

A Zero-Variance-Based Scheme for Variance Reduction in Monte Carlo Criticality

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Abstract

A zero-variance scheme is derived and proven theoretically for criticality cases, and a simplified transport model is used for numerical demonstration. It is shown in practice that by appropriate biasing of the transition and collision kernels, a significant reduction in variance can be achieved. This is done using the adjoint forms of the emission and collision densities, obtained from a deterministic calculation, according to the zero-variance scheme. By using an appropriate algorithm, the figure of merit of the simulation increases by up to a factor of 50, with the possibility of an even larger improvement. In addition, it is shown that the biasing speeds up the convergence of the initial source distribution.

1. Introduction

The aim of a Monte Carlo simulation in nuclear reactor physics is to calculate the response of a detector (which can be a physical detector or a hypothetical detector providing a response) at a point $P = (r, \Omega, E)$ according to

$$R = \int \eta_\phi(P)\phi(P)dP \quad (1)$$

where $\phi(P) = \phi(r, \Omega, E)$ is the neutron flux at point P , while $\eta_\phi(P)$ is the detector response function with respect to the flux. However, the flux is the solution of the analytical transport equation, and therefore hard to simulate by a random process. Therefore, we prefer to use measurable physical quantities, such as the collision density $\psi(P)$, where

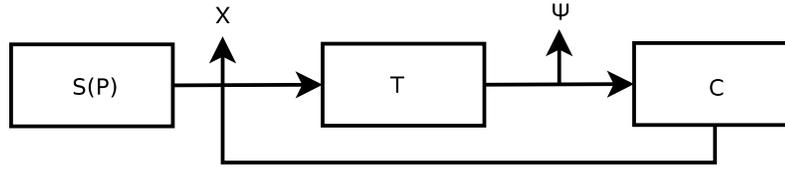
$$\psi(P) = \Sigma_t(P)\phi(P) \quad (2)$$

or the emission density $\chi(P)$. The detector response will now be

$$R = \int \eta_\chi(P)\chi(P)dP = \int \eta_\psi(P)\psi(P)dP \quad (3)$$

where $\eta_\chi(P), \eta_\psi(P)$ are the detector response functions with respect to $\chi(P)$ and $\psi(P)$. This response is calculated by simulating many statistically independent particle histories and averaging their scores, as calculated by the detector response function.

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Figure 1: Schematic diagram of particle transport


1.1 Monte Carlo sampling

A particle will start a flight path which is sampled by the so called transition kernel T , where

$$T(r' \rightarrow r, \Omega', E')dV$$

is the probability that a particle starting a flight path at r' will have its next collision in dV at r . After the new collision point has been sampled, the collision process must be sampled. This is done by the collision kernel C , where

$$C(r', \Omega' \rightarrow \Omega, E' \rightarrow E)d\Omega dE$$

is the probability that a particle will exit a collision at r' with direction Ω in $d\Omega$ and energy E in dE . Via this scheme, it is easy to visualize the sampling of the collision and emission densities. Such a scheme is shown in Fig. 1.

Using these kernels we can now sample $\psi(P)$ and $\chi(P)$, since $\psi(r, \Omega, E)dV$ is now the expected number of particles going into a collision at a point r in dV , while $\chi(r, \Omega, E)d\Omega dE$ is the expected number of particles coming out of the collision with direction Ω in $d\Omega$ and energy E in dE . The concepts of transition and scattering kernels are also used in order to directly interpret the Boltzmann equation in terms of a Monte Carlo calculation. Note that from the Boltzmann transport equation, we define $\chi(P)$ as

$$\chi(P) = S(P) + \int T(r' \rightarrow r, \Omega', E')C(r, \Omega' \rightarrow \Omega, E' \rightarrow E)\chi(P')dP' \quad (4)$$

where $S(P)$ is source of the particles at P . We can see that if we start at a point P' , we can sample the emission density of the next point P by first sampling the transition kernel $T(r' \rightarrow r, \Omega', E')$ in order to select a new collision point, and after that we sample the collision kernel $C(r, \Omega' \rightarrow \Omega, E' \rightarrow E)$ in order to get the next sample of the emission density. If we want to sample the collision density $\psi(P)$, where

$$\psi(P) = S_1(P) + \int C(r', \Omega' \rightarrow \Omega, E' \rightarrow E)T(r' \rightarrow r, \Omega, E)\psi(P')dP' \quad (5)$$

We can see from the diagram that we start by sampling the collision kernel (since we are entering a collision, we already know the position of the collision) and then sample the transition kernel for the next collision. Also note that we use the term $S_1(P)$ instead of $S(P)$ since in this case the source density cannot be the initial source density, but the source of first collisions. In order to make the formulation easier, we can combine the transition and collision kernels into the transport kernel K , where

$$K(P' \rightarrow P) = T(r' \rightarrow r, \Omega', E')C(r, \Omega' \rightarrow \Omega, E' \rightarrow E) \quad (6)$$

or a kernel L , where

$$L(P' \rightarrow P) = C(r', \Omega' \rightarrow \Omega, E' \rightarrow E)T(r' \rightarrow r, \Omega, E) \quad (7)$$

So now the integral equations for $\chi(P)$ and $\psi(P)$ will be as follows:

$$\chi(P) = S(P) + \int K(P' \rightarrow P)\chi(P')dP' \quad (8)$$

$$\psi(P) = S_1(P) + \int L(P' \rightarrow P)\psi(P')dP' \quad (9)$$

Through the sampling of particles we can now obtain the collision or emission density and through use of Eq. 3 finally reach an estimate of the detector response R .

2. The Zero-Variance principle

The Zero-Variance principle is the idea on which most variance reduction schemes are based. According to this scheme, by biasing the source and transport kernel with appropriate adjoint functions, one is able to obtain zero-variance results. This is based on the concept of an adjoint simulation; If we try to recreate an adjoint form of a particle history, we can think of it as follows: a hypothetical adjoint particle begins its history at the detector response site, and it has its first collision where the real particle would be last emitted. Then, following the reverse path, the particle ends up ‘scoring’ where the initial particle was created. By matching the real history with the adjoint history, we can see that the most likely path of a scoring particle is the opposite path of the adjoint particle. This means that adjoint equations should be candidates for importance functions when trying to lower the variance of a calculation, and this claim has been proven some time ago [1, 2]. Although the scheme is mostly of theoretical value, it can be used in order to improve variance of both criticality and shielding calculations. In our case, the scheme was developed for a criticality case, using the model of a homogeneous slab reactor with half-width a , isotropic fission and anisotropic scattering. Towards this goal we made use of the two-direction model [3].

In a multiplying system, we can express the eigenvalue k_{eff} as the ratio of source neutrons of two successive neutron generations:

$$k_{eff} = \frac{\int S_{n+1}(P)dP}{\int S_n(P)dP} \quad (10)$$

For generation n we solve the equation

$$\chi(P) = S_n(P) + \int K(P' \rightarrow P)\chi(P')dP' \quad (11)$$

In order to sample the kernel K , the transition kernel is sampled first, followed by the collision kernel. Starting with a normalized source $S_n(P)$, we can regard k_{eff} as the detector response

$$R = \int S_{n+1}(P)dP = \int \frac{1}{4\pi}\chi_f(E) \int \int \frac{\nu\Sigma_f}{\Sigma_t}\psi_n(r, \Omega', E')d\Omega'dE'dP = \int \frac{\nu\Sigma_f}{\Sigma_t}\psi(P)dP \quad (12)$$

where $\chi_f(E)$ is the fission energy spectrum, ν is the expected number of neutrons produced by one fission and Σ_f is the fission cross-section. This means that for a certain generation, we in

fact treat a criticality simulation as a source-detector problem with the response function shown above. Now, if we follow the standard method of determining the adjoint equation, the source term in the adjoint equation for ψ^* becomes $\eta_\psi = \frac{\nu\Sigma_f}{\Sigma_t}$ and the adjoint function we are looking for is given by

$$\psi^*(P) = \frac{\nu\Sigma_f}{\Sigma_t} + \int L(P \rightarrow P')\psi^*(P')dP' \quad (13)$$

which is also an (adjoint) source-detector problem. The (forward) kernel $L(P' \rightarrow P)$ is analogous to $K(P' \rightarrow P)$, but the collision kernel has to be sampled first and the transition kernel afterwards. On this point we will base our variance reduction scheme, in order to reduce the variance of the virtual detector's response, ie k_{eff} . Note that the adjoint function from Eq. 13 is different from the adjoint eigenfunction of the criticality problem.

2.1 Proof of the Zero-Variance Behaviour

We can denote with $\bar{\kappa}(P)$ the biased non-absorption probability of a particle entering a collision point at P' .

$$\bar{\kappa}(P') = \int \bar{L}(P' \rightarrow P)dP \quad (14)$$

where \bar{L} is the biased transport kernel, ie

$$\bar{L}(P' \rightarrow P) = L(P' \rightarrow P) \frac{\psi^*(P)}{\psi^*(P')} \quad (15)$$

Using Eq. 13 with $\eta_\psi(P) = \frac{\nu\Sigma_f}{\Sigma_t}$ gives us

$$\int \bar{L}(P' \rightarrow P)dP = \frac{1}{\psi^*(P')} \int L(P' \rightarrow P)\psi^*(P)dP = 1 - \frac{\eta_\psi(P')}{\psi^*(P')}. \quad (16)$$

This is the biased analogue of the non-absorption probability in a forward calculation

$$\kappa(P) = 1 - \frac{\Sigma_s}{\Sigma_t}$$

If we use an implicit capture model, we can therefore see that $\bar{\kappa}(P)$ should be used as a modifying weight factor of a particle exiting a collision, in order to compensate for the absence of an absorption probability in the system. In an implicit capture model without a lower cut-off point for the particle weight, the history will never terminate. In that case, the contribution to the estimator from that history will be

$$\hat{R}_{col} = \sum_{i=1}^{\infty} \bar{\kappa}(P_1)\bar{\kappa}(P_2) \dots \bar{\kappa}(P_{i-1}) \frac{\eta_\psi(P_i)}{\psi^*(P_i)} R. \quad (17)$$

Note that there is no collision at the phase-space point P_0 , the particle source, therefore for $i = 1$ the formula above will reduce to

$$\hat{R}_{col,1} = \frac{\eta_\psi(P_1)}{\psi^*(P_1)} R. \quad (18)$$

Now, if we calculate $1 - \widehat{R}_{col}/R$ using Eq. 16 we get:

$$\begin{aligned}
 1 - \widehat{R}_{col}/R &= \\
 &= \bar{\kappa}(P_1) - (1 - \bar{\kappa}(P_2))\bar{\kappa}(P_1) - (1 - \bar{\kappa}(P_3))\bar{\kappa}(P_1)\bar{\kappa}(P_2) - \dots \\
 &= \bar{\kappa}(P_1) - \bar{\kappa}(P_1) + \bar{\kappa}(P_1)\bar{\kappa}(P_2) - \bar{\kappa}(P_1)\bar{\kappa}(P_2) + \bar{\kappa}(P_1)\bar{\kappa}(P_2)\bar{\kappa}(P_3) - \dots \\
 &= \bar{\kappa}(P_1)\bar{\kappa}(P_2)\bar{\kappa}(P_3)\dots = 0
 \end{aligned} \tag{19}$$

since $\bar{\kappa}(P_1) < 1$ for an infinite number of collision points. Therefore, at all histories, $\widehat{R}_{col} = R$, and the variance will be zero. However, in practice we cannot use infinitely long histories, therefore we use a lower weight for history termination, after which Russian roulette is applied.

3. Demonstration of the Scheme

3.1 The Two-Direction Model

The two-direction model, proposed by Hoogenboom, is a model that limits the transport of particles to the $\pm x$ direction. That way, although it remains a true transport model, the equations describing the particle transport become differential, diffusion type equations. This means that both forward and adjoint solutions can be obtained analytically, which makes the model an excellent one for testing theories for variance reduction. Also, as the numerical results for a given case can easily be obtained full benchmarking of the model, both against theoretical results and against established Monte Carlo codes is possible.

By limiting our transport to the $\pm x$ directions, the transition and scattering kernels become extremely simple, especially if we assume a monoenergetic case. In that case, the position vector r simply becomes $s = |x - x'|$, while for the scattering kernel all we need to specify is a direction $\mu = \pm 1$. Finally, in a monoenergetic case, we can completely drop the energy variable E . We can now give the simplified versions of the two kernels (for a homogeneous medium) as follows:

The transition kernel will be

$$T(x' \rightarrow x) = \Sigma_t e^{-\Sigma_t |x - x'|} \tag{20}$$

while the scattering kernel becomes equal to

$$C(x, \mu' \rightarrow \mu) = \begin{cases} \frac{\Sigma_{\rightarrow}}{\Sigma_t} & \mu' \mu = +1 \\ \frac{\Sigma_{\leftarrow}}{\Sigma_t} & \mu' \mu = -1 \end{cases} \tag{21}$$

where Σ_{\rightarrow} and Σ_{\leftarrow} are the forwards and backwards scattering cross section respectively, with

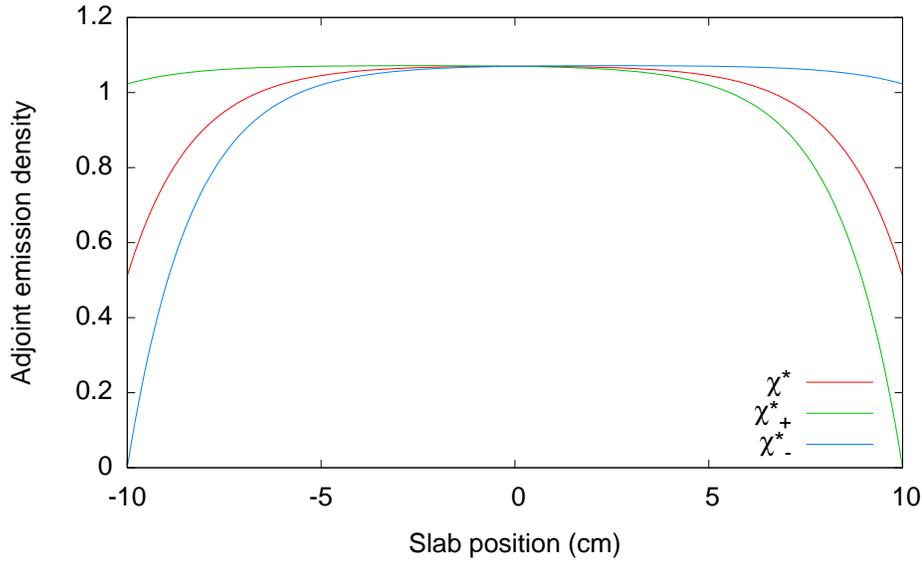
$$\Sigma_{\rightarrow} + \Sigma_{\leftarrow} = \Sigma_s \tag{22}$$

It is clear that the model simplifies sampling of these kernels significantly. This still applies to a heterogeneous system, although the analytical solutions will become more involved. However, we also need to obtain the adjoint functions in order to bias the above kernel if we want to implement the zero-variance scheme in the model.

3.2 Adjoint equations

As we stated above, the 2-direction model allows us to simplify the integro-differential form of the Boltzmann equation into a diffusion type differential equation. For a homogeneous system, it can be shown that the differential equation of $\phi^*(x)$ is

$$-\frac{1}{\Sigma_{tr}} \frac{d^2 \phi^*(x)}{dx^2} + \Sigma_a \phi^*(x) = \eta_\phi \tag{23}$$

Figure 2: Adjoint emission density for a slab reactor


It can be shown that $\chi^*(x)$ has exactly the same form, which makes the 2-direction model an excellent selection for testing the input of deterministic codes (which will usually output $\phi^*(x)$).

In Fig. 2 we can see the form of $\chi^*(x)$ for a slab reactor with half-width $a = 10\text{cm}$ in the 2-direction model. As $\chi_{\pm}^*(x)$, the adjoint *emission* density for the $\pm x$ direction, becomes zero at the left and right boundary, respectively, it is clear that the weight probability of particles to escape the system becomes extremely small. This, coupled with the lowering of the Russian roulette cut-off weight, provide maximum efficiency in our detector response.

By transformation of the kernels, we can relate the two adjoint densities as:

$$\psi_{\pm}^*(x) = \eta_{\psi} + \frac{\Sigma_{\rightarrow}}{\Sigma_t} \chi_{\pm}^*(x) + \frac{\Sigma_{\leftarrow}}{\Sigma_t} \chi_{\mp}^*(x) \quad (24)$$

In order to obtain a k_{eff} response using this scheme, we need to properly bias the source, transition and scattering kernels and then sample from the biased kernels. By applying the fact that the optimum weighting factor is the adjoint emission density we can show that the optimum source biasing is equal to

$$\bar{S}_{\pm}(x) = S_{\pm}(x) \times \frac{\chi_{\pm}^*(x)}{R} \quad (25)$$

with the factor R included to have a normalized biased source. In order to apply to zero-variance scheme on the transition kernel, we have to bias it by the adjoint *collision* density, since it determines the importance of the particles that are going to have a collision on the next point x . The biased transition kernel will be equal to

$$\begin{aligned} \bar{T}_{\pm}(x' \rightarrow x) &= T_{\pm}(x' \rightarrow x) \frac{\psi_{\pm}^*(x)}{\chi_{\pm}^*(x')} \\ &= \Sigma_t e^{-\Sigma_t |x-x'|} \frac{\eta_{\psi} + \Sigma_{\rightarrow} \chi_{\pm}^*(x) + \Sigma_{\leftarrow} \chi_{\mp}^*(x)}{\chi_{\pm}^*(x')} \end{aligned} \quad (26)$$

where $\chi_{\pm}^*(x')$ is a normalization factor for the kernel \bar{T} . In order to select from the biased kernel, we have:

$$\rho = P(x) = \int_{x'}^x \bar{T}(x' \rightarrow x'') dx'' \quad (27)$$

where ρ is a random number, uniformly distributed between 0 and 1. We can now calculate the value of x using a root-finding iterative method, such as the regula falsi method, until x converges.

For the biasing of the scattering kernel, we use the adjoint emission density, since we are interested in the importance of particles coming out of a collision with a specific direction μ . The normalized biased scattering kernel \bar{C} will be:

$$\begin{aligned} \bar{C}(x, \mu' \rightarrow \mu) &= C(x, \mu' \rightarrow \mu) \frac{\chi_{\mu}^*(x)}{\psi_{\mu'}^*(x)} \frac{\psi_{\mu'}^*(x)}{\psi_{\mu'}^*(x) - \eta_{\psi}} \\ &= C(x, \mu' \rightarrow \mu) \frac{\chi_{\mu}^*(x)}{\psi_{\mu'}^*(x) - \eta_{\psi}} \end{aligned} \quad (28)$$

where the weight correction is the non-absorption probability $\bar{\kappa}(P)$. By use of Eq. 24 & 28 we arrive at the final form of the biased collision kernel \bar{C}' :

$$\bar{C}'(x, \mu' \rightarrow \mu) = \begin{cases} \frac{\Sigma_{\rightarrow} \chi_{+}^*(x)}{\Sigma_{\rightarrow} \chi_{+}^*(x) + \Sigma_{\leftarrow} \chi_{-}^*(x)} & \mu : +1 \rightarrow +1 \\ \frac{\Sigma_{\leftarrow} \chi_{-}^*(x)}{\Sigma_{\rightarrow} \chi_{+}^*(x) + \Sigma_{\leftarrow} \chi_{-}^*(x)} & \mu : +1 \rightarrow -1 \\ \frac{\Sigma_{\rightarrow} \chi_{+}^*(x)}{\Sigma_{\rightarrow} \chi_{-}^*(x) + \Sigma_{\leftarrow} \chi_{+}^*(x)} & \mu : -1 \rightarrow +1 \\ \frac{\Sigma_{\leftarrow} \chi_{-}^*(x)}{\Sigma_{\rightarrow} \chi_{-}^*(x) + \Sigma_{\leftarrow} \chi_{+}^*(x)} & \mu : -1 \rightarrow -1 \end{cases} \quad (29)$$

We can select from the scattering kernel by simply calculating the probability of a particle to change direction or not after a collision, since we are only interested in the $+x$ and $-x$ directions. Note that, since we bias the kernels, in order to reach an unbiased k_{eff} estimate, we have to appropriately modify the statistical weight of the sampled particles, which is done after the sampling of each kernel.

3.3 Numerical Demonstration

In order to demonstrate the zero-variance scheme, we have written a simple code that simulates a Monte Carlo criticality calculation. Using this code, we can test the principle of the zero-variance scheme and also compare the results of the true, analytically derived adjoints with those using adjoints generated by a computational method. The equations used are exactly the same ones as for a shielding calculation, but using the detector response $\eta_{\psi} = \frac{\nu \Sigma_f}{\Sigma_t}$. The biasing of the kernels was initially done by using the exact analytical forms of the adjoint equations and later by input of discrete values and their interpolation, while the analytically calculated converged neutron source is used.

In Table 1 we can see the results of such a calculation, using isotropic scattering ($\bar{\mu}_0 = 0$), 10^4 particles per batch, constant artificial cross-sections and lowering the Russian Roulette threshold for each calculation. The results are taken after the 2nd batch for the different Russian roulette threshold weights. It is obvious that, by using an appropriately low weight threshold, we can approximate zero-variance rather quickly. Of course, the lower thresholds cost more in terms of CPU time, so it is necessary to decide whether absolute minimum variance is preferred to a possibly higher figure of merit and modify the input weight thresholds accordingly.

Table 1: k_{eff} results for varying RR weight threshold

RR Weight threshold	k_{eff}
2.5E-02	$0.958854 \pm 5.3259E-03 \%$
2.5E-03	$0.958771 \pm 9.3465E-04 \%$
2.5E-04	$0.958782 \pm 1.3711E-04 \%$
2.5E-05	$0.958788 \pm 4.3961E-06 \%$
Theoretical value	0.958788

The results look very promising indeed and confirm the theory of the zero-variance scheme. However, it is important to remember that we are here using the exact forms of the adjoint equations, and in all but the simplest cases, the analytical forms are very hard to solve. Therefore, another method must be used in order to acquire the adjoint functions. To that end, the XSDRN code [4] was used for the 2-direction model. XSDRN is a 1-D discrete-ordinates transport code which can, upon option, solve the adjoint forms of the 1-D transport equation. The output of such a calculation is the angular and total $\phi^*(x)$. However, since in this case $\phi^*(x) = \chi^*(x)$, we can directly use the output of XSDRN in order to bias the source and transport kernel.

XSDRN could easily accommodate the 2-direction model, since the only change required was the blocking of any possible angle cosine when selecting direction except -1 and +1, each being selected with probability 1/2. As the geometry of our system was simple, XSDRN gave excellent results for the values of the adjoints, that compared well with the analytical solutions, both in isotropic and anisotropic scattering calculations.

3.4 Numerical results and discussion

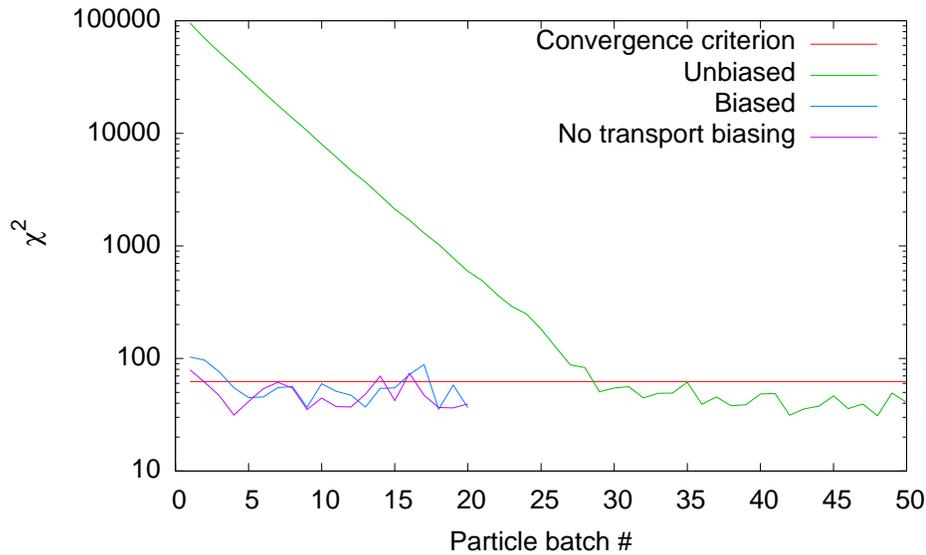
In order to investigate the performance of the biasing scheme, we applied it to the simple 1-dimensional slab reactor described above, using $\Sigma_t = 1.05cm^{-1}$, $\Sigma_s = 0.55cm^{-1}$, $\nu\Sigma_f = 0.625cm^{-1}$ and $\bar{\mu}_0 = 0.75$. The threshold for application of Russian roulette was set to 10^{-3} . A flat initial source was assumed.

Initially, we only considered the comparison between a fully biased calculation and a fully unbiased one. However, since collision biasing does not require a root finding method, its tax on CPU time should be much smaller than the transition biasing, therefore we also investigated a case where no biasing is applied to the transition kernel, but normal biasing is applied to the collision kernel. From Fig. 2 we can see that for a large part of our slab reactor the adjoints remain relatively constant, so we expect this change not to have a large effect on the behaviour of the biasing.

Since the calculation begins with a flat source distribution assumed, it is important to know when we have achieved a converged source distribution, since meaningful results for k_{eff} can only be acquired using a converged source. In order to investigate the evolution of the source and the effect of biasing on convergence we have used a χ^2 goodness-of-fit test [5]. This was possible since, because of the simplicity of the model, we could analytically calculate the converged source distribution. We have used an exceeding probability of 1% in order to calculate the accepted convergence limit shown in Fig. 3.

As we can see, the unbiased scheme needs a much larger number of batches before it can match our criterion, while the biased cases fare much better. What is surprising is that the case where no transition kernel biasing was used behaves almost identically to the full biasing one.

Figure 3: χ^2 test for source convergence determination



Although it was expected that transport biasing would effect the new fission locations more than this, it seems that the flat adjoints over a large area of the detector played a role in the convergence. The fast convergence meant that only a small number of batches was discarded for the biased calculations, which means that, assuming the same total number of batches, much better statistics can be obtained from the biased simulations. In fact, in the unbiased calculation, we have used 10^5 particles in order to reach source convergence in a reasonable number of batches and allow for better statistics.

Table 2: Comparison of biased and unbiased simulations

Particles	k_{eff}	Batches until source convergence	Total # of batches used	Relative FOM
100000 (Unbiased)	1.0819 ± 0.0005	30	50	1
1000 (No Trans. Bias)	1.0816 ± 0.0029	8	20	50
1000	1.0814 ± 0.0012	7	20	19
Theoretical value	1.8016			

The results can be seen in Table 2. We can see that, although we do not use the exact adjoints and a source normalization is required, the biased case already provides an advantage in the figure of merit over the unbiased simulation. The smaller standard deviation in the unbiased case is because of the number of particles used, by using 1000 particles the standard deviation is around one order of magnitude higher, as expected. The resulting improvement is rather surprising, especially since in a very simple case like this, the unbiased calculation should have a considerable advantage in computing time.

One important thing to note is that the nature of the scheme requires many recalculations and interpolations of the adjoints in order to calculate the ψ^* and χ^* at every point of the

simulation. This means that the performance is heavily dependent on the computational scheme used. During our numerical tests, we managed to raise the figure of merit by a whole order of magnitude, by simply optimizing the algorithm for calculating the adjoint at a point x . Another option considered for further optimization is the biasing of transport kernel based on the slope of the adjoint function. That way, biasing would be applied only where needed (near interfaces, voids etc) while in large homogenized regions it would be omitted for gain in CPU time.

The acceleration of the source convergence is also a valuable result of the scheme. It is interesting to research whether it can be used in conjunction with other acceleration schemes (such as the fission matrix scheme), since the convergence acceleration obtained by the scheme during a particle batch simulation can directly benefit another scheme.

4. Conclusion

It can be concluded that for a simple model, the zero-variance derived scheme shown here can provide a significant reduction in the variance of a criticality Monte Carlo calculation, and a corresponding increase in the total figure of merit of the calculation, when compared to an unbiased scheme. The scheme also improves the convergence of the particle source and the fundamental k_{eff} mode. The scheme can be extended to a full 3-dimensional transport model, however it remains a question whether the CPU time will be significantly taxed from the calculation of the angle-dependent adjoints.

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