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Discrete Ordinates Prediction of the Forced-Collision Variance Reduction Technique in Slab Geometry

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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:

$$f_c(x) = \frac{\Sigma_t e^{-\Sigma_t x}}{1 - e^{-\Sigma_t \ell}}, \quad 0 \leq x < \ell(\mathbf{x}, \hat{\Omega}).$$

- 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

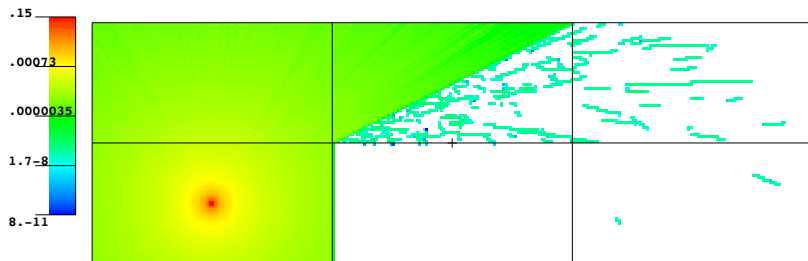
$$w_t = \rho_t w, \quad \rho_t = 1 - \rho_c = e^{-\Sigma_t \ell}.$$

Motivation

- 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

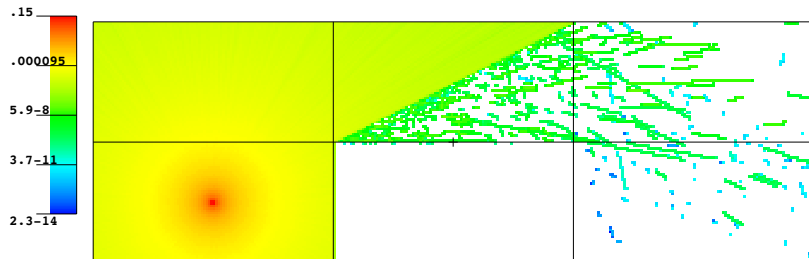
- 200 keV photon source in air in lower-left part of problem, shielded by thick tungsten block; want to find flux in lower-right part
- Analog MCNP:



- Calculations by Eric Pearson at Univ. of Michigan.

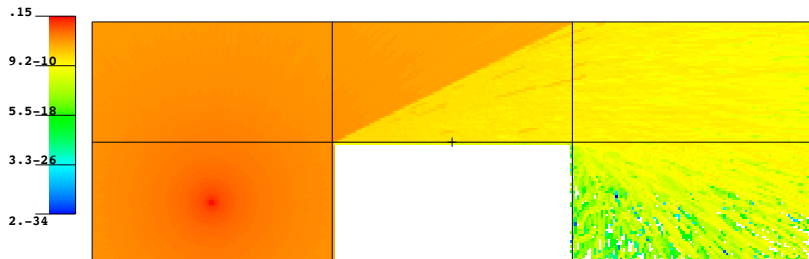
Motivating Test Problem

- 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)



History Score Density Equations

- Consider a problem with or without regions with forced collisions and a surface current estimator.
- Define augmented phase space $\mathbf{p} = (\mathbf{r}, w) = (\mathbf{x}, \hat{\Omega}, E, w)$. Here w is the statistical weight factor. (In analog transport $w = 1$ always.)
- Define the history score probability density function:

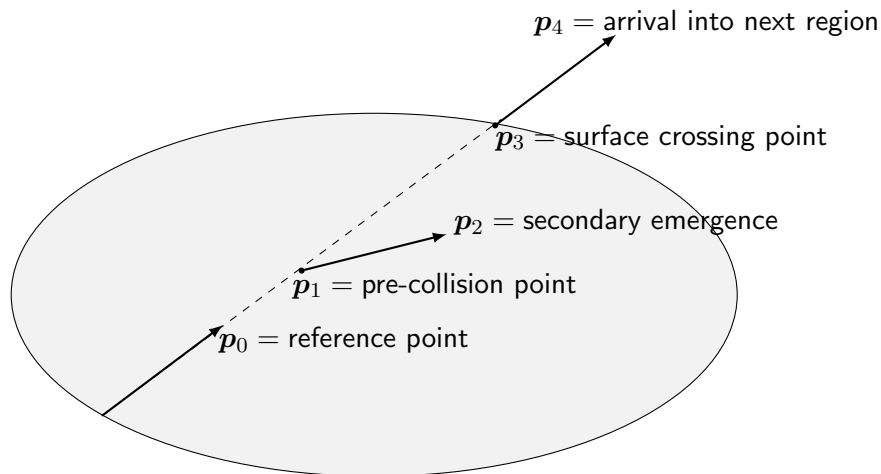
$\psi(\mathbf{p}, s)ds$ = probability that a particle at phase space \mathbf{p} will contribute a score in ds about s .

- 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: Ψ_1 is the adjoint flux ψ^\dagger .

Phase Space Indexing



Analog History Score Density Equation

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

$$\begin{aligned}
 \psi(\mathbf{p}_0, s) = & \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \psi(\mathbf{p}_2, s) && \text{collision event} \\
 & + \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \psi(\mathbf{p}_4, s). && \text{surface crossing event}
 \end{aligned}$$

Diagram illustrating the components of the equation:

- free flight** (top left) points to $\mathcal{T}(\mathbf{p}_0, \mathbf{p}_1)$
- collide** (top center) points to $\mathcal{K}(\mathbf{p}_1)$
- scatter emergence** (top right) points to $\mathcal{E}(\mathbf{p}_1, \mathbf{p}_2)$
- free flight** (bottom left) points to $\mathcal{T}(\mathbf{p}_0, \mathbf{p}_3)$
- reach surface** (bottom center) points to $\mathcal{S}(\mathbf{p}_3)$
- arrival at adjacent region** (bottom right) points to $\mathcal{A}(\mathbf{p}_3, \mathbf{p}_4)$

- Note + between events denotes one or the other occurs.

Analog History Score Density Equation

- Analog history score density with surface current tally:

$$\psi(\mathbf{p}_0, s) = \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1)\mathcal{K}(\mathbf{p}_1)\mathcal{E}(\mathbf{p}_1, \mathbf{p}_2)\psi(\mathbf{p}_2, s) \\ + \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3)\mathcal{S}(\mathbf{p}_3) \int_0^\infty f(\mathbf{p}_3, s_3)\mathcal{A}(\mathbf{p}_3, \mathbf{p}_4)\psi(\mathbf{p}_4, s-s_3)ds_3.$$

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

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

and integral over the possible scores s_3 at \mathbf{p}_3 . Scoring is done before arrival into adjacent region.

- The term $\psi(\mathbf{p}_4, s - s_3)$ are the additional scores after crossing surface.

Analog First Statistical Moment Equation

- Multiply by s and integrate over all scores to get first statistical moment (adjoint transport) equation:

$$\Psi_1(\mathbf{p}_0) = \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1)\mathcal{K}(\mathbf{p}_1)\mathcal{E}(\mathbf{p}_1, \mathbf{p}_2)\Psi_1(\mathbf{p}_2) + \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3)\mathcal{S}(\mathbf{p}_3) \left[\bar{s}(\mathbf{p}_3) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4)\Psi_1(\mathbf{p}_4) \right].$$

expected score after collision

expected (mean) score at surface

expected score after arrival into adjacent region

Analog Second Statistical Moment Equation

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

$$\Psi_2(\mathbf{p}_0) = \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1)\mathcal{K}(\mathbf{p}_1)\mathcal{E}(\mathbf{p}_1, \mathbf{p}_2)\Psi_2(\mathbf{p}_2) + \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3)\mathcal{S}(\mathbf{p}_3) \left[\overline{s^2}(\mathbf{p}_3) + 2\overline{s}(\mathbf{p}_3)\mathcal{A}(\mathbf{p}_3, \mathbf{p}_4)\Psi_1(\mathbf{p}_4) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4)\Psi_2(\mathbf{p}_4) \right].$$

second moment after collision

mean squared score at surface **second moment after arrival into adjacent region** **product of mean score at surface and mean score after arrival**

Forced Collision Operators

- We define the following operators for forced collisions:

$\mathcal{B}_c(\mathbf{p}, \mathbf{p}')$ = operator for particles entering a forced-collision region at \mathbf{p} and undergoing forced-collision processing: moving the particle to \mathbf{p}' , initiating a collision, and reducing its weight by ρ_c ;

$\mathcal{B}_t(\mathbf{p}, \mathbf{p}')$ = operator for particles entering a forced-collision region at \mathbf{p} and being transported to \mathbf{p}' on the exterior surface and having its weight reduced by ρ_t .

Forced Collision History Score Density Equation

- Forced collision history score density with surface current tally:

$$\begin{aligned} \psi(\mathbf{p}_0, s) = & \mathcal{B}_c(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \int_0^\infty \psi(\mathbf{p}_2, s_2) \\ & \times \mathcal{B}_t(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) \int_0^\infty f(\mathbf{p}_3, s_3) \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \psi(\mathbf{p}_4, s - s_2 - s_3) ds_3 ds_2. \end{aligned}$$

- The transmission operators \mathcal{T} have been replaced by \mathcal{B}_c and \mathcal{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.**

Forced Collision First Statistical Moment Equation

- Multiply by s and integrate over all scores to get first statistical moment (adjoint transport) equation:

$$\begin{aligned}\Psi_1(\mathbf{p}_0) &= \mathcal{B}_c(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{p}_2) \\ &\quad + \mathcal{B}_t(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) [\bar{s}(\mathbf{p}_3) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{p}_4)].\end{aligned}$$

- The equation should be identical to the analog process,

$$\begin{aligned}\Psi_1(\mathbf{p}_0) &= \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{p}_2) \\ &\quad + \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) [\bar{s}(\mathbf{p}_3) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{p}_4)],\end{aligned}$$

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:

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

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

- Recall that the weight of the collided and transmitted parts are modified to ρ_c and ρ_t respectively.
- For the collided part of the forced collision equation:

$$\begin{aligned} & \mathcal{B}_c(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{p}_2) \\ &= \rho_c \mathcal{B}_c(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{r}_2, 1) \\ &= \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{r}_2, 1), \end{aligned}$$

with $\rho_c \mathcal{B}_c$ reducing to \mathcal{T} because the process is otherwise identical except for the modified weight.

Forced Collision First Statistical Moment Equation

- Since all scoring functions are modified by weight as well

$$\overline{s^k}(\mathbf{p}) = w^k \overline{s^k}(\mathbf{r}, 1),$$

- Therefore the transmitted part of the forced collision equation:

$$\begin{aligned} & \mathcal{B}_t(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) [\overline{s}(\mathbf{p}_3) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{p}_4)] \\ &= \mathcal{B}_t(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) [\rho_t \overline{s}(\mathbf{r}_3, 1) + \rho_t \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{r}_4, 1)] \\ &= \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) [\overline{s}(\mathbf{r}_3, 1) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{r}_4, 1)]. \end{aligned}$$

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

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:

$$\begin{aligned} \Psi_2(\mathbf{p}_0) = & \rho_c \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_2(\mathbf{r}_2, 1) \\ & + \rho_t \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) \left[\overline{s^2}(\mathbf{r}_3, 1) + 2\bar{s}(\mathbf{r}_3, 1) \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{r}_4, 1) \right. \\ & \quad \left. + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_2(\mathbf{r}_4, 1) \right] \\ & + 2 \left[\mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{r}_2, 1) \right] \\ & \times \left[\mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) (\bar{s}(\mathbf{r}_3, 1) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{r}_4, 1)) \right]. \end{aligned}$$

- 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.

$$\begin{aligned} & \rho_c \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_2(\mathbf{r}_2, 1) \\ & \rho_t \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) \left[\overline{s^2}(\mathbf{r}_3, 1) + 2\overline{s}(\mathbf{r}_3, 1) \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \right. \\ & \quad \left. + \Psi_1(\mathbf{r}_4, 1) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_2(\mathbf{r}_4, 1) \right] \end{aligned}$$

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

$$\begin{aligned} & 2 \left[\mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{r}_2, 1) \right] \\ & \times \left[\mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) (\overline{s}(\mathbf{r}_3, 1) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{r}_4, 1)) \right] \end{aligned}$$

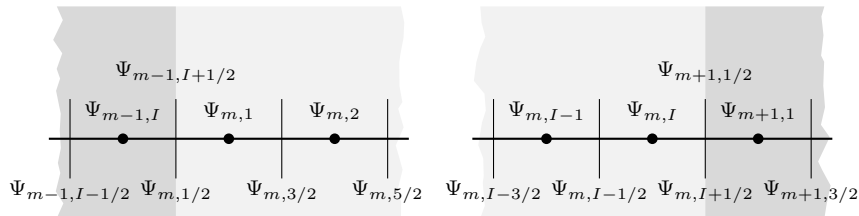
Discrete Ordinates Indexing

- 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 th statistical moment of the history scoring density function in spatial region m with local spatial element i traveling in direction n .

Discrete Ordinates Spatial Discretization

- 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

- Second statistical moment sweep is similar except the region interface condition (for the right-to-left sweep) is

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

- 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:

$$\rho_c \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_2(\mathbf{r}_2, 1),$$

scaling the resulting value by ρ_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:

$$\rho_t \mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) \left[\overline{s^2}(\mathbf{r}_3, 1) + 2\overline{s}(\mathbf{r}_3, 1) \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \right. \\ \left. + \Psi_1(\mathbf{r}_4, 1) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_2(\mathbf{r}_4, 1) \right]$$

scaling the resulting value by ρ_t .

Second Statistical Moment Sweep

- Store separated first statistical moment sweeps with only collision source and zero boundary source and vice versa for cross term:

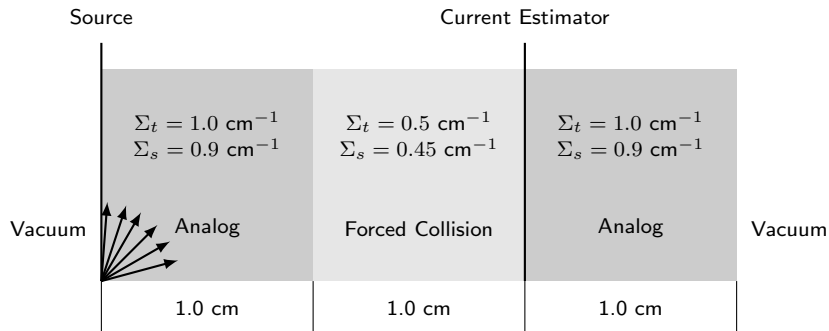
$$2 \left[\mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1) \mathcal{E}(\mathbf{p}_1, \mathbf{p}_2) \Psi_1(\mathbf{r}_2, 1) \right] \\ \times \left[\mathcal{T}(\mathbf{p}_0, \mathbf{p}_3) \mathcal{S}(\mathbf{p}_3) (\bar{s}(\mathbf{r}_3, 1) + \mathcal{A}(\mathbf{p}_3, \mathbf{p}_4) \Psi_1(\mathbf{r}_4, 1)) \right],$$

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.



Test Problem Description

- The k th statistical moment of the response current is calculated by integrating Ψ_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 ω_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.

	Analog		Forced Collision	
	R_1	R_2	R_1	R_2
Discrete Ordinates	0.551288	1.212050	0.551288	0.865821
Monte Carlo	0.551112	1.211550	0.551160	0.865341

- 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

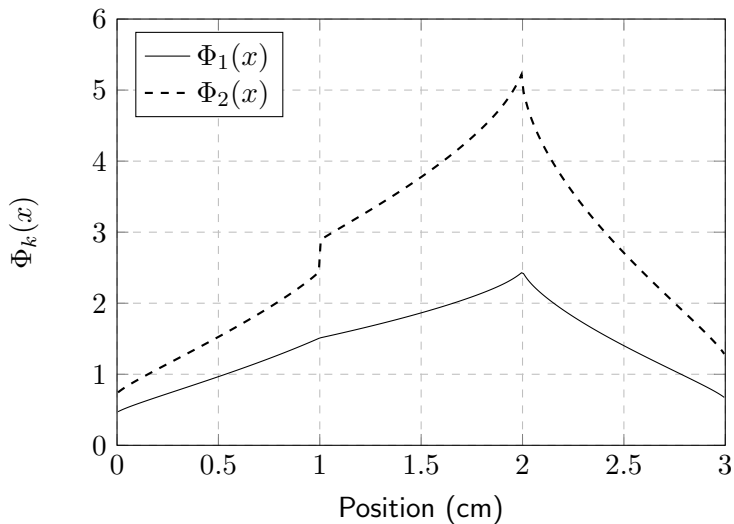
- Also calculate the scalar first and second statistical moments from the S_N calculation

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

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



Scalar Flux Statistical Moment Discussion

- The first scalar flux statistical moment Φ_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 Φ_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 Φ_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.

Acknowledgments

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Questions?

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