Progress in NUCLEAR SCIENCE and TECHNOLOGY, Vol. 2, pp.722-731 (2011)

ARTICLE

A Priori Efficiency Calculations for Monte Carlo Applications in Neutron Transport

Andreas J. VAN WIJK and J. Eduard HOOGENBOOM*

Delft University of Technology, Mekelweg 15, 2629 JB Delft, The Netherlands

In this paper a general derivation is given of equations describing the variance of an arbitrary detector response in a Monte Carlo simulation and the average number of collisions a particle will suffer until its history ends. The theory is validated for a simple slab system using the two-direction transport model and for a two-group infinite system, which both allow analytical solutions. Numerical results from the analytical solutions are compared with actual Monte Carlo calculations, showing excellent agreement. These analytical solutions demonstrate the possibilities for optimizing the weight window settings with respect to variance. Using the average number of collisions as a measure for the simulation time a cost function inversely proportional to the usual Figure of Merit is defined, which allows optimization with respect to overall efficiency of the Monte Carlo calculation. For practical applications it is outlined how the equations for the variance and average number of collisions can be solved using a suitable existing deterministic neutron transport code with adapted number of energy groups and scattering matrices.

KEYWORDS: Monte Carlo, neutron transport, efficiency, variance, moment equations

I. Introduction

The Monte Carlo technique is widely recognized as a powerful tool for simulating neutron transport. In many situations simple analog simulation will not suffice and therefore variance reduction and/or efficiency boosting schemes are implemented.

Although 'rules of thumb' exist for the implementation of such non-analog schemes, especially for setting weight window parameters like Russian roulette and splitting thresholds, a rigorous theoretical basis for these rules of thumb is lacking; both for rules regarding the reduction of variance and boosting the Figure of Merit (FOM).

Normally the variance or standard deviation of the result of the Monte Carlo calculation is estimated together with the desired quantity. However, for a proper choice of weight window parameters it is useful to be able to calculate *a priori* the variance and FOM for a given choice of weight window parameters in order to make an optimum choice. To this end in Section II the equations determining the first moment (requested quantity) and the second moment (averaged squared value) are derived to obtain the variance of the Monte Carlo result. The FOM, or rather its inverse, is approximated by the product of variance and a function describing the average number of collisions during a particle history. The equation for the average number of collisions is also derived in Section II. Analytical results are obtained for a one-group slab system using the two-direction transport model and for a two-group infinite system in Section III. Numerical results of the analytic formulas and comparison with Monte Carlo calculations are shown in Section IV. The numerical solution of the second moment equation with an existing transport code and the modifications needed in the input to the code are discussed in Section V.

As the amount of information that can be given in this paper is limited, the reader is referred to Reference 1 for more details and results.

II. Moments Equations

1. The Integral Form of the Transport Equation

The Monte Carlo simulation of neutron or photon transport is governed by sampling of the source $S(P)=S(\boldsymbol{r},E,\boldsymbol{\Omega})$ and successive sampling of the transition kernel $T(\boldsymbol{r}'\rightarrow\boldsymbol{r},E',\boldsymbol{\Omega}')$ to select the next collision point $\boldsymbol{r}$ starting at $\boldsymbol{r}'$ and the collision kernel $C(\boldsymbol{r},E'\rightarrow E,\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega})$ to select the energy E and direction $\boldsymbol{\Omega}$ after scattering. Then the collision density $\psi(P)$ is given by the integral transport equation

$$\psi(P) = S_1(P) + \int K(P'\rightarrow P)\psi(P')dP' \tag{1}$$

with $S_1(P)$ the source of first collisions, given by

$$S_1(P) = \int T(\boldsymbol{r}'\rightarrow\boldsymbol{r},E,\boldsymbol{\Omega})S(\boldsymbol{r}',E,\boldsymbol{\Omega})dV' \tag{2}$$

and the full transport kernel $K(P'\rightarrow P)$ defined by

$$K(P'\rightarrow P) = C(\boldsymbol{r}',E'\rightarrow E,\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega})T(\boldsymbol{r}'\rightarrow\boldsymbol{r},E,\boldsymbol{\Omega}). \tag{3}$$

The non-absorption probability for a particle entering a collision at P' is

$$\kappa(P') = \int K(P'\rightarrow P'')dP'' = \int C(\boldsymbol{r}',E'\rightarrow E'',\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega}'')dE''d\Omega''. \tag{4}$$

*Corresponding author, E-mail: j.e.hoogenboom@tudelft.nl

This probability is used in an analog Monte Carlo simulation to select a scattering event (instead of capture or absorption) or is used as a weight factor to reduce the particle weight in case of a non-analog simulation with implicit capture. In the following we will omit the dependence of κ on P' in light of notational convenience if no confusion is possible.

The aim of a calculation will be to determine the response R of an actual or hypothetical detector, being some average over the collision density $\psi(P)$ as follows

$$R = \int \eta_\psi(P)\psi(P)dP \tag{5}$$

with $\eta_\psi(P)$ the averaging function or detector response function.

2. The Score Probability Equation

To derive the moment equations, especially for the second moment of the estimate of R, we introduce the score probability function $\pi(P,W,s)ds$ along the lines of Lux and Koblinger,[2] but with the modification of Hoogenboom[3] as the probability of a neutron *entering a collision* at P with statistical weight W to give a total score s in ds. To take into account the possibility of splitting and Russian roulette in a non-analog simulation we apply a weight window after a collision with splitting if the particle weight after collision is above the threshold W_{split} and with Russian roulette if the particle weight after collision is below the threshold W_{RR}. The weight window settings may be space and energy dependent. The Russian roulette and splitting can be arranged in different ways with different survival probabilities and corresponding particle weights. Here we use a survival weight W_{surv} after the Russian roulette, independent of the particle weight before the Russian roulette and in case of splitting a particle is always split in N_{split} particles (N_{split}>1). As the particle weight after implicit capture is $\kappa(P)W$, we have the conditional probability that exactly one particle will be alive after application of the weight window

$$z_1(P,\kappa W) = \begin{cases} 0 & \kappa W \geq W_{split} \\ 1 & W_{RR} < \kappa W < W_{split} \\ \dfrac{\kappa W}{W_{surv}} & \kappa W \leq W_{RR}. \end{cases} \tag{6}$$

and the probability $z_0(P,\kappa W)=1-\kappa W/W_{surv}$ for $\kappa W \leq W_{RR}$ to get no particle out of the weight window.

The probability to have N_{split}>1 particles resulting after applying the weight window is

$$z_N(P,\kappa W) = \begin{cases} 1 & \kappa W \geq W_{split} \\ 0 & W_{RR} < \kappa W < W_{split} \\ 0 & \kappa W \leq W_{RR}. \end{cases} \tag{7}$$

Then the weight after application of the weight window is

$$W^*(P,\kappa W) = \begin{cases} \dfrac{\kappa W}{N_{split}} & \kappa W \geq W_{split} \\ \kappa W & W_{RR} < \kappa W < W_{split} \\ W_{surv} & \kappa W \leq W_{RR}. \end{cases} \tag{8}$$

Normally the ratio between the Russian roulette survival weight W_{surv} and the threshold W_{RR} as well as the ratio between the boundaries of the weight windows is a fixed value:

$$\frac{W_{surv}}{W_{RR}} = \alpha \qquad \frac{W_{split}}{W_{RR}} = \beta \tag{9}$$

with α often a value of 2 and β a value of 4 to 10.

We can now derive the equation for the score probability considering a particle with weight W entering a collision.[3] The particle will give anyway a contribution to the score of $W\eta_\psi(P)$ as $\eta_\psi(P)$ is the scoring function from Eq. (5) for the collision density. In a non-analog simulation there will always be implicit capture, reducing the weight to κW. Then the weight window will be applied giving a probability $1\text{-}z_1$ that no particle will survive and the total score s remains $W\eta_\psi(P)$, hence a function $\delta(s\text{-}W\eta_\psi(P))$ represents the score in case of a terminal collision. In case that one particle comes out of the weight window application, it will have a probability $K_n(P\rightarrow P')=K(P\rightarrow P')/\kappa(P)$ to enter the next collision at P'. Then the total score s is a convolution of the former δ–function and the score probability at P' with weight $W^*(P,\kappa W)$. Another mutually exclusive possibility is to have N_{split} particles after the weight window application. Then the total score is a convolution of the δ–function with the multiple convolution of the score probabilities of all N_{split} particles. Hence,

$$\begin{aligned} \pi(P,W,s) &= (1-z_1(P,\kappa W))\delta(s-W\eta_\psi) \\ &+ z_1(P,\kappa W)\int K_n(P\rightarrow P')\delta(s-W\eta_\psi) \\ &\quad * \pi(P',W^*(P,\kappa(P)W),s)dP' \\ &+ z_N(P,\kappa W)\int K_n(P\rightarrow P')\delta(s-W\eta_\psi) \\ &\quad * \prod_{j=1}^{N_{split}} * \pi(P',W_j^*(P,\kappa(P)W),s)dP'. \end{aligned} \tag{10}$$

with $*$ denoting convolution and $\prod_{j=1}^{N} *$ multiple convolutions.[4]

3. Average and Variance

The first and second moment of the score are defined by

$$\begin{aligned} M_1(P,W) &= \langle s \rangle = \int_{-\infty}^{\infty} s\pi(P,W,s)ds \\ M_2(P,W) &= \langle s^2 \rangle = \int_{-\infty}^{\infty} s^2\pi(P,W,s)ds. \end{aligned} \tag{11}$$

with the integration starting at $-\infty$ for convenience.

For application to Eq. (10) we need the following properties of multiple convolutions[4)]

$$< s >_{f_1 * f_2 * \ldots f_N} = \int_{-\infty}^{\infty} s \prod_{j=1}^{N} * f_j(s) ds = \sum_{j=1}^{N} < s >_{f_j} \quad (12)$$

and

$$< s^2 >_{f_1 * f_2 * \ldots f_N} = \int_{-\infty}^{\infty} s^2 \prod_{j=1}^{N} * f_j(s) ds =$$
$$\sum_{j_i = 0,1,2} \frac{2!}{j_1! j_2! \cdots j_N!} < s^{j_1} >_{f_1} < s^{j_2} >_{f_2} \cdots < s^{j_N} >_{f_N} \quad (13)$$
$$\text{with } j_i \in (0,1,2) \text{ such that } \sum_{i=1}^{N} j_i = 2 .$$

Noting that

$$\left\{ z_1(P, \kappa W) + z_N(P, \kappa W) N_{split} \right\} W^*(P, \kappa W) = \kappa(P) W, \quad (14)$$

we arrive at

$$M_1(P,W) = W \eta_\psi(P) + \kappa(P) W \int K_n(P \to P') \psi(P') dP'. \quad (15)$$

For the first moment it holds that[2)]

$$M_1(P,W) = W M_1(P, W=1) = W M_1(P) \quad (16)$$

and we see that M_1 satisfies the adjoint transport equation

$$M_1(P) = \psi^*(P) = \eta_\psi(P) + \int K(P \to P') \psi^*(P') dP'. \quad (17)$$

When we take the average over all particles entering their first collision we see

$$E[M_1(P)] = \int S_1(P) M_1(P) dP = \int S_1(P) \psi^*(P) dP = R. \quad (18)$$

For the second moment we find

$$\begin{aligned} M_2(P,W) &= W^2 I_0(P) \\ &+ \left\{ z_1(P, \kappa W) + z_N(P, \kappa W) N_{split} \right\} \\ &\times \int K_n(P \to P') M_2(P', W^*(P, \kappa(P) W) dP' \\ &+ z_N(P, \kappa W) W^2 \frac{N_{split} - 1}{N_{split}} \\ &\times \kappa \int K(P \to P') M_1^2(P') dP' \end{aligned} \quad (19)$$

with

$$I_0(P) = \eta_\psi(P) \left[2 M_1(P) - \eta_\psi(P) \right]. \quad (20)$$

This is also an adjoint type equation with the arguments of the kernel K_n reversed compared to a forward equation like Eq. (1), but with a complicated source term including the integral term with M_1^2 and an additional factor to the kernel K_n. The variance in the estimate of R for a particle with initial weight W_{init} can now be obtained from

$$Var(W_{init}) = \int S_1(P) \frac{M_2(P, W_{init})}{W_{init}^2} dP - R^2 . \quad (21)$$

For the non-analog simulation without splitting and Russian roulette, but only implicit capture we can set in Eq. (19) $z_N = 0$ and $z_1 = 1$ and obtain

$$M_2^{ic}(P,W) = W^2 I_0(P) + \frac{1}{\kappa} \int K(P \to P') M_2^{ic}(P', \kappa(P) W) dP'. \quad (22)$$

As the simulation process at each collision is independent of the particle weight, we have in this case $M_2^{ic}(P,W) = W^2 M_2^{ic}(P, W=1) = W^2 M_2^{ic}(P)$ and

$$M_2^{ic}(P) = I_0(P) + \kappa \int K(P \to P') M_2^{ic}(P') dP'. \quad (23)$$

For the fully analog game we always have W=1 and can drop the weight dependence. For the derivation of the second-moment equation we have to consider that the particle history ends with the absorption probability 1-κ and continues with probability κ. This results in

$$M_2^{an}(P) = I_0(P) + \int K(P \to P') M_2^{an}(P') dP' . \quad (24)$$

Comparing Eq. (24) with Eq. (23) we see that the second moment and hence the variance with implicit capture is always smaller than for the analog simulation. However, using only implicit capture without Russian roulette may result in long histories with particle weights getting progressively smaller, especially in a system with low leakage. The resulting increase in CPU time will deteriorate the FOM. As it is hardly possible to model the CPU time of a Monte Carlo simulation we will use the number of collisions as a substitute. For an alternative see Reference 5.

4. The Number of Collisions

The score probability equation for the number of collisions for the case with a weight window can be derived along the same lines as for the score itself, taking into account that for a neutron entering a collision the number of collisions is 1 if no particle survives the weight window. This leads to

$$\begin{aligned} \pi^c(P,W,s) &= (1 - z_1(P, \kappa W)) \delta(s-1) \\ &+ z_1(P, \kappa W) \int K_n(P \to P') \delta(s-1) \\ &\quad * \pi^c(P', W^*(P, \kappa(P) W), s) dP' \\ &+ z_N(P, \kappa W) \int K_n(P \to P') \delta(s-1) \\ &\quad * \prod_{j=1}^{N_{split}} * \pi^c(P', W_j^*(P, \kappa(P) W), s) dP' \end{aligned} \quad (25)$$

with the score variable s and the convolutions now being discrete. The expected number of collisions $n_c(P,W)$ for a neutron entering a collision at P with weight W is obtained by summation over s leading to

$$n_c(P,W) = 1 + \left\{ z_1(P,\kappa W) + z_N(P,\kappa W) N_{split} \right\} \times \int K_n(P \to P') n_c(P', W^*(P,\kappa(P)W)) dP'. \tag{26}$$

For the case of only implicit capture this becomes

$$n_c^{ic}(P) = 1 + \frac{1}{\kappa} \int K(P \to P') n_c^{ic}(P') dP', \tag{27}$$

independent of the initial weight. For analog simulation it becomes

$$n_c^{an}(P) = 1 + \int K(P \to P') n_c^{an}(P') dP'. \tag{28}$$

The averaged number of collisions over all particle histories is obtained from

$$N_c(W_{init}) = \int S_1(P) n_c(P, W_{init}) dP. \tag{29}$$

5. Cost Function

We now proceed with the definition of the cost function as a product of variance and number of collisions.

$$Cost(W_{init}) = Var(W_{init}) N_c(W_{init}). \tag{30}$$

The cost function may be interpreted as being proportial to the inverse of the Figure of Merit. It may be used to compare different simulation implementations and it should be minimized to find optimum weight window parameters. It is independent of the computer used to perform the Monte Carlo calculation and the programming of the Monte Carlo code.

III. Analytical Solutions

To validate the theory presented in Section II it will be useful to apply the theory to a case for which analytical solutions can be obtained. This is hardly possible in general, but using the simplified two-direction transport model[6] upon simple cases, a true Monte Carlo calculation is still possible and one can obtain the desired analytical solutions.

1. The Two-Direction Transport Model

In the two-direction transport model we consider only particles moving into the $+x$ or $-x$ direction. Differentiation of the integral equations for both directions and combining the results leads to a diffusion-type differential equation for the scalar flux

$$-\frac{d}{dx}\frac{1}{\boldsymbol{\Sigma}_{tr}(x)}\frac{d\phi(x)}{dx} + \boldsymbol{\Sigma}_a(x)\phi(x) = S(x), \tag{31}$$

with the transport cross section as usual defined by

$$\Sigma_{tr} = \Sigma_t - \bar{\mu}_0 \Sigma_s. \tag{32}$$

The boundary conditions at boundary x_b can be derived to be

$$\left| \frac{d\phi(x_b)}{dx} \right| = \boldsymbol{\Sigma}_{tr}\phi(x_b). \tag{33}$$

In case of the two-direction model the collision kernel C simplifies to

$$\Sigma_s(x, \mu' \to \mu) = \begin{cases} \Sigma_{\rightarrow}(x) & \mu'\mu = +1 \\ \Sigma_{\leftarrow}(x) & \mu'\mu = -1 \end{cases} \tag{34}$$

with $\Sigma_{\rightarrow}$ the cross section for scattering into the same direction as before the collision and $\Sigma_{\leftarrow}$ for scattering into the opposite direction. Then the mean cosine of the scattering angle becomes

$$\bar{\mu}_0 = \frac{\Sigma_{\rightarrow} - \Sigma_{\leftarrow}}{\Sigma_s}. \tag{35}$$

The transition kernel T becomes

$$T(x' \to x, \mu = \pm 1) = \begin{cases} \boldsymbol{\Sigma}_t e^{-\boldsymbol{\Sigma}_t |x-x'|} & \mu(x-x') > 0 \\ 0 & \mu(x-x') < 0. \end{cases} \tag{36}$$

For simplicity of notation we will consider in the following only the case of isotropic scattering or $\bar{\mu}_0 = 0$.

2. Homogeneous Slab System with Weight Window

(1) General quantities

We consider a homogeneous slab of half-width b with a constant source S over the full width of the slab. Then the solution for the collision density $\psi(x) = \Sigma_t \phi(x)$ is

$$\psi(x) = S\frac{\Sigma_t}{\Sigma_a}\left\{1 - \frac{\Sigma_{tr}\cosh kx}{\Sigma_{tr}\cosh kb + k\sinh kb}\right\}, \tag{37}$$

with a relaxation length given by

$$k = \sqrt{\boldsymbol{\Sigma}_a \boldsymbol{\Sigma}_{tr}}. \tag{38}$$

Taking a hypothetical detector registering the total flux over the slab we have $\eta_\psi = 1/\Sigma_t$ and

$$R = \int_{-b}^{b} \phi(x)dx = \int_{-b}^{b} \frac{1}{\Sigma_t}\psi(x)dx = \frac{2S}{k\Sigma_a}\left\{kb - \frac{\Sigma_{tr}\sinh kb}{\Sigma_{tr}\cosh kb + k\sinh kb}\right\}. \tag{39}$$

The first moment of the score is the solution of the adjoint equation which reads in our case

$$-\frac{1}{\boldsymbol{\Sigma}_{tr}}\frac{d^2\psi^*(x)}{dx^2} + \boldsymbol{\Sigma}_a(x)\psi^*(x) = \boldsymbol{\Sigma}_t\eta_\psi(x) \tag{40}$$

with boundary condition[5]

$$\left| \frac{d\psi^*}{dx} \right|_{\pm b} = \boldsymbol{\Sigma}_{tr}\psi^*(\pm b) - \boldsymbol{\Sigma}_{tr}\eta_\psi(\pm b) \tag{41}$$

and solution

$$\psi^*(x) = \eta_\psi \frac{\Sigma_t}{\Sigma_a}\left\{1 - \frac{\Sigma_s}{\Sigma_t}\frac{\Sigma_{tr}\cosh kx}{\Sigma_{tr}\cosh kb + k\sinh kb}\right\}. \quad (42)$$

The source of first collisions from Eq. (2) is

$$S_1(x) = S\left\{1 - e^{-\Sigma_t b}\cosh kx\right\}, \quad (43)$$

from which we can verify the detector response according to Eq. (18).

(2) Analog simulation and implicit capture

Transforming the integral equation (24) into a differential equation we get

$$-\frac{1}{\boldsymbol{\Sigma}_{tr}}\frac{d^2M_2^{an}(x)}{dx^2} + \boldsymbol{\Sigma}_a M_2^{an}(x) = -\frac{1}{\boldsymbol{\Sigma}_{tr}}\frac{d^2I_0(x)}{dx^2} + \boldsymbol{\Sigma}_t I_0(x) \quad (44)$$

with solution

$$M_2^{an}(x) = C_0^{an} + C_1^{an}\cosh kx + C_2^{an} x\sinh kx. \quad (45)$$

The solution for the implicit capture case is

$$M_2^{ic}(x) = C_0^{ic} + C_1^{ic}\cosh kx + C_2^{ic} x\cosh\sqrt{\Sigma_t^2 - \Sigma_s^2}\,x. \quad (46)$$

Expressions for all coefficients can be found in the Appendix.

The differential equation for the number of collision n_c becomes for the analog case

$$-\frac{1}{\boldsymbol{\Sigma}_{tr}}\frac{d^2n_c^{an}(x)}{dx^2} + \boldsymbol{\Sigma}_a n_c^{an}(x) = \boldsymbol{\Sigma}_t\eta_\psi(x) \quad (47)$$

with solution

$$n_c^{an}(x) = \frac{\Sigma_t}{\Sigma_a}\left\{1 - \frac{\Sigma_s\cosh kx}{\Sigma_t\cosh kb + k\sinh kb}\right\}. \quad (48)$$

The solution for the implicit capture case is

$$n_c^{ic}(x) = 1 + \Sigma_t b + \frac{1}{2}\Sigma_t^2\left(b^2 - x^2\right). \quad (49)$$

(3) Using weight windows

The integral equation (19) for the second moment is more difficult to solve as M_2 in the integral shows up at a different weight than at the left hand side. For the following derivation we assume $\kappa W_{surv}<W_{RR}$, which means that it takes only one collision for a particle with weight W_{surv} to have its weight reduced to below the Russian roulette threshold W_{RR}. Then it is necessary to solve the equation in steps:

(1) for the weight $W=W_{surv}$, because then there is no splitting and $W^*=W_{surv}$,

(2) for the range $\kappa W<W_{RR}$,

(3) for $W_{RR}/\kappa<W<W_{RR}/\kappa^2$

(4) and so on, until the weight becomes above the splitting threshold.

Likewise, Eq. (26) for the number of collisions must be solved in steps.

The solution for $W=W_{surv}$ becomes

$$M_2(x, W_{surv}) = C_0^{surv} + C_1^{surv}\cosh kx + C_2^{surv} x\sinh kx \quad (50)$$

$$n_c(x, W_{surv}) = \frac{\Sigma_t}{\Sigma_a}\left\{1 - \frac{\Sigma_s\cosh kx}{\Sigma_t\cosh kb + k\sinh kb}\right\}. \quad (51)$$

For the range $W_{RR}/\kappa^m<W<W_{RR}/\kappa^{m+1}$ and $\kappa W<W_{RR}$, we have $z_N=0$, $z_1(\kappa^{m+1}W)=\kappa^{m+1}W/W_{surv}$, $W^*(\kappa^{m+1}W)=W_{RR}$, $z_1(\kappa^m W)=\kappa^m W/W_{surv}$, and $W^*(\kappa^m W)=\kappa^{m+1}W$. With these relations we can derive a recursive equation for the second moment and the number of collisions using the following integral functions

$$I_{j+1}(x) = \int K(x\to x')I_j(x')dx' \quad (52)$$

with $I_0(x)$ given by Eq. (20) and

$$\varsigma_{j+1}(x) = \int K(x\to x')\varsigma_j(x')dx' \quad (53)$$

with $\varsigma_0=1$. The solutions can now be written as

$$M_2(x,W) = W\sum_{j=0}^{m}\left(W\kappa^j - W_{surv}\right)I_j(x) + \frac{W}{W_{surv}}M_2(x,W_{surv}) \quad (54)$$

and

$$n_c(x,W) = \sum_{j=0}^{m}\left(\kappa^{-j} - \frac{W}{W_{surv}}\right)\varsigma_j(x) + \frac{W}{W_{surv}}n_c(x,W_{surv}). \quad (55)$$

Explicit expressions for the functions $I_j(x)$ and $\varsigma_j(x)$ can be found in the Appendix. See Reference 1 for the solutions for $\kappa W>W_{split}$ when splitting occurs. If the assumption $\kappa W_{surv}<W_{RR}$ is not satisfied and hence two or more collisions are necessary to have the particle weight from W_{surv} reduced to below the Russian roulette threshold, one also has to consider successive weight ranges below W_{surv}.

3. Two-Group Infinite System

Another type of system that can be treated analytically and reveals some interesting features is a 2-group infinite system. There is no space dependence in this situation, but there is a group dependence. Considering only down-scattering from group 1 to group 2, using the first subscript of M for the first or second moment, and using a second subscript for the group, we have from Eq. (17)

$$M_{11}=\eta_{\psi 1}+\frac{\Sigma_s^{11}}{\Sigma_t^1}M_{11}+\frac{\Sigma_s^{12}}{\Sigma_t^1}M_{12}$$
$$M_{12}=\eta_{\psi 2}+\kappa_2 M_{12} \tag{56}$$

which has solutions

$$M_{12}=\frac{\eta_{\psi 2}}{1-\kappa_2}$$
$$M_{11}=\frac{\eta_{\psi 1}\Sigma_t^1(1-\kappa_2)+\eta_{\psi 2}\Sigma_s^{12}}{\Sigma_t^1(1-\kappa_2)+\Sigma_s^{11}(1-\kappa_2)}. \tag{57}$$

The solution for the second moment is more complicated as scattering from group 1 to group 2 introduces new weight range possibilities. Furthermore, the weight window for the two groups may be different. To keep matters manageable we assume that the boundaries of the weight window for the first group differ by a constant factor γ from those of the second group, i.e. $W_{RR1}=\gamma W_{RR2}$, $W_{split1}=\gamma W_{split2}$ and $W_{surv1}=\gamma W_{surv2}$.

The equations for the second moment and for the number of collisions can be written as[1]

$$M_{2g}(W)=W^2 I_{0g}+\left(z_1(\kappa_g W)+N_{split}z_N(\kappa_g W)\right)\times\kappa_g^{-1}\sum_{g'}\frac{\Sigma_s^{gg'}}{\Sigma_t^g}M_{2g'}(W^*(\kappa_g W))+z_N(\kappa_g W)\frac{N_{split}-1}{N_{split}}W^2\kappa_g\sum_{g'}\frac{\Sigma_s^{gg'}}{\Sigma_t^g}M_{1g'}^2, \tag{58}$$

$$n_g(W)=1+\left(z_1(\kappa_g W)+N_{split}z_N(\kappa_g W)\right)\times\kappa_g^{-1}\sum_{g'}\frac{\Sigma_s^{gg'}}{\Sigma_t^g}n_{g'}(W^*(\kappa_g W)). \tag{59}$$

As for the finite slab system solutions can be found starting at $W=W_{surv}$, first for group 2. From the solution for $W=W_{surv}$ the solution for the range $\kappa_2 W_{surv}<W<W_{surv}$ can be obtained. Next, solutions at successive higher ranges for the particle weight $W_{surv}/\kappa_2^m<W<W_{surv}/\kappa_2^{m+1}$ can be obtained. Finally, all solutions for group 1 can be obtained. Complete derivations and solutions can be found in Reference 1.

The response R, variance, number of collisions and cost function can be expressed as

$$R=\sum_g S_g M_{1g}$$
$$Var(W)=\sum_g S_g\frac{M_{2g}(W)}{W^2}-R^2$$
$$N_c(W)=\sum_g S_g n_g(W) \tag{60}$$
$$Cost(W)=Var(W)N_c(W)$$

with S_g the source for group g.

IV. Numerical Results

1. Homogeneous Slab System with Weight Window

To validate the theory and solutions presented in Section III, we calculated the variance and standard deviation as well as the average number of collisions and the cost function from the above formulas and compared the results with a Monte Carlo calculation. To this end we developed a simple Monte Carlo program for a slab system with implementation of the two-direction transport model and all variance reduction methods treated in the theory. **Table 1** shows the parameters used.

Monte Carlo calculations were performed with $N=10^7$ particle histories to ensure that the Monte Carlo estimate of the theoretical variance and number of collisions of a particle history was sufficiently accurate. **Table 2** shows the results from the Monte Carlo calculations and the analytical results for an analog simulation and a non-analog simulation with implicit capture only.

From Table 2 we can conclude that there is a very good agreement between the analytical and Monte Carlo results for all quantities. The table also demonstrates that implicit capture reduces the variance, but (without Russian roulette) increases the number of collisions and hence the CPU time considerably, resulting in a higher cost function and lower efficiency, as particle histories only end by escape from the (relatively thick) system.

When applying a weight window we keep the Russian roulette threshold W_{RR} fixed and vary the initial weight of the particle as well as the parameters α and β according to Eq. (9), which together with W_{RR} and N_{split}, determines the

Table 1 Parameters used in slab calculation

quantity	symbol	value
Total cross section	Σ_t	1.1 cm^{-1}
Scattering cross section	Σ_s	0.5 cm^{-1}
Average cosine of scattering angle	$\bar{\mu}_0$	0
Slab half width	b	10 cm
Non-absorption probability	$\kappa=\Sigma_s/\Sigma_t$	0.4545 cm^{-1}
Relaxation length	$k=\sqrt{(\Sigma_a\Sigma_{tr})}$	0.8124 cm^{-1}
RR threshold	W_{RR}	0.5

Table 2 Results for analog simulation and implicit capture (IC)

Method	R	Var
Analog MC	$7.745\ 10^{-2} \pm 2\ 10^{-5}$	$3.0771\ 10^{-3}$
Analog analytically	$7.743322725\ 10^{-2}$	$3.07151277\ 10^{-3}$
IC MC	$7.7434\ 10^{-2} \pm 6\ 10^{-6}$	$3.4063\ 10^{-4}$
IC analytically	$7.743322725\ 10^{-2}$	$3.4005285\ 10^{-4}$
	N_c	$Cost$
Analog MC	1.7038	$5.243\ 10^{-3}$
Analog analytically	1.703530999	$5.23241721\ 10^{-3}$
IC MC	51.315	$1.748\ 10^{-2}$
IC analytically	51.33333335	$1.74560465\ 10^{-2}$

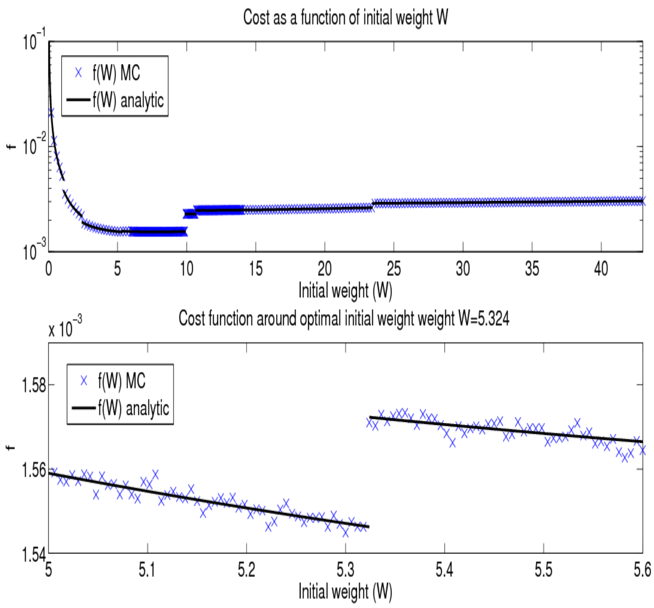

Fig. 1 Cost function dependence on initial particle weight for the slab system with a detailed view around the minimum at W_{init}=5.324

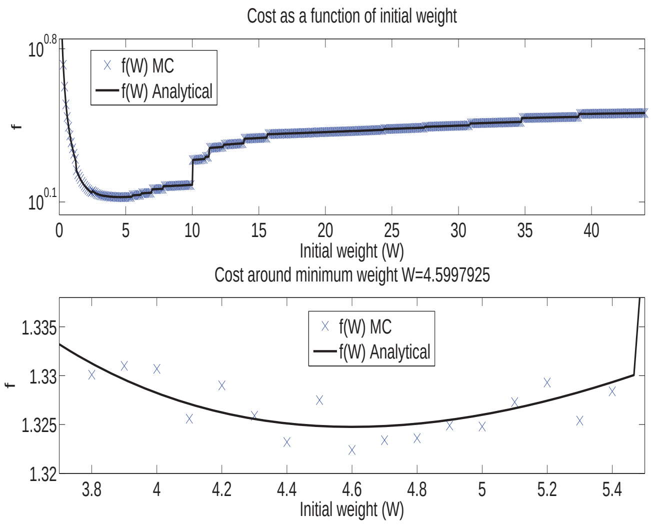

Fig. 2 Cost function dependence on initial particle weight for the infinite system with a detailed view around the minimum at W_{init} =4.5998.

Table 3 Comparison of results for the slab system

	Optimum weight window	Implicit capture	Analog
W	5.324	n.a.	n.a.
Var	4.3061 10^{-4}	3.4005 10^{-4}	4.3061 10^{-3}
Nc	3.54589	51.3333	1.70353
Cost	1.54624 10^{-3}	1.7456 10^{-2}	5.23242 10^{-3}

Table 4 Parameters used for the two-group infinite system

parameter	value	parameter	value
Σ_{t1}	1 cm^{-1}	Σ_{t2}	1 cm^{-1}
Σ_s^{11}	0.2 cm^{-1}	Σ_s^{22}	0.4 cm^{-1}
Σ_s^{12}	0.25 cm^{-1}	Σ_s^{21}	0 cm^{-1}
S_1	0.7	S_2	0.3
M_{11}	0.5208333	M_{12}	1.666667
κ_1	0.45	κ_2	0.4
R	0.864583	W_{RR}	0.5

weight window. Numerous computations were performed with varying parameters which show that the parameters α, β and N_{split} are of marginal influence in the overall cost as long as reasonable values are chosen and extreme values avoided. We therefore chose α=2, β=9 and N_{split}=2. Monte Carlo results are obtained from 400 runs with different initial particle weights. **Figure 1** shows the behavior of the cost function by varying initial weight. The discontinuities occur when the particle needs an additional collision to reach the Russian roulette or splitting threshold. The minimum cost is at the discontinuity for an initial weight W_{init} =5.324 where it takes a particle just 3 collisions to arrive at the Russian roulette threshold. As the boundaries of the weight window were fixed in this calculation, it means that for an initial weight of unity the optimum Russian roulette threshold is at 0.5/5.324=0.0939. **Table 3** compares results for the optimum weight window with the implicit capture and analog case. It is clear that the weight window performs much better in terms of cost.

2. Two-Group Infinite System

For the two-group infinite system we used the parameters as specified in **Table 4** with the detector response equal to the flux in the second group, hence $R=\psi_2/\Sigma_{t2}$.

Results for the cost function at varying initial particle weight were obtained from the analytical results in Section III.3 and 200 Monte Carlo runs with 10^7 neutron histories each.

Figure 2 shows the results for the cost function using the following parameters for the weight window: α=2, β=9 and the ratio between the weight boundaries of the first and second group γ=1. In this case there are many more discontinuities due to the different series of weights a particle can have when scattering in the first or second group and the fact that a neutron can change from group 1 to group 2 at any collision in group 1. However, the minimum of the cost function no longer occurs at a discontinuity but shows a true global minimum. The minimum of the cost function (1.3248) is much lower than for the analog calculation with a cost function value of 3.5094. The case of implicit capture *only* has no meaning here since the variance is zero and the number of collisions infinite without escape from the system.

V. Numerical Solutions with a Transport Code

As there are no realistic systems for which analytical solutions of the transport and moment equation can be obtained, it is of importance to see whether the moment equations can be solved numerically by an existing deterministic transport code. This should be the case for the first-moment equation as it is a normal adjoint equation.

In order to see how we have to interpret the second-moment equation to solve it by a deterministic transport code, we need to transform the integral equations (19) and (26) to the more usual integro-differential form solved in deterministic transport codes. A discrete-ordinates code like PARTISN[7] solves the adjoint transport equation for an adjoint function $X^*(P)$ of the form

$$-\boldsymbol{\Omega}\cdot\nabla X^*(\boldsymbol{r},E,\boldsymbol{\Omega})+\Sigma_t(\boldsymbol{r},E)X^*(\boldsymbol{r},E,\boldsymbol{\Omega}) = \Sigma_t(\boldsymbol{r},E)Y^*(\boldsymbol{r},E,\boldsymbol{\Omega}) \quad (61)$$

with Y^* the source term including scattering related to X^* according to

$$\Sigma_t(\boldsymbol{r},E)Y^*(\boldsymbol{r},E,\boldsymbol{\Omega}) = S^*(\boldsymbol{r},E,\boldsymbol{\Omega}) + \iint\tilde{\Sigma}_s(\boldsymbol{r},E\to E',\boldsymbol{\Omega}\to\boldsymbol{\Omega}')X^*(\boldsymbol{r},E',\boldsymbol{\Omega}')dE'd\Omega'. \quad (62)$$

Applying an exponential integrating function, Eq. (61) can be transformed into[8]

$$X^*(\boldsymbol{r},E,\boldsymbol{\Omega}) = \int T(\boldsymbol{r}\to\boldsymbol{r}',E,\boldsymbol{\Omega})Y^*(\boldsymbol{r}',E,\boldsymbol{\Omega})dV'. \quad (63)$$

Now we need to write our integral equations for the first and second moment and for the number of collisions in the form of Eqs. (62) and (63). To illustrate this for the second-moment equation (19), we define

$$\Lambda(P,W) = W^2 I_0(P) + z_N(P,\kappa W)W^2\frac{N_{split}-1}{N_{split}} \times\kappa(P)\int K(P\to P')M_1^2(P')dP' \quad (64)$$

and use for simplicity of notation the following abbreviation

$$z(P,W) = \kappa^{-1}(P)\left\{z_1(P,\kappa W)+z_N(P,\kappa W)N_{split}\right\}. \quad (65)$$

Then we can rewrite Eq. (19) as

$$\begin{aligned} M_2(P,W) &= \Lambda(P,W) \\ &+ z(P,W)\iint C(\boldsymbol{r},E\to E',\boldsymbol{\Omega}\to\boldsymbol{\Omega}') \\ &\times Q(\boldsymbol{r},E',\boldsymbol{\Omega}',W^*(P,\kappa W))dE'd\Omega' \\ Q^*(r,E,\boldsymbol{\Omega},W) &= \\ &\int T(r\to r',E,\boldsymbol{\Omega})M_2(r',E,\boldsymbol{\Omega},W)dV'. \end{aligned} \quad (66)$$

As a deterministic transport code solves the transport equation in multi-group form, we have to interpret Eq. (66) also in multi-group form. Then we can interpret every discrete value of W as representing an additional energy subgroup and the appearance of a different weight $W^*(P,\kappa W)$ in the integral at the right-hand side as scattering from another energy subgroup. Hence, the number of energy groups and the artificial scattering matrix to be entered to the transport equation solver must be defined in such a way as prescribed by Eq. (66). The transport code gives the function Q^* as its solution.

The first moment function M_1 is easier to calculate by PARTISN as its equation is a true adjoint transport equation without weight dependence. Only the correct source term has to be entered. The solution for the number of collisions function needs again special interpretation of its equation.

The averaged first and second moments are integrals over the source of first collisions as given by Eqs. (18) and (21). By rewriting these integrals using Eq. (2), we have (for instance) for the second moment

$$\begin{aligned} < R^2(W) > &= \int S_1(P)\frac{M_2(P,W)}{W^2}dP \\ &= \int S(P)\frac{Q^*(P,W)}{W^2}dP. \end{aligned} \quad (67)$$

Hence the averaged moments and the variance can easily be calculated once the solution for Q^* has been obtained.

This procedure was applied to the slab problem with weight windows. The PARTISN code solved the adjoint function Q^* as well as analogous functions for the first moment and the number of collisions. For the first moment a run with only one energy group is needed. For the calculation of Q^* one energy group is needed to calculate $Q^*(P,W_{surv})$. A second energy group is needed to obtain $Q^*(P,W_{surv}/\kappa)$ which is related to $Q^*(P,W_{surv})$. A third energy group is used to obtain $Q^*(P,W_{surv}/\kappa^2)$, which is related to $Q^*(P,W_{surv}/\kappa)$, and so on. From $Q^*(P,W_{surv})$ the averaged squared value $<R^2(W_{surv})>$ is obtained. Moreover, from $<R^2(W_{surv})>$, also $<R^2(W)>$ can be obtained for all values $W<W_{surv}$ by an algebraic relation as $Q^*(P,W)$ can be related to $Q^*(P,W_{surv})$ by an algebraic relation following from Eq. (19) for $W= W_{surv}$.

Proper application of the input to PARTISN and calculation of the average second moment from Eq. (67) by simple numerical integration over space of the scalar adjoint output yielded numerical results for R, Var, and N_c that agreed with the analytical results of Section IV.1 at various initial weights to four significant digits.

VI. Conclusions and Discussion

Integral equations have been derived for the second moment of the detector response estimated by a Monte Carlo calculation for a particle entering a collision. Besides the cases of analog and implicit capture simulations, the case when applying a weight window is considered. The integral equations for the expected number of collisions were also derived. Integrating these functions multiplied by the source of first collisions $S_1(\boldsymbol{r})$ over all space results in the average first or second moment of the quantity to be estimated, from which the variance in the estimate is obtained. Likewise, the average number of collisions is obtained. From these quantities a cost function is obtained that can be minimized with respect to the weight window parameters.

From the comparison of analytical solutions with Monte Carlo calculations for two cases using a simplified particle transport model, it is concluded that the theory is correct and applicable to Monte Carlo simulations employing a weight window.

The sample problems also demonstrate the possibility of optimizing the weight window parameters, especially the setting of the Russian roulette threshold value a priori to the Monte Carlo calculation.

The example two-group problem (for an infinite system) opens the possibility for optimization of source biasing. The formulas for source biasing are not given here, but can be found in Reference 1, along with numerical results. They show that the optimum choice of source biasing is close to, but not identical to the often used values of the inverse adjoint functions.

As there are only very few cases where analytical solutions can be obtained, it is shown how the derived equation for the second moment can be cast into a form suitable for solution with an existing transport code. This opens the way for optimization studies of weight window parameters a priori to the Monte Carlo calculation, as the time required by a deterministic transport code to solve such cases will be small compared to the Monte Carlo calculation. This extension is not limited to the two-direction transport model, nor to homogeneous systems, but can be applied more general to heterogeneous system and/or different weight window bounds in different regions of a system. The theory of Section V can be extended to deal with multigroup problems. In that case for each energy group, multiple pseudo groups are needed to obtain the required quantities for different weight ranges.

Application to realistic systems and optimization of the weight window settings in different regions and energy groups will open the way to determine what can be gained in the Figure of Merit with respect to well performing variance reduction methods like the CADIS methodology.[9)]

The solutions of the equations for the first and second moment and the expected number of collisions with a deterministic transport code requires the usual approximations with respect to the use of multi-energy groups and possibly homogenization of complex geometry zones. However, it is expected that such deterministic calculations of the variance and cost function will be sufficiently accurate (and fast) for realistic optimization of weight window parameters in much more complex systems than those treated in the demonstration problems.

Although not discussed in this paper, the theory derived here can be extended to include biasing of the transition and collision kernel. Then the results may be used to test theories about optimum variance reduction. This already applies with the presented theory to the often-postulated statement that the optimum value for weight window boundaries is inversely proportional to the adjoint function for the relevant energy and space region. Including a possible biasing of the transport kernels in the theory makes it possible to investigate also other variance reduction methods than those based on weight windows.

References

1) A. J. van Wijk, *A priori efficiency calculations for Monte Carlo applications in neutron transport*, MSc thesis PNR-131-2010-001, Delft University of Technology, Delft, The Netherlands (2010).
2) I. Lux, L. Koblinger, *Monte Carlo Particle Transport Methods: Neutron and Photon Calculations*, CRC Press, Boca Raton (1991).
3) J. E. Hoogenboom, "Theoretical and practical study of the variance and efficiency of a Monte Carlo calculation due to Russian roulette," *Proc. Int. Conf. on The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments (Physor 2004),* Chicago, USA, April 25-29 (2004).
4) C. A. Laury-Micoulaut, "The nth centred moment of a multiple convolution and its applications in an intercloud gas model," *Astron. Astrophys.*, **51**, 343-346 (1976).
5) C. Solomon *et al.*, An S_n approach to predicting Monte Carlo cost with weight dependent variance reduction," in ANS Winter Meeting, Las Vegas, Nevada, November 7-11 2010, American Nuclear Society, LaGrange Park, IL (2010), [CD-ROM].
6) J. E. Hoogenboom, "The two-direction neutral particle transport model: a useful tool for research and education," *Transp. Th. Stat. Phys.*, **37**, 65-108 (2008).
7) R. E. Alcouffe, R. S. Baker, *PARTISN: A time-dependent, parallel neutral particle transport code system*, LA-UR-05-3925, Los Alamos National Laboratory (LANL) (2005).
8) G. I. Bell, S. Glasstone, *Nuclear Reactor Theory*, Van Nostrand Rheinhold, New York (1970).
9) A. Haghigat, J.C. Wagner, "Monte Carlo variance reduction with deterministic importance functions," *Prog. Nucl. Energy*, **42**, 25-53 (2003).

Appendix: Expansion Coefficients for Various Functions

The expressions given in this Appendix apply to the two-direction model with isotropic scattering for the slab system defined in Section III.2.

From Eq. (20) we get for the two-direction model with $M_1(x)=\psi^*(x)$ according to Eq. (42)

$$I_0(x) = \eta_\psi \left\{2M_1(x) - \eta_\psi\right\} = C_0 + D_0 \cosh kx \qquad \text{(A.1)}$$

with

$$C_0 = \eta_\psi^2 \frac{\Sigma_t + \Sigma_s}{\Sigma_a} \qquad \text{(A.2)}$$

and

$$D_0 = -2\eta_\psi^2 \frac{\Sigma_s}{\Sigma_a} \frac{\Sigma_t}{\Sigma_t \cosh kb + k \sinh kb}. \qquad \text{(A.3)}$$

From the definition of the functions $I_n(x)$ according to Eq. (52), we obtain the system of differential equations

$$\frac{d^2 I_n(x)}{dx^2} + \boldsymbol{\Sigma}_t^2 I_n(x) = -\boldsymbol{\Sigma}_t \boldsymbol{\Sigma}_s I_{n-1}(x) \qquad n \geq 1 \qquad \text{(A.4)}$$

with boundary conditions

$$\frac{dI_n}{dx}\Big|_{x=\pm b} = \mp \boldsymbol{\Sigma}_t I_n(x = \pm b). \qquad \text{(A.5)}$$

With $I_0(x)$ from Eq. (A.1) we have

$$I_n(x) = C_n + D_n \cosh kx + \sum_{j=0}^{n-1} x^j \left\{ E_{n,j} \cosh \Sigma_t x + F_{n,j} \sinh \Sigma_t x \right\} \quad \text{(A.6)}$$

with the coefficients given by

$$C_n = \left(\frac{\Sigma_s}{\Sigma_t}\right)^n C_0 \qquad D_n = D_0. \quad \text{(A.7)}$$

The functions $\varsigma_n(x)$ obey the same differential equation as $I_n(x)$ but start with $\varsigma_0(x)$ =1, from which one obtains

$$\varsigma_n(x) = A_n + \sum_{j=0}^{n-1} x^j \left\{ B_{n,j} \cosh \Sigma_t x + C_{n,j} \sinh \Sigma_t x \right\} \quad \text{(A.8)}$$

with A_0=1 and the other coefficients given by

$$A_n = \left(\frac{\Sigma_s}{\Sigma_t}\right)^n. \quad \text{(A.9)}$$

For the coefficients $B_{n,j}$, $C_{n,j}$, $E_{n,j}$ and $F_{n,j}$, it holds that

$$\begin{aligned} &B_{n,j} = E_{n,j} = 0, \quad j \text{ odd} \\ &C_{n,j} = F_{n,j} = 0, \quad j \text{ even} \end{aligned} \quad j \le n-1$$
$$B_{n,n} = C_{n,n} = E_{n,n} = F_{n,n} = 0, \qquad n \ge 0 \quad \text{(A.10)}$$

and the following recurrent relations (j=1, …, n-1; n>1) hold

$$\begin{aligned} B_{n,j} &= -\frac{\Sigma_t\Sigma_s C_{n-1,j-1} + j(j+1)C_{n,j+1}}{2j\Sigma_t} \\ C_{n,j} &= -\frac{\Sigma_t\Sigma_s B_{n-1,j-1} + j(j+1)B_{n,j+1}}{2j\Sigma_t} \\ E_{n,j} &= -\frac{\Sigma_t\Sigma_s F_{n-1,j-1} + j(j+1)F_{n,j+1}}{2j\Sigma_t} \\ F_{n,j} &= -\frac{\Sigma_t\Sigma_s E_{n-1,j-1} + j(j+1)E_{n,j+1}}{2j\Sigma_t}. \end{aligned} \quad \text{(A.11)}$$

The coefficients $B_{n,0}$ and $E_{n,0}$ can be found from the boundary conditions of Eq. (A.5)

$$\begin{aligned} B_{n,0} = -\frac{e^{-\Sigma_t b}}{\Sigma_t}\Big[&\Sigma_t A_n \\ &+ \sum_{j=0}^{n-1} B_{n,j} \left\{ (jb^{j-1} + \Sigma_t b^j)\cosh \Sigma_t b + \Sigma_t b^j \sinh \Sigma_t b \right\} \\ &+ \sum_{j=0}^{n-1} C_{n,j} \left\{ (jb^{j-1} + \Sigma_t b^j)\sinh \Sigma_t b + \Sigma_t b^j \cosh \Sigma_t b \right\} \Big] \end{aligned} \quad \text{(A.12)}$$

$$\begin{aligned} E_{n,0} = -\frac{e^{-\Sigma_t b}}{\Sigma_t}\Big[&\Sigma_t C_n + D_n (k \cosh kb + \Sigma_t \sinh kb) \\ &+ \sum_{j=0}^{n-1} E_{n,j} \left\{ (jb^{j-1} + \Sigma_t b^j)\cosh \Sigma_t b + \Sigma_t b^j \sinh \Sigma_t b \right\} \\ &+ \sum_{j=0}^{n-1} F_{n,j} \left\{ (jb^{j-1} + \Sigma_t b^j)\sinh \Sigma_t b + \Sigma_t b^j \cosh \Sigma_t b \right\} \Big]. \end{aligned} \quad \text{(A.13)}$$

Then all coefficients can be determined.

The second moment $M_2^{an}(x)$ for an analog game is given by Eq. (45). Its coefficients are

$$C_0^{an} = \frac{\Sigma_t^2}{k^2} C_0 \quad \text{(A.14)}$$

$$C_1^{an} = \frac{1}{\Sigma_{tr} \cosh kb + k \sinh kb} \left\{ \Sigma_t (C_0 - C_0^{an}) + (kD_0 - \Sigma_t b C_2^{an} - C_2^{an}) \sinh kb + (\Sigma_t D_0 - bkC_2^{an}) \cosh kb \right\} \quad \text{(A.15)}$$

$$C_2^{an} = -\frac{\Sigma_s \Sigma_t}{2k} D_0. \quad \text{(A.16)}$$

The coefficients for the second moment for implicit capture according to Eq. (46) are

$$C_0^{ic} = \frac{\Sigma_t^2}{l^2} C_0 \quad \text{(A.17)}$$

$$\begin{aligned} C_1^{ic} = &\frac{1}{\Sigma_{tr} \cosh kb + k \sinh kb} \\ &\times \Big\{ \Sigma_t (C_0 - C_0^{ic}) + kA_1 \sinh kb + \Sigma_t D_0 \cosh kb \\ &- \sqrt{\Sigma_t^2 - \Sigma_s^2}\, C_2^{ic} \sinh \sqrt{\Sigma_t^2 - \Sigma_s^2}\, b - \Sigma_t C_2^{ic} \cosh \sqrt{\Sigma_t^2 - \Sigma_s^2}\, b \Big\} \end{aligned} \quad \text{(A.18)}$$

$$C_2^{ic} = \frac{D_0}{\Sigma_a}. \quad \text{(A.19)}$$

The second moment when applying Russian roulette $M_2(x, W_{surv})$ with weight equal to the survival weight is given by Eq. (50). Its coefficients are in this case equal to those for the analog case:

$$\begin{aligned} C_0^{surv} &= C_0^{an} = \frac{\Sigma_t^2}{k^2} C_0 \\ C_1^{surv} &= C_1^{an} \\ C_2^{surv} &= C_2^{an} = -\frac{\Sigma_s \Sigma_t}{2k} D_0. \end{aligned} \quad \text{(A.20)}$$