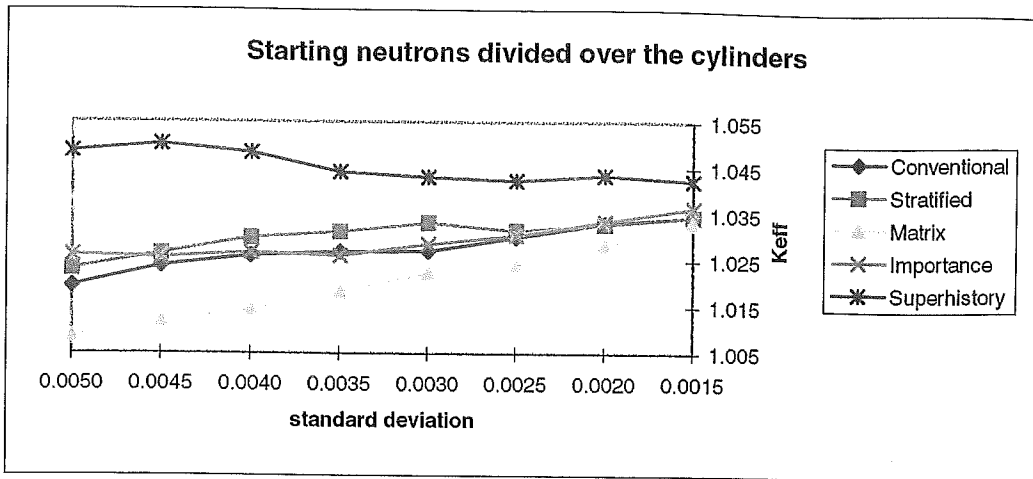


Figure 6.6. k_{eff} as a function of the standard deviation for Smith's geometry and the starting neutrons divided over the four cylinders

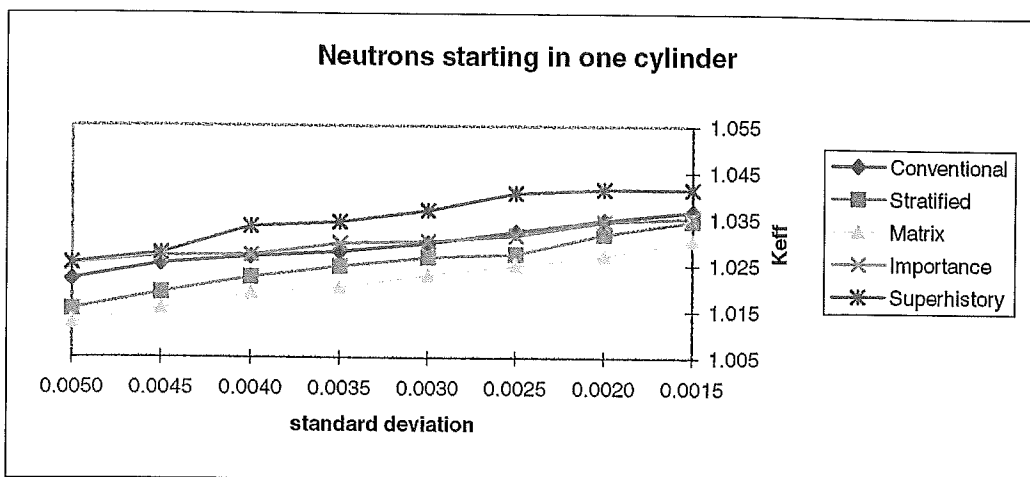


Figure 6.7. k_{eff} as a function of the standard deviation for Smith's geometry and all neutrons starting from one of the cylinders

6.3.2 Variable number of starting neutrons

The results found for the calculations with variable number of starting neutrons are given in figure 6.8.

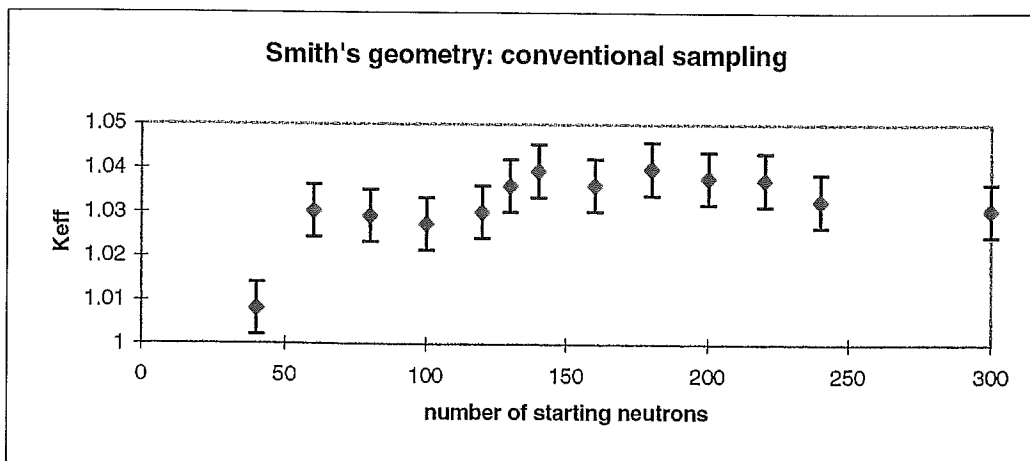


Figure 6.8. Dependence of k_{eff} when varying the number of starting neutrons in calculations with Smith's geometry

6.3.3 Suppressing settling iterations

As was done for the results found for Whitesides' geometry, for Smith's geometry, with neutrons starting in one of the cylinders, being one of the worst starting guesses, the test has also been performed to find the minimal standard deviation when suppressing iterations. The results can be found in table 6.1 (superhistory powering: $k_{\text{eff}}=1.04150$, $\sigma=204$ pcm).

Table 6.1. Values found for k_{eff} and σ with and without suppressing generations for Smith's geometry

Smith -1 cyl.	k_{eff}	$\sigma(\text{pcm})$	gen. suppr.	k_{eff}^s	$\sigma^s(\text{pcm})$
Conventional	1.03187	247	29	1.04158	155
Matrix	1.02601	207	18	1.03179	142
Importance	1.03080	292	28	1.03831	235
Stratified	1.03061	215	19	1.03706	149

6.3.4 Fission matrix, eigenvalues and eigenvector

In table 6.2 are given the fission matrix, the eigenvalues and the eigenvector corresponding to the largest eigenvalue for Smith's geometry. The volumes 1-4 represent the cylinders and number 5 the uranium sphere.

Table 6.2. The (reduced) fission matrix, the eigenvalues and the eigenvector corresponding to the largest eigenvalue for Smith's geometry.

Fission matrix	Eigenvalues	Eigenvector
$\begin{pmatrix} 0.572 & 0.060 & 0.048 & 0.057 & 0.070 \\ 0.058 & 0.560 & 0.057 & 0.044 & 0.072 \\ 0.042 & 0.056 & 0.579 & 0.058 & 0.071 \\ 0.059 & 0.044 & 0.060 & 0.579 & 0.069 \\ 0.008 & 0.007 & 0.010 & 0.008 & 1.033 \end{pmatrix}$	$\begin{pmatrix} 1.041 \\ 0.726 \\ 0.499 \\ 0.531 \\ 0.527 \end{pmatrix}$	$\begin{pmatrix} 0.120 \\ 0.118 \\ 0.121 \\ 0.120 \\ 0.522 \end{pmatrix}$

6.4 Discussion of results

6.4.1 Convergence

For this geometry the superhistory powering appears to converge as fastest. The final estimate of k_{eff} is in all cases the highest one, and in some cases even in conflict with the other results. However, when settling iterations are being suppressed, the results for the other methods, except for the fission matrix method, do seem to agree better with the result found with the superhistory powering (although no stages have been suppressed for this result). The contribution of the first generations, having a very low estimate of k_{eff} , obviously lowers the final estimate. It is surprising that, where the superhistory powering had a very slow start for Whitesides' geometry, it does very well for this geometry.

The fission matrix method does not show a faster convergence in this case as it did for Whitesides' geometry, but it does give too low results again. Except for the case of all neutrons starting in the sphere, it does always give the lowest result, and these results remain so when calculations are repeated with other random numbers. When generations are being suppressed the results are clearly in conflict with the other methods. This aspect of the fission matrix method needs to be investigated thoroughly.

One of the things that can be looked at is the convergence in the iteration used to find the highest eigenvalue. If the first two highest eigenvalues are very close to each other, this might lead to problems.

6.4.2 Variable number of starting neutrons

The results found when varying the number of simulated neutrons seem to indicate that it would be advisable to take more than 150 neutrons, but the results found with 300 neutrons is comparable to those with 60 to 120 neutrons. More calculations, with up to a 1000 neutrons, should be performed to get a better view of a minimal amount of neutrons needed.

6. CONCLUSION AND RECOMMENDATIONS

The goal of this research was to compare four possible ways of improving the analog Monte Carlo simulation for nuclear criticality studies in weakly coupled cases, and to improve the code MORET with the conclusion drawn from this comparison. In the first place the four methods have been compared using a simple one-dimensional model. All methods did indeed appear to improve the convergency of the Monte Carlo simulation. In this simple case the fission matrix method was extremely effective.

When the different methods had been included in MORET different calculations have been performed using three different geometries. The results were not always coherent and none of the methods satisfied in all cases. The problem investigated thus still remains, but improvements have been found in certain cases. The effect of the different methods appeared to vary for the different geometries. In further research there should be investigated what the physical phenomena are behind the differences caused by the various geometries.

One of the aspects that should be considered, is the performance of the methods as a function of how weakly coupled the system is. For example the element k_{ij} for two neighbouring volumes indicates the number of neutrons produced in one due to a neutron emitted in the other, and thus quantifies in some way how weakly coupled the system is. In the three geometries that have been looked at, these values were very different. In Kadotani's geometry the k_{ij} for two neighbouring spheres was of the order of 10^{-2} , in Whitesides' geometry it was of the order of 10^{-4} , and in Smith's geometry these values were of the order 10^{-3} for neutrons emitted in one of the cylinders and producing neutrons in the sphere, and of the order 10^{-2} for neutrons produced in one of the cylinders. Results with the different methods could be compared when the distance between the spheres in Kadotani's and Whitesides' is varied.

Other problems for which solution many more calculations will be necessary, are the problem of the minimal amount of neutrons that have to be simulated and the number of generations that should be skipped in the calculation of k_{eff} .

An aspect that deserves a lot of attention, but not necessarily needs many calculations, is the estimator of k_{eff} . The way k_{eff} has been calculated using the superhistory powering is fundamentally different from the way it has been calculated in the other methods. Lux and Koblinger^[3] propose an even different estimate of the ratio.

MORET should be able to benefit from the methods implemented, but for a good comparison between the methods more data is needed. A combination of the methods should not be excluded as a possibility.

8. LITERATURE

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APPENDIX A: The nuclear fuel cycle and criticality concerns

Nuclear criticality safety plays an important role in all nuclear fuel cycle steps where accidental criticality is credible. A generic fuel cycle diagram including uranium and thorium material flows and recycle of ^{233}U , ^{235}U and plutonium is given in figure a. Steps where criticality safety is required are indicated.

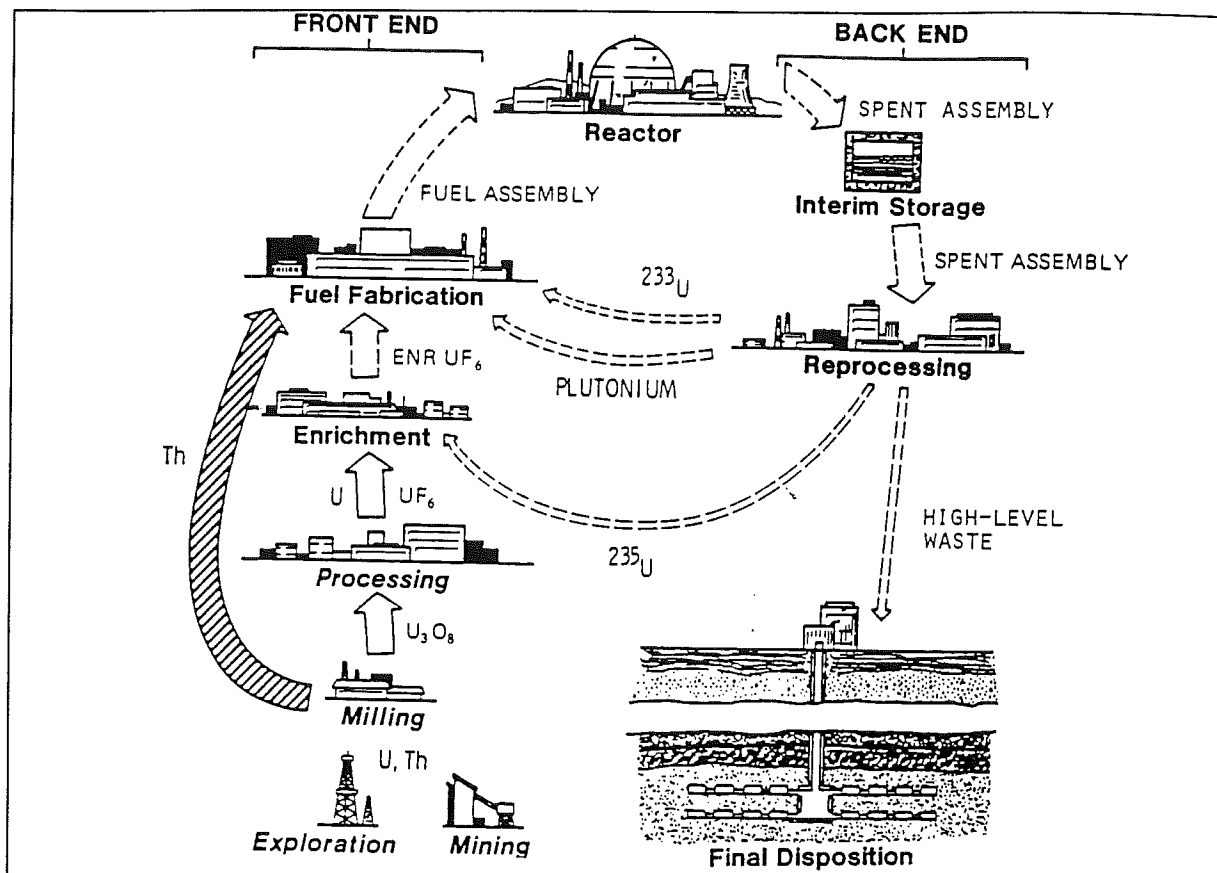


Figure a. Nuclear fuel cycle. Operation and transportation steps where accidental criticality is credible are indicated by bold labels and dashed arrows, respectively.

The mining, milling, and processing steps of uranium fuel cycle have no credible criticality safety concerns. This also applies to fabrication and fuel storage for heavy-water reactors and gas-cooled reactors that use natural uranium fuel. Natural uranium can support a self-sustaining chain reaction only under very special conditions of moderation and geometric arrangement. Although it is theoretically possible for a natural uranium and water system to achieve criticality, the prerequisites of extremely high purity, precise heterogeneous arrangements, and large size could not be met by accident. The other usual moderators, heavy water, beryllium, and graphite, are not present in fuel cycle facilities in sufficient purity and quantity to result in a critical configuration with natural uranium. The thorium stream, being essentially all nonfissile isotope ^{232}Th , by itself poses no criticality concern.

Criticality in the slightly enriched uranium of the enrichment and fabrication steps of the LWR fuel cycle requires water moderation. With highly enriched ^{235}U or ^{233}U for the high-temperature gas-cooled reactor, plutonium, or one of more of these fissile species in other commercial or military fuel cycles, dry criticality is an additional possibility.

Fuel in the reactor itself is generally excluded from the purview of nuclear criticality safety. However, a significant exception exists at Three Mile Island Unit 2 where accident-damaged fuel is to be removed

Fresh LWR fuel assemblies at reactor sites may be stored and handled in air or water in initial full-core or reload batches. Spent fuel is generally stored and handled underwater to provide both cooling and shielding as required by the radiation from its fission product inventory. Maintaining adequate spacing between fuel assemblies is an effective criticality control measure.

Reprocessing operations start with spent fuel assemblies, separate fuel material from fission product and transuranic wastes, and separate fuel constituent from each other. While the products of the LWR fuel cycle are slightly enriched uranium and plutonium, cycles that contain thorium produce ^{233}U . The resulting diversity of forms leads to interesting criticality control strategies. However, the shielding and containment required for the fission products already in the fuel could be expected to mitigate the radiological consequences of most potential criticality accidents.

Criticality concerns for high-level reprocessing wastes are relatively minor since the content of fissile materials is intentionally very low. However, long-term concentration effects in disposal media must be assessed. The situation is more extreme if spent fuel elements are the waste form. The latter require controls similar to those for spent fuel storage in the short term as well as evaluations for long-term effects.

Transportation among all appropriate nuclear fuel cycle steps requires criticality controls conceptually similar to those applied to the same material within the facility. Specially designed containers for each fuel form must also account for possibilities of accidents, which, for example could result in substantial geometry changes as well as water flooding with the inherent changes in neutron moderation.^[1]

APPENDIX B: Quota sampling

In quota sampling the total domain is cut into sub-domains as it was in the case of stratified sampling, but the number of samples to be taken from each subdomain is selected such as to obtain a minimum - or, in practice, near-minimum - variance. Regions of large variances should be sampled more often.^[3]

The procedure of calculation is almost equal to the one described for systematic sampling, but the probability density function is now defined as:

$$p_i^g = \frac{S_i \sigma_i}{\sum_{j=1}^J S_j \sigma_j}$$

where σ_i is the variance.

Since the σ_i variances are generally not known in advance, an iterative method has to be applied: first, calculations are made by best-guess estimates of M_i -s and the corresponding empirical variances are calculated from:

$$\sigma_i^{g+1} = \frac{1}{g(g-1)} \left[\sum_{\gamma=1}^g S_i^2 - \frac{1}{g} \left(\sum_{\gamma=1}^g S_i \right)^2 \right]$$

where g indicates the number of generations over which the variance is calculated.

The σ_i values are then the bases for selecting a better set of M_i -s according to equation: $M_i^g = M_0 \cdot p_i^g$

The method has not been used because simulations with the one-dimensional model showed that all neutrons were put rapidly in the most reactive parts of the system. This can be seen in figure b. The sudden jump at the 100th generation is due to the fact that the program suppressed the first 100 generations for the calculation of k_{eff} .

Examining the situation for the conventional sampling showed that the most reactive box did not only have the highest production, but it also had the highest variance at any time. This resulted in the fact that all neutrons would rapidly be simulated starting from this box, and the value found for k_{eff} was incorrect.

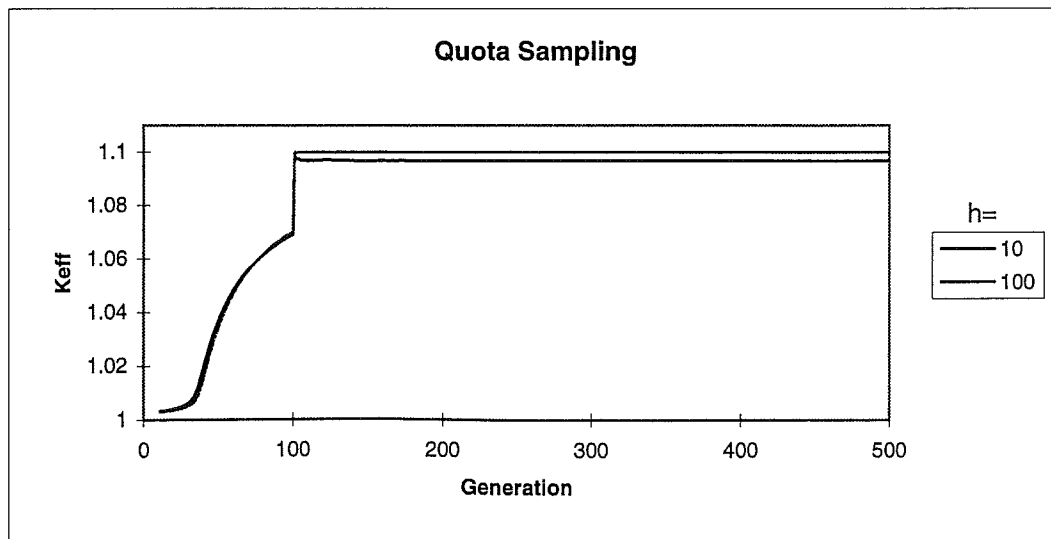


Figure b. Results found for the one-dimensional model with quota-sampling

APPENDIX C: Superhistory powering and reserve store

The results for the simulations done on the one-dimensional model for the cases of superhistory powering with and without reserve store can be found in figure c. They have been compared to a normal simulation with the conventional sampling method.

When the reserve store is used the new neutrons have received a weight of 10 or 100 times the old neutrons that were already in the reserve store. This is indicated by $d*10$ or $d*100$.

The simulations have been done for the case with $h=100$, and the results show clearly that the reserve store slows down the convergence.

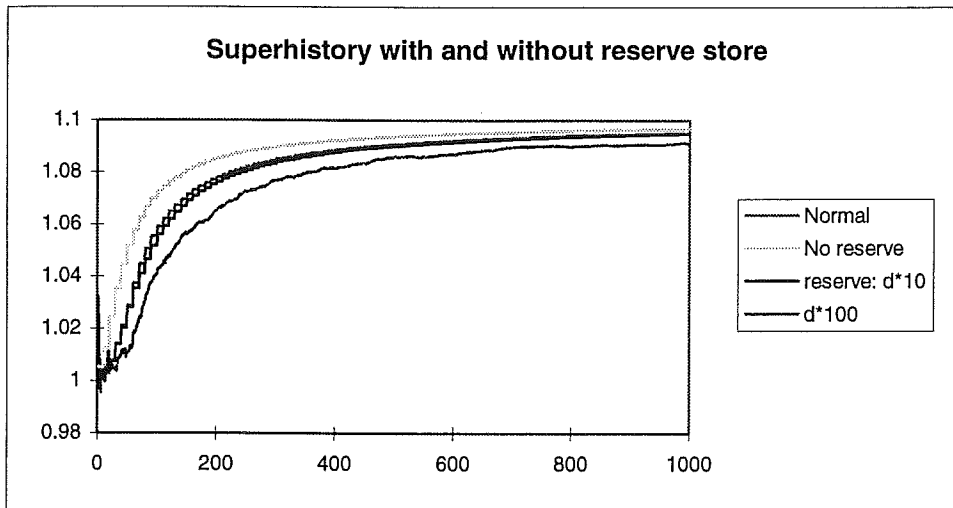


Figure c. Superhistory powering simulations with the one-dimensional with and without reserve store

APPENDIX D: Eigenvalues of the fission matrix for a system consisting of two units

In the case of two units the characteristic equation can be written as:

$$\lambda^2 - (k_{11} + k_{22})\lambda + k_{11}k_{22} - k_{12}k_{21} = 0$$

This leaves two roots:

$$\lambda_1 = \frac{k_{11} + k_{22} + \sqrt{(k_{11} - k_{22})^2 + 4k_{12}k_{21}}}{2} \quad \text{and} \quad \lambda_2 = \frac{k_{11} + k_{22} - \sqrt{(k_{11} - k_{22})^2 + 4k_{12}k_{21}}}{2}$$

By using the following normalization:

$$S_1 + S_2 = 1$$

the components of the eigenvector associated two each of the eigenvalues are given by:

$$S_1 = \frac{k_{21}}{\lambda + k_{21} - k_{11}} \quad \text{and} \quad S_2 = \frac{\lambda - k_{11}}{\lambda + k_{21} - k_{11}}$$

The second root (λ_2) is positive if $k_{11}k_{22} \geq k_{12}k_{21}$, but despite this fact this root cannot be accepted. In fact, if in the equations for S_1 and S_2 λ is being replaced by λ_2 the components of the eigenvector can be written as:

$$\begin{cases} S_1 = \frac{2k_{21}}{(k_{22} - k_{11}) + 2k_{21} - \sqrt{(k_{22} - k_{11})^2 + 4k_{12}k_{21}}} \\ S_2 = \frac{(k_{22} - k_{11}) - \sqrt{(k_{22} - k_{11})^2 + 4k_{12}k_{21}}}{(k_{22} - k_{11}) + 2k_{21} - \sqrt{(k_{22} - k_{11})^2 + 4k_{12}k_{21}}} \end{cases}$$

According to these expressions, one of the components becomes negative and the other superior to 1 (since $S_1 + S_2 = 1$ and the product $S_1 \cdot S_2$ is negative), and this is physically not acceptable.

In the same way it can be proven that the largest eigenvalue is necessarily superior to the maximum of the k_{ii} . In fact, if one supposes that $\max(k_{11}, k_{22}) = k_{11} > \lambda$, two cases can present themselves:

$$\lambda + k_{21} - k_{11} > 0 \Rightarrow S_2 < 0 \quad \text{and} \quad S_1 > 1$$

$$\lambda + k_{21} - k_{11} < 0 \Rightarrow S_2 > 1 \quad \text{and} \quad S_1 < 0$$

which are both physically not acceptable.