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Predicting Monte Carlo Tally Variance and Calculation Time when Using Forced-flight Variance Reduction—Theory

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Outline

Introduction & Terminology

Forced-flight Variance Reduction Overview

History-score Moment Equations

- Transport Operators

- Scoring Functions

- Forced-flight & Modified Free-flight Biasing Operators

Future-time Equation

Summary & Future Work

Introduction & Terminology

Objective: perform computational-cost optimization of Monte Carlo calculations using forced-flight variance reduction

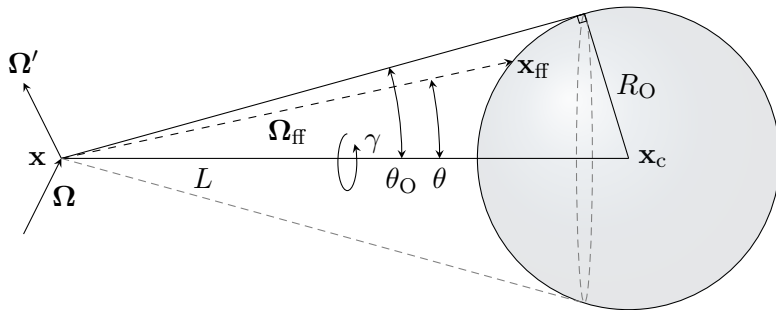
- ▶ Process overview
 - ▶ Deduce biasing operator(s) for forced-flight variance reduction
 - ▶ Construct history-score probability density function (HSPDF, $\psi(\mathbf{p}, s)$)
 - ▶ Derive history-score moment equations (HSMEs, $\Psi_{1,2}(\mathbf{p})$)
 - ▶ Construct future-time probability density function (FTPDF, $v(\mathbf{p})$)
 - ▶ Derive future-time equation (FTE, $\Upsilon(\mathbf{p})$)
 - ▶ Calculate computational cost

$$\$(\mathbf{p}) = \frac{[\Psi_2(\mathbf{p}) - \Psi_1^2(\mathbf{p})] \Upsilon(\mathbf{p})}{\Psi_1^2(\mathbf{p})}. \quad (1)$$

Forced-flight Variance Reduction Overview

- ▶ Forced-flight: directly biases particle direction of flight
- ▶ “DXTRAN” in the MCNP code
 - ▶ Developed in the late 1970s, not clear by who
 - ▶ Best reference: MCNP theory manual (X-5 Monte Carlo Team, 2008)
- ▶ “Forced flight” in the MCBEND code
 - ▶ (Chucas et al., 1994; Shuttleworth et al., 2000)
- ▶ “Forced scattering” in a research version of the EGSnrc code
 - ▶ (Tickner, 2009; Kawrakow et al., 2017)
- ▶ Diverse fields of use
 - ▶ Medical physics
 - ▶ Research reactor irradiation beam port flux characterization
 - ▶ Neutron generator device design
 - ▶ Spacecraft nuclear propulsion
 - ▶ Inertial confinement fusion reactor design

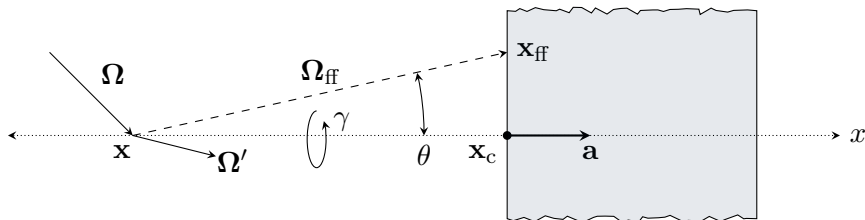
Simplified Spherical Forced-flight Variance Reduction



- ▶ User-defined geometry cell-wise rouletting fraction, β_c (i.e., DXC)
- ▶ Occurs following every valid non-absorptive collision
 - ▶ Weight balance by terminating particles entering the sphere
- ▶ No rouletting on transmission for weight control; no weight cutoffs

$$w_{\text{ff}} = \frac{w g(\mu) \exp[-\lambda(\mathbf{x}, \mathbf{x}_{\text{ff}}, E)]}{\beta_c \tilde{g}(\mu)} \quad (2)$$

1-D Cartesian Forced-flight Region

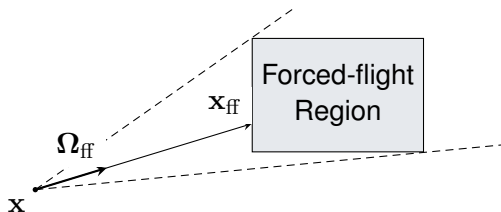


- ▶ User-defined geometry cell-wise rouletting fraction, β_c (i.e., DXC)
- ▶ Occurs following every valid non-absorptive collision
- ▶ No rouletting on transmission for weight control; no weight cutoffs

$$w_{\text{ff}} = \frac{w g(\mu) \exp[-\lambda(\mathbf{x}, \mathbf{x}_{\text{ff}}, E)]}{\beta_c \tilde{g}(\mu)} \frac{1}{1} \quad (3)$$

- ▶ Kulesza et al. (2018)

2-D Cartesian Forced-flight Region



- ▶ User-defined geometry cell-wise rouletting fraction, β_c (i.e., DXC)
- ▶ Occurs following every valid non-absorptive collision
- ▶ No rouletting on transmission for weight control; no weight cutoffs

$$w_{\text{ff}} = \frac{w}{\beta_c} \frac{g(\mu) \exp[-\lambda(\mathbf{x}, \mathbf{x}_{\text{ff}}, E)]}{\tilde{g}(\mu)} \quad (4)$$

- ▶ Kulesza et al. (2018)

HSME Methodology Overview

- ▶ History-score moment equations (HSMEs)
 - ▶ Describe Monte Carlo random walk statistical moments
 - ▶ HSME-based methods are Monte Carlo code agnostic
- ▶ Specific implementations are **directly** related to a Monte Carlo code
 - ▶ Descriptions of geometry, materials, tallies, sources, etc.
 - ▶ VR technique availability & implementation
 - ▶ Must deterministically model Monte Carlo transport code processes
- ▶ Different random walks available
 - ▶ Terminates with absorptive collision, continues with collision with emergence, continues with surface crossing
 - ▶ Modified as a function of variance reduction
- ▶ First, assemble history-score probability distribution function (HSPDF)
 - ▶ Probability of contributing score ds about s from \mathbf{p}

$$\psi(\mathbf{p}, s) ds = \sum_i \psi_i(\mathbf{p}, s) ds \quad (5)$$

HSME Components: Transport Operators

- ▶ HSPDF is constructed from **transport operators** and **scoring functions**
- ▶ Transport operators
 - ▶ Describe particles undergoing phase-space change

$\mathcal{T}(\mathbf{p}, \mathbf{p}')$ for particles undergoing free flight from \mathbf{p} to \mathbf{p}'

$\mathcal{S}(\mathbf{p}, \mathbf{p}')$ for particles crossing a Monte Carlo surface (combining \mathcal{S} and \mathcal{A} from Kiedrowski et al. (2019))

$\mathcal{K}(\mathbf{p}, \mathbf{p}')$ for particles undergoing collision

$\mathcal{E}(\mathbf{p}, \mathbf{p}')$ for particles undergoing emergence (e.g., scattering) from a non-absorptive collision

$\mathcal{A}(\mathbf{p})$ for particles undergoing absorption, which is considered terminal in this work

$\mathcal{B}_{\text{ff}}(\mathbf{p}, \mathbf{p}')$ for the forced-flight process

$\mathcal{T}_{\text{ff}}(\mathbf{p}, \mathbf{p}')$ for free flight, with truncation, following forced-flight

HSME Components: Scoring Functions

- ▶ Scoring functions
 - ▶ Probability density functions giving history-scoring behavior
 - ▶ Surface-crossing tally scoring function:

$$f_S(\mathbf{p}, s) = \delta(s - w), \mathbf{x} \in \partial\Gamma_S, \boldsymbol{\Omega} \cdot \mathbf{n} > 0, \quad (6)$$

- ▶ Expected track-length tally scoring function (Solomon, 2010):

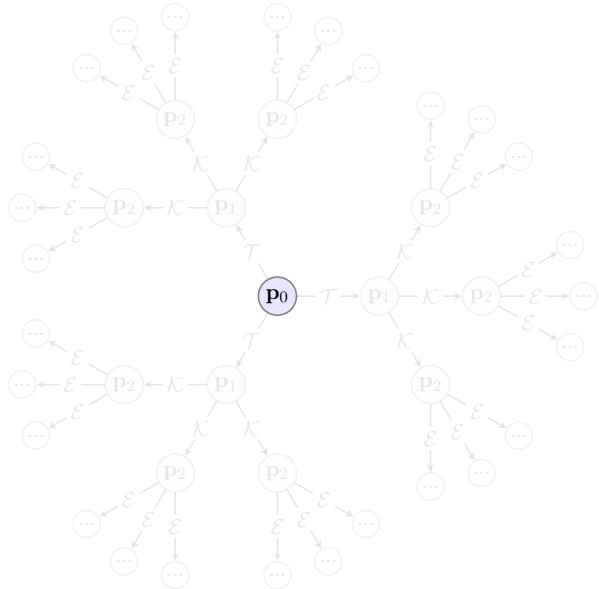
$$f_T(\mathbf{p}, s) = \delta\left(s - \frac{w}{V\Sigma_t(\mathbf{x})} [1 - \exp(-d(\mathbf{x}, \boldsymbol{\Omega}) \cdot \Sigma_t(\mathbf{x}))]\right), \mathbf{x} \in \Gamma_T, \quad (7)$$

- ▶ Construct HSPDF from transport operators and scoring functions, e.g., analog collision with emergence:

$$\begin{aligned} \psi_E(\mathbf{p}_0, s) &= \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \\ &\times \int ds_T f_T(\mathbf{p}_3, s_T) \psi(\mathbf{p}_3, s - s_T). \end{aligned} \quad (8)$$

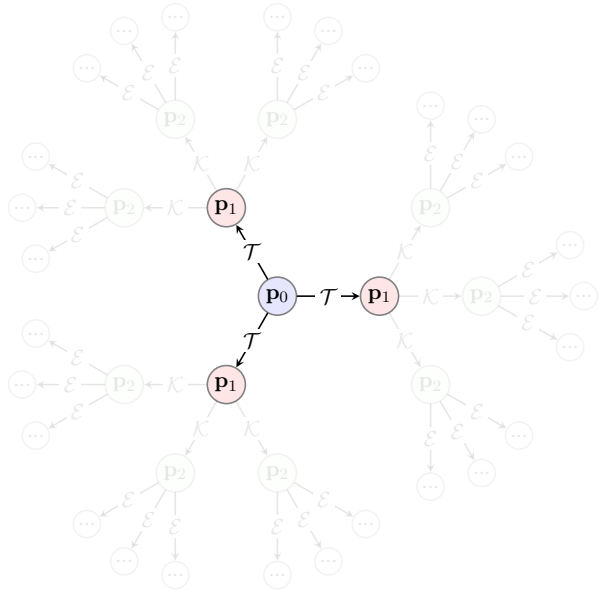
Forward Random Walk Interpretation (→)

$$\begin{aligned} \psi_{\mathcal{E}}(\mathbf{p}_0, s) = & \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \\ & \times \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\ & \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \\ & \times \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \\ & \times \psi(\mathbf{p}_3, s - s_{\mathcal{T}}) \end{aligned}$$



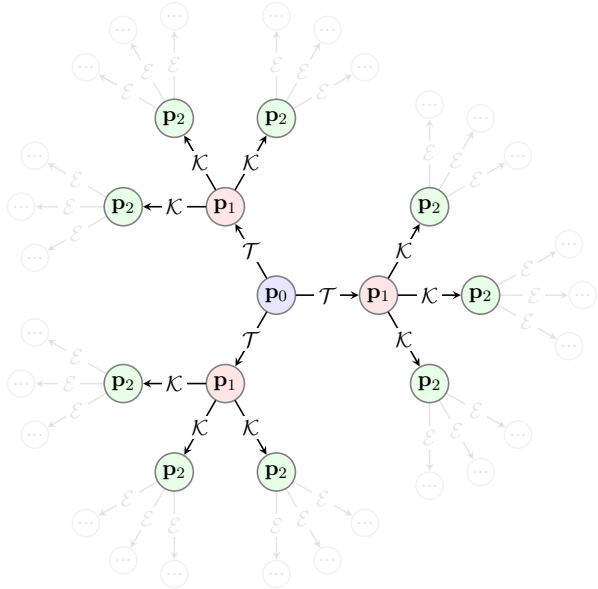
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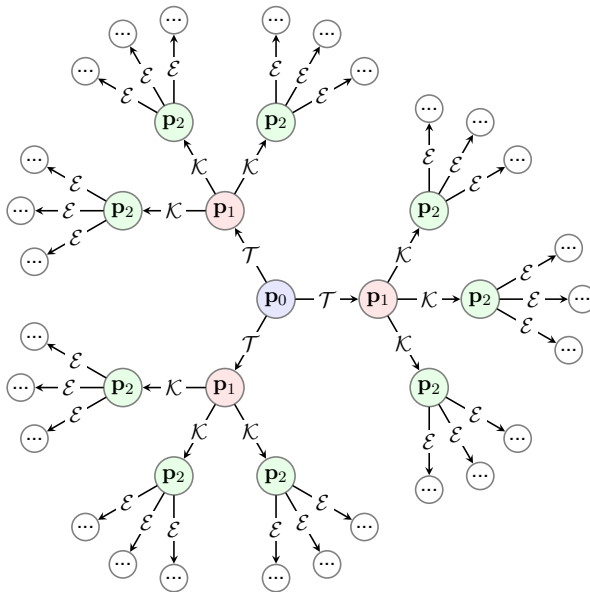
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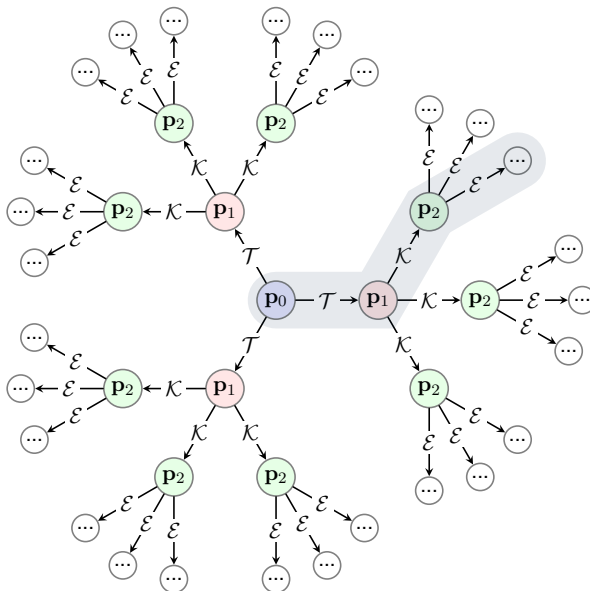
Forward Random Walk Interpretation (→)

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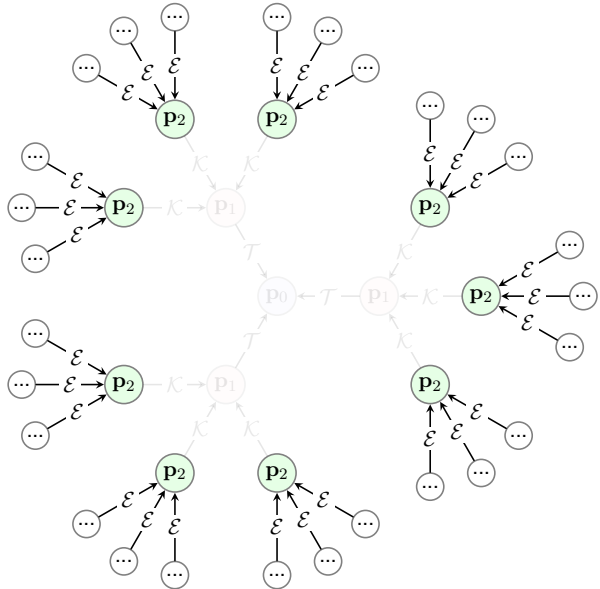
Forward Random Walk Interpretation (→)

$$\begin{aligned}
 \psi_{\mathcal{E}}(\mathbf{p}_0, s) = & \\
 & \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \\
 & \times \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\
 & \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \\
 & \times \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \\
 & \times \psi(\mathbf{p}_3, s - s_{\mathcal{T}})
 \end{aligned}$$



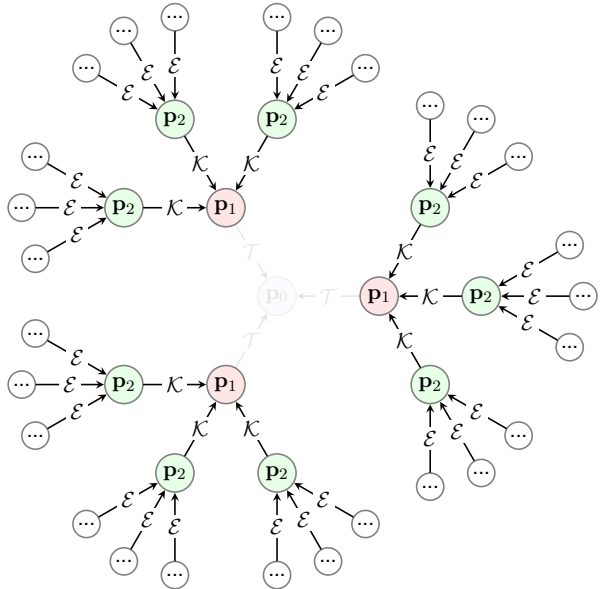
Adjoint Random Walk Interpretation (←)

$$\begin{aligned} \psi_{\mathcal{E}}(\mathbf{p}_0, s) = & \\ & \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \\ & \times \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\ & \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \\ & \times \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \\ & \times \psi(\mathbf{p}_3, s - s_{\mathcal{T}}) \end{aligned}$$



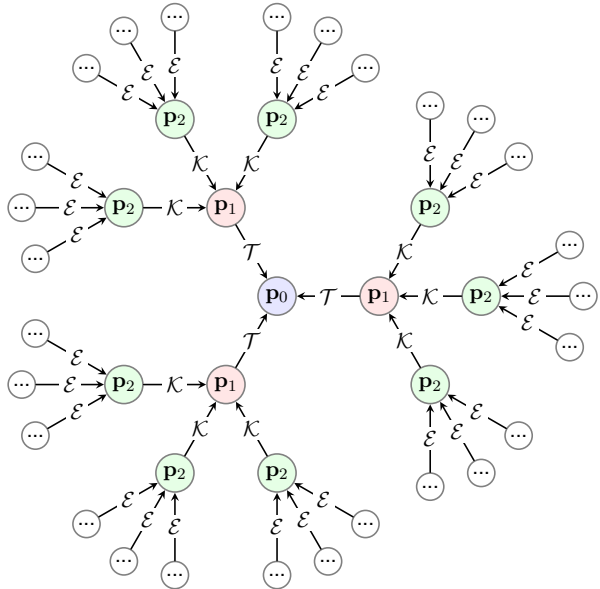
Adjoint Random Walk Interpretation (←)

$$\begin{aligned} \psi_{\mathcal{E}}(\mathbf{p}_0, s) = & \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \\ & \times \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\ & \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \\ & \times \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \\ & \times \psi(\mathbf{p}_3, s - s_{\mathcal{T}}) \end{aligned}$$



Adjoint Random Walk Interpretation (\leftarrow)

$$\begin{aligned} \psi_{\mathcal{E}}(\mathbf{p}_0, s) = & \\ & \mathcal{T}(\mathbf{p}_0, \mathbf{p}_1) \\ & \times \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\ & \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \\ & \times \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \\ & \times \psi(\mathbf{p}_3, s - s_{\mathcal{T}}) \end{aligned}$$



HSME Calculation and Use

- ▶ The m moments of the history-score distribution are:

$$\Psi_m(\mathbf{p}_0) = \int_{-\infty}^{\infty} s^m \psi(\mathbf{p}_0, s) ds \quad (9)$$

- ▶ For $m = 1$: comparable to adjoint integral transport equation
- ▶ Associated tally responses (with physical source term $Q(\mathbf{p}_0)$) are:

$$M_m = \int \Psi_m(\mathbf{p}_0) Q(\mathbf{p}_0) d\mathbf{p}_0 \quad (10)$$

- ▶ Population variance is:

$$\sigma^2 = M_2 - M_1^2 \quad (11)$$

- ▶ Difficulty of solving for $\Psi_{m>1}(\mathbf{p}_0)$ affected by VR techniques used

Forced-flight Biasing & Transmission Kernels

- ▶ Forced-flight biasing kernel (for notational convenience):

$$\begin{aligned} \mathcal{B}_{\text{ff}}(\mathbf{p}, \mathbf{p}') &\equiv \int dV' \int d\Omega' \int dE' \int dw' \\ &\mathbb{1}(\mathbf{x} \notin \{\mathbf{x}_{\text{ff}}\}) \delta(\mathbf{x}' - \mathbf{x}_{\text{ff}}(\mathbf{x}, \Omega')) \\ &\times \tilde{g}(\Omega, E \rightarrow \Omega', E') \\ &\times \left[\beta(\mathbf{x}) \delta\left(w' - \frac{w}{\beta(\mathbf{x})} \frac{g(\Omega, E \rightarrow \Omega', E')}{\tilde{g}(\Omega, E \rightarrow \Omega', E')} \exp[-\lambda(\mathbf{x}, \mathbf{x}_{\text{ff}}, E)]\right) \right. \\ &\quad \left. + (1 - \beta(\mathbf{x})) \delta(w' - 0) \right] \end{aligned}$$

where

$\mathbb{1}(\mathbf{x} \notin \{\mathbf{x}_{\text{ff}}\})$ indicator function whether original position is inside or on surface of forced-flight region

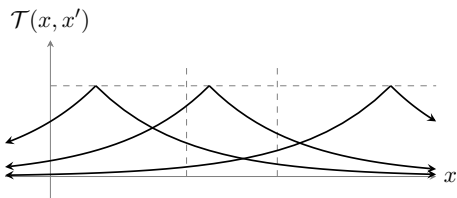
$\delta(\cdot)$ Dirac delta

$\mathbf{x}_{\text{ff}}(\mathbf{x}, \Omega')$ nearest boundary point of forced flight to x along Ω'

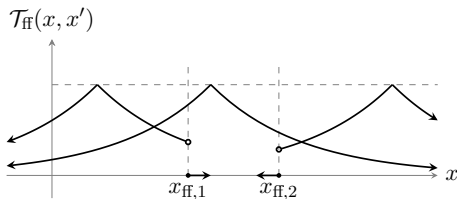
Forced-flight Biasing & Transmission Kernels

- Complementary 1-D forced-flight-associated free-flight transmission kernel

$$\mathcal{T}_{\text{ff}}(\mathbf{p}, \mathbf{p}') = \begin{cases} 0, & \left[\begin{array}{l} \mathbf{x} \notin \{\mathbf{x}_{\text{ff}}\} \text{ and} \\ \frac{\mathbf{x}' - \mathbf{x}}{\|\mathbf{x}' - \mathbf{x}\|} \cdot \frac{\mathbf{h}}{\|\mathbf{h}\|} = 1 \text{ and} \\ \|\mathbf{x}' - \mathbf{x}\| \geq \|\mathbf{h}\| \end{array} \right] \forall \mathbf{h} \in \{\mathbf{x}_{\text{ff}} - \mathbf{x}\} \\ \mathcal{T}(\mathbf{p}, \mathbf{p}'), & \text{otherwise} \end{cases} \quad (12)$$

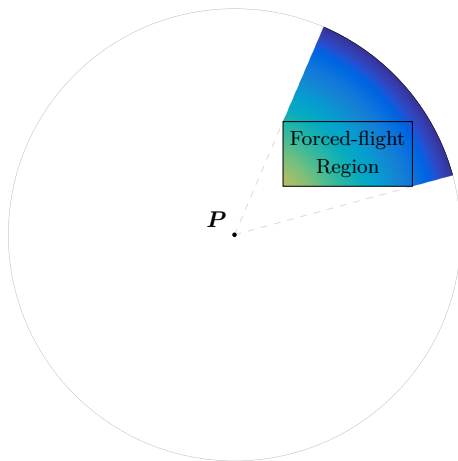
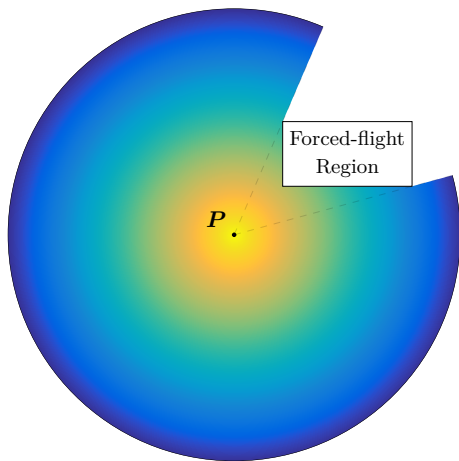


Analog



Forced Flight

Forced-flight Biasing & Transmission Kernels



Random Walk Incorporating Forced-flight

- ▶ The Monte Carlo random walk with forced-flight is:

$$\begin{aligned}\psi_{\text{ff}}(\mathbf{p}_0, s) &= \mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\ &\quad \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \int ds_{\mathcal{E}} \psi(\mathbf{p}_3, s_{\mathcal{E}}) \\ &\quad \times \mathcal{B}_{\text{ff}}(\mathbf{p}_2, \mathbf{p}_4) \psi(\mathbf{p}_4, s - s_{\mathcal{T}} - s_{\mathcal{E}}),\end{aligned}\tag{13}$$

- ▶ Forced-flight acts as a conditional splitting process
 - ▶ Applied in concert with analog non-absorptive collision and surface crossing
- ▶ Truncating transmission kernel applies for all random walks

Forced-flight Second HSME Solution Approach

- ▶ Operate on both sides as $\int ds s^2 (\cdot)$
- ▶ Substitute $u = s - s_{\mathcal{T}}$ so $s = u + s_{\mathcal{T}}$ and $ds = du$ to obtain

$$\begin{aligned}\Psi_{2,\text{ff}}(\mathbf{p}_0) &= \mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \\ &\quad \times \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \int ds_{\mathcal{T}} f_{\mathcal{T}}(\mathbf{p}_3, s_{\mathcal{T}}) \int ds_{\mathcal{E}} \psi(\mathbf{p}_3, s_{\mathcal{E}}) \\ &\quad \times \mathcal{B}_{\text{ff}}(\mathbf{p}_2, \mathbf{p}_4) \int du (u + s_{\mathcal{E}} + s_{\mathcal{T}})^2 \psi(\mathbf{p}_4, u). \quad (14)\end{aligned}$$

- ▶ Distribute the binomial and perform the integrations to obtain moments
- ▶ Separate into $\Psi_{2,\text{ff}}$ and Q_2 to ease incorporation into solver
 - ▶ Result on next slide

Forced-flight Second HSME Result

$$\begin{aligned}\Psi_{2,\text{ff}}(\mathbf{p}_0) &= \mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \Psi_2(\mathbf{p}_3) \\ &\quad + \mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \mathcal{B}_{\text{ff}}(\mathbf{p}_2, \mathbf{p}_4) \Psi_2(\mathbf{p}_4) \\ &\quad + Q_{2,\text{ff}}(\mathbf{p}_0)\end{aligned}\tag{15a}$$

$$\begin{aligned}Q_{2,\text{ff}}(\mathbf{p}_0) &= \mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \overline{s^2_{\mathcal{T}}}(\mathbf{p}_3) \\ &\quad + 2\mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \Psi_1(\mathbf{p}_3) \overline{s_{\mathcal{T}}}(\mathbf{p}_3) \\ &\quad + 2\mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \mathcal{B}_{\text{ff}}(\mathbf{p}_2, \mathbf{p}_4) \overline{s_{\mathcal{T}}}(\mathbf{p}_3) \Psi_1(\mathbf{p}_4) \\ &\quad + 2\mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) \underbrace{\mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) \Psi_1(\mathbf{p}_3) \mathcal{B}_{\text{ff}}(\mathbf{p}_2, \mathbf{p}_4) \Psi_1(\mathbf{p}_4)}_{\text{Cross term}}\end{aligned}\tag{15b}$$

Future Time Equation (FTE)

- ▶ Each event e requires some processing time τ_e , which is represented by a time “scoring” function

$$f_e(\mathbf{p}, \tau) = \delta(\tau - \tau_e) \quad (16)$$

from the events

- τ_{tally} time to process a tally event,
- τ_{col} time to process a collision event,
- τ_{xs} time to process a cross-section lookup,
- τ_{geom} time to perform transmission along a free-flight trajectory,
- τ_{rt} time to perform ray tracing, per Monte Carlo surface, for forced-flight variance reduction,
- τ_{ff} time to perform all other forced-flight variance reduction processing,
- τ_{surf} time to process surface-crossing,
- τ_{bank} time to process a particle bank event, and
- τ_{src} time to process a forward source event as noted previously.

Future Time Equation (FTE), cont.

- ▶ Construct FTPDF

$$v(\mathbf{p}_0, \tau) = v_S(\mathbf{p}_0, \tau) + v_{\text{ff}}(\mathbf{p}_0, \tau) + v_{\mathcal{A}}(\mathbf{p}_0, v) \quad (17)$$

compared with the analog FTPDF

$$v(\mathbf{p}_0, \tau) = v_S(\mathbf{p}_0, \tau) + v_{\mathcal{E}}(\mathbf{p}_0, \tau) + v_{\mathcal{A}}(\mathbf{p}_0, v) \quad (18)$$

- ▶ Integrate to get the first moment, the future-time equation (FTE)

$$\Upsilon(\mathbf{p}_0) = \int d\tau \tau v(\mathbf{p}_0, \tau) \quad (19)$$

- ▶ The partial forced-flight biased FTE is:

$$\begin{aligned} \Upsilon_{\text{ff}}(\mathbf{p}_0) = & \mathcal{T}_{\text{ff}}(\mathbf{p}_0, \mathbf{p}_1) \{ \overline{\tau}_{\text{geom}}(\mathbf{p}_2) + \mathcal{K}(\mathbf{p}_1, \mathbf{p}_2) [\overline{\tau}_{\text{col}}(\mathbf{p}_2) \\ & + \mathcal{B}_{\text{ff}}(\mathbf{p}_2, \mathbf{p}_4) [\beta(\mathbf{p}_4) \overline{\tau}_{\text{ff}}(\mathbf{p}_4) + \beta(\mathbf{p}_4) n_{\text{surf}}(\mathbf{p}_4) \overline{\tau}_{\text{rt}}(\mathbf{p}_4) + \Upsilon(\mathbf{P}_4)] \\ & + \mathcal{E}(\mathbf{p}_2, \mathbf{p}_3) [\overline{\tau}_{\text{tally}}(\mathbf{p}_3) + \overline{\tau}_{\text{xs}}(\mathbf{p}_3) + \Upsilon(\mathbf{P}_3)] \} . \end{aligned} \quad (20)$$

Summary & Future Work

- ▶ History-score moment equations
 - ▶ Biasing kernel deduced, HSPDF constructed, HSMEs derived
 - ▶ Show reasonable moment-ordered quantities and cross terms
- ▶ Future time scales according to
 - ▶ Local forced flight rouletting parameter, β
 - ▶ Number of Monte Carlo surfaces along forced-flight trajectory
- ▶ Future work:
 - ▶ Apply forced-flight variance reduction to source-emission events
 - ▶ Analyze multiple forced-flight regions
 - ▶ Incorporate forced-flight weight cutoffs

Questions?

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Backup Slides

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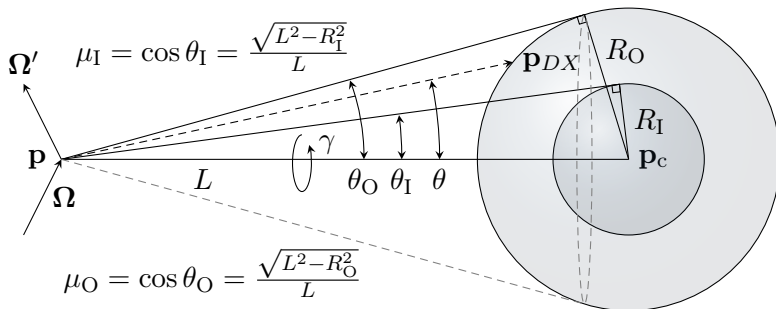
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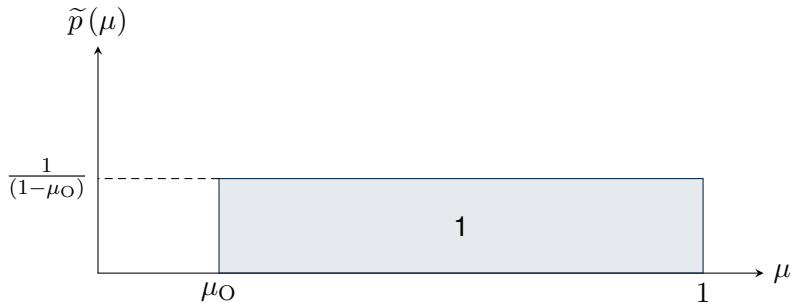
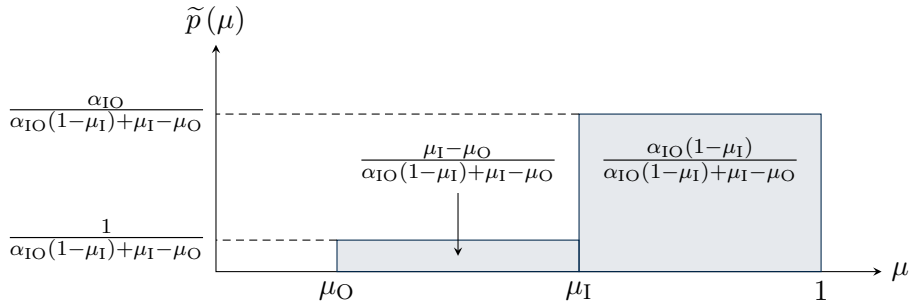
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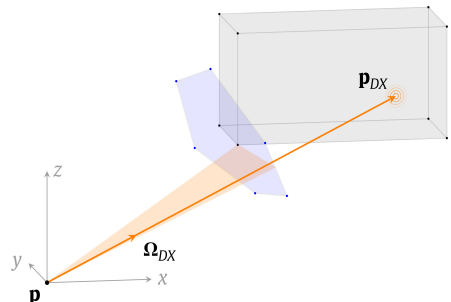
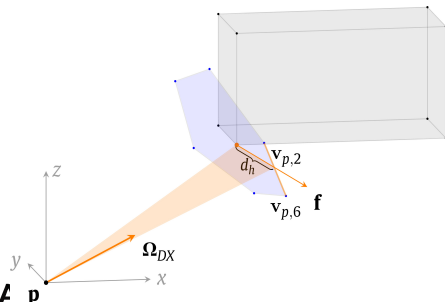
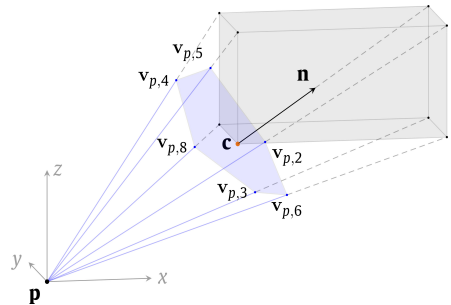
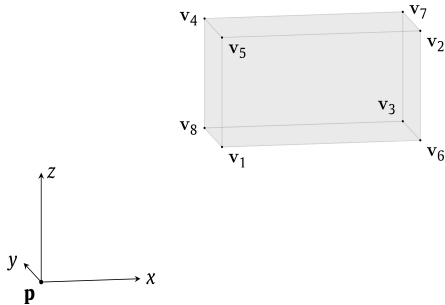
Full DXTRAN Treatment



Inner/Outer Sphere Polar Cosine Biasing PDF



Arbitrary Convex Polyhedral DXTRAN Process



CADIS & FW-CADIS Overview

Adjoint Solution

Forward flux, $\mathbf{M}^* \psi^* = \Sigma_d$

Total response, $R = \langle q, \psi^* \rangle$

CADIS

Adjoint flux, $\mathbf{M}^* \psi^* = \Sigma_d$

Total response, $R = \langle q, \psi^* \rangle$

Weight targets, $w = R/\psi^*$

Biased source, $\tilde{q} = \psi^* q/R$

Forward Solution

Forward flux, $\mathbf{M} \psi = q$

Total response, $R = \langle \Sigma_d, \psi \rangle$

FW-CADIS

Forward flux, $\mathbf{M} \psi = q$

Adjoint flux, $\mathbf{M}^* \psi^* = \Sigma_d / \langle \Sigma_d, \psi \rangle_{E, \Omega}$

Total response, $R = \langle q, \psi^* \rangle$

Weight targets, $w = R/\psi^*$

Biased source, $\tilde{q} = \psi^* q/R$

History-Score-Moment Equation Weight Separability

- ▶ Weight separability¹ with weight-independent VR techniques:

$$\Psi_m(\mathbf{R}, aw) = a^m \Psi_m(\mathbf{R}, w) = a^m w^m \Psi_m(\mathbf{R}, w = 1) \quad (21)$$

- ▶ This separability shows that weight-independent techniques do not require a discretized weight mesh for any moments
 - ▶ Reduced memory requirements
 - ▶ Reduced deterministic solver computational time
 - ▶ Permits easier incorporation into pre-existing deterministic solver

¹ T. E. Booth et al., Nucl. Sci. & Eng., vol. 71, pp. 128–142, Aug. 1979.