Disclaimer:
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.
Discrete Ordinates Prediction of the Forced-Collision Variance Reduction Technique in Slab Geometry

Brian C. Kiedrowski\textsuperscript{1}, Joel A. Kulesza\textsuperscript{2}, Clell J. Solomon\textsuperscript{2}

\textsuperscript{1}Department of Nuclear Engineering and Radiological Sciences, University of Michigan
\textsuperscript{2}Computational Physics Division, Los Alamos National Laboratory

M\&C 2019, Portland, OR, USA

August 25-29, 2019
Overview

- Derive transport equations for the first and second statistical moments that describe the mean and variance of the forced-collision process
- Develop discrete ordinates ($S_N$) scheme for solving the equations in slab geometry
- Show agreement of $S_N$ calculation with Monte Carlo reference solution for illustrative test problem
Forced Collision Variance Reduction

- Upon entering a designated region (cell), the particle history is split into two parts: collided and transmitted.
- The collided part is forced to undergo a collision prior to exiting the cell
  - Distance to collision sampled from truncated exponential distribution:
    \[
    f_c(x) = \frac{\Sigma_te^{-\Sigma_t x}}{1 - e^{-\Sigma_t \ell}}, \quad 0 \leq x < \ell(x, \hat{\Omega}).
    \]
  - Weight modified by collision probability:
    \[
    w_c = \rho_c w, \quad \rho_c = 1 - e^{-\Sigma_t \ell}.
    \]
- The transmitted part is transported to the next region without collision, with weight modified by transmission probability
  \[
  w_t = \rho_t w, \quad \rho_t = 1 - \rho_c = e^{-\Sigma_t \ell}.
  \]
Hybrid deterministic-Monte Carlo methods are used to accelerate convergence of Monte Carlo calculations.

Current state-of-the-art methods (e.g., CADIS) may produce suboptimal results in problems where collisions are improbable and important.

Forced collisions are effective in these cases, but currently no automated method exists for applying them.

Creating equations for forced collisions is the first step in developing such an automated approach.
Motivating Test Problem

- 200 keV photon source in air in lower-left part of problem, shielded by thick tungsten block; want to find flux in lower-right part
- Analog MCNP:

Calculations by Eric Pearson at Univ. of Michigan.
Motivating Test Problem

- 200 keV photon source in air in lower-left part of problem, shielded by thick tungsten block; want to find flux in lower-right part
- MCNP with optimized weight windows (only): (FOM improvement 4x)
Motivating Test Problem

- 200 keV photon source in air in lower-left part of problem, shielded by thick tungsten block; want to find flux in lower-right part
- MCNP with optimized weight windows with forced collisions: (FOM improvement 35x)
Consider a problem with or without regions with forced collisions and a surface current estimator.

Define augmented phase space $\mathbf{p} = (\mathbf{r}, w) = (x, \hat{\Omega}, E, w)$. Here $w$ is the statistical weight factor. (In analog transport $w = 1$ always.)

Define the history score probability density function:

$$\psi(\mathbf{p}, s)ds = \text{probability that a particle at phase space } \mathbf{p} \text{ will contribute a score in } ds \text{ about } s.$$

From the history score PDF we can calculate statistical moments (for mean and variance):

$$\Psi_k(\mathbf{p}) = \int_0^\infty s^k \psi(\mathbf{p}, s)ds.$$

Note: $\Psi_1$ is the adjoint flux $\psi^\dagger$. 
Phase Space Indexing

\( p_0 = \) reference point

\( p_1 = \) pre-collision point

\( p_2 = \) secondary emergence

\( p_3 = \) surface crossing point

\( p_4 = \) arrival into next region
Analog History Score Density Equation

- Write integral transport equation for history score density function for analog physics with no local tallies in operator form:

\[ \psi(p_0, s) = T(p_0, p_1)K(p_1)E(p_1, p_2)\psi(p_2, s) + T(p_0, p_3)S(p_3)A(p_3, p_4)\psi(p_4, s). \]

- Note $+$ between events denotes one or the other occurs.
Analog history score density equation with surface current tally:

\[
\psi(p_0, s) = T(p_0, p_1)K(p_1)E(p_1, p_2)\psi(p_2, s) \\
+ T(p_0, p_3)S(p_3) \int_0^\infty f(p_3, s_3)A(p_3, p_4)\psi(p_4, s-s_3)ds_3.
\]

- Now contains an additional surface current scoring function \( f(p, s) \),

\[
f(p, s) = \delta(s - w), \quad x \in \partial\Gamma_m, \quad \hat{\Omega} \cdot \hat{n} > 0,
\]

- and integral over the possible scores \( s_3 \) at \( p_3 \). Scoring is done before arrival into adjacent region.

- The term \( \psi(p_4, s - s_3) \) are the additional scores after crossing surface.
Multiply by $s$ and integrate over all scores to get first statistical moment (adjoint transport) equation:

$$
\Psi_1(p_0) = T(p_0, p_1)K(p_1)E(p_1, p_2)\Psi_1(p_2)
+ T(p_0, p_3)S(p_3) \left[ \bar{s}(p_3) + A(p_3, p_4)\Psi_1(p_4) \right].
$$
Analog Second Statistical Moment Equation

- Multiply by $s^2$ and integrate over all scores to get second statistical moment equation:

$$\Psi_2(p_0) = T(p_0, p_1)K(p_1)E(p_1, p_2)\Psi_2(p_2)$$

$$+ T(p_0, p_3)S(p_3)\left[ s^2(p_3) + 2s(p_3)A(p_3, p_4)\Psi_1(p_4) \right.$$  

$$+ A(p_3, p_4)\Psi_2(p_4) \right].$$

- $\Psi_2(p_0)$: Mean squared score at surface after arrival into adjacent region
- $T(p_0, p_1)K(p_1)E(p_1, p_2)\Psi_2(p_2)$: Second moment after collision
- $T(p_0, p_3)S(p_3)$: Product of mean score at surface and mean score after arrival
- $s^2(p_3)$: Second moment after collision
- $2s(p_3)A(p_3, p_4)\Psi_1(p_4)$: Second moment after arrival into adjacent region
- $A(p_3, p_4)\Psi_2(p_4)$: Product of mean score at surface and mean score after arrival
Forced Collision Operators

We define the following operators for forced collisions:

\[ B_c(p, p') = \text{operator for particles entering a forced-collision region at } p \text{ and undergoing forced-collision processing: moving the particle to } p', \text{ initiating a collision, and reducing its weight by } \rho_c; \]

\[ B_t(p, p') = \text{operator for particles entering a forced-collision region at } p \text{ and being transported to } p' \text{ on the exterior surface and having its weight reduced by } \rho_t. \]
Forced Collision History Score Density Equation

- Forced collision history score density with surface current tally:

\[
\psi(p_0, s) = B_c(p_0, p_1)K(p_1)\mathcal{E}(p_1, p_2) \int_0^\infty \psi(p_2, s_2) \times B_t(p_0, p_3)S(p_3) \int_0^\infty f(p_3, s_3)A(p_3, p_4)\psi(p_4, s - s_2 - s_3)ds_3ds_2. 
\]

- The transmission operators \(T\) have been replaced by \(B_c\) and \(B_t\) in the collision and surface crossing events respectively.
- The \(\times\) replaces the \(+\) because both events occur.
- There is an integral over \(s_2\), the scores accrued after the collision, as well as \(s_3\), the scores accrued after crossing into the adjacent region.
- Note: this equation only applies for particles that have just entered a forced collision region.
Multiply by \( s \) and integrate over all scores to get first statistical moment (adjoint transport) equation:

\[
\Psi_1(p_0) = B_c(p_0, p_1)K(p_1)\mathcal{E}(p_1, p_2)\Psi_1(p_2) + B_t(p_0, p_3)S(p_3)\left[\bar{s}(p_3) + A(p_3, p_4)\Psi_1(p_4)\right].
\]

The equation should be identical to the analog process,

\[
\Psi_1(p_0) = T(p_0, p_1)K(p_1)\mathcal{E}(p_1, p_2)\Psi_1(p_2) + T(p_0, p_3)S(p_3)\left[\bar{s}(p_3) + A(p_3, p_4)\Psi_1(p_4)\right],
\]

as all valid variance reduction schemes should preserve the mean.

This is straightforward to show.
Forced collision first statistical moment equation

- Forced collisions are done independent of statistical weight, so we can apply the relationship:

$$\Psi_k(p) = w^k \Psi_k(r, 1),$$

where $$\Psi_k(r, 1)$$ is the $$k$$th statistical moment for the analog process.

- Recall that the weight of the collided and transmitted parts are modified to $$\rho_c$$ and $$\rho_t$$ respectively.

- For the collided part of the forced collision equation:

$$B_c(p_0, p_1) K(p_1) E(p_1, p_2) \Psi_1(p_2)$$

$$= \rho_c B_c(p_0, p_1) K(p_1) E(p_1, p_2) \Psi_1(r_2, 1)$$

$$= T(p_0, p_1) K(p_1) E(p_1, p_2) \Psi_1(r_2, 1),$$

with $$\rho_c B_c$$ reducing to $$T$$ because the process is otherwise identical except for the modified weight.
Since all scoring functions are modified by weight as well

\[ \bar{s}^k(p) = w^k \bar{s}^k(r, 1), \]

Therefore the transmitted part of the forced collision equation:

\[ \mathcal{B}_t(p_0, p_3)S(p_3) \left[ \bar{s}(p_3) + A(p_3, p_4)\Psi_1(p_4) \right] \]
\[ = \mathcal{B}_t(p_0, p_3)S(p_3) \left[ \rho_t \bar{s}(r_3, 1) + \rho_t A(p_3, p_4)\Psi_1(r_4, 1) \right] \]
\[ = \mathcal{T}(p_0, p_3)S(p_3) \left[ \bar{s}(r_3, 1) + A(p_3, p_4)\Psi_1(r_4, 1) \right]. \]

Therefore the mean of the forced collision and analog processes are identical.
Theory

Forced Collision Second Statistical Moment Equation

- Multiply by $s^2$ integrate over all scores, and apply properties to put in terms of analog process to obtain second statistical moment equation:

$$\Psi_2(p_0) = \rho_c \mathcal{T}(p_0, p_1) \mathcal{K}(p_1) \mathcal{E}(p_1, p_2) \Psi_2(r_2, 1)$$

$$+ \rho_t \mathcal{T}(p_0, p_3) \mathcal{S}(p_3) \left[ s^2(r_3, 1) + 2\bar{s}(r_3, 1)A(p_3, p_4)\Psi_1(r_4, 1) \right.$$ 

$$+ A(p_3, p_4)\Psi_2(r_4, 1) \right]$$

$$+ 2 \left[ \mathcal{T}(p_0, p_1) \mathcal{K}(p_1) \mathcal{E}(p_1, p_2) \Psi_1(r_2, 1) \right]$$

$$\times \left[ \mathcal{T}(p_0, p_3) \mathcal{S}(p_3) \left( \bar{s}(r_3, 1) + A(p_3, p_4)\Psi_1(r_4, 1) \right) \right].$$

- Differences from analog equation highlighted in red.
Forced Collision Second Statistical Moment Equation

The collided and transmitted terms are now scaled by the collision and transmission probabilities respectively.

$$\rho_c T(p_0, p_1) K(p_1) E(p_1, p_2) \Psi_2(r_2, 1)$$

$$\rho_t T(p_0, p_3) S(p_3) \left[ s^2(r_3, 1) + 2s(r_3, 1) A(p_3, p_4) \right]$$

$$+ \Psi_1(r_4, 1) + A(p_3, p_4) \Psi_2(r_4, 1)$$

There is a cross term from the product of the first statistical moment terms for both the collided and transmitted events.

$$2 \left[ T(p_0, p_1) K(p_1) E(p_1, p_2) \Psi_1(r_2, 1) \right]$$

$$\times \left[ T(p_0, p_3) S(p_3) (s(r_3, 1) + A(p_3, p_4) \Psi_1(r_4, 1)) \right]$$
The first and second statistical moment equations are solved in 1-D slab geometry to demonstrate the idea.

Since the problem needs to map onto Monte Carlo regions with scoring occurring upon a forward particle leaving the region (or adjoint entering), the calculation involves separate regions.

The following indexing convention is used:

\[ \Psi_{k,m,i,n} = k\text{th statistical moment of the history scoring density function in spatial region } m \text{ with local spatial element } i \text{ traveling in direction } n. \]
Use the standard discretization and indexing in slab geometry with cell-centered and cell-edge quantities (statistical moment and direction indices suppressed):

Note the overlapping element at region edges, which is important for handling the location of the scoring.
Sweep Algorithm

- Solution method for both statistical moments uses source iteration with reverse sweeps involving the diamond difference method.
- The right-to-left sweep ($\mu_n > 0$):
  \[
  \Psi_{k,m,i,n} = \left[ \Psi_{k,m,i+1/2,n} + \frac{q_{k,m,i,n} \Delta m}{2|\mu_n|} \right] \cdot \left[ 1 + \frac{\Sigma_{t,m} \Delta m}{2|\mu_n|} \right]^{-1},
  \]
  \[
  \Psi_{k,m,i-1/2,n} = 2\Psi_{k,m,i,n} - \Psi_{k,m,i+1/2,n}.
  \]
- Here $q_{k,m,i,n}$ is the scattering source for the $k$th statistical moment.
First Statistical Moment Sweep

- The region interface condition for the first statistical moment (for the right-to-left sweep) is

\[ \Psi_{1,m,I+1/2,n} = \delta_{m,I+1/2} + \Psi_{1,m+1,1/2,n} \]

where \( \delta_{m,I+1/2} \) is one if a surface current estimator is present on the right edge and zero otherwise. (Analogous for left-to-right sweep.)

- Otherwise equivalent to the backwards sweeping scheme used to find the adjoint flux in a fixed-source calculation.
Second statistical moment sweep is similar except the region interface condition (for the right-to-left sweep) is

\[ \Psi_{2,m,I+1/2,n} = \delta_{m,I+1/2}(1 + 2\Psi_{1,m+1/2},n) + \Psi_{2,m+1/2},n. \]

Forced collision regions require special sweeps for computing the edge values of adjoint particles exiting forced collision regions, i.e.,

\[ \Psi_{2,m,1/2,n}, \quad \mu_n > 0, \]
\[ \Psi_{2,m,I+1/2,n}, \quad \mu_n < 0 \]

(corresponding to forward particles entering forced collision regions).
Second Statistical Moment Sweep

- Perform a special sweep from one edge of the forced collision region to the other with only collision source and zero boundary source for the collided term:

\[ \rho_c \mathcal{T}(p_0, p_1) \mathcal{K}(p_1) \mathcal{E}(p_1, p_2) \Psi_2(r_2, 1), \]

scaling the resulting value by \( \rho_c \).

- Perform another special sweep from one edge of the forced collision region to the other with only boundary source and zero collision source for the transmitted term:

\[ \rho_t \mathcal{T}(p_0, p_3) \mathcal{S}(p_3) \left[ \bar{s}^2(r_3, 1) + 2\bar{s}(r_3, 1) \mathcal{A}(p_3, p_4) \right. \]

\[ \left. + \Psi_1(r_4, 1) + \mathcal{A}(p_3, p_4) \Psi_2(r_4, 1) \right] \]

scaling the resulting value by \( \rho_t \).
Store separated first statistical moment sweeps with only collision source and zero boundary source and vice versa for cross term:

\[
2 \left[ T(p_0, p_1) K(p_1) E(p_1, p_2) \Psi_1(r_2, 1) \right. \\
\times \left. \left[ T(p_0, p_3) S(p_3) (\bar{s}(r_3, 1) + A(p_3, p_4) \Psi_1(r_4, 1)) \right] \right],
\]

taking twice the product of their resulting values.

Add the result of the three terms together to get the exiting (in adjoint sense) edge value for a forced collision region.
Test Problem Description

- Test problem selected to ensure each of the three terms in the forced-collision second statistical moment equation have a significant impact on the overall solution.

<table>
<thead>
<tr>
<th>Source</th>
<th>Current Estimator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vacuum</td>
<td>Analog</td>
</tr>
</tbody>
</table>
|        | $\Sigma_t = 1.0 \text{ cm}^{-1}$  
$\Sigma_s = 0.9 \text{ cm}^{-1}$ |
| 1.0 cm | 1.0 cm            |
| Forced Collision | 1.0 cm |
| Analog | Vacuum            |
| $\Sigma_t = 0.5 \text{ cm}^{-1}$  
$\Sigma_s = 0.45 \text{ cm}^{-1}$ |
| 1.0 cm | 1.0 cm            |
| $\Sigma_t = 1.0 \text{ cm}^{-1}$  
$\Sigma_s = 0.9 \text{ cm}^{-1}$ |

*$\Sigma$ values in cm$^{-1}$.
The $k$th statistical moment of the response current is calculated by integrating $\Psi_k$ with the forward boundary source (normalized with intensity of two) over directions $\mu_n > 0$,

$$R_k = 2 \sum_{n=1}^{N/2} \omega_n \mu_n \Psi_{k,1,1/2,n}.$$  

Here $\omega_n$ are the Gauss-Legendre quadrature weights.

Discrete ordinates calculations were run with the $S_{64}$ Gauss-Legendre angular quadrature with 100 spatial cells in each region.

Reference Monte Carlo calculation is continuous in space and direction and run with $10^8$ histories, which is sufficient to converge the estimates of $R_1$ and $R_2$. 

Particle Current Statistical Moments Comparison

Test problem is run in both analog-only mode and also with forced collisions turned on using both $S_N$ and Monte Carlo.

<table>
<thead>
<tr>
<th></th>
<th>Analog</th>
<th>Forcde Collision</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$R_1$</td>
<td>$R_2$</td>
</tr>
<tr>
<td>Discrete Ordinates</td>
<td>0.551288</td>
<td>1.212050</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>0.551112</td>
<td>1.211550</td>
</tr>
</tbody>
</table>

The $R_2$ results for the forced-collision case have an error of 0.055%.

Analog versus forced collisions have the $R_1$ values, as expected; however, $R_2$ is reduced using forced collisions (again, expected).
Scalar Flux Statistical Moments

- Also calculate the scalar first and second statistical moments from the $S_N$ calculation

$$\Phi_{k,m,i} = \sum_{n=1}^{N} \omega_n \Psi_{k,m,i,n}$$

- corresponding to the spatially-dependent, directionally-integrated expected contribution to the first and second statistical moment of the response.

- Results provided forced collisions. No Monte Carlo comparison was performed; however, should illustrate the mathematics of the Monte Carlo simulation.
Scalar Flux Statistical Moments

\[ \Phi_k(x) \]

\[ \Phi_1(x) \]

\[ \Phi_2(x) \]
Scalar Flux Statistical Moment Discussion

- The first scalar flux statistical moment $\Phi_1$ increases toward the estimator. Function is continuous with discontinuous derivatives at interfaces. (Expected behavior for adjoint scalar flux.)

- The second scalar flux statistical moment $\Phi_2$ exhibits a similar increase, but is discontinuous at the interface of the forced collision region. (Very apparent on left edge, but very small on the right edge for this problem).

- This discontinuity in $\Phi_2$ at the forced collision region interface is expected since particles in the region to the left of the forced collision region are much more likely to experience a forced collision and have a reduced variance of the estimator than those to the right of the interface which do not.
Summary

- Equations for the first and second statistical moments of the forced collision problem were derived.
- A numerical scheme to solve these equations using $S_N$ was developed for 1-D slab geometry.
- Results of an illustrative test problem of the $S_N$ equation show agreement ($\ll 1\%$ error) with those from a reference Monte Carlo calculation.
Future Work

- Apply algorithm to a greater variety of scenarios of greater complexity, e.g., 2/3D, cell flux estimators, include rouletting on collided particles, allow collided particles to undergo forced collisions, etc.
- Combine with other variance reduction techniques.
  - See Kulesza’s talk for these techniques applied to the forced flight (DXTRAN) variance reduction technique.
- Develop automated approaches to optimally apply forced collisions and other variance reduction techniques beyond weight windows.
This work is supported by the Department of Energy National Nuclear Security Administration (NNSA) under Award Number(s) DE-NA0002576 from the NNSA Office of Defense Nuclear Nonproliferation R&D through the Consortium for Nonproliferation Enabling Capabilities.
Questions?

- Contact Brian Kiedrowski (Email: bckiedro@umich.edu).