A GENERAL TRANSFORM FOR VARIANCE REDUCTION IN MONTE CARLO SIMULATIONS

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ABSTRACT

This paper describes a general transform to reduce the variance of the Monte Carlo estimate of some desired solution, such as flux or biological dose. This transform implicitly includes many standard variance reduction techniques, including source biasing, collision biasing, the exponential transform for path-length stretching, and weight windows. Rather than optimizing each of these techniques separately or choosing semi-empirical biasing parameters based on the experience of a seasoned Monte Carlo practitioner, this General Transform unites all these variance techniques to achieve one objective: a distribution of Monte Carlo particles that attempts to optimize the desired solution. Specifically, this transform allows Monte Carlo particles to be distributed according to the user’s specification by using information obtained from a computationally inexpensive deterministic simulation of the problem. For this reason, we consider the General Transform to be a hybrid Monte Carlo/Deterministic method. The numerical results confirm that the General Transform distributes particles according to the user-specified distribution and generally provide reasonable results for shielding applications.

Key Words: Monte Carlo, general transform, weight window, hybrid, variance reduction, shielding

1. INTRODUCTION

Accurate Monte Carlo simulations of neutron and gamma transport problems require that many Monte Carlo particles undergo the events that represent the desired output. This is problematic for optically thick problems with a localized source, in which detailed information is sought in numerous spatial regions far from the source. Standard Monte Carlo simulations of such problems typically require the use of some variance reduction techniques such as weight windows, geometric importances, source biasing, or path-length stretching to efficiently “steer” Monte Carlo particles from the source region to a specific detector region. However, if N detector responses are desired, then either N Monte Carlo simulations of this type must be run, each with
its own biasing parameters, or the N detectors must be partitioned into S groups of detectors and S Monte Carlo simulations run, with each group having its own biasing parameters. Historically, the biasing parameters for such problems have been chosen (often laboriously, with significant trial and error) by a code user. Due to the tedious and ill-defined nature of manually choosing these parameters, automated techniques have been developed that remove much of the burden from the code user. Particularly, weight windows have been developed for detector problems as well as global problems, in which a solution is desired in every spatial location, that utilize a cheap deterministic solution to set the weight window center. These weight window techniques fall within the class of variance reduction techniques referred to as hybrid Monte Carlo/Deterministic techniques [1–4].

The General Transform is a variance reduction technique that unites many of the variance reduction techniques utilized in deep-penetration (shielding) problems into a single mathematical expression for optimizing the distribution of Monte Carlo particles. The transform implicitly includes source biasing, collision biasing, the exponential transform for path-length stretching, and weight windows. In this paper, we describe the General Transform as a new variance reduction technique that seeks to optimize the desired solution by distributing Monte Carlo particles in a specified way. We then discuss how each of the individual variance reduction techniques is incorporated into the transform in order to demonstrate the flexible nature of the transform. Finally, we provide numerical results that demonstrate that the General Transform distributes Monte particles according to a specified distribution and that it can be used to solve a variety of shielding problems.

2. THE GENERAL TRANSFORM

The General Transform is a variance reduction technique for distributing Monte Carlo particles throughout phase-space according to some user specification. To achieve this distribution, it utilized two fundamental procedures:

- Modify the fundamental physics in order to “steer” the particles (in space, energy, and angle) toward a more optimal particle distribution. Variance reduction techniques that modify the particle physics include implicit capture, path-length stretching, and source biasing. These techniques require adjustments in the Monte Carlo weight to maintain an unbiased estimate of the solution.

- Impose a condition on the weight of the Monte Carlo particle to selectively filter particles (in space, energy, and angle) to obtain a more optimal particle distribution. Variance reduction techniques that impose these filtering conditions include weight windows and geometric/energy importances.

Thus, the General Transform consists of two components: a transform function to advantageously modify the particle physics, and a weight window to selectively filter particles in phase-space.

Mathematically, the modification of the particle physics is accomplished by the following transform:

$$\psi(x, \Omega, E) = T(x, \Omega, E)f(x, \Omega, E),$$  \hspace{1cm} (1)
where $T(x, \Omega, E)$ is the transform function and $\psi(x, \Omega, E)$ is the angular flux defined by the Boltzmann equation for steady-state, neutral-particle transport:

$$\mathbf{\Omega} \cdot \nabla \psi(x, \Omega, E) + \Sigma_t(x, E)\psi(x, \Omega, E) = \int_0^\infty \int_{4\pi} \Sigma_s(x, \Omega') \cdot \Omega', E' \rightarrow E)\psi(x, \Omega', E')d\Omega'dE' + Q(x, \Omega, E),$$

$$x \in \mathcal{V}, \quad \Omega \in 4\pi, \quad 0 < E < \infty,$$  

(2a)

with boundary condition

$$\psi(x, \Omega, E) = \psi_b(x, \Omega, E), \quad x \in \partial\mathcal{V}, \quad \Omega \cdot n(x) < 0, \quad 0 < E < \infty.$$  

(2b)

The transformed angular flux $f(x, \Omega, E)$ is then defined by substituting Eq. (1) into Eq. (2):

$$\mathbf{\Omega} \cdot \nabla f(x, \Omega, E) + \hat{\Sigma}_t(x, \Omega, E)f(x, \Omega, E)$$

$$= \int_0^\infty \int_{4\pi} \hat{\Sigma}_s(x, \Omega') \cdot \Omega', E' \rightarrow E)f(x, \Omega', E')d\Omega'dE' + \hat{Q}(x, \Omega, E),$$

$$x \in \mathcal{V}_e, \quad \Omega \in 4\pi, \quad E_g < E < E_{g-1},$$  

(3a)

with boundary condition

$$f(x, \Omega, E) = \hat{\psi}_b(x, \Omega, E), \quad x \in \partial\mathcal{V}_e, \quad \Omega \cdot n(x) < 0, \quad 0 < E < \infty,$$  

(3b)

and continuity condition

$$T(x, \Omega, E)|_{x \in \mathcal{V}^-_e} = T(x, \Omega, E)|_{x \in \mathcal{V}^+_e}.$$  

(3c)

The continuity condition is required where the transform function $T(x, \Omega, E)$ is discontinuous in phase-space. The notation $\mathcal{V}_e^-$ and $\mathcal{V}_e^+$ denotes that these elements are adjacent to one another and the discontinuity exists on their shared boundary. We have also made the following definitions:

$$\hat{\Sigma}_t(x, \Omega, E) = \Sigma_t(x, E) + \mathbf{\Omega} \cdot \nabla \ln[T(x, \Omega, E)],$$  

(4a)

$$\hat{\Sigma}_s(x, \Omega' \cdot \Omega, E' \rightarrow E) = \Sigma_s(x, \Omega' \cdot \Omega, E' \rightarrow E)\frac{T(x, \Omega', E')}{T(x, \Omega, E)},$$  

(4b)

$$\hat{Q}(x, \Omega, E) = \frac{Q(x, \Omega, E)}{T(x, \Omega, E)},$$  

(4c)

$$\hat{\psi}_b(x, \Omega, E) = \frac{\psi_b(x, \Omega, E)}{T(x, \Omega, E)}.$$  

(4d)

Just as the Boltzmann transport equation describes the interaction of neutral particles in a medium, the transformed transport equation [Eq. (3)] describes the interaction of “f-particles” in a medium. It is apparent that the form of the transformed transport equation is identical to the neutron transport equation, except that the cross-sections and fixed sources have been modified. Each term in the transformed transport equation shares the same meaning as in the neutron transport equation – streaming, collision, scattering source, interior source, and boundary source. The solution to this transformed equation $f(x, \Omega, E)$ remains positive if the transform function is positive.
The transformed transport equation [Eq. (3)] is then simulated using the Monte Carlo method with a weight window imposed. The details of this simulation, including a description of the modified particle physics under which Monte Carlo particles interact in a medium as well as the means by which to recover the physical flux, will be described in a later section. But first we turn our attention to understanding how the application of this transform function along with a weight window determines the distribution of Monte Carlo particles in a simulation.

### 2.1 The Monte Carlo Particle Distribution

The distribution of Monte Carlo particles throughout phase-space (or in some particular domain of phase-space) can be represented in a variety of ways, either directly as a particle density or indirectly through some quantity such as particle flux. Since the General Transform is used to distribute Monte Carlo particles according to a user specification, it is important to decide which quantity to specify – the Monte Carlo particle density or the particle flux. It may seem more natural to distribute Monte Carlo particles by density rather than flux; however, since the desired solutions (e.g. flux and response) always include the physical flux, it is more consistent that the Monte Carlo particles be distributed according to the particle flux. In fact, in a Monte Carlo simulation of the Boltzmann transport equation [Eq. (2)], the angular neutral-particle flux \( \psi(x, \Omega, E) \) is related to the weight-dependent angular Monte Carlo particle flux \( M(x, \Omega, E, w) \) by the integral

\[
\psi(x, \Omega, E) = \int_0^{\infty} w M(x, \Omega, E, w) dw, \tag{5}
\]

where \( w \) is the weight of the Monte Carlo particle. Hence, wherever the Monte Carlo particle distribution is discussed in this paper, it refers to the Monte Carlo particle flux.

In a Monte Carlo simulation of the transformed transport equation [Eq. (3)], a similar relation to Eq. (5) exists:

\[
f(x, \Omega, E) = \int_0^{\infty} w M(x, \Omega, E, w) dw. \tag{6}
\]

Since a weight window is imposed in the General Transform, the weight-dependent angular Monte Carlo particle flux can be approximated by

\[
M(x, \Omega, E, w) \approx m(x, \Omega, E) \delta[w - w(x, \Omega, E)], \tag{7}
\]

where \( m(x, \Omega, E) \) is the angular Monte Carlo particle flux and \( w(x, \Omega, E) \) is the weight window center. Substituting this approximation into Eq. (6), we obtain:

\[
f(x, \Omega, E) \approx w(x, \Omega, E) m(x, \Omega, E). \tag{8}
\]

Finally, substituting Eq. (8) into Eq. (1), we obtain:

\[
\psi(x, \Omega, E) \approx T(x, \Omega, E) w(x, \Omega, E) m(x, \Omega, E). \tag{9}
\]

This expression enables the user to choose the transform function \( T(x, \Omega, E) \) and a weight window \( w(x, \Omega, E) \) to ensure that the Monte Carlo particles are distributed throughout phase-space according to the user’s prescription. The ability to choose the transform function and the weight window center provides the user with the flexibility to decide whether to use a weight
window to achieve the user-specified Monte Carlo particle flux, to modify the particle physics to achieve the desired distribution, or some combination of both. In a later section, we discuss several types of problems and the Monte Carlo particle distributions that work well to optimize the solution.

### 2.2 Features of the General Transform

Many features of the General Transform resemble other variance reduction techniques, such as weight windows, importance sampling, path-length stretching, and collision biasing. These techniques are often applied and optimized with no governing objective except to obtain a reasonable solution; this generally results in the practitioner massaging the biasing parameters until a reasonable solution is achieved, with a vague understanding of the consequences on the total simulation. The General Transform has a clear governing objective: distribute Monte Carlo particles throughout phase-space according to a user-specified distribution that statistically seems to optimize the desired solution. In this case, the user knows exactly how phase-space is populated by Monte Carlo particles and whether this distribution is sufficient or may lead to poor results due to inadequate sampling.

Even though we do not view the General Transform as a collection of variance reduction techniques, but rather as a means to optimally distribute Monte Carlo particles, we consider it useful to connect it to the familiar variance reduction techniques and demonstrate the similarities and differences.

#### 2.2.1 The Standard Weight Window

The flexibility of the General Transform allows it to function as a simple weight window. To see this, we define the transform function to be unity [i.e. $T(x, \Omega, E) = 1$]; then Eq. (1) reduces to $\psi(x, \Omega, E) = f(x, \Omega, E)$, implying that the transformed transport equation is the standard Boltzmann transport equation. The Monte Carlo particle flux, described by Eq (9), reduces to

$$\psi(x, \Omega, E) \approx w(x, \Omega, E)m(x, \Omega, E).$$  \hspace{1cm} (10)

This expression can be used in two ways:

- To define the weight window required to achieve a user-specified Monte Carlo distribution $m(x, \Omega, E)$. In this case, Eq. (10) is written as

$$w(x, \Omega, E) = \frac{\psi(x, \Omega, E)}{m(x, \Omega, E)}. \hspace{1cm} (11)$$

- To determine the Monte Carlo distribution resulting from the application of a particular weight window $w(x, \Omega, E)$. The relevant form of Eq. (10) is

$$m(x, \Omega, E) = \frac{\psi(x, \Omega, E)}{w(x, \Omega, E)}. \hspace{1cm} (12)$$

In the standard application of weight windows, the adjoint flux $\psi^*(x, \Omega, E)$ is used to set the weight window center: $w(x, \Omega, E) = 1/\psi^*(x, \Omega, E)$. Applying Eq. (11), we obtain the Monte Carlo distribution resulting from the standard weight window:

$$m(x, \Omega, E) = \psi(x, \Omega, E)\psi^*(x, \Omega, E),$$

$$= \psi^c(x, \Omega, E), \quad (13)$$

where $\psi^c(x, \Omega, E)$ is the contribution flux [5]. The contribution flux is a well-known and understood quantity within the shielding community and represents the relative contribution of particles at a point in phase space to the detector response. To our knowledge, this relationship between the standard weight window and a Monte Carlo particle distribution that is proportional to the contribution flux has not been described in the literature.

### 2.2.2 Source Biasing

The General Transform source from Eqs. (3) and (4) is sampled by the distribution $p_{\text{src}}(x, \Omega, E)$, with an initial particle weight $w_{\text{src}}$:

$$p_{\text{src}}(x, \Omega, E) = \frac{Q(x, \Omega, E)T^{-1}(x, \Omega, E)w^{-1}(x, \Omega, E)}{\int_{V_{\text{src}}} \int_0^{4\pi} \int_0^\infty Q(x, \Omega, E)T^{-1}(x, \Omega, E)w^{-1}(x, \Omega, E)dEd\Omega dx}, \quad (14a)$$

$$w_{\text{src}} = w(x, \Omega, E). \quad (14b)$$

where the weight window is included in the distribution to ensure that the Monte Carlo particle is born with a weight within the weight window. If this probability distribution is too computationally expensive to sample, then a modified form may be used:

$$p_{\text{src}}(x, \Omega, E) = \frac{Q(x, \Omega, E)w^{-1}(x, \Omega, E)}{\int_{V_{\text{src}}} \int_0^{4\pi} \int_0^\infty Q(x, \Omega, E)w^{-1}(x, \Omega, E)dEd\Omega dx}, \quad (15a)$$

$$w_{\text{src}} = w(x, \Omega, E)T^{-1}(x, \Omega, E). \quad (15b)$$

In this case, the weight of the Monte Carlo particle may be outside the weight window, which means that all the work is pushed to the weight window to selectively filter particles. It should be clear that the transform function may be split between the probability distribution and the initial particle weight in whatever way the user determines is most convenient and efficient.

For standard source biasing, Eq. (14) adequately describes the probability distribution for sampling the source, with $T(x, \Omega, E)$ set to the adjoint flux or some other reasonable distribution, and the weight window set to unity (if no weight window is used). Source biasing has primarily been used in Monte Carlo simulations to initially “direct” particles (in energy and angle) toward the detector in an attempt to improve detector response statistics. The General Transform biases the source as part of a comprehensive approach to achieve a user-specified Monte Carlo particle distribution.
### 2.2.3 Collision Biasing

The General Transform collision process described by Eqs. (3) and (4) is sampled by the distribution $p_{\text{col}}(x, \Omega, E)$, with a multiplicative weight change $w_{\text{col}}$:

$$p_{\text{col}}(x, \Omega, E) = \frac{\Sigma_s(x, \Omega', \Omega, E' \rightarrow E)T^{-1}(x, \Omega, E)}{\int_{4\pi} \int_0^\infty \Sigma_s(x, \Omega', \Omega, E' \rightarrow E'')T^{-1}(x, \Omega'', E'')dE''d\Omega''},$$  \hspace{1cm} (16a)

$$w_{\text{col}} = \int_{4\pi} \int_0^\infty \Sigma_s(x, \Omega', \Omega, E' \rightarrow E'')T^{-1}(x, \Omega', E'')dE''d\Omega'' \cdot T(x, \Omega', E') \cdot \frac{\Sigma_t(x, E') + \Omega' \cdot \nabla \ln[T(x, \Omega', E')]}{\Sigma_t(x, E') + \Omega' \cdot \nabla \ln[T(x, \Omega', E')]},$$  \hspace{1cm} (16b)

where $(x, \Omega', E', w)$ is the initial state of the particle, and $(x, \Omega, E, w * w_{\text{col}})$ is the final state of the particle. The transform function $T(x, \Omega, E)$ can be chosen such that the multiplicative weight change $w_{\text{col}}$ is near unity; however, the resulting probability distribution can be difficult to sample or at least implement in a pre-existing Monte Carlo code. In this case, a modified form of the probability distribution and multiplicative weight change may be used:

$$p_{\text{col}}(x, \Omega, E) = \frac{\Sigma_s(x, \Omega', \Omega, E' \rightarrow E)}{\Sigma_s(x, E')},$$  \hspace{1cm} (17a)

$$w_{\text{col}} = \frac{T(x, \Omega', E')T^{-1}(x, \Omega, E)}{\Sigma_t(x, E') + \Omega' \cdot \nabla \ln[T(x, \Omega', E')]}. \hspace{1cm} (17b)$$

Just as in source biasing, this pushes all the work to the weight window to selectively filter Monte Carlo particles. It should again be clear that the transform function can be split between the probability distribution and the multiplicative weight change in whatever way the user determines is most convenient and efficient.

Collision biasing has seen limited use in Monte Carlo codes due to the difficulties described above and from the limited benefits that have been witnessed. Where it has been implemented, it has been implemented as in Eqs. (16) with the transform function set to the adjoint function or some other reasonable importance function and a slightly modified multiplicative weight change. Just like source biasing, collision biasing has primarily been used in Monte Carlo simulations to “direct” particles (in energy and angle) toward the detector in an attempt to improve detector response statistics; whereas, the General Transform biases the collision process as part of a comprehensive approach to achieve a user-specified Monte Carlo particle distribution.

### 2.2.4 The Exponential Transform: Path-Length Stretching

The General Transform distance-to-next collision is determined by solving the left-hand side of Eq. (3) with a unit point source at $x_0$. The resulting probability distribution describing the probability of a Monte Carlo particle streaming from $x_0$ to $x_0 + \Omega s$ with a collision at $x_0 + \Omega s$ is given as

$$p(s \mid x_0, \Omega, E) = \hat{\Sigma}_t(x_0 + \Omega s, \Omega, E) \exp \left[ -\int_0^s \hat{\Sigma}_t(x_0 + \Omega s', \Omega, E)ds' \right],$$  \hspace{1cm} (18)
where \( \hat{\Sigma}_t(x, \Omega, E) = \Sigma_t(x, E) + \Omega \cdot \nabla \ln[T(x, \Omega, E)] \). There is no explicit weight adjustment that results from this biasing; however, the collision biasing implicitly includes weight adjustments due to this distance-to-next collision modification.

The probability distribution for the standard form of the exponential transform is given by substituting \( T(x, \Omega, E) = h(E, \Omega) \exp[-\lambda(E)\Sigma_t(E)x \cdot \omega(E)] \) into Eq. (18), where the magnitude of \( \lambda(E) \) determines how strongly a particle is biased toward the unit direction \( \omega(E) \). This results in the following probability distribution:

\[
p(s | x_0, \Omega, E) = \Sigma_t(E)[1 - \lambda(E)\Omega \cdot \omega(E)]e^{-\Sigma_t(E)[1 - \lambda(E)\Omega \cdot \omega(E)]s}.
\] (19)

To sample from this distribution, the cumulative probability distribution is inverted to obtain:

\[
s = \frac{\ln(\xi)}{\Sigma_t(E)[1 - \lambda(E)\Omega \cdot \omega(E)]},
\] (20)

where \( \xi \in (0, 1) \) is a random number. Unlike the General Transform, a weight adjustment \( w_{\text{dist}} \) is explicitly applied at the collision site to account for the biasing:

\[
w_{\text{dist}} = \frac{e^{-\Sigma_t(E)\lambda(E)\Omega \cdot \omega(E)s}}{1 - \lambda(E)\Omega \cdot \omega(E)}.
\] (21)

The angle-dependent cross-section causes a particle to travel farthest when its direction, \( \Omega \), is equal to \( \omega(E) \); it travels the shortest distance when its direction is equal to \( -\omega(E) \). For most shielding problems the vector \( \omega(E) \) points toward the deep regions of the problem (such as in the direction of a detector), and thus particles have a tendency to stream farther when traveling toward the deep regions of the problem. Similar to source biasing and collision biasing, the standard exponential transform has primarily been used in Monte Carlo simulations to “direct” particles (in angle) toward the detector in an attempt to improve detector response statistics [6]; whereas, the General Transform biases the distance-to-next collision process as part of a comprehensive approach to achieve a user-specified Monte Carlo particle distribution.

### 2.3 Tally Estimators

To obtain estimates of the quantities of interest, such as the scalar flux \( \phi(x, E) \) or a response \( R(x) = \int_0^\infty \Sigma_{R,E}(E)\phi(x, E)dE \), the General Transform requires a modified path-length estimator and a modified collision estimator. The bin structure is defined for the energy range by the boundaries \( \{E_g\}_{g=0}^G \) and spatially by the set \( \{V_e\}_{e=1}^N \) with each spatial element having a volume \( V_e \).

The total modified source \( \hat{Q}_T \), necessary for defining each estimator, is determined by the source biasing. If Eq. (14) is used to sample the source, then \( \hat{Q}_T \) is defined as

\[
\hat{Q}_T = \int_{V_{src}} \int_{4\pi} \int_0^\infty Q(x, \Omega, E)T^{-1}(x, \Omega, E)w^{-1}(x, \Omega, E)dEd\Omega dV.
\] (22)

If the source is sampled using Eq. (15), \( \hat{Q}_T \) is defined as

\[
\hat{Q}_T = \int_{V_{src}} \int_{4\pi} \int_0^\infty Q(x, \Omega, E)w^{-1}(x, \Omega, E)dEd\Omega dV
\] (23)
A General Transform

The estimated mean $H_e$ and variance of the mean $\text{Var}[H_e]$ have the standard definitions:

$$H_e = \frac{1}{N} \sum_{n=1}^{N} H_{e,n},$$  \hspace{1cm} (24)

$$\text{Var}[H_e] = \frac{1}{N-1} \sum_{n=1}^{N} (H_{e,n} - H_e)^2,$$  \hspace{1cm} (25)

where $H_{e,n}$ is the estimate of the mean provided by the $n$th simulation particle. For our problems, $H_e$ represents an estimate of the mean scalar flux (i.e. $H_e = \phi_{e,g}$) or the mean response (i.e. $H_e = R_e$). For both the path-length estimator and the collision estimator, the $H_{e,n}$ estimates are defined below.

2.3.1 Path-Length Estimator

The $n$th simulation particle provides path-length estimates for the scalar flux $\phi(x, E)$ and the response $R(x)$ that are given by the following for $E_i \in (E_g, E_{g-1}]$ and $x_i \in V_e$:

$$\phi^{\text{path}}_{e,g,n} = \hat{Q}_T \frac{I_{e,g,n}}{V_e} \sum_{i=1}^{l_i} w_i \int_{0}^{l_i} \hat{T}(x_i + s\Omega_i, \Omega_i, E_i) ds,$$  \hspace{1cm} (26)

$$R^{\text{path}}_{e,n} = \hat{Q}_T \frac{G}{V_e} \sum_{g=1}^{G} \sum_{i=1}^{l_i} w_i \Sigma_{R,e}(E_i) \int_{0}^{l_i} \hat{T}(x_i + s\Omega_i, \Omega_i, E_i) ds,$$  \hspace{1cm} (27)

where $\hat{Q}_T$ is the total modified source rate, $I_{e,g,n}$ is the number of track lengths generated by the $n$th simulation particle in spatial element $V_e$ (with volume $V_e$) and in energy group $g$, $E_i$ is the particle’s energy, $\Omega_i$ is the particle’s direction, $w_i$ is the particle’s weight, and $x_i$ is the initial spatial location of the $i$th streaming path, which has length $l_i$. $\Sigma_{R,e}(E)$ is the response parameter in spatial element $V_e$.

2.3.2 Collision Estimator

The $n$th simulation particle provides collision estimates for the scalar flux $\phi(x, E)$ and the response $R(x)$ that are given by the following for $E_i \in (E_g, E_{g-1}]$ and $x_i \in V_e$:

$$\phi^{\text{coll}}_{e,g,n} = \hat{Q}_T \frac{I_{e,g,n}}{V_e} \sum_{i=1}^{l_i} w_i \frac{\hat{T}(x_i, \Omega_i, E_i)}{\hat{\Sigma}_{t,e}(\Omega_i, E_i)},$$  \hspace{1cm} (28)

$$R^{\text{coll}}_{e,n} = \hat{Q}_T \frac{G}{V_e} \sum_{g=1}^{G} \sum_{i=1}^{l_i} w_i \Sigma_{R,e}(E_i) \frac{\hat{T}(x_i, \Omega_i, E_i)}{\hat{\Sigma}_{t,e}(\Omega_i, E_i)},$$  \hspace{1cm} (29)

where $\hat{Q}_T$ is the total modified source rate, $I_{e,g,n}$ is the number of collisions generated by the $n$th simulation particle in spatial element $V_e$ (with volume $V_e$) and in energy group $g$, $E_i$ is the particle’s energy when it collides, $\Omega_i$ is the particle’s direction when it collides, $w_i$ is the particle’s weight when it collides, $x_i$ is the particle’s spatial location when it collides, and $\hat{\Sigma}_{t,e}(\Omega, E)$ is the effective total cross-section. $\Sigma_{R,e}(E)$ is the response parameter in spatial element $V_e$. 
2.4 Sample Problems

In this paper, we investigate the two types of problems at the extremes of solution space:

- **The Global Flux Problem**: the scalar flux $\phi(x, E)$ is desired at all spatial locations and for all energies.
- **The Source-Detector Response Problem**: the response $R_D = \int_{V_D} \int_0^\infty \Sigma_R(x, E) \phi(x, E) dEdV$ due to a localized source is desired in a detector region $V_D$.

To solve these problems using the General Transform, we first specify the Monte Carlo particle distribution $m(x, \Omega, E)$ that seems to optimize the solution and then apply Eq. (9) to determine the way in which to use the transform function and weight window to solve the problem. As a reminder, Eq. (9) is given by

$$
\psi(x, \Omega, E) \approx T(x, \Omega, E)w(x, \Omega, E)m(x, \Omega, E).
$$

We investigate each of these problems in detail in the following sections.

2.4.1 The Global Flux Problem

To determine the scalar flux at every spatial location and for all energies, we distribute Monte Carlo particles in phase-space according to their relative contribution to the scalar flux. A distribution that achieves this objective is given by

$$
m(x, \Omega, E) = C \frac{\psi(x, \Omega, E)}{\phi(x, E)},
$$

where $C$ is an arbitrary constant that may be used to scale the weight window and the transform function, as well as to ensure each quantity has the correct units. Substituting this into Eq. (9), we obtain

$$
T(x, \Omega, E)w(x, \Omega, E) = C^{-1} \tilde{\phi}(x, E),
$$

where $\tilde{\phi}(x, E)$ represents a deterministic estimate of the scalar flux. We are now free to choose the transform function and the weight window to best suit our needs. To demonstrate the extreme cases, we solve this problem in two ways (and present the solutions in the numerical results section):

- **The Standard Weight Window**: set $T(x, \Omega, E) = 1$ and $w(x, \Omega, E) = C^{-1} \tilde{\phi}(x, E)$.
- **The Complete Transform Function**: set $w(x, \Omega, E) = 1$ and $T(x, \Omega, E) = C^{-1} \tilde{\phi}(x, E)$.

For shielding problems, we represent $\tilde{\phi}(x, E)$ by the functional form:

$$
\tilde{\phi}(x, E) = A_{e,g} e^{-\lambda_{e,g} \Sigma_{t,e,g}(x - x_e) \cdot \omega_{e,g}}, \quad x \in V_e, \quad E_g < E \leq E_{g-1},
$$

where $A_{e,g}$ is the amplitude of the scalar flux, $\lambda_{e,g}$ is the exponential attenuation coefficient, $\omega_{e,g}$ is a unit vector proportional to the gradient of the scalar flux, and $x_e$ is some reference point in the spatial element $V_e$. 

2.4.2 The Source-Detector Response Problem

It is well-known within the shielding community that the contributon flux \( \psi_c(x, \Omega, E) \) describes the important locations in phase space for a source-detector response problem. That is, the contributon flux describes the relative contribution of each location in phase space to the detector response. Therefore, it seems reasonable to assume that a good variance reduction strategy would distribute Monte Carlo particles according to the contributon flux:

\[
m(x, \Omega, E) = C \psi(x, \Omega, E) = C \psi(x, \Omega, E) \psi^*(x, \Omega, E), \quad (33)
\]

where \( C \) is again an arbitrary constant that may be used to scale the weight window and the transform function, as well as to ensure each quantity has the correct units. Substituting this into Eq. (9), we obtain

\[
T(x, \Omega, E)w(x, \Omega, E) = \frac{C^{-1}}{\tilde{\psi}^*(x, \Omega, E)}, \quad (34)
\]

where \( \tilde{\psi}^*(x, \Omega, E) \) represents a deterministic estimate of the adjoint flux. For this problem, the adjoint flux is defined by the following adjoint transport equation:

\[
-\Omega \cdot \nabla \psi^*(x, \Omega, E) + \Sigma_t(x, E) \psi^*(x, \Omega, E)
= \int_0^\infty \int_{4\pi} \Sigma_s(x, \Omega \cdot \Omega', E \to E') \psi^*(x, \Omega', E')d\Omega'dE' + \frac{\Sigma_R(x, E)}{4\pi},
\]

with boundary condition

\[
\psi^*(x, \Omega, E) = 0, \quad x \in \partial \mathcal{V}, \quad \Omega \cdot n(x) > 0, \quad 0 < E < \infty. \quad (35a)
\]

Just as in the global flux problem, we solve this problem in two ways (and present the solutions in the numerical results section):

- The Standard Weight Window: set \( T(x, \Omega, E) = 1 \) and \( w(x, \Omega, E) = C^{-1}/\tilde{\psi}^*(x, \Omega, E) \).
- The Complete Transform Function: set \( w(x, \Omega, E) = 1 \) and \( T(x, \Omega, E) = C^{-1}/\tilde{\psi}^*(x, \Omega, E) \).

For shielding problems, we represent \( \tilde{\psi}^*(x, \Omega, E) \) by the functional form:

\[
\tilde{\psi}^*(x, \Omega, E) = \frac{A_{e,g}}{1 - \lambda_{e,g} \Omega \cdot \omega_{e,g}} e^{-\lambda_{e,g} \Sigma_{t,e,g}(x - x_e) \cdot \omega_{e,g}}, \quad x \in \mathcal{V}_e, \quad E_g < E \leq E_{g-1}, \quad (36)
\]

where \( A_{e,g} \) is the amplitude of the scalar flux, \( \lambda_{e,g} \) is the exponential attenuation coefficient, \( \omega_{e,g} \) is a unit vector proportional to the gradient of the scalar flux, and \( x_e \) is some reference point in the spatial element \( \mathcal{V}_e \). To ensure the denominator does not become negative, either a condition must be imposed on \( \lambda_{e,g} \) (i.e. \( |\lambda_{e,g}| \leq \lambda_{\text{max}} < 1 \)) or the denominator approximated as \( 1 - \lambda_{e,g} \Omega \cdot \omega_{e,g} \approx \exp(-\lambda_{e,g} \Omega \cdot \omega_{e,g}) \).
3. NUMERICAL TEST PROBLEM

To verify that the General Transform performs as the theory predicts, and to compare the two extremes of the General Transform (i.e. the Standard Weight Window and the Complete Transform Function described in Section 2.4) for efficiency and statistical quality, we consider a relatively simple multigroup shielding problem that 1) assesses how well these two versions of the General Transform perform on the Global Flux Problem and the Source-Detector Response Problem (also described in Section 2.4), and 2) verifies that the methods perform as the theory predicts. Specifically, we consider a homogeneous 3-group cube with a localized source in the center that emits particles in the top energy group.

3.1 PROBLEM DESCRIPTION

For this homogenous 3-group problem, the geometry is chosen to be a 50 cm homogeneous cube with a 2 cm cubic source at its center and vacuum boundaries. Because this problem is symmetric, we only need to obtain a solution in one octant; we do this by imposing symmetric (reflecting) boundaries that pass through the center of the source. Figure 1 demonstrates this geometry: a 25 cm homogeneous cube with a 1 cm cubic source in the corner, symmetric boundary conditions at the planes that cut through the source, and vacuum boundaries at the exterior planes. The source is a unit source (1 cm$^{-3}$s$^{-1}$), in the first energy group only. The total cross-section is set equal to unity throughout space and energy (i.e. $\Sigma_{t,g} = 1$ cm$^{-1}$). The scattering matrix is provided in the material data table of Figure 1.

For the source-detector problem, we placed a 1 cm cubic detector near the furthest corner from the source, 1.5 cm from all three vacuum boundaries. The detector was not placed directly on the boundary of the system to avoid edge effects. The detector is shown in Figure 1.

![Figure 1: Problem Geometry and Material Properties](image)
Figure 2 demonstrates that this problem is indeed a shielding problem, with the scalar flux being attenuated by 20 orders of magnitude in the first energy group, 18 orders of magnitude in the second group, nearly 16 orders of magnitude in the third group, and roughly 17 orders of magnitude in the energy-integrated (total) flux. As can be seen in Figure 2, the total flux is composed mostly of group-1 flux near the source and mostly of group-3 flux near the detector.

![Scalar Flux plots](image)

Figure 2: Scalar Flux along the plane \(x = y\)

The objective of the global flux problem is to obtain the scalar flux \(\phi_{e,g}\) for all \(g\) at every spatial element \(V_e\) in the mesh, where \(\phi_{e,g}\) is defined as

\[
\phi_{e,g} = \frac{1}{V_e} \int_{V_e} \int_{E_{g-1}}^{E_g} \phi(x, E) dE dV.
\]  

(37)

The objective of the source-detector response problem is to obtain the response \(R_D\) in the detector, defined by the space \(V_D\). We investigate a special response, the energy-integrated (total) flux, denoted simply as \(\phi_D\) and defined as

\[
\phi_D = \sum_{g=1}^{3} \phi_{D,g}.
\]  

(38)

(For this response, we set \(\Sigma_R(x, E) = 1\).)

To analyze the results, we plot the simulated scalar Monte Carlo particle flux, the theoretically predicted scalar Monte Carlo particle flux, and the figure of merit for both versions of the General Transform – the Standard Weight Window and the Complete Transform Function –
and for both types of problems – the Source-Detector Response Problem and the Global Flux Problem.

The energy-dependent scalar Monte Carlo particle flux $\mathcal{M}_{e,g}$ and the energy-integrated scalar Monte Carlo particle flux $\mathcal{M}_e$ are volume-averaged quantities determined directly from the Monte Carlo simulation. These scalar Monte Carlo particle flux quantities are defined as

$$\mathcal{M}_{e,g} = \frac{1}{V_e} \int V_e \int_{E_g}^{E_g-1} \int_{4\pi} \int \psi(x, \Omega, E) d\Omega dE dV, \quad (39)$$

$$\mathcal{M}_e = \sum_{g=1}^{G} \mathcal{M}_{e,g}. \quad (40)$$

For this simulation, the path-length estimator described in Section 2.3.1 provides these estimates for the Monte Carlo particle flux by setting the particle weight $w_i$ and the transform function $T(x, \Omega, E)$ to unity in Eq. (26). The Monte Carlo particle flux in the detector is obtained by summing the values corresponding to the spatial elements $V_e$ that comprise the detector $V_D$.

For the Global Flux Problem, the theoretically predicted scalar Monte Carlo particle flux quantities are obtained by substituting the theoretical angular Monte Carlo particle flux $m(x, \Omega, E)$ into Eq. (39). Eq. (30) defines $m(x, \Omega, E)$ for the Global Flux Problem, but must be modified to reflect the reality that a Monte Carlo simulation estimates the scalar flux in spatial elements and within energy groups $\phi_{e,g}$ rather than as a continuous function of space and energy $\phi(x, E)$. Hence, the theoretical angular Monte Carlo particle flux is defined as:

$$m(x, \Omega, E) = C \frac{\psi(x, \Omega, E)}{\phi_{e,g}}. \quad (41)$$

Substituting this expression into Eq. (39), results in the following theoretically predicted scalar Monte Carlo particle flux quantities:

$$\tilde{\mathcal{M}}_{e,g} = C, \quad (42)$$

$$\tilde{\mathcal{M}}_e = CG. \quad (43)$$

That is, each group and spatial element should have the same scalar Monte Carlo particle flux in order to achieve similar statistical quality of the scalar flux.

For the Source-Detector Response Problem, the theoretically predicted scalar Monte Carlo particle flux quantities are obtained by substituting the theoretical angular Monte Carlo particle flux $m(x, \Omega, E)$ given by Eq. (33) into Eq. (39):

$$\tilde{\mathcal{M}}_{e,g} = \frac{C}{V_e} \int V_e \int_{E_g}^{E_g-1} \int_{4\pi} \psi^{*}(x, \Omega, E) d\Omega dE dV$$

$$= \frac{C}{V_e} \int V_e \int_{E_g}^{E_g-1} \int_{4\pi} \psi(x, \Omega, E) \psi^{*}(x, \Omega, E) d\Omega dE dV$$

$$\approx C \phi_{e,g} \Phi_{e,g}^{*}, \quad (44)$$

$$\tilde{\mathcal{M}}_e \approx C \sum_{g=1}^{G} \phi_{e,g} \Phi_{e,g}^{*}, \quad (45)$$
A General Transform

where $\phi_{e,g}$ is the Monte Carlo estimate of the forward scalar flux and is treated as the “exact” solution, and $\Phi^*_{e,g}$ is the deterministic estimate of the adjoint scalar flux. Due to the inaccuracy in the approximation of the above integral, we expect slight differences between the simulated and theoretical Monte Carlo particle flux.

The figures of merit (FOM) in each spatial element $V_e$ are defined as

$$FOM_{e,g} = \frac{1}{\text{Var}[\phi_{e,g}] T_{cpu}},$$

$$FOM_e = \frac{1}{\text{Var}[\phi_e] T_{cpu}},$$

where $T_{cpu}$ is the total run time, and $\phi_{e,g}$, $\phi_e$, and the corresponding variances are volume-averaged quantities obtained directly from the Monte Carlo simulation.

### 3.2 NUMERICAL RESULTS

Figures 3 - 5 include the simulated Monte Carlo particle flux, the theoretically predicted Monte Carlo particle flux, and the figure of merit for the Global Flux Problem for each energy group using two versions of the General Transform – the Standard Weight Window (SWW) and the Complete Transform Function (CTF). Figure 6 includes the same data for the Source-Detector Response Problem for the (energy-integrated) total flux. For clarity, all the 2D figures for the Source-Detector Response Problem have a black rectangle in the upper right corner to denote the detector region and a dashed line tracing out the diagonal from the source to the detector (i.e. the line $x = y = z$). The values are computed on a uniform 0.5 cm grid that is imposed on the problem geometry. Thus, the system consists of 125,000 spatial elements, each denoted by $V_e$. (The source and detector each consist of eight spatial elements.)

Table I: The mean global FOM and mean detector FOM for the Global Flux Problem and Source-Detector Response Problem, respectively

<table>
<thead>
<tr>
<th>Problem</th>
<th>Method</th>
<th>Mean FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Group 1</td>
</tr>
<tr>
<td>Flux ($\phi_{e,g}$)</td>
<td>SWW</td>
<td>0.081</td>
</tr>
<tr>
<td></td>
<td>CTF</td>
<td>0.154</td>
</tr>
<tr>
<td>Response ($\phi_D$)</td>
<td>SWW</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>CTF</td>
<td>–</td>
</tr>
</tbody>
</table>

For the global problem, Figures 3 - 5 indicate that the Standard Weight Window and the Complete Transform Function yield results consistent with the theory: they both nearly uniformly distribute particles across the entire problem space and in every energy group. Although the theory does not specifically predict that the FOM will also be nearly uniform, we see that the FOM is positively correlated to the particle distribution. For this problem type, the Table I data demonstrate that both methods produce comparable results; although, the CTF approach yields better results in the first energy group, in which the greatest attenuation occurs.
For the source-detector problem, Figure 6 demonstrates a particle distribution that is consistent with one that likely maximizes the detector response. That is, the majority of particles travel along the diagonal from the source to the detector. For this problem, the Table I data indicate that the CTF approach performs significantly better than the SWW approach. This is most likely the result of the modified physics being better able to direct particles in space and energy to the most important portions of phase space; the SWW approach uses the simple procedure of filtering particles in space and energy with a weight window, which clearly is not as effective. We again note that although the theory does not specifically predict that the FOM will follow the particle distribution, there is a clear correlation between the two.

Figure 3: Group 1 Simulated MC Particle Flux, Predicted MC Particle Flux, and the FOM for the Global Flux Problem obtained from the Standard Weight Window (SWW) and the Complete Transform Function (CTF) along the plane $x = y$
4. CONCLUSIONS

In this paper, we have described a General Transform that allows Monte Carlo practitioners to disperse Monte Carlo particles throughout phase-space according to a user-specified distribution. The General Transform accomplishes the user-specified distribution by two means: 1) comprehensively modifying the underlying particle physics through the introduction of a specific transform function into the neutron transport equation and 2) selectively filtering Monte Carlo particles in phase-space using a weight window. We derived an expression that relates the Monte Carlo particle distribution to a transform function and a weight window center that accomplishes these objectives.

The General Transform has been applied to the two extremes of shielding applications – the classic Source-Detector Response Problem and the Global Flux Problem. For each of these problems, a particular Monte Carlo particle distribution is specified that likely optimizes the solution; then, the General Transform is applied by using this particle distribution to set the transform function and weight window center in whatever way is the most convenient and efficient. The results presented here indicate that the General Transform performs according to the theoretical specification, by dispersing Monte Carlo particles according to a user-specified distribution, and that it yields good results for difficult shielding problems. Although we provide no theoretical expression that relates the Monte Carlo particle flux and the figure of merit, there seems to be a positive correlation between the two. Even without a theoretical link between the two, Monte Carlo particles exist within the system with some distribution; it seems better to have tools that allow the user to prescribe these distributions clearly.

REFERENCES


Figure 4: Group 2 Simulated MC Particle Flux, Predicted MC Particle Flux, and the FOM for the Global Flux Problem obtained from the Standard Weight Window (SWW) and the Complete Transform Function (CTF) along the plane $x = y$. 
Figure 5: Group 3 Simulated MC Particle Flux, Predicted MC Particle Flux, and the FOM for the Global Flux Problem obtained from the Standard Weight Window (SWW) and the Complete Transform Function (CTF) along the plane $x = y$. 

$FOM = \frac{\text{Simulated Flux}}{\text{Predicted Flux}}$
Figure 6: Total Simulated MC Particle Flux, Predicted MC Particle Flux, and the FOM for the Source-Detector Response Problem obtained from the Standard Weight Window (SWW) and the Complete Transform Function (CTF) along the plane $x = y$