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Adjoint-Weighted Tallies for k -Eigenvalue Calculations with Continuous-Energy Monte Carlo

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Abstract – A Monte Carlo method is developed that performs adjoint-weighted tallies in continuous-energy k -eigenvalue calculations. Each contribution to a tally score is weighted by an estimate of the relative magnitude of the fundamental adjoint mode, by way of the iterated fission probability, at the phase space location of the contribution. The method is designed around the power iteration method such that no additional random walks are necessary, resulting in a minimal increase in computational time. The method is implemented in the Monte Carlo N-Particle (MCNP) code. These adjoint-weighted tallies are used to calculate adjoint-weighted fluxes, point reactor kinetics parameters, and reactivity changes from first-order perturbation theory. The results are benchmarked against discrete ordinates calculations, experimental measurements, and direct Monte Carlo calculations.

Keywords – criticality; kinetics parameters; perturbation theory

1 Introduction

The Monte Carlo method is applied successfully to many types of reactor physics calculations[1]. However, one area where continuous-energy Monte Carlo methods have been lacking[2] for reactor problems is in the area of adjoint functions (often colloquially called adjoint fluxes) or importances[3]. Many quantities in reactor physics, such as those found in reactor kinetics or perturbation theory, are ratios of integrals of adjoint-weighted quantities[4][5]. A new method is developed using a forward simulation that weights particles by the iterated fission probability[6], a quantity proportional to the adjoint function.

Historically, adjoint methods in Monte Carlo have involved a “backwards” approach. Physically, the adjoint equation describes particles traversing backwards from detector to source. This can be simulated through inversion of the random walk: particles stream in the opposite direction and scatter opposite to the normal energy transfer[7]. These are rarely used in production codes because inverting the scattering laws used in continuous-energy-angle calculations is complicated.

Recently, there has been interest in adjoint weighting in k -eigenvalue calculations. Early work uses an approximate importance weighting factor, a one generation approximation of the iterated fission probability, to weight tally scores. A multigroup code KENO that is part of the SCALE code system[8] spawns artificial secondary pseudo-particles each track, follows them only in the current generation, computes an estimate of k based on their tracks, and uses this as the importance weighting factor for the track that spawned the pseudo-particles[9]. Other efforts[10][11] use the probability of a track having a fission neutron as a weighting factor to compute kinetics parameters using continuous-energy physics in a modified version of the Monte Carlo N-Particle (MCNP) code[12].

More recent work[13][14] uses the correct importance weighting factor[6]. The authors in [13] compute adjoint functions by varying the initial source in a k -eigenvalue calculation. The iterated fission probability (adjoint function at the source location) is estimated by looking at the product of collision estimates of k from the initial source. In [14], the authors manually fold multigroup results with fluxes in a converged k -eigenvalue calculation to compute multigroup estimates of neutron generation times. Unfortunately, this approach does not produce continuous-energy estimates despite using a continuous-energy simulation because of the post processing of region averaged quantities.

A method is developed for k -eigenvalue problems that performs adjoint weighting of tallies during a forward power iteration method. Furthermore, with the appropriate accounting and definitions, there is no need for any additional random walks; the increased computational time is small. This paper specifically focuses on the theory and methods of computing adjoint-weighted quantities. Specifically, much attention is focused upon the development of the tallies for computing reactor kinetics parameters and reactivity changes

using perturbation theory. Results, along with validation and verification are summarized here; additional calculations illustrating practical examples to a reactor physicist are given in [15].

2 Method Development

Before developing the method to perform adjoint weighting, theoretical background of the adjoint function in a k -eigenvalue problem is reviewed. Specifically, the iterated fission probability is shown to be proportional to the importance or adjoint function. With these insights, it is possible to apply this theory to develop a method that weights each tally contribution (e.g., an individual track length) in a continuous-energy Monte Carlo simulation by its importance. Finally, details of the algorithm that fits nearly seamlessly within the production code, MCNP5, are discussed.

2.1 Adjoint Functions in k -Eigenvalue Problems

Before developing the specific method, it is first important to understand the nature of the k -eigenvalue problem:

$$\mathbf{H}\psi = \frac{1}{k}\mathbf{F}\psi. \quad (1)$$

\mathbf{H} is the transport operator containing the terms for streaming, collisions, and scattering. \mathbf{F} is the fission operator for both prompt and delayed emission. ψ is the angular flux and k is the eigenvalue.

This equation can be solved with the power iteration method given some initial condition on the fission source in the zeroth generation. Assuming the reactor is critical, $k = 1$, these source neutrons will have progeny. Eventually, these progeny will be distributed throughout the reactor corresponding to the fundamental eigenmode. The shape is independent of the source; however, the amplitude of the fundamental mode does depend upon the initial condition[4].

The adjoint k -eigenvalue equation,

$$\mathbf{H}^\dagger\psi^\dagger = \frac{1}{k}\mathbf{F}^\dagger\psi^\dagger, \quad (2)$$

is quite similar. The adjoint function, ψ^\dagger , corresponds to the expected contribution to some prescribed detector response resulting from neutrons at the current location and all its progeny. In the adjoint equation, the role of source and detector are reversed. Also, time or generations move in the opposite direction[16].

The physical interpretation of (2) can be obtained with a heuristic example. Suppose a detector is placed in a large reactor (the mean distance a neutron traverses within a generation is small relative to the reactor

size) and prescribed to take a reading exclusively in some generation called the detector (or asymptotic) generation. In generations just prior the detector generation, the neutrons whose progeny will be most likely to contribute will be nearest the detector. Conversely, neutrons far away are less likely have their progeny reach the detector in the specific generation when it is accepting contributions. For very many generations prior to the detector generation, the neutrons that are more able to form persisting fission chains are more likely to have their progeny contribute to the detector; a chain that goes extinct will not be able to contribute. Further, in a sufficient generation prior to the detector generation, a neutron has had sufficient “time” to reach any other point in the reactor and is therefore independent of its proximity to the detector. Thus, only the ability to produce a persisting chain matters with respect to contributing to the detector, and therefore this corresponds to the importance or fundamental adjoint mode.

Formally, the iterated fission probability interpretation of the adjoint function can be demonstrated by considering the time-dependent^a forward and adjoint transport equations:

$$\frac{1}{v} \frac{\partial \psi}{\partial t} + \mathbf{H}\psi = \mathbf{F}\psi, \quad (3)$$

$$-\frac{1}{v} \frac{\partial \psi^\dagger}{\partial t} + \mathbf{H}^\dagger \psi^\dagger = \mathbf{F}^\dagger \psi^\dagger. \quad (4)$$

v is the neutron speed and t is time. Multiply (3) by ψ^\dagger , and multiply (4) by ψ . Integrate the results over all position \mathbf{r} , energy E , direction $\hat{\Omega}$, and time from $t = 0$ to $t = t_d$ where $t_d \gg 0$, and take the difference. Because of the adjoint relationship (where \mathbf{A} is a generic linear operator and the brackets denote an inner product integration of position, direction, and energy),

$$\langle \psi^\dagger, \mathbf{A}\psi \rangle = \langle \psi, \mathbf{A}^\dagger \psi^\dagger \rangle, \quad (5)$$

the transport and fission terms cancel out, and the following relationship remains:

$$\left\langle \psi^\dagger, \frac{1}{v} \psi \right\rangle_{t=0} = \left\langle \psi^\dagger, \frac{1}{v} \psi \right\rangle_{t=t_d}. \quad (6)$$

This generic relationship will be applied to a reactor in a critical configuration. For systems that are not critical, the forward and adjoint functions are, in general, time-dependent even though the relationship in Eq. (6) holds. Only the critical case need be considered in the context of the k -eigenvalue problem because neutron balance from one generation to the next is enforced artificially by the application of the $1/k$ factor.

^aWhile the k -eigenvalue equation is time independent. It is only the asymptotic behavior that is of interest, and late times and generations are equivalent.

An arbitrary detector with response function $R(\mathbf{r}, \hat{\mathbf{\Omega}}, E)$ is turned on during the time interval $t_d - dt$ to t_d , after which the detector is turned off forever. This leads to the final condition on the adjoint function,

$$\psi^\dagger(\mathbf{r}, \hat{\mathbf{\Omega}}, E, t_d) = R(\mathbf{r}, \hat{\mathbf{\Omega}}, E). \quad (7)$$

The initial condition on the forward equation must be specified as well. For this, a point source is introduced into the reactor at $t = 0$, which can be expressed mathematically as

$$\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E, 0) = v_0 \delta(\mathbf{r} - \mathbf{r}_0) \delta(\hat{\mathbf{\Omega}} - \hat{\mathbf{\Omega}}_0) \delta(E - E_0). \quad (8)$$

δ is the Dirac delta function. While the source is still arbitrary, the reason for selecting a point source is to solve for the fundamental adjoint function at a single point in phase space. Since t_d is sufficiently large, only the fundamental modes of the forward and adjoint equations will remain at $t = t_d$ and $t = 0$ respectively:

$$\psi(\mathbf{r}, \hat{\mathbf{\Omega}}, E, t_d) = A(\mathbf{r}_0, \hat{\mathbf{\Omega}}_0, E_0) \psi_0(\mathbf{r}, \hat{\mathbf{\Omega}}, E), \quad (9)$$

$$\psi^\dagger(\mathbf{r}, \hat{\mathbf{\Omega}}, E, 0) = C \psi_0^\dagger(\mathbf{r}, \hat{\mathbf{\Omega}}, E), \quad (10)$$

A is the amplitude that depends only upon the location of the initial source[4]. Likewise, C is some constant whose value depends only upon the detector response function R . ψ_0^\dagger is independent of the detector response R as ψ_0 is independent of the initial source.

Substitute equations (8), (9), and (10) into (6) to find:

$$\psi_0^\dagger(\mathbf{r}_0, \hat{\mathbf{\Omega}}_0, E_0) = \frac{1}{C} A(\mathbf{r}_0, \hat{\mathbf{\Omega}}_0, E_0) \left\langle R, \frac{1}{v} \psi_0 \right\rangle. \quad (11)$$

The fundamental adjoint mode at some location in phase space $(\mathbf{r}_0, \hat{\mathbf{\Omega}}_0, E_0)$ is proportional to the amplitude A induced by a unit source at that point and some integral of the neutron density multiplied by the detector response. Since the fundamental adjoint shape is independent of the choice of the detector, R only impacts the magnitude of the multiplicative constant C . In other words, the choice of detector does not impact the fundamental adjoint shape.

An interesting choice is to make the detector response unity everywhere, $R = 1$. The inner product in (11) is the total neutron population in the entire reactor. The term within the integrals is then a constant related to the prescribed power level of the reactor. For this choice, the adjoint is proportional to only the

amplitude function A . This is sometimes called the iterated fission probability interpretation of the adjoint function and forms the basis for the adjoint weighting method.

The normalization of the forward and adjoint eigenfunctions is arbitrary and only impact their physical meaning and units. The absolute magnitude of either eigenfunction at any one location of phase space is, other than for the aforementioned reasons, meaningless. What is meaningful are their magnitudes relative to those at other phase space locations.

2.2 The Adjoint-Weighted Tally

The goal of the method will be to weight an arbitrary tally contribution T (could be flux in a region, current crossing a surface, or just about anything else) by the adjoint function at the phase-space location of that contribution. This tally contribution must be remembered, and the expected detector response of its progeny R many generations in the future must then be found. The tally contribution is weighted by the detector response of the progeny to form the score for the adjoint-weighted tally.

The choice of the detector response is arbitrary so long as the function is well-behaved and non-negative everywhere. The convenient choice, however, is the iterated fission probability case of counting the neutron production everywhere in the reactor in some sufficiently distant generation, or asymptotic population.

This is chosen in the design for a few practical reasons. First, the choice of detector is irrelevant so long as a well behaved one is chosen. Secondly, the iterated fission probability has historical application to early methods for reactivity changes with perturbation theory[6]. The third, and more important, reason relates to statistical convergence. Having the “detector” cover the entire reactor yields many more responses than if it is localized. From a statistical point of view, more scores to a tally are typically better than fewer and are less prone to noise. Therefore faster statistical convergence can be achieved by this choice. Another important reason is that global quantities tend to approach a steady state value faster than localized ones (for example, k almost always converges faster than the detailed fundamental fission source shape), so fewer generations are required between scoring tally contributions and detector responses.

The series of fission generations over which the calculation is performed is called a *block*. The neutrons in the first generation, or *original generation*, of the block are called *progenitors* (a more rigorous definition is forthcoming in Sec. 2.3) because they may go on to have progeny, and their ancestry is important in performing the adjoint weighting. In the original generation, neutrons that contribute to a tally that needs importance weighting have their contributions T recorded as if there is to be no importance weighting, and these neutrons are tagged with a progenitor index p . This progenitor index is passed on to all subsequent progeny. The generation where the asymptotic population (detector response R) is calculated is called the *asymptotic generation* because it is assumed that the expected population has converged by that generation.

The generations in between these are called *latent generations*, since the progeny are simply “waiting” to achieve asymptotic behavior; nothing is done in these generations other than what occurs in a standard calculation.

The score S for progenitor p to an adjoint-weighted tally is

$$S_p = R_p T_p. \quad (12)$$

The tally contribution T_p is an arbitrary tally score in a standard Monte Carlo calculation, but only for neutron paths with a progenitor index p . R_p is the corresponding asymptotic population. This quantity is scored by summing the neutron production estimates for all tracks of all neutron histories in the asymptotic generation having inherited a progenitor index p . The estimator for R_p can be expressed mathematically as

$$R_p = \sum_{\tau \in p} \nu \Sigma_f w \ell. \quad (13)$$

The detector contribution sums over all tracks τ in the asymptotic generation that have progenitor index p . ν is the average number of neutrons per fission, and Σ_f is the macroscopic fission cross section of the current material at the current particle energy. w is the current particle weight, and ℓ is the length of track τ . The units of the asymptotic population, and hence the adjoint weighting factor, are fission neutrons per progenitor neutron (or dimensionless). The Monte Carlo implementation discussed in this paper preserves these units; however, it is possible to normalize the adjoint weighting factor in other ways.

2.3 Definition of the Progenitor

Before providing an example of how T_p and R_p are estimated to compute S_p , it is first important to formally define the progenitor. The concept of importance gives the expected detector response for a neutron introduced at a point in phase space. For a given Monte Carlo history, all points within a track can be considered a random trial to be importance weighted. Since these points share a common future (and therefore a common random estimate of the asymptotic population) it makes sense to assign the same progenitor index p to all points along the track.

However, n,2n reactions, implicit capture, particle splitting, and other variance reduction techniques create branches in the fission chain. These branching events necessitate a splitting of the progenitors within a history such that they form a tree-like structure. It does not make causal sense to weight the tally contributions in one branch of a particle history by the detector responses caused by another. Therefore, some rigorous notion of the progenitor must be defined that preserves the causality of the random walk, and

therefore the result of the adjoint-weighted tally.

First, consider each random walk state within a single history X_i containing all state information: position, direction, energy, weight, etc. These random walk states are enumerated such that X_0 is the fission source state. Next, define a set Ξ_0 that contains only the state X_0 , and other sets Ξ that contain all ordered states in between each source, branching, or fission neutron producing event (such as from implicit capture) within the random walk sequence.

The set of random walk states defining a progenitor with set Π consist of unions of various sets Ξ . Criteria are defined such that the tallied importance weights are multiplied in causal ways. These criteria are:

1. The progenitor Π_0 is always a progenitor containing only Ξ_0 regardless of other criteria.
2. All sets Ξ must be causal and within the same fission generation.
3. The causal sets Ξ always extend back to the fission source set Ξ_0 .
4. The progenitor may only terminate upon the production of a fission neutron for the next generation.
5. The progenitor must be unique.

To illustrate this, consider an example in Figures 1 and 2. A neutron is emitted from the source and undergoes an n,2n reaction. One of the branches goes on to produce a fission neutron and then terminates from the weight cutoff. The other produces a fission neutron, goes on (because of implicit capture) to have a scattering event followed by another fission neutron production, and then continues to leak out of the system.

For this example, there are six sets Ξ illustrated in Figure 1 and four progenitors Π displayed in Figure 2. To explain, Π_0 contains set $\{\Xi_0\}$ because of condition 1. Π_1 contains sets $\{\Xi_0, \Xi_1, \Xi_2\}$ and Π_2 contains sets $\{\Xi_0, \Xi_1, \Xi_3\}$ because they form causal chains going back to the fission source specified by conditions 2 and 3, and terminate with a fission neutron production because of condition 4. Conversely, $\{\Xi_2, \Xi_3\}$ is not a progenitor because this union is neither causal nor does it extend back to the fission source. Also, $\{\Xi_0, \Xi_1, \Xi_3, \Xi_4, \Xi_5\}$ is not a progenitor either because it does not terminate with a fission neutron production as demanded by condition 4. Finally, there are no duplicates because of condition 5.

With this definition, this gives all of the progenitor states that need to be assigned. The definition is chosen such that the minimum number of progenitors is used: all are uniquely numbered with a different random walk sequence in the original generation. Note Π_0 which is kept as a common point to score all progeny in the asymptotic generation.

An example of a block illustrating progenitors and the various generation types is given in Fig. 3. The history in the original generation has one branching event from implicit capture, necessitating two progenitor

indices enumerated as 1 and 2. Tally contributions T_i and asymptotic populations R_j are displayed in Fig. 3. Table I provides an example of the calculation of the two adjoint-weighted scores S_p .

2.4 Overview of the Algorithm

The template for the adjoint weighting algorithm is the power iteration method. The iterations following convergence are broken into blocks containing an original generation, L latent generations ($L \geq 0$), and an asymptotic generation for a total of $L+2$ generations in each block. The computational operations performed will depend upon the type of generation.

During an original generation, a progenitor candidate is spawned for every source, branching, and fission neutron producing event. The original tally contributions T_p are recorded for each progenitor candidate; for reference, a list of tally contributions is given in Table II. The specific nomenclature is defined in the given reference section. The brackets without a subscript denote integration over all position, angle, and energy. Those with are averaged over a particular region. When a new progenitor candidate is required, the current tally contributions are copied to the new candidate to preserve the sequence of contributions back to the fission source site. Each fission neutron produced for the next iteration must have its progenitor index associated with it. At the end of the generation, only the progenitor candidates that actually produced fission neutrons are saved.

For latent generations, the neutrons must remember their progenitor index. While no new progenitor candidates are created, the neutrons still must pass the information about their progenitors onto their progeny.

During the asymptotic generation, the detector response (asymptotic population) R_p for all neutrons sharing a common progenitor is tabulated. At the end of the iteration, the adjoint-weighted scores are found by taking the products of T_p and R_p and adding these products to the global tally accumulator.

The score itself is the sum over all products tally contribution T and detector response R for all progeny resulting from the history in the original generation (hence some unique number for the initial source state in the original generation is kept). This is somewhat different than usual tallies that group scores according to the history in the current generation. Because the ordering of fission neutrons is not necessarily guaranteed, progenitors will need to be grouped according to the history they belonged to in the original generation.

Following this, all progenitor information is cleared and the next iteration begins as an original generation. The process repeats with a new block and continues to do so until the end of the simulation.

The selected algorithm is not the only possible approach, but represents a compromise between computational expense and memory usage.

It is possible to have multiple overlapping blocks such that neutrons carry a progenitor index for each

cycle. However, the memory requirements for the current (no overlapping blocks) implementation can be burdensome depending upon the problem, especially if space-energy resolution in the adjoint-weighted tallies is required. While starting a block every cycle may indeed be more computationally efficient, the memory requirements may become too large for many problems when the computational resource available is a modern desktop computer.

Another proposed implementation is to perform the importance weighting via “pseudoneutrons”. For every tally contribution (possibly every track), a particle called a pseudoneutron is generated that affects the calculation in no other way than to estimate an importance weight. This pseudoneutron and its subsequent progeny are followed some number of generations, and the tally score is multiplied by the scored asymptotic population from the spawned pseudoneutron. While this is almost free in terms of memory usage, many problems such as those with significant scattering will run orders of magnitude slower if this implementation is employed. This implementation was not pursued because such a large potential slowdown is usually considered unacceptable.

2.5 Further Considerations

A subtle detail is reconciling the impact of a non-analog simulation with the forward interpretation of the adjoint function. In an analog simulation, what occurs in the next event only depends upon the current state in phase space (a purely Markov process) – the effect of taking any state of the neutron in its random walk and following it to calculate a response is the same as if the neutron had been introduced into that point. Unfortunately, in non-analog simulations, the behavior of the random walk depends upon previous states through the particle weight w and is, strictly speaking, non-Markovian with respect to the traditional phase space. The weighting is done in such a way to preserve the expected scores, but it is no longer permissible to equate taking a snapshot of a neutron in a forward random walk with introducing a hypothetical neutron at that point because of this extra information carried in the particle weight. It can be shown that the expected number of eventual progeny produced (detector response) between the analog and non-analog cases are different by a factor of particle weight w and that this equivalence can be restored by a factor of C/w at the moment of recording the tally contribution T_p where C is some normalization constant and, for convenience, will be taken to be unity. This factor of $1/w$ is applied to each component of T_p making the tally contributions appear to be not multiplied by particle weight.

Another important consideration is how many generations it takes for the expected detector response measurement to converge. The answer is not addressed in this paper, but is similar to the issue of fission source convergence[17] in standard Monte Carlo k -eigenvalue calculations. A few results will be offered pertaining to convergence, but the exact number of generations required is going to be, like with the conver-

gence of the fission source, problem dependent. For the test problems in this paper, except where noted, the number of generations until measuring the detector response is ten. The question of testing for convergence remains an open topic of research.

3 Applications

The applications of adjoint-weighted fluxes, kinetics parameters, and perturbation theory are used to validate and verify the method. The validation and verification of the the method is performed with other calculations with the Monte Carlo N-Particle (MCNP) code and the discrete ordinates Partisn code[18].

3.1 Adjoint-Weighted Flux

Two verification problems are performed. The first is a mono-energetic, bare 1-D slab problem. The adjoint scalar “flux” and the forward scalar flux are equivalent for the one-speed transport equation[3]. The scalar flux as a function of position is computed by MCNP, and this is taken to be the reference adjoint function solution. The adjoint-weighted flux is estimated using the adjoint-weighting routines in MCNP, and an estimate of the adjoint function is found from the crude approximation,

$$\psi_j^\dagger \approx \frac{\langle \psi^\dagger, \psi \rangle_r}{\langle 1, \psi \rangle_r}. \quad (14)$$

ψ is the fundamental mode of the forward flux. The brackets denote an integration where the subscript indicates phase space region r (generally containing a spatial zone and an energy group). This approximation is only valid when neither the flux nor the adjoint vary too much within the spatial zone of r . Also, the forward and adjoint function must be isotropic because of the angular integration.

Computing the numerator in equation (14) requires an adjoint weighted flux tally in region r . In fact, this will be used as the denominator as well. There are many ways to compute a flux in a Monte Carlo simulation. A preferred method that works generally well is a track-length estimator:

$$\langle 1, \psi \rangle_r = \frac{1}{V_r} \sum_{\tau} w \ell \delta_{sr}. \quad (15)$$

The estimator sums over all tracks τ that are within region r . The current phase space region of the track is s and δ_{sr} is the Kronecker delta function defined to be one if $s = r$ and zero otherwise. w is the particle weight, ℓ is the length of track τ , and V_r is the physical volume of region r .

Relating this to the general form in equation (12), T_p is the track-length flux estimator given in (15) but modified by the weight factor $1/w$, and R_p is the usual resulting detector response (asymptotic population)

measured in some distant generation. The adjoint-weighted flux tally takes the following form:

$$C \langle \psi^\dagger, \psi \rangle_r = \frac{1}{N} \frac{1}{V_r} \sum_p R_p \sum_{\tau \in p} \ell \delta_{sr} \quad (16)$$

N is the total source weights of all the progenitor histories in the original generation. Note the constant C is arbitrary and depends upon the characteristics of the detector response function. In doing comparisons with other calculations, some normalization is needed to get results to match.

To help facilitate the validity of the approximation, the following cross sections are chosen for a 1-D slab: $\Sigma_t = 1.0 \text{ cm}^{-1}$, $\Sigma_\gamma = 0.1 \text{ cm}^{-1}$, $\Sigma_f = 0.2 \text{ cm}^{-1}$, $\Sigma_{s0} = 0.7 \text{ cm}^{-1}$, $\nu = 1.5$. Σ_t is the macroscopic total cross section, Σ_γ is the macroscopic capture cross section, and Σ_{s0} is the macroscopic cross section for isotropic scattering. A slab with a half-thickness of 10 cm is used. The mean free path in this slab is 1.0 cm and scattering is isotropic; the adjoint solution should be valid in about the inner 8 cm half-width of the slab. The outer 2 cm are expected to be in error because of anisotropy from leakage.

The slab calculation is run by varying the number of generations. The results for various generations are given in Figure 4. The solid line is the adjoint function (equivalent to the flux for 1-group) computed with Monte Carlo. The dots represent an approximate estimate of the adjoint function obtained from the forward calculation by waiting some number of generations ($L - 1$ latent generations). For small L , the adjoint-weighted flux shows poor agreement, but by around 20 generations, it appears the adjoint function is converging to the correct result.

This calculation shows that, for localized quantities, very many generations will be needed to get accurate importance weighting factors. This specific problem, which is 20 mean free paths thick (when both halves are included), takes at least 20 generations for the asymptotic population to settle. Problems with a very high dominance ratio may require even more. Fortunately, it will be seen by empirical example in the subsequent section that global quantities, such as the kinetics parameters, need far fewer iterations to converge.

The next test looks at a multigroup problem. The model used is a reflected 1-D slab. The three group data (χ is the fission emission spectrum and $\Sigma_{sg'g}$ is the macroscopic scattering cross section for scatter from energy group g' to g) are given in Table III. The inner (core) region of the slab has a 10 cm half-thickness, and the slab (core and reflector) has a total half-thickness of 40 cm.

Results are calculated in both MCNP and Partisn. The discrete ordinates results are computed by calculating angular forward and adjoint functions and manually integrating them to produce the scalar adjoint-weighted flux. The curves are then normalized such that the total area under the curves summed over the three energy groups is unity. The comparison is given in Figure 5, (the dashed lines represent the discrete ordinates results, and the dots represent those from Monte Carlo) and agreement within statistical

bounds is observed between the two methods.

3.2 Kinetics Parameters

The neutron generation time Λ is defined by

$$\Lambda = \frac{\langle \psi^\dagger, \frac{1}{v}\psi \rangle}{\langle \psi^\dagger, \mathbf{F}\psi \rangle}. \quad (17)$$

The integrations are taken over all phase space within the reactor. The neutron lifetime measures the mean time for a neutron to produce one additional neutron and represents a time constant for a transient in a nuclear reactor. Note that the neutron generation time is related to the neutron lifetime (or removal time) t_r by $\Lambda = t_r/k$. Traditionally, these are computed by inserting a $1/v$ absorber uniformly throughout the system[19] to measure the time-absorption or α -eigenvalue. In Monte Carlo, two calculations must be performed: a reference case and another with the artificial absorber. Since this method is only correct where the artificial insertion is small, such an approach is often hampered by the fact that the statistical uncertainty of the difference is often larger than the difference itself. The adjoint-weighted approach does not suffer from this because no subtraction of stochastic numbers is required.

To compute the generation time with this method, the numerator and denominator each need to be tallied separately. The numerator, the adjoint-weighted neutron density, can be obtained by

$$C \left\langle \psi^\dagger, \frac{1}{v}\psi \right\rangle = \frac{1}{N} \sum_p R_p \sum_{\tau \in p} \frac{1}{v} \ell, \quad (18)$$

where v is the neutron speed. The tally contribution T_p is the sum of individual contributions from all tracks τ sharing progenitor index p . The individual contribution is almost exactly like a track-length flux estimator except it is divided by neutron speed v to get a neutron density. This tally functions exactly like an adjoint-weighted flux estimator.

The denominator is the adjoint-weighted fission source. Computing the non-adjoint weighted fission source over a region in Monte Carlo power iteration simply involves counting up the source weight emitted in that region and normalizing to the overall power. To find the adjoint-weighted fission source over a region (in this case the entire reactor), each neutron score is the source weight times its importance. In many respects, this is significantly easier than the adjoint-weighted flux tallies. All that is required is to weight each source neutron (having weight w_0 that is divided out producing unity) by the detector response or asymptotic population:

$$C \left\langle \psi^\dagger, \frac{1}{k} \mathbf{F} \psi \right\rangle = \frac{1}{N} \sum_p R_p. \quad (19)$$

There is an additional factor of $1/k$ within the tally. This comes from the normalization of the fission source that occurs every generation; the neutron population is divided by the current estimate of k to keep the population stable. To match the denominator in (17), some estimate of k needs to be applied to each score. MCNP normalizes by the collision estimator of k every iteration[12]. For this implementation, the most self-consistent way is to multiply by the geometric mean of all k estimates within the block of iterations containing the original, latent, and asymptotic generations. There are many ways to do this and the “best” approach probably depends on the specifics of how the power iteration normalization is performed.

The effective delayed neutron fraction, β_{eff} can be found by

$$\beta_{\text{eff}} = \frac{\langle \psi^\dagger, \mathbf{B} \psi \rangle}{\langle \psi^\dagger, \mathbf{F} \psi \rangle}. \quad (20)$$

\mathbf{B} is the delayed emission source operator. The denominator is estimated much like with the total fission source in equation (19) except for one small modification. The form of the tally is

$$C \left\langle \psi^\dagger, \frac{1}{k} \mathbf{B} \psi \right\rangle = \frac{1}{N} \sum_p R_p (1 - \delta_{i0}). \quad (21)$$

Here i is the index of the precursor, where $i = 0$ denotes a prompt neutron. Like with the adjoint-weighted fission source tally, this tally contains a $1/k$ factor. The approach of multiplying each score by the geometric mean of the corresponding collision estimates of k is used.

Rossi- α , a common parameter measured in criticality experiments, is defined by

$$\alpha = -\frac{\beta_{\text{eff}}}{\Lambda} = -\frac{\langle \psi^\dagger, \mathbf{B} \psi \rangle}{\langle \psi^\dagger, \frac{1}{v} \psi \rangle}. \quad (22)$$

Like with Λ , this can often be estimated by inserting a uniform $1/v$ absorber and measuring the time-absorption eigenvalues. Also, some Monte Carlo codes can perform an iterative α -eigenvalue search to help find Rossi- α [20].

For verification, a two-group, infinite medium problem[21] is compared. MCNP is further modified to accept multigroup delayed neutron data. The delayed neutron fractions are independent of incident energy and have values of $\beta_1 = 1/4$ and $\beta_2 = 1/8$. The total delayed neutron fraction is therefore $\beta = 3/8$. The rest of the nuclear data is given in Table IV. Speed is given in ns and macroscopic cross sections in cm^{-1} . The removal cross section for group g is defined as $\Sigma_{Rg} = \Sigma_{tg} - \Sigma_{sgg}$. To simplify notation, ξ_g is defined as

the sum, over precursor index i , of all $\chi_{ig}\beta_i$.

The forward and adjoint functions are normalized such that $\psi_1 = 1$ and $\psi_2^\dagger = 1$. The ratios of the forward and adjoint functions are

$$\frac{\psi_2}{\psi_1} = \frac{\Sigma_{s12}}{\Sigma_{R2} - \frac{1}{k}\xi_2\nu\Sigma_f}, \quad (23)$$

$$\frac{\psi_1^\dagger}{\psi_2^\dagger} = \frac{\Sigma_{s12}}{\Sigma_{R1}}. \quad (24)$$

The solution for k is

$$k = [(1 - \beta) + \xi_1] \frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R1}\Sigma_{R2}} + \frac{\xi_2\nu\Sigma_f}{\Sigma_{R2}} = 1. \quad (25)$$

Analytic solutions are obtained for Λ , β_{eff} , and α :

$$\Lambda = \frac{\frac{1}{v_1} \frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2} \frac{\Sigma_{s12}}{\Sigma_{R2} - \xi_2\nu\Sigma_f}}{\left\{ \frac{\Sigma_{s12}}{\Sigma_{R1}} [(1 - \beta) + \xi_1] + \xi_2 \right\} \frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2} - \xi_2\nu\Sigma_f}} = 44/3 \text{ ns}, \quad (26)$$

$$\beta_{\text{eff}} = \frac{\frac{\Sigma_{s12}}{\Sigma_{R1}} \xi_1 + \xi_2}{\frac{\Sigma_{s12}}{\Sigma_{R1}} [(1 - \beta) + \xi_1] + \xi_2} = 1/2, \quad (27)$$

$$\alpha = -\frac{\left[\frac{\Sigma_{s12}}{\Sigma_{R1}} \xi_1 + \xi_2 \right] \frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2} - \xi_2\nu\Sigma_f}}{\frac{1}{v_1} \frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2} \frac{\Sigma_{s12}}{\Sigma_{R2} - \xi_2\nu\Sigma_f}} = -3/88 \text{ ns}^{-1}. \quad (28)$$

The results from MCNP are compared to the analytic solutions in Table V (C/R is the calculated to reference or analytic solution) and show agreement within the 2- σ confidence band and well within a tenth of a percent.

Eight 1-D, multigroup slab and sphere problems are described in Table VI where G denotes the number of energy groups.. More detailed information, such as the system dimensions and the artificial cross section data, can be found in [22]. Λ is computed with both MCNP and Partisn, and the results are compared. The cross section data is fictitious and does not represent any particular physical problem; however, it is consistently used by both the discrete ordinates and Monte Carlo calculations. The results of the test problems are given in Table VII. The C/R denotes the calculated to reference (Partisn) solutions. The comparisons appear to be within or near the 2- σ confidence interval and are all well within one percent of the values predicted by discrete ordinates.

Also in Table VII is the importance impact factor I , which is the ratio of the importance weighted to the

non-importance weighted values predicted by Partisn. In five of these problems, the impact of importance weighting is greater than ten percent, meaning a non-importance weighted value will be incorrect by at least that amount. Of particular note is problem 3, which is particularly pathological. In this case, not factoring in the importance weighting leads to a prediction of Λ that is orders of magnitude too large. Even with such extreme cases, these methods can predict the correct value within less than a tenth of a percent.

Like with the adjoint-weighted flux, it would be useful to get some measure of convergence for a global parameter such as the neutron generation time. For this calculation, a detailed 2-D Pressurized Water Reactor model[23] is used with ENDF/B-VII.0 nuclear data[24]. The neutron generation time is calculated for various numbers of latent generations. These results are displayed in Figure 6.

It appears convergence in Λ is not observed until around twenty latent generations. Notice the statistical noise increases dramatically as the number of latent generations increases. This is because the tallies score less frequently, and the length of the runs must increase substantially with the increase in the number of latent generations to have statistically meaningful results. However, the difference between the two latent generation case and that of twenty is less than one percent. This suggests for a typical power reactor, somewhere around ten to twenty generations is probably appropriate. Even with fewer, the discrepancy is likely to be small and probably outside of the ability of instrumentation to detect. This supports the assertion that global (or integrated) quantities are far less sensitive to getting an exact importance function than a local quantity and would explain the fairly accurate effective delayed neutron results seen in [10] and [11] for using a one-generation next fission probability as a detector response.

This also demonstrates that there is a tradeoff between accuracy (more generations means smaller truncation error) and statistical precision. At a certain point, there are diminishing returns where the increase in accuracy is more than offset by the increase in statistical noise in the tally result. The large uncertainty bars (for the cases of more than 15 latent generations) observed in Figure 6 illustrate this. In other words, the increased cost of losing such statistical precision at the benefit of marginally increasing accuracy is rarely justified.

Continuous-energy MCNP calculations of Rossi- α (using ENDF/B-VII.0 nuclear data) are validated against experimental measurements for seven OECD/NEA benchmarks[25]. Models from the MCNP criticality validation suite[26] are used for the calculations. The comparisons are given in Table VIII.

The MCNP calculated values of Rossi- α agree with experimental measurements for benchmarks containing U-235/238 and Pu within two percent. The Rossi- α values for both the U-233 benchmarks do not agree as well. Jezebel-233 and Flattop-233 are in error by about seven and eight percent respectively. While it would be premature to draw too many conclusions from two calculations, the consistency in the errors of both suggests that the discrepancies are likely caused by inaccuracies in the U-233 nuclear data.

3.3 Perturbation Theory

A first-order estimate of the change in reactivity caused by a small perturbation can be estimated by[3]

$$\Delta\rho = -\frac{\langle\psi^\dagger, (\Delta\Sigma_t - \Delta\mathbf{S} - \frac{1}{k}\mathbf{F})\psi\rangle}{\langle\psi^\dagger, \mathbf{F}'\psi\rangle}. \quad (29)$$

The reactivity ρ is defined in the usual manner,

$$\rho = \frac{k - 1}{k}. \quad (30)$$

There are three terms on the right side of the inner product in the numerator. From left to right, when operating on the flux, the terms correspond to the change in the total collision rate, the change in the scattering source, and the normalized change in the fission source. The term in the denominator is the perturbed fission source^b. Each of these four terms will require a tally.

The term for the change in the collision rate is a fairly easy extension from the adjoint-weighted flux estimator. It takes the following form

$$C \langle\psi^\dagger, \Delta\Sigma_t\psi\rangle = \frac{1}{N} \sum_p R_p \sum_{\tau \in p} \Delta\Sigma_t \ell. \quad (31)$$

$\Delta\Sigma_t$ is the change in the total cross section in the region of track τ . This term represents how much the loss rate from collisions changes.

The other three terms involve finding the change in either the scattering or fission sources. Recall that to tally a non-adjoint weighted fission source over a region, the source weight of every fission neutron emitted in that region is tallied. Normally, the fission source weight is the same for every source neutron within an iteration because of the renormalization. This does not have to be the case. In theory, it would be possible to emit particles uniformly with different weights to reflect the local intensity of the fission source. Another interpretation of particle weight involves thinking of each trajectory as consisting of numerous particles with the weight reflecting the population.

A local increase in the fission cross section by $\Delta\Sigma_f$ would increase the number of fission neutrons produced locally. In effect, the source weight could be increased relative to the unperturbed source weight. This would be done in such a way to bias the source such that the same path could be followed as if it is unperturbed, but contribute more to tallies and further multiplication.

This is very similar to a variance reduction technique called source biasing used in fixed source problems.

^bMany derivations have fission source unperturbed in the denominator. This is a further approximation that makes this a fully linear estimate.

In effect, one source is being made to look like another. In that case, the motivation is to preserve the physical source through numerical weighting, but simulate a different one to gain calculational efficiency. Consider an isotropic point source where neutrons in the rightward direction are three times as important as those in the leftward direction. The calculation is more efficient if three times as many neutron histories are simulated in the rightward direction as the leftward one. The particle source weights must be modified to preserve the expected tally scores. In this case, rightward neutrons have a source weight of two-thirds while leftward neutrons have a source weight of two. In terms of weight, the source is still isotropic – equal weight, on average, is carried by neutrons emitted in both directions.

With this application, the objective is to make the unperturbed, simulated source look like a perturbed source. In reality, the source weight itself will not be perturbed at all, but this biasing factor will be used in the tally contributions for the perturbed sources. For the fission source, the number of neutrons produced at a collision is

$$\eta = \frac{1}{k} w \frac{\nu \Sigma_f}{\Sigma_t}. \quad (32)$$

w/Σ_t is a collision estimate of the flux, which is not perturbed in first-order perturbation theory. The bias factor (or new weight) for the perturbed fission source is the ratio of the number of neutrons produced in the perturbed case to the number produced in the unperturbed case. For a first-order perturbation, the new weight for the fission source would be

$$w'_0 = w_0 \frac{(\nu \Sigma_f)'}{\nu \Sigma_f}. \quad (33)$$

This is the modified weight that can be inserted into the term for the perturbed fission source,

$$C \left\langle \psi^\dagger, \frac{1}{k} \mathbf{F}' \psi \right\rangle = \frac{1}{N} \sum_p R_p \frac{(\nu \Sigma_f)'}{\nu \Sigma_f}. \quad (34)$$

The change in the fission source is the expected change in source weight $w'_0 - w_0$:

$$\Delta w_0 = w_0 \left[\frac{(\nu \Sigma_f)'}{\nu \Sigma_f} - 1 \right] = w_0 \frac{\Delta(\nu \Sigma_f)}{\nu \Sigma_f}. \quad (35)$$

Therefore, the change in the fission source is

$$C \left\langle \psi^\dagger, \frac{1}{k} \Delta \mathbf{F} \psi \right\rangle = \frac{1}{N} \sum_p R_p \frac{\Delta(\nu \Sigma_f)}{\nu \Sigma_f}. \quad (36)$$

Likewise, similar arguments can be made for the change in the scattering source,

$$C \langle \psi^\dagger, \Delta \mathbf{S} \psi \rangle = \frac{1}{N} \sum_p R_p \sum_{s \in p} \frac{\Delta(\Sigma_s)}{\Sigma_s}. \quad (37)$$

The tally contribution is made every scattering event s with progenitor p within the history in the original generation.

The new tallies can be combined as in equation (29) to find an estimate of the change in reactivity $\Delta\rho$. There are a couple caveats here. The first is that nothing is done to account for changes in the fission emission spectra or the scattering laws. Only the bulk change in $\nu\Sigma_f$ and Σ_s at the incident energy of collision is considered and not the relative change in the energy-angle transfer probabilities. The second is an assumption with source biasing. To bias a source correctly, all regions of phase space that would be sampled in the perturbed source need to be sampled in the simulated (unbiased) source. This is not necessarily always the case, and this method will produce incorrect results in perturbation where, for example, fissile material is added to a region that is nominally vacuum.

To validate the method, the Godiva benchmark[25], a bare high-enriched uranium sphere (approximately 93.8 weight percent uranium-235) is given two different perturbations. The first is changing density in the outer 0.1 cm of the sphere. This problem is selected because the standard technique used for continuous-energy perturbations in Monte Carlo, the differential operator method[27], cannot accurately predict the change in reactivity without accounting for a perturbation in the fission source[28]. A reference discrete ordinates solution (using MENDF6 nuclear data[29]) is published in [30]. The first-order perturbation Monte Carlo results (using ENDF/B-VII.0 nuclear data) should closely match the first-order discrete ordinates solution.

The results are displayed in Figure 7. The reference solution is an exact change in reactivity computed from two direct Partisn calculations. The first-order Partisn reactivity changes are estimated with equation (29). The first-order (adjoint-weighted) Monte Carlo and discrete ordinates match very well. Note that all of the perturbations were performed in MCNP with one calculation using the exact same set of random numbers. There is a consistent $1\text{-}\sigma$ difference between the two calculations, but the deviation is consistent with the first-order discrete ordinates results.

In the next test, the Godiva sphere has its cross section library perturbed. The reference change in k is estimated by two direct computations; one uses ENDF/B-VI.5 cross sections[31] and the other uses ENDF/B-VII.0 cross sections. The first-order approximation is done by doing a material substitution perturbation by replacing one set of nuclear cross sections with another. Note that the discrete ordinates method requires a not insignificant amount of perturbed isotopes be present in the unperturbed material. As such, the differential operator technique cannot perform cross section library perturbations. Results for Δk for the

reference and first-order solutions are given in Table IX and compare well. While outside the $2\text{-}\sigma$ confidence band, the difference in k is 0.00014, which is small compared to the typical deficiencies in k from experimental results. The discrepancy is likely the result of not accounting for the differences in the angular distributions of inelastic scattering reactions.

Additional perturbations involving changes in enrichment, changes in moderator density, buildup of xenon-135 in fuel, and control rod worth calculations are given in [15].

4 Summary & Future Work

A method is developed that weights tally scores by adjoint weighting factors. The score of an adjoint-weighted tally is defined by the product, for each progenitor, of the contributions to a tally within a generation and the detector response in some distant, future generation. A definition of the progenitor is given that is consistent with the physical meaning of the adjoint; this accounts for branching in a neutron history as well as the issues involving weight in the multiplication. An overview of the algorithms, which can be inserted into a standard power iteration method, is given.

Values of adjoint functions and adjoint-weighted fluxes are verified against discrete ordinates or Monte Carlo one-group solutions. The kinetics parameters Λ (neutron generation time) and Rossi- α are compared with discrete ordinates calculations and experimental measurements respectively. The validation to discrete ordinates comes out very well, and the validation tests against experimental measurements compare well for most of the benchmarks. A couple perturbations are run comparing first-order Monte Carlo reactivity changes to those estimated by first-order discrete ordinates and direct Monte Carlo. The edge density variation and a cross section library perturbation compare well with reference solutions.

The question of how many generations need to pass between measuring the tally contributions and the detector response requires quantification. A couple calculations are performed that produce some ad hoc rules-of-thumb, but a more rigorous method of assessing convergence is needed.

Closely related to the perturbations is the analysis of sensitivity and uncertainty of cross section data[32]. This is of particular interest to criticality safety where uncertainty margins for computations need to be calculated. Also, extending the routines to calculate fixed source adjoint-weighted fluxes may be possible as well.

Finally, there are yet unresolved question of quantifying biases in results from source normalization in the iteration scheme relate to adjoint-weighted tallies. While these questions are yet unresolved for standard, spatially-dependent tallies and it is unlikely that much progress can be made on spatially-dependent, adjoint-weighted tallies until this is resolved, there may be some useful results attainable for the adjoint-weighted

integrated quantities such as the point kinetics parameters. Empirical observations show that biases are negligible for batch sizes of several thousand or more, as expected for non-adjoint-weighted tallies.

References

- [1] F.B. Brown, "Monte Carlo Lectures," Los Alamos National Laboratory, LA-UR-05-4983 (2005).
- [2] F.B. Brown, W.R. Martin, and R.D. Mosteller "Monte Carlo - Advances and Challenges," *Workshop at PHYSOR 2008, International Conference on the Physics of Reactors*, Interlaken, Switzerland (2008).
Also: LA-UR-08-05891, Los Alamos National Laboratory.
- [3] J.D. Lewins, *Importance: The Adjoint Function*, Pergamon Press, Oxford, UK (1965).
- [4] G.I. Bell and S. Glasstone, *Nuclear Reactor Theory*, Van Norstrand Reinhold, New York, NY (1970).
- [5] G.R. Keepin, *Physics of Nuclear Kinetics*, Addison-Wesley, Reading, MA (1965).
- [6] H. Hurwitz in *Naval Reactor Physics Handbook*, A. Radkowsky (ed.), vol. 1, pp. 864-849, Naval Reactors, U.S. Atomic Energy Commission (1964).
- [7] J.E. Hoogenboom, "Methodology of Continuous-Energy Adjoint Monte Carlo for Neutron, Photon, and Coupled Neutron-Photon Transport," *Nuclear Science and Engineering*, **143** pp. 99-120 (2003).
- [8] *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, ORNL/TM-2005/39, Version 5.1, Vols. I-III, Oak Ridge National Laboratory (2006).
- [9] B.T. Rearden and M.L. Williams, "Eigenvalue Contribution Estimator for Sensitivity Calculations with TSUNAMI-3D," *Proc. of the 8th International Conference on Nuclear Criticality Safety*, St. Petersburg, Russia, May 28 - Jun. 1 (2007).
- [10] Y. Nauchi and T. Kameyama, "Proposal of Direct Calculation of Kinetic Parameters β_{eff} and Λ Based on Continuous-Energy Monte Carlo Method," *Journal of Nuclear Science and Technology*, **42**, No. 6, pp. 503-514 (2005).
- [11] R. Meulekamp and S.C. van der Marck, "Calculating Effective Delayed Neutron Fraction with Monte Carlo," *Nuclear Science and Engineering*, **152** pp. 142-148 (2006).
- [12] X-5 Monte Carlo Team, "MCNP - A General N-Particle Transport Code, Version 5, Volume I: Overview and Theory," Los Alamos National Laboratory, LA-UR-03-1987 (2003).
- [13] S.A.H. Fegghi, M. Shahriari, and H. Afarideh, "Calculation of Neutron Importance Function in Fissionable Assemblies using Monte Carlo Method," *Annals of Nuclear Energy*, **34** pp. 514-520 (2007).
- [14] S.A.H. Fegghi, M. Shahriari, and H. Afarideh, "Calculation of the Importance-Weighted Neutron Generation Time using MCNIC Method," *Annals of Nuclear Energy*, **35** pp. 1397-1402 (2008).

- [15] B.C. Kiedrowski, F.B. Brown, and P.P.H. Wilson, “Calculating Kinetics Parameters and Reactivity Changes using Continuous-Energy Monte Carlo,” *Proc. of PHYSOR 2010: Advances in Reactor Physics to Power the Nuclear Renaissance*, Pittsburgh, PA, May 14-19, 2010 (2010).
- [16] J.D. Lewins, “The Time-Dependent Importance of Neutrons and Precursors,” *Nuclear Science and Engineering*, **7** pp. 268-274 (1960).
- [17] F.B. Brown, “A Review of Best Practices for Monte Carlo Criticality Calculations,” *Proc. of the 2009 ANS Nuclear Criticality Safety Division Topical Meeting on Realism, Robustness, and the Nuclear Renaissance*, Richland, WA, Sep. 13-17 (2009).
- [18] R.E. Alcouffe, R.S. Baker, J.A. Dahl, S.A. Turner, and R.C. Ward “Partisn: A Time-Dependent, Parallel Neutral Particle Transport Code System,” Los Alamos National Laboratory, LA-UR-08-7258 (2008).
- [19] W.B. Verboomen, “Monte Carlo Calculation of Effective Neutron Generation Time,” *Annals of Nuclear Energy*, **33** pp. 911-916 (2006).
- [20] D. Brockway, P. Soran, and P. Whalen in *Monte Carlo Methods and Applications in Neutronics, Photonics and Statistical Physics*, pp. 378-387, Springer-Verlag, Berlin, Germany (1985).
- [21] B.C. Kiedrowski, “Analytic, Infinite-Medium Solutions for Point Reactor Kinetics Parameters and Reactivity Perturbations,” Los Alamos National Laboratory, LA-UR-10-01803 (2010).
- [22] B.C. Kiedrowski, “Theory, Interface, Verification, Validation, and Performance of the the Adjoint-Weighted Point Reactor Kinetics Parameter Calculations in MCNP,” Los Alamos National Laboratory, LA-UR-10-01700 (2010).
- [23] M. Nakagawa and T. Mori, “Whole Core Calculations of Power Reactors by use of Monte Carlo Method,” *Journal of Nuclear Science and Technology*, **30**, no. 7 pp. 692-701 (1993).
- [24] M.B. Chadwick, et. al. “ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology,” *Nuclear Data Sheets*, **107** pp. 2931-3060 (2006).
- [25] J. Blair Briggs (ed.), *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, Nuclear Energy Agency, NEA/NSC/DOC(95)03/I, Paris, France (2004).
- [26] R.D. Mosteller, “Validation Suites for MCNP,” *Proc. of 12th Biennial Meeting of the Radiation Protection and Shielding Division*, Santa Fe, New Mexico, Apr. 14-17 (2002).

- [27] H. Rief, "Generalized Monte Carlo Perturbation Algorithms for Correlated Sampling and a Second-Order Taylor Series Approach," *Annals of Nuclear Energy*, **11** pp. 455 (1984).
- [28] Y. Nagaya and F.B. Brown, "Estimation in the Change of k -effective due to Perturbed Fission Source Distribution in MCNP," *Proc. of M&C 2003, ANS Mathematics and Computation Meeting*, Gatlinburg, TN, Apr. 6-10 (2003).
- [29] R.C. Little "MENDF6: A 30-Group Neutron Cross-Section Library Based on ENDF/B-VI," Los Alamos National Laboratory, XTM:96-82(U) (1996).
- [30] J.A. Favorite, "Second-Order Reactivity Worth Estimates Using an Off-the-Shelf Multigroup Discrete Ordinates Transport Code," *Proc. of PHYSOR 2008, International Conference on the Physics of Reactors*, Interlaken, Switzerland, Sep. 14-19 (2008).
- [31] J.M. Campbell, S.C. Frankle, R.C. Little "ENDF66: A Continuous-Energy Neutron Data Library for MCNP4C," *Proc. of 12th Biennial Meeting of the Radiation Protection and Shielding Division*, Santa Fe, NM, Apr. 14-18 (2002).
- [32] E. Greenspan, "Developments in Perturbation Theory," in *Advances in Nuclear Science and Technology*, E.J. Henley and J.D. Lewins (eds.), **9** pp. 181-268 (1976).

Table I: Adjoint-weighted scoring quantities for the example in Fig. 3.

p	T_p	R_p	S_p
1	T_1	$R_2 + R_3$	$T_1 (R_2 + R_3)$
2	$T_1 + T_2 + T_3$	R_1	$(T_1 + T_2 + T_3) R_1$

Table II: Adjoint-weighted tally types used within this paper.

Adjoint-Weighted:	Equation	T	See section:
Flux	$\langle \psi^\dagger, \psi \rangle$	ℓ	3.1
Neutron Density	$\langle \psi^\dagger, \frac{1}{\nu} \psi \rangle$	$\frac{1}{\nu} \ell$	3.2
Fission Source	$\langle \psi^\dagger, \frac{1}{k} \mathbf{F} \psi \rangle$	1	3.2
Delayed Source	$\langle \psi^\dagger, \frac{1}{k} \mathbf{B} \psi \rangle$	$(1 - \delta_{i0})$	3.2
Collision Rate Change	$\langle \psi^\dagger, \Delta \Sigma_t \psi \rangle$	$\Delta \Sigma_t \ell$	3.3
Scatter Source Change	$\langle \psi^\dagger, \Delta \mathbf{S} \psi \rangle$	$\frac{\Delta(\Sigma_s)}{\Sigma_s}$	3.3
Fission Source Change	$\langle \psi^\dagger, \frac{1}{k} \Delta \mathbf{F} \psi \rangle$	$\frac{\Delta(\nu \Sigma_f)}{\nu \Sigma_f}$	3.3
Perturbed Fission Source	$\langle \psi^\dagger, \frac{1}{k} \mathbf{F}' \psi \rangle$	$\frac{(\nu \Sigma_f)'}{\nu \Sigma_f}$	3.3

Table III: Artificial data for 1-D reflected slab problem.

	g	Σ_t	$\bar{\nu}\Sigma_f$	Σ_γ	χ	$\Sigma_{sg'1}$	$\Sigma_{s,g'2}$	$\Sigma_{s,g'3}$
Core	1	0.05	0	0	1	0.05	0	0
	2	0.15	0	0.01	0	0	0.14	0
	3	0.15	0.0238	0	0	0	0	0.14
Refl	1	0.2	0	0	-	0.15	0.05	0
	2	0.2	0	0	-	0	0.05	0.15
	3	0.2	0	0	-	0	0	0.199

Table IV: Cross section data for analytic test problem of the kinetics parameters.

g	v_g	Σ_t	Σ_γ	Σ_R	$\nu\Sigma_f$	χ_p	χ_1	χ_2	ξ	Σ_{sg1}	Σ_{sg2}
1	10	2	1	3/2	0	1	3/4	1/2	1/4	1/2	1/2
2	5	3	1	2	5/24	0	1/4	1/2	1/8	0	1

Table V: Comparisons of kinetics parameter results from MCNP with analytic solutions.

	Analytic	MCNP	C/R
Λ (ns)	14.66667	14.66548 ± 0.00110	0.99992
β_{eff}	0.50000	0.50003 ± 0.00005	1.00006
α (ns ⁻¹)	-3.40909×10^{-2}	$-3.40955 \pm 0.00044 \times 10^{-2}$	1.00013

Table VI: Test problem descriptions used in verifying Λ .

Problem	G	Description
1	4	Bare fast slab
2	4	Metallic slab with a moderating reflector
3	2	Metallic slab, strong thermal absorber, and moderating reflector
4	8	Bare intermediate spectrum slab
5	4	Bare fast sphere
6	4	Reflected fast sphere
7	4	Subcritical bare fast slab ($k = 0.78$)
8	4	Supercritical bare fast slab ($k = 1.14$)

Table VII: Partisn/MCNP Λ comparisons for multigroup test problems.

Problem	Partisn	MCNP	C/R	I
1	9.79325 ns	9.79675 ± 0.00188 ns	1.00036	0.99021
2	135.19020 us	135.22164 ± 0.03384 μ s	1.00023	1.14537
3	49.16822 ns	49.20663 ± 0.01863 ns	1.00078	0.00488
4	112.05232 us	112.29905 ± 0.13692 μ s	1.00220	1.11580
5	1.72115 ns	1.72121 ± 0.00032 ns	1.00003	0.86498
6	10.18997 ns	10.18794 ± 0.00233 ns	0.99980	0.56477
7	10.17161 ns	10.17110 ± 0.00230 ns	0.99995	1.05365
8	9.67254 ns	9.67168 ± 0.00166 ns	0.99990	0.96534

Table VIII: Comparisons of Monte Carlo (MCNP) calculations and experimental measurements of Rossi- α (in ms^{-1}).

	Experiment	MCNP	C/R
Godiva	-1100 ± 20	-1139.57 ± 2.35	1.017
Jezebel-239	-640 ± 10	-640.238 ± 2.374	1.000
BIG TEN	-117 ± 1	-115.518 ± 0.219	0.987
Jezebel-233	-1000 ± 10	-1071.18 ± 3.50	1.071
Flattop-233	-271 ± 3	-292.401 ± 0.808	1.079
Stacy-29	-0.122 ± 0.004	-0.122155 ± 0.00296	1.001
WINCO Slab Tank	-1.1093 ± 0.0003	-1.11723 ± 0.00311	1.007

Table IX: Cross section library perturbation (ENDF/B-VI.5 to ENDF/B-VII.0) for Godiva.

k (ENDF/B-VI.5)	0.99646 +/- 0.00004
Reference Δk	0.00344 +/- 0.00006
First-Order Δk	0.00358 +/- 0.00006

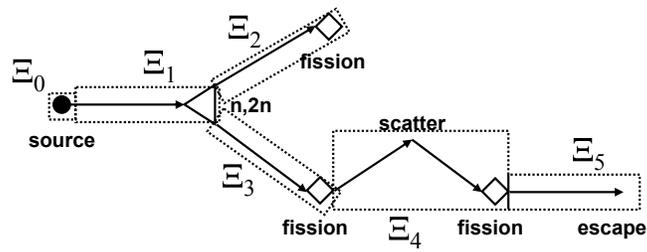


Figure 1: Example of a neutron history. The sets Ξ for the random walks are specified.

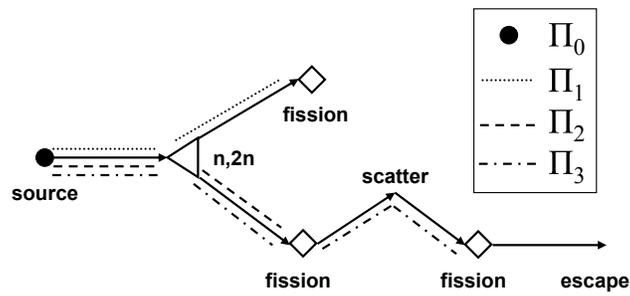


Figure 2: Example of a neutron history. The four progenitor sets Π for this history are specified.

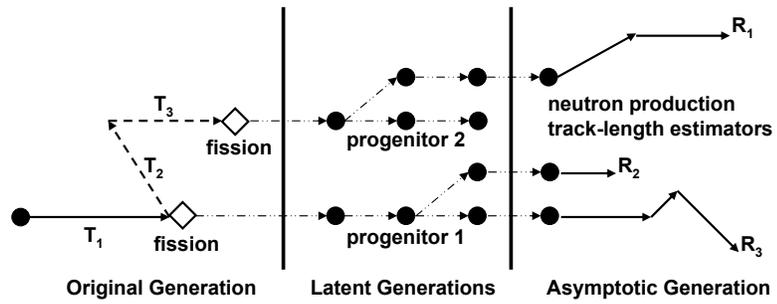


Figure 3: Example of a random walk of a single history in the original generation and subsequent generations within a block.

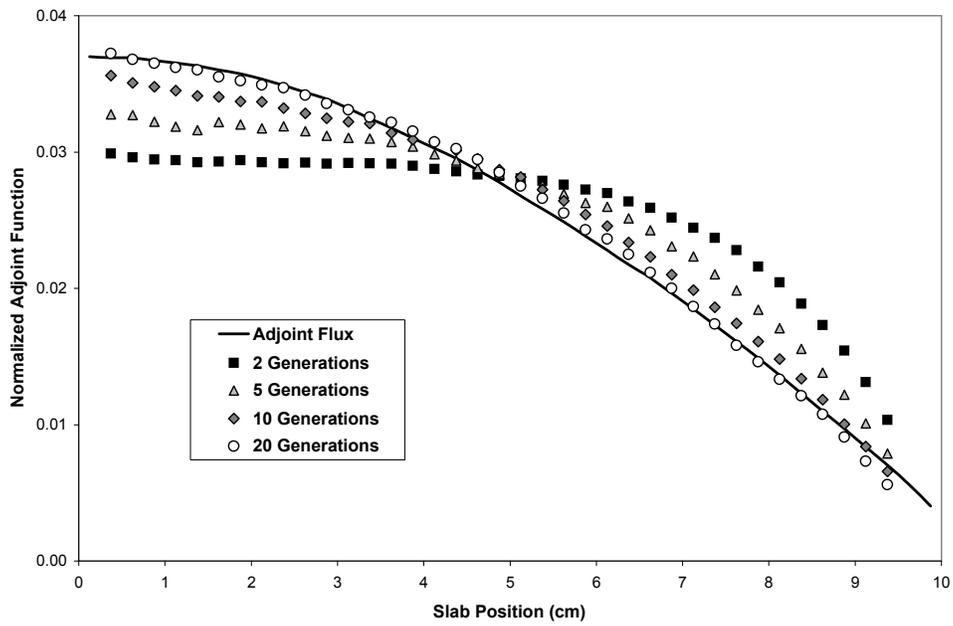


Figure 4: Number of latent generations it takes the adjoint function to converge to its fundamental shape for a mono-energetic, 1-D bare slab reactor.

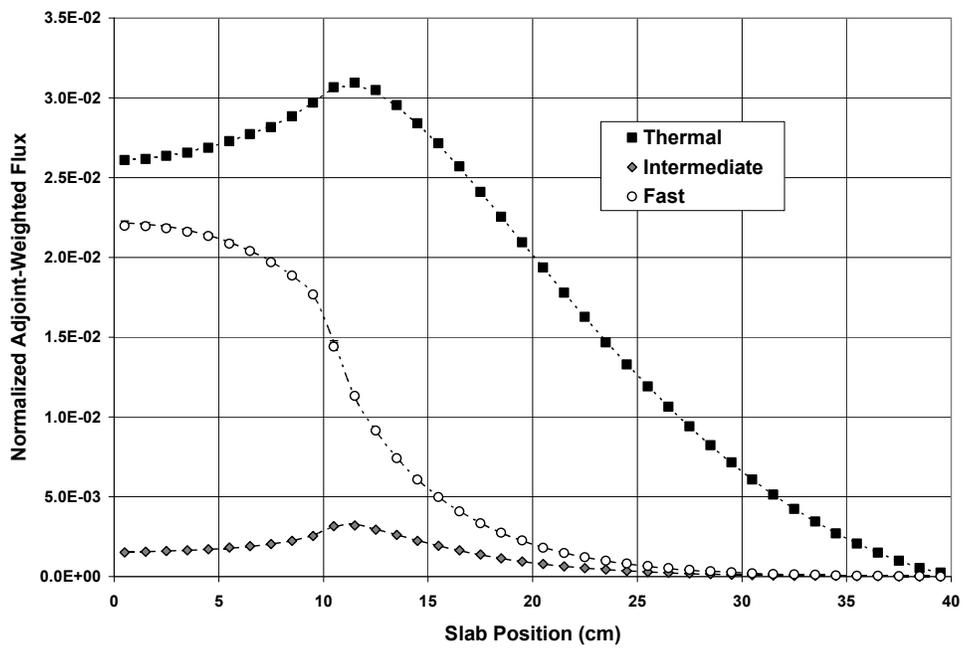


Figure 5: Adjoint-weighted fluxes calculated by discrete ordinates (Partisn) and Monte Carlo (MCNP).

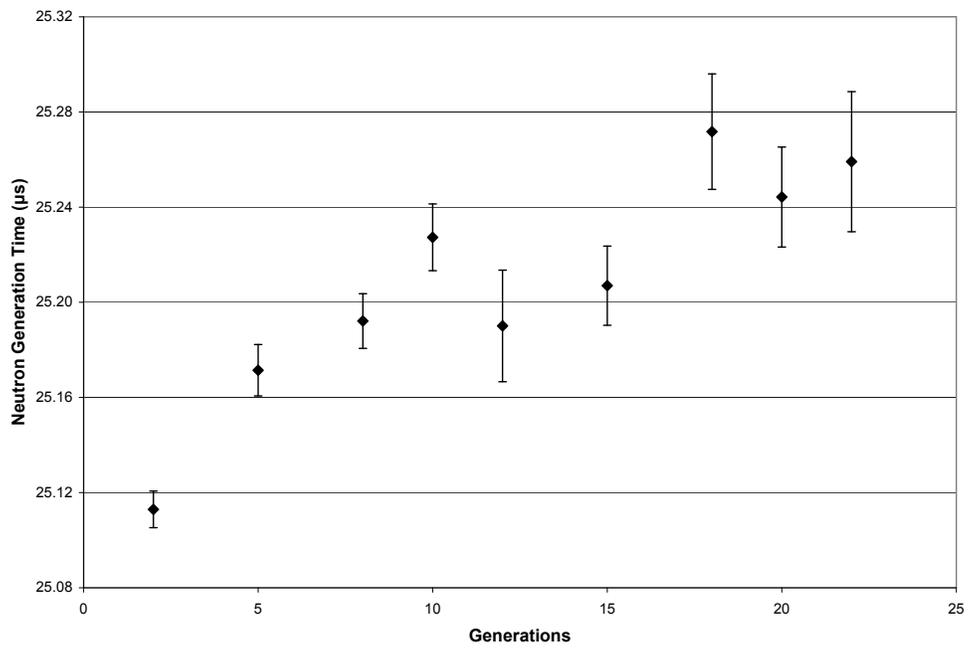


Figure 6: Calculated values of neutron generation time for varied numbers of latent generations in the 2-D PWR problem.

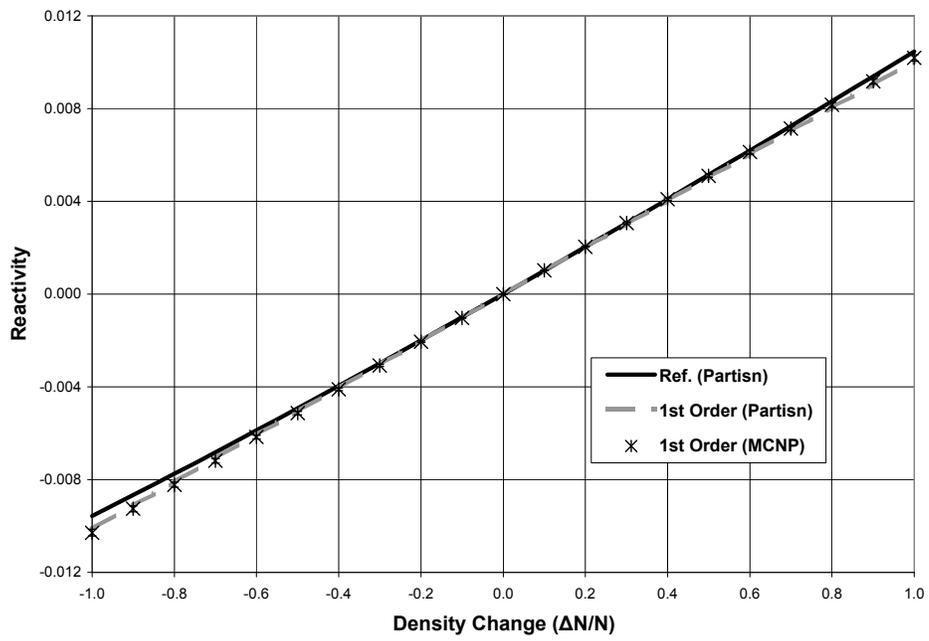


Figure 7: Calculated change in reactivity $\Delta\rho$ for density perturbations to the outer 0.1 cm of Godiva.