Los Alamos
NATIONAL LABORATORY
— EST.1943 —

LA-UR-21-25127
Approved for public release; distribution is unlimited.

Title:	Derivation of the Future Time Equation for Analog, Non-Multiplying Monte Carlo Simulation
Author(s):	Pearson, Eric John Kulesza, Joel A. Kiedrowski, Brian Christopher
Intended for:	Report
Issued:	2021-05-27

Derivation of the Future Time Equation
for Analog, Non-Multiplying Monte Carlo Simulation

Eric J. Pearson, Joel A. Kulesza, and Brian C. Kiedrowski

May 24, 2021

Introduction

The expected computational time required to simulate a particle from a point in phase space through a Monte Carlo history, termed the expected future time, is found by solving the Future Time Equation (FTE). The expected future time may be useful when generating variance reduction parameters for a Monte Carlo simulation with a method such as Consistent Adjoint Driven Importance Sampling (CADIS). This report presents a detailed derivation of the Future Time Probability Density Function (FTPDF) and FTE for neutral particle Monte Carlo transport to aid future researchers. For simplicity, this derivation only considers analog transport in non-multiplying media.

The FTPDF describes the probability of the simulation of a complete history starting from some point in phase space requiring a given computational time and the FTE is the first time moment of the FTPDF. In analog neutral particle transport, the only routines (hereafter referred to as events) needed in a Monte Carlo code to describe a particle history are the following:

`source event`, the event in which the distributions that define each dimension of the source are sampled to construct a particle;

`transition event`, the event in which the distribution that describes the respective likelihoods of each transport event is sampled and the particle is transmitted to the sampled event;

`collision event`, the event in which a particle collision is processed; and

`surface-crossing event`, the event in which a particle crossing a constructive solid geometry surface is processed.

Describing the Monte Carlo simulation with only these events is possible because the many computations necessary for a useful simulation such as tallying and looking up cross sections are abstracted under the above events. A flowchart depicting the possible steps in one history of the simulation with the previously stated simplifications is given in Fig. 1.

1 Derivation of the Future Time Probability Density Function

Transport operator notation is used as in Ref. [1] and, as noted there, this notation breaks from previous work but does not change conclusions. See Ref. [2–4] for transport kernel notation used in similar derivations.
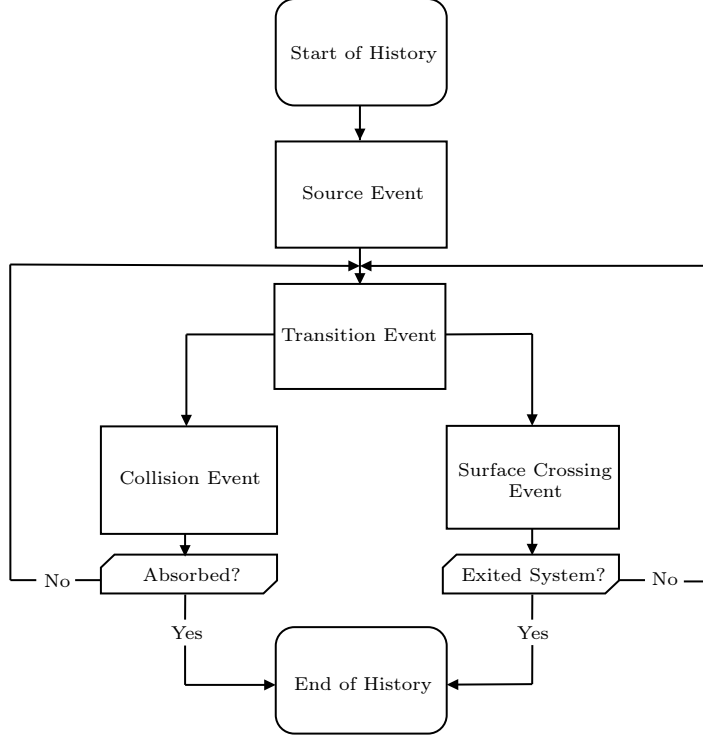
Figure 1: Flowchart depicting all possible steps in one history of an analog neutral particle Monte Carlo simulation in non-multiplying media.

1.1 Definitions

In the following sections five operators are defined to describe the random walk a particle may take in a simulated history. Next, probability density functions (PDFs) governing the contribution of computational time at several points in transport are defined. The FTPDF is then formed using these definitions. The particle phase space considered for all definitions includes position (x, y, z), direction (μ, γ), energy (E), and statistical weight (w) and is denoted as

$$\boldsymbol{p} \equiv (\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) \equiv (x, y, z, \mu, \gamma, E, w). \tag{1}$$

Note that the statistical weight of a particle gives the number of physical particles being represented by the simulation particle and is modified from the analog value to preserve the expected value of estimated quantities when using variance reduction techniques. This work does not consider variance reduction techniques; however, statistical weight is still considered so that a particle at the end of simulation can be represented with a weight of zero.

1.1.1 Event Transition Operator

After any non-terminal event, the next event that a particle transitions to must be sampled. The following operators account for all possible phase spaces that the particle may transition into as the result of the next sampled event and weight these phase spaces with the probability of free-flight to them. The particle streaming from some position, $\boldsymbol{x}$ in $\boldsymbol{p}$, along the direction of flight of the particle, $\hat{\boldsymbol{\Omega}}$ in $\boldsymbol{p}$, may either cross the surface bounding the cell it currently resides in or first undergo a collision. The particle colliding at some

point, $\boldsymbol{x}'$ in $\boldsymbol{p}'$, before reaching the next surface is governed by the *transition-to-collision operator*,

$$\mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}') = \int dx' \int d\Omega' \int dE' \int \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}'\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)$$
$$\times \delta(\hat{\boldsymbol{\Omega}}' - \hat{\boldsymbol{\Omega}})\delta(E' - E)\delta(w' - w)dw', \qquad \frac{\|\boldsymbol{x} - \boldsymbol{x}'\|}{\|\boldsymbol{x} - \boldsymbol{x}_s\|} < 1, \quad (2)$$

where $\boldsymbol{x}_s$ is the point of intersection between the particle-direction vector and the surface bounding the cell the particle resides in, $\Sigma_t(\boldsymbol{p})$ is the total macroscopic cross section, and $\mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}') = 0$ for all positions outside of the current cell. There is a set of phase spaces supported by the transition-to-collision operator. Each phase space in this set is identical to the initial phase space except that the position is in the set of all points along the particle direction inside the current cell, $(\{\boldsymbol{x}_\ell\}, \hat{\boldsymbol{\Omega}}, E, w)$ where $\{\boldsymbol{x}_\ell\}$ is the set of all points that lay on the ray connecting $\boldsymbol{x}$ and $\boldsymbol{x}_s$. Streaming to the next surface in the simulation and intersecting at point $\boldsymbol{x}_s$ in $\boldsymbol{p}'$ is governed by the *transition-to-surface operator*,

$$\mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}') = \int dx' \int d\Omega' \int dE' \int \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}'\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)$$
$$\times \delta(\boldsymbol{x}' - \boldsymbol{x}_s)\delta(\hat{\boldsymbol{\Omega}}' - \hat{\boldsymbol{\Omega}})\delta(E' - E)\delta(w' - w)dw'. \quad (3)$$

Note that $\boldsymbol{x}_s$ will always exist because the particle is not simulated after leaving the system, i.e., leaving the system is a terminal event. There is only one phase space supported by the transition-to-surface operator. This phase space is identical to the initial phase space except that the position is at the point of intersection between the particle-direction vector and the bounding surface of the current cell, $(\boldsymbol{x}_s, \hat{\boldsymbol{\Omega}}, E, w)$.

These operators may be interpreted as attenuating some probability from all phase spaces with support back to the current phase space of the particle. Note that this interpretation is adjoint in that it considers particles moving backwards along the particle-direction vector, i.e., backwards in time. Considering the operators together implies that a simulation particle cannot transition past the surface of the cell in which it currently resides in one event.

1.1.2 Collision Event Operator

Given that a collision has been transitioned to, the possibilities of a particle continuing on or terminating must be considered depending on the reaction that the particle undergoes at the collision. Analog transport in non-multiplying media implies that a particle only continues on after scattering and is otherwise absorbed in the collision, terminating the history. The total macroscopic cross section is

$$\Sigma_t(\boldsymbol{p}) = \Sigma_s(\boldsymbol{p}) + \Sigma_a(\boldsymbol{p}), \quad (4)$$

where $\Sigma_s(\boldsymbol{p})$ and $\Sigma_a(\boldsymbol{p})$ are the scattering and absorption macroscopic cross sections, respectively. A particle undergoing a collision event, scattering, and then continuing on is governed by the *scattering collision operator*,

$$\mathcal{C}_S(\boldsymbol{p}, \boldsymbol{p}') = \int dx' \int d\Omega' \int dE' \int \Sigma_s(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\delta(\boldsymbol{x}' - \boldsymbol{x})\delta(w' - w)dw', \quad (5)$$

where $\Sigma_s(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')$ is the double-differential scattering cross section corresponding to the product of the scattering cross section and the probability density function governing the outgoing angle and energy,

$$\Sigma_s(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E') = \Sigma_s(\boldsymbol{p})P(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E'). \quad (6)$$

The phase spaces supported by the scattering collision operator are all directions and energies at the particle position and weight, $(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}', E', w)$, $\hat{\boldsymbol{\Omega}}' \in 4\pi$, $E' \in [0, \infty)$. All outgoing directions and energies are considered

3

valid because the double-differential scattering cross section may be zero. Likewise, a particle undergoing a collision event, being absorbed, and terminating the history is governed by the *absorptive collision operator*,

$$\mathcal{C}_A(\boldsymbol{p}, \boldsymbol{p}') = \int dx' \int d\Omega' \int dE' \int \Sigma_a(\boldsymbol{x}, E)\delta(\boldsymbol{x}' - \boldsymbol{x})\delta(\hat{\boldsymbol{\Omega}}' - \hat{\boldsymbol{\Omega}})\delta(E' - E)\delta(w' - 0)dw'. \tag{7}$$

The only supported phase space resulting from the absorptive collision operator is identical to the incident particle phase space except for a statistic weight of zero denoting a terminated history, $(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, 0)$.

These operators may be interpreted as accounting for all phase spaces with support resulting from a reaction of the type denoted by the operator subscript at the particle phase space and weighting these phase spaces by the corresponding reaction cross section. Note that this interpretation is again adjoint in that it considers all resulting phase spaces being tracked back to the incident phase space. To extend this work to consider more reaction types, such as fission or collision-related variance-reduction processing, additional collision operators may be defined and applied similarly throughout the derivation. As discussed in Sec. 1.1.4, these additional operators should be accompanied with the computational time required to process the event they govern.

1.1.3 Surface-Crossing Event Operator

Given that a surface-crossing event has been transitioned to, the particle exiting the current cell is processed. A surface-crossing event does not alter the particle position in the simulation, instead it alters the current cell that the particle resides in, which is a neglected dimension in the phase space (as defined herein). However, processing crossing a surface requires computational time, so it must be considered. If the surface being crossed is a system boundary, the history is terminated; otherwise, the particle continues on into the next cell. A particle undergoing a surface-crossing event is governed by the *surface-crossing operator*,

$$\mathcal{S}(\boldsymbol{p}, \boldsymbol{p}') = \begin{cases} \int dx' \int d\Omega' \int dE' \int \delta(\boldsymbol{x}' - \boldsymbol{x})\delta(\hat{\boldsymbol{\Omega}}' - \hat{\boldsymbol{\Omega}})\delta(E' - E)\delta(w' - w)dw', & \boldsymbol{x} \in \{\boldsymbol{x}_{\text{Internal Surfaces}}\}, \\ \int dx' \int d\Omega' \int dE' \int \delta(\boldsymbol{x}' - \boldsymbol{x})\delta(\hat{\boldsymbol{\Omega}}' - \hat{\boldsymbol{\Omega}})\delta(E' - E)\delta(w' - 0)dw', & \boldsymbol{x} \in \{\boldsymbol{x}_{\text{Boundary Surfaces}}\}, \\ 0, & \text{otherwise}, \end{cases} \tag{8}$$

where $\{\boldsymbol{x}_{\text{Internal Surfaces}}\}$ is the set of all points that lay on the internal surfaces of the system, i.e., surfaces with cells on either side, and $\{\boldsymbol{x}_{\text{Boundary Surfaces}}\}$ is the set of all points that lay on the boundary surfaces of the system, i.e., surfaces with a cell only on one side. Note that this operator is an indicator of whether a surface is crossed, similar to the arrival operator used in Ref. [5]. This operator may be interpreted as accounting for all supported phase spaces that result from a surface crossing. Trivially, the only supported phase space is that of the incident particle, $(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w)$, given that the particle is on an internal surface, $\boldsymbol{x} \in \{\boldsymbol{x}_{\text{Internal Surfaces}}\}$ or that of the incident particle except with zero weight, $(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, 0)$, given that that particle is on a boundary surface, $\boldsymbol{x} \in \{\boldsymbol{x}_{\text{Boundary Surfaces}}\}$.

1.1.4 Time Contribution Probability Density Functions

For any event to be processed, the computational time required is contributed to the total amount of time required by the simulation. The exact time required per event call varies because of a number of factors including problem specification, code configuration, system hardware, etc. For discussion on how representative times per event call may be found using profiling tools see Ref. [3, 4]. It is also possible to find representative values using timing routines embedded in the Monte Carlo transport code, such as how this work is implemented in the University of Michigan's hybrid deterministic-Monte Carlo Hammer code [6, 7]. For this derivation, the average time per call determined empirically by some means will be assumed to have been found and is defined as:

τ_{src}, the time required to process a `source event`;

τ_{trans},   the time required to process a `transition event`;

τ_{surf},   the time required to process a `surface-crossing event`;

$\tau_{\text{col},S}$,   the time required to process a scattering `collision event`;

$\tau_{\text{col},A}$,   the time required to process an absorptive `collision event`.

The probability density function for contributing a time τ_e at some event e is defined as

$$f_e(\boldsymbol{p}, \tau) = \delta(\tau - \tau_e), \tag{9}$$

denoting that if event e is processed, a time of τ_e is contributed. The dependence on the phase space of the particle is included in Eq. 9 so that it may be more easily extended to less trivial forms in future work.

1.2 Future Time Probability Density Function

Using the transport operators and time contribution functions defined above, the FTPDF may be defined in an integral form by defining partial FTPDFs for surface-crossing and collision events and summing the two.

The partial FTPDF describing the probability of time τ being required to simulate a particle at phase space $\boldsymbol{p}$ that first undergoes a collision is denoted as

$$
\begin{aligned}
\upsilon_{\mathcal{C}}(\boldsymbol{p}, \tau) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) &\int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans})} \\
&\times \Bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \int f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) \delta(\tau - \tau_{\text{trans}} - \tau_{\text{col},A}) d\tau_{\text{col},A} \\
&+ \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau_{\text{col},S} \Bigg),
\end{aligned} \tag{10}
$$

where $\upsilon(\boldsymbol{p}, \tau)$ is the FTPDF, to be defined later. The term following the absorptive collision operator,

$$\int f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) \delta(\tau - \tau_{\text{trans}} - \tau_{\text{col},A}) d\tau_{\text{col},A},$$

accounts for the probability of requiring exactly τ time from processing a transition and absorptive collision event as enforced by the Dirac delta function evaluated at time $\tau - \tau_{\text{trans}} - \tau_{\text{col},A}$. Note that the transition and absorptive collision events are processed at different phase spaces. The absorptive collision operator accounts for this probability at all supported phase spaces following an absorptive collision and weights it according to the probability of entering that phase space through an absorbing event. The term following the scattering collision operator,

$$\int f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau_{\text{col},S},$$

accounts for the probability of the history requiring exactly τ time from simulating the particle through all events to the end of the history from phase space $\boldsymbol{p}_3$ after processing a transition event and scattering collision event. This is enforced by the FTPDF evaluated at the phase space $\boldsymbol{p}_3$ and time $\tau - \tau_{\text{trans}} - \tau_{\text{col},S}$. The scattering collision operator accounts for this probability at all supported phase spaces following a scattering collision and weights it according to the probability of entering that phase space through a scattering event. The first term on the right-hand side,

$$\mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}),$$

acting on the above terms weights the probability of contributing time τ through any collision event at all valid phase spaces according to the probability of transitioning to that phase space. It is then apparent that

5

Eq. 10 accounts for the probability of simulating a particle at phase space $\boldsymbol{p}$ requiring computational time τ given that it undergoes a collision event before crossing the surface bounding the cell it resides in.

Similarly, the partial FTPDF describing the probability of time τ being required to simulate a particle at phase space $\boldsymbol{p}$ that first undergoes a surface crossing is denoted as

$$v_{\mathcal{S}}(\boldsymbol{p}, \tau) = \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4) \int d\tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})$$
$$\times \mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5) \int f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}}) v(\boldsymbol{p}_5, \tau - \tau_{\text{trans}} - \tau_{\text{surf}}) d\tau_{\text{surf}}. \tag{11}$$

Reading Eq. 11 right to left, the probability of the history requiring exactly τ time from simulating the particle through all events to the end of the history from phase space $\boldsymbol{p}_5$ after processing a transition and surface-crossing event is accounted for by the FTPDF evaluated at $(\boldsymbol{p}_5, \tau - \tau_{\text{trans}} - \tau_{\text{surf}})$ in the term following the surface-crossing operator,

$$\int f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}}) v(\boldsymbol{p}_5, \tau - \tau_{\text{trans}} - \tau_{\text{surf}}) d\tau_{\text{surf}}.$$

The surface-crossing operator acting on this term accounts for this probability at all supported phase spaces following a surface crossing and weights it according to the probability of entering that phase space through a surface crossing. Finally, the leftmost term on the right-hand side,

$$\mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4) \int d\tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}}),$$

acting on the above terms weights the probability of contributing time τ from a surface-crossing event at all supported phase spaces according to the probability of transitioning to that phase space. This confirms that Eq. 11 accounts for the probability of a particle simulated at phase space $\boldsymbol{p}$ requiring computational time τ given that it crosses the surface bounding the cell it resides in before it undergoes a collision.

Because a particle may only transition to a surface-crossing event or a collision event, the FTPDF is formed by summing the probabilities of these disjoint events, given by Eqs. 10 and 11, and is found to be

$$v(\boldsymbol{p}, \tau) d\tau = v_{\mathcal{C}}(\boldsymbol{p}, \tau) d\tau + v_{\mathcal{S}}(\boldsymbol{p}, \tau) d\tau \tag{12a}$$

with the associated boundary condition

$$v(\boldsymbol{p}, \tau) = \delta(\tau - 0), \; w = 0, \tag{12b}$$

which arises because no computational effort is expended on terminated particles. See Fig. 2 for a diagram of the way all possible events are connected in the random walk.

2 Derivation of the Future Time Equation

The Future Time Equation (FTE) is the first time moment of Eq. 12:

$$\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \Upsilon(\boldsymbol{p}) = \int \tau v(\boldsymbol{p}, \tau) d\tau. \tag{13}$$

This moment represents the expected computational time to simulate a hypothetical particle introduced at phase-space position $\boldsymbol{p}$. From the FTE, one may compute the expected time per history as

$$T = \int (\Upsilon(\boldsymbol{p}) + \tau_{\text{source}}) Q(\boldsymbol{p}) d\boldsymbol{p}, \tag{14}$$

where $Q(\boldsymbol{p})$ is the source distribution and τ_{source} is defined in Sec. 1.1.4. The FTE is derived in integral form by finding the expected value of the collision and surface-crossing FTPDFs given in Eqs. 10 and 11 separately and summing the results. This derivation follows that given in Ref. [3, Sec. 4.3] closely. After the FTE is derived in integral form, it is converted to integro-differential form, which has the form of an adjoint neutron transport equation as it is typically expressed before discretization and solution but with unique source terms.
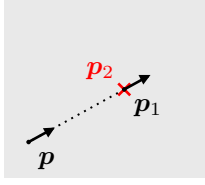
(a) Phase spaces connected by transition-to-collision and absorptive collision events.
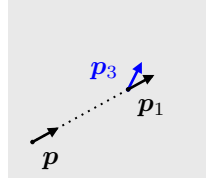
(b) Phase spaces connected by transition-to-collision and scattering collision events.
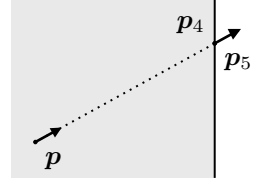
(c) Phase spaces connected by transition-to-surface and surface-crossing events.

Figure 2: Representation of the connections between phase spaces accounted for in analog, non-multiplying neutral particle future time considerations where the light gray region is a cell and the vertical black line is the cell boundary. Note that phase space subscripts map directly to those used in Eq. 25.

2.1 Expected Collision Event Time

The expected time required by a particle simulated at phase space $\boldsymbol{p}$ given that it undergoes a collision event before crossing the surface bounding the cell it resides in is found by taking the first time moment of the collision event probability density function,

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \int \tau \upsilon_{\mathcal{C}}(\boldsymbol{p}, \tau) d\tau. \tag{15}$$

Substituting in the definition of $\upsilon_{\mathcal{C}}(\boldsymbol{p}, \tau)$ from Eq. 10,

$$
\begin{aligned}
\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \int \tau \Bigg(& \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) \\
& \times \Bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \int f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) \delta(\tau - \tau_{\text{trans}} - \tau_{\text{col},A}) d\tau_{\text{col},A} \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int f_{\mathcal{C}_S}(\boldsymbol{p}_2, \tau_{\text{col},S}) \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau_{\text{col},S} \Bigg) \Bigg) d\tau.
\end{aligned}
\tag{16a}
$$

Distributing the integration over τ,

$$
\begin{aligned}
\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \int & d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) \\
\times \Bigg(& \mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \int d\tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) \int \tau \delta(\tau - \tau_{\text{trans}} - \tau_{\text{col},A}) d\tau \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int \tau \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau \Bigg).
\end{aligned}
\tag{16b}
$$

Using $\delta(\tau - \tau_{\text{trans}} - \tau_{\text{col},A}) = \delta(\tau - (\tau_{\text{trans}} + \tau_{\text{col},A}))$,

$$
\begin{aligned}
\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \int & d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) \\
\times \Bigg(& \mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \int f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A})(\tau_{\text{trans}} + \tau_{\text{col},A}) d\tau_{\text{col},A} \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int \tau \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau \Bigg).
\end{aligned}
\tag{16c}
$$

7

Distributing $(\tau_{\text{trans}} + \tau_{\text{col},A})$,

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})$$

$$\times \Bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \bigg(\tau_{\text{trans}} \int f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} \bigg)$$

$$+ \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int \tau \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau \Bigg). \tag{16d}$$

Using $\int f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} = 1$ because it is a probability density function,

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})$$

$$\times \Bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \bigg(\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} \bigg)$$

$$+ \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int \tau \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau \Bigg). \tag{16e}$$

Distributing the integration over τ_{trans},

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}}$$

$$+ \mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \int f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A}$$

$$+ \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int \tau \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau \bigg). \tag{16f}$$

Using $\int f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} = 1$ and collecting terms,

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \bigg(\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} \bigg)$$

$$+ \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int \tau \upsilon(\boldsymbol{p}_3, \tau - \tau_{\text{trans}} - \tau_{\text{col},S}) d\tau \bigg). \tag{16g}$$

Setting $q = \tau - \tau_{\text{trans}} - \tau_{\text{col},A}$,

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \bigg(\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} \bigg)$$

$$+ \int d\tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int d\tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) \int (q + \tau_{\text{trans}} + \tau_{\text{col},S}) \upsilon(\boldsymbol{p}_3, q) dq \bigg). \tag{16h}$$

Distributing $(q + \tau_{\text{trans}} + \tau_{\text{col},S})$,

$$\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1) \bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2) \bigg(\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A}) d\tau_{\text{col},A} \bigg)$$

$$+ \int f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) d\tau_{\text{col},S} \int q \upsilon(\boldsymbol{p}_3, q) dq$$

$$+ \int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) d\tau_{\text{col},S} \int \upsilon(\boldsymbol{p}_3, q) dq$$

$$+ \int f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}}) d\tau_{\text{trans}} \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3) \int \tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S}) d\tau_{\text{col},S} \int \upsilon(\boldsymbol{p}_3, q) dq \bigg). \tag{16i}$$

8

Using $\Upsilon(\boldsymbol{p}) = \int q\upsilon(\boldsymbol{p}, q)d\tau$, $\int f_e(\boldsymbol{p}, \tau_e)d\tau_e = 1$, and $\int \upsilon(\boldsymbol{p}, q)dq = 1$,

$$
\begin{aligned}
\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = {} & \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)\bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2)\bigg(\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A})d\tau_{\text{col},A}\bigg) \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\Upsilon(\boldsymbol{p}_3) \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})d\tau_{\text{trans}} \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\int \tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S})d\tau_{\text{col},S}\bigg).
\end{aligned}
\tag{16j}
$$

Collecting terms yields the final result,

$$
\begin{aligned}
\Upsilon_{\mathcal{C}}(\boldsymbol{p}) = {} & \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)\bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2)\bigg(\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A})d\tau_{\text{col},A}\bigg) \\
& + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\bigg(\Upsilon(\boldsymbol{p}_3) + \int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S})d\tau_{\text{col},S}\bigg)\bigg).
\end{aligned}
\tag{17}
$$

Eq. 17 can be interpreted in the forward sense as a particle being transmitted to a collision and undergoing either an absorption or scattering event. If an absorption event takes place, the expected time required to process a transmission and absorption event is contributed. If a scattering event takes place, the expected time required to process a transmission and scattering event as well as to continue on in the simulation is contributed. Alternatively, Eq. 17 may also be interpreted in the adjoint sense identically to Eq. 10 except that the absorptive and scattering operators now act on the expected execution time of events rather than the probability of events requiring some execution time.

2.2 Expected Surface-Crossing Event Time

The expected time required by a particle simulated at phase space $\boldsymbol{p}$ given that it crosses the surface bounding the cell it resides in before it undergoes a collision is found by taking the first time moment of the surface-crossing event probability density function,

$$
\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = \int \tau\upsilon_{\mathcal{S}}(\boldsymbol{p}, \tau)d\tau.
\tag{18}
$$

Substituting the definition of $\upsilon_{\mathcal{S}}(\boldsymbol{p}, \tau)$ from Eq. 11,

$$
\begin{aligned}
\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = {} & \int \tau\bigg(\mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\int d\tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}}) \\
& \times \mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\int f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})\upsilon(\boldsymbol{p}_5, \tau - \tau_{\text{trans}} - \tau_{\text{surf}})d\tau_{\text{surf}}\bigg)d\tau.
\end{aligned}
\tag{19a}
$$

Distributing the integration over τ,

$$
\begin{aligned}
\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = {} & \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\int d\tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}}) \\
& \times \mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\int d\tau_{\text{surf}} f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})\int \tau\upsilon(\boldsymbol{p}_5, \tau - \tau_{\text{trans}} - \tau_{\text{surf}})d\tau.
\end{aligned}
\tag{19b}
$$

Setting $q = \tau - \tau_{\text{trans}} - \tau_{\text{surf}}$,

$$
\begin{aligned}
\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = {} & \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\int d\tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}}) \\
& \times \mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\int d\tau_{\text{surf}} f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})\int (q + \tau_{\text{trans}} + \tau_{\text{surf}})\upsilon(\boldsymbol{p}_5, q)dq.
\end{aligned}
\tag{19c}
$$

Distributing $(q + \tau_{\text{trans}} + \tau_{\text{surf}})$,

$$\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\bigg(\int f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})d\tau_{\text{trans}}\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5) \int f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})d\tau_{\text{surf}} \int qv(\boldsymbol{p}_5, q)dq$$

$$+ \int \tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})d\tau_{\text{trans}}\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5) \int f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})d\tau_{\text{surf}} \int v(\boldsymbol{p}_5, q)dq \tag{19d}$$

$$+ \int f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})d\tau_{\text{trans}}\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5) \int \tau_{\text{surf}} f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})d\tau_{\text{surf}} \int v(\boldsymbol{p}_5, q)dq \bigg).$$

Using $\Upsilon(\boldsymbol{p}) = \int qv(\boldsymbol{p}, q)d\tau$, $\int f_e(\boldsymbol{p}, \tau_e)d\tau_e = 1$, and $\int v(\boldsymbol{p}, q)dq = 1$,

$$\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\bigg(\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\Upsilon(\boldsymbol{p}_5)$$

$$+ \mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5) \int \tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})d\tau_{\text{trans}} \tag{19e}$$

$$+ \mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5) \int \tau_{\text{surf}} f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})d\tau_{\text{surf}} \bigg).$$

Collecting terms yields the final result,

$$\Upsilon_{\mathcal{S}}(\boldsymbol{p}) = \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\bigg(\Upsilon(\boldsymbol{p}_5) + \int \tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{surf}} f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})d\tau_{\text{surf}} \bigg). \tag{20}$$

Eq. 20 can be interpreted in the forward sense as a particle being transmitted to a surface-crossing event. This process contributes the computational time required to process transmitting the particle and crossing the surface as well as the time required to continue the simulation on the other side of the surface (which, by the definition of the surface-crossing operator and Eq. 12b, is zero after crossing a system boundary). Alternatively, Eq. 20 may also be interpreted in the adjoint sense identically to Eq. 11 except that the surface-crossing operator now acts on the expected execution time of events rather than the probability of events requiring some execution time.

2.3 Future Time Equation in Integral Form

The FTPDF given in Eq. 12 is the sum of the collision FTPDF given in Eq. 10 and the surface-crossing FTPDF given in Eq. 11. The expected value of the FTPDF is then the sum of the expected value of the collision and surface-crossing FTPDFs. For ease of notation define

$$\overline{\tau}_e(\boldsymbol{p}) = \int \tau f_e(\boldsymbol{p}, \tau)d\tau \tag{21}$$

and note that by the definitions given in Sec. 1.1.4,

$$\overline{\tau}_e(\boldsymbol{p}) = \int \tau \delta(\tau - \tau_e)d\tau = \tau_e. \tag{22}$$

The FTE is then given by

$$\Upsilon(\boldsymbol{p}) = \Upsilon_{\mathcal{C}}(\boldsymbol{p}) + \Upsilon_{\mathcal{S}}(\boldsymbol{p}). \tag{23}$$

Using Eq. 10 and 11,

$$\Upsilon(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)\bigg(\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2)\bigg(\int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{col},A} f_{\mathcal{C}_A}(\boldsymbol{p}_2, \tau_{\text{col},A})d\tau_{\text{col},A} \bigg)$$

$$+ \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\bigg(\Upsilon(\boldsymbol{p}_3) + \int \tau_{\text{trans}} f_{\mathcal{T}_C}(\boldsymbol{p}_1, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{col},S} f_{\mathcal{C}_S}(\boldsymbol{p}_3, \tau_{\text{col},S})d\tau_{\text{col},S} \bigg)\bigg) \tag{24a}$$

$$+ \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\bigg(\Upsilon(\boldsymbol{p}_5) + \int \tau_{\text{trans}} f_{\mathcal{T}_S}(\boldsymbol{p}_4, \tau_{\text{trans}})d\tau_{\text{trans}} + \int \tau_{\text{surf}} f_{\mathcal{S}}(\boldsymbol{p}_5, \tau_{\text{surf}})d\tau_{\text{surf}} \bigg).$$

Using $\int \tau f_e(\boldsymbol{p}, \tau) d\tau = \tau_e$,

$$
\begin{aligned}
\Upsilon(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)\Big(&\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2)(\tau_{\text{trans}} + \tau_{\text{col},A}) \\
&+ \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)(\Upsilon(\boldsymbol{p}_3) + \tau_{\text{trans}} + \tau_{\text{col},S})\Big) \\
&+ \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)(\Upsilon(\boldsymbol{p}_5) + \tau_{\text{trans}} + \tau_{\text{surf}}).
\end{aligned}
\tag{24b}
$$

This may be rewritten in the form

$$
\Upsilon(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)\mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\Upsilon(\boldsymbol{p}_3) + \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\Upsilon(\boldsymbol{p}_5) + Q_\Upsilon(\boldsymbol{p}),
\tag{25a}
$$

where

$$
\begin{aligned}
Q_\Upsilon(\boldsymbol{p}) = \mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)(&\mathcal{C}_A(\boldsymbol{p}_1, \boldsymbol{p}_2)(\tau_{\text{trans}} + \tau_{\text{col},A}) + \mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)(\tau_{\text{trans}} + \tau_{\text{col},S})) \\
&+ \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)(\tau_{\text{trans}} + \tau_{\text{surf}}).
\end{aligned}
\tag{25b}
$$

In the above form, $\Upsilon(\boldsymbol{p})$ governs how computational time moves through phase space as a result of transition, collision, and surface-crossing events while $Q_\Upsilon(\boldsymbol{p})$ acts as a fixed source contributing the time required to process these events.

2.4 Future Time Equation in Integro-differential Form

The integro-differential form of the FTE is found by first restricting it to be defined over a single Monte Carlo cell, Γ. The integral form of the FTE may then be expressed in expanded notation, cast into characteristic coordinates, and simplified. This simplified integral formulation is then transformed into the integro-differential form.

2.4.1 Characteristic Future Time Equation in Integral Form

Eq. 25a with the source term temporarily neglected to ease notation may be written as

$$
\begin{aligned}
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = &\mathcal{T}_C(\boldsymbol{p}, \boldsymbol{p}_1)\mathcal{C}_S(\boldsymbol{p}_1, \boldsymbol{p}_3)\Upsilon(\boldsymbol{p}_3) \\
&+ \mathcal{T}_S(\boldsymbol{p}, \boldsymbol{p}_4)\mathcal{S}(\boldsymbol{p}_4, \boldsymbol{p}_5)\Upsilon(\boldsymbol{p}_5).
\end{aligned}
\tag{26}
$$

After restricting the FTE to a single cell, Γ, operators are expanded,

$$
\begin{aligned}
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = &\int dx_1 \int d\Omega_1 \int dE_1 \int dw_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \\
&\times \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})\delta(E_1 - E)\delta(w_1 - w) \\
&\times \int dx_3 \int d\Omega_3 \int dE_3 \int \Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E_1 \to E_3)\Upsilon(\boldsymbol{x}_3, \hat{\boldsymbol{\Omega}}_3, E_3, w_3) \\
&\times \delta(\boldsymbol{x}_3 - \boldsymbol{x}_1)\delta(w_3 - w_1)dw_3 \\
&+ \int dx_4 \int d\Omega_4 \int dE_4 \int dw_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_4\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \\
&\times \delta(\boldsymbol{x}_4 - \boldsymbol{x}_s)\delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})\delta(E_4 - E)\delta(w_4 - w) \\
&\times \int dx_5 \int d\Omega_5 \int dE_5 \int \Upsilon(\boldsymbol{x}_5, \hat{\boldsymbol{\Omega}}_5, E_5, w_5)\delta(\boldsymbol{x}_5 - \boldsymbol{x}_4)\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4)\delta(E_5 - E_4)\delta(w_5 - w_4)dw_5.
\end{aligned}
\tag{27a}
$$

Note that because $\delta(w_5 - w_4)$ is used, it is implied by the definition of the surface-crossing operator that the first surface intersected by the particle-direction vector is an internal surface rather than a boundary surface. The case of a boundary surface is later accounted for by the boundary condition of Eq. 39. In the meantime,

evaluating integrals with Dirac delta functions on the statistical weight variables of integration, w_i,

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \int d\Omega_1 \int dE_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})\delta(E_1 - E)
$$
$$
\times \int dx_3 \int d\Omega_3 \int \Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E_1 \to E_3)\Upsilon(\boldsymbol{x}_3, \hat{\boldsymbol{\Omega}}_3, E_3, w)\delta(\boldsymbol{x}_3 - \boldsymbol{x}_1)dE_3
$$
$$
+ \int dx_4 \int d\Omega_4 \int dE_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_4\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\boldsymbol{x}_4 - \boldsymbol{x}_s)\delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})\delta(E_4 - E)
$$
$$
\times \int dx_5 \int d\Omega_5 \int \Upsilon(\boldsymbol{x}_5, \hat{\boldsymbol{\Omega}}_5, E_5, w)\delta(\boldsymbol{x}_5 - \boldsymbol{x}_4)\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4)\delta(E_5 - E_4)dE_5.
$$

(27b)

Evaluating integrals with Dirac delta functions on the position variables of integration, $\boldsymbol{x}_i$,

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \int d\Omega_1 \int dE_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})\delta(E_1 - E)
$$
$$
\times \int d\Omega_3 \int \Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E_1 \to E_3)\Upsilon(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_3, E_3, w)dE_3
$$
$$
+ \int d\Omega_4 \int dE_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})\delta(E_4 - E)
$$
$$
\times \int d\Omega_5 \int \Upsilon(\boldsymbol{x}_s, \hat{\boldsymbol{\Omega}}_5, E_5, w)\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4)\delta(E_5 - E_4)dE_5.
$$

(27c)

Evaluating integrals with Dirac delta functions on the energy variables of integration, E_i,

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \int d\Omega_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})
$$
$$
\times \int d\Omega_3 \int \Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)\Upsilon(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_3, E_3, w)dE_3
$$
$$
+ \int d\Omega_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})
$$
$$
\times \int d\Omega_5 \Upsilon(\boldsymbol{x}_s, \hat{\boldsymbol{\Omega}}_5, E, w)\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4).
$$

(27d)

Evaluating integrals with Dirac delta functions on the direction variables of integration, $\hat{\boldsymbol{\Omega}}_i$, yields the simplified result,

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)
$$
$$
\times \int d\Omega_3 \int \Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)\Upsilon(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_3, E_3, w)dE_3
$$
$$
+ \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\Upsilon(\boldsymbol{x}_s, \hat{\boldsymbol{\Omega}}, E, w).
$$

(27e)

Now defining $\boldsymbol{x}_1 = \boldsymbol{x} + a\hat{\boldsymbol{\Omega}}$ and a_s to be the distance along $\hat{\boldsymbol{\Omega}}$ to the boundary of Γ, equal to $\|\boldsymbol{x} - \boldsymbol{x}_s\|$, yields

$$
\begin{aligned}
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} &\exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}-a\hat{\boldsymbol{\Omega}}\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \\
&\times \int d\Omega_3 \int dE_3 \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}_3, E_3, w)da \\
&+ \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w).
\end{aligned} \tag{27f}
$$

Simplifying the integral bounds within the exponential functions,

$$
\begin{aligned}
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} &\exp\left(-\int_0^{a} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \\
&\times \int d\Omega_3 \int dE_3 \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}_3, E_3, w)da \\
&+ \exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w).
\end{aligned} \tag{28}
$$

This process is repeated for the source term starting with Eq. 25b. Expanding operator notation,

$$
\begin{aligned}
Q_\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 &\int d\Omega_1 \int dE_1 \int dw_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \\
&\times \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})\delta(E_1 - E)\delta(w_1 - w) \\
&\times \left(\int dx_2 \int d\Omega_2 \int dE_2 \int (\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x}_1, E_1)\right. \\
&\times \delta(\boldsymbol{x}_2 - \boldsymbol{x}_1)\delta(\hat{\boldsymbol{\Omega}}_2 - \hat{\boldsymbol{\Omega}}_1)\delta(E_2 - E_1)\delta(w_2 - 0)dw_2 \\
&+ \int dx_3 \int d\Omega_3 \int dE_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E_1 \to E_3) \\
&\left.\times \delta(\boldsymbol{x}_3 - \boldsymbol{x}_1)\delta(w_3 - w_1)dw_3\right) \\
&+ \int dx_4 \int d\Omega_4 \int dE_4 \int dw_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_4\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \\
&\times \delta(\boldsymbol{x}_4 - \boldsymbol{x}_s)\delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})\delta(E_4 - E)\delta(w_4 - w) \\
&\times \int dx_5 \int d\Omega_5 \int dE_5 \int (\tau_{\text{trans}} + \tau_{\text{surf}})\delta(\boldsymbol{x}_5 - \boldsymbol{x}_4)\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4)\delta(E_5 - E_4)\delta(w_5 - w_4)dw_5.
\end{aligned} \tag{29a}
$$

Evaluating integrals with Dirac delta functions on the statistical weight variables of integration, w_i,

$$Q_{\Upsilon}(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \int d\Omega_1 \int dE_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})\delta(E_1 - E)$$

$$\times \left(\int dx_2 \int d\Omega_2 \int (\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x}_1, E_1)\delta(\boldsymbol{x}_2 - \boldsymbol{x}_1)\delta(\hat{\boldsymbol{\Omega}}_2 - \hat{\boldsymbol{\Omega}}_1)\delta(E_2 - E_1)dE_2 \right.$$

$$\left. + \int dx_3 \int d\Omega_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E_1 \to E_3)\delta(\boldsymbol{x}_3 - \boldsymbol{x}_1)dE_3 \right)$$

$$+ \int dx_4 \int d\Omega_4 \int dE_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_4\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\boldsymbol{x}_4 - \boldsymbol{x}_s)\delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})\delta(E_4 - E)$$

$$\times \int dx_5 \int d\Omega_5 \int (\tau_{\text{trans}} + \tau_{\text{surf}})\delta(\boldsymbol{x}_5 - \boldsymbol{x}_4)\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4)\delta(E_5 - E_4)dE_5.$$

$$(29b)$$

Evaluating integrals with Dirac delta functions on the position variables of integration, $\boldsymbol{x}_i$,

$$Q_{\Upsilon}(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \int d\Omega_1 \int dE_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})\delta(E_1 - E)$$

$$\times \left(\int d\Omega_2 \int (\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x}_1, E_1)\delta(\hat{\boldsymbol{\Omega}}_2 - \hat{\boldsymbol{\Omega}}_1)\delta(E_2 - E_1)dE_2 \right.$$

$$\left. + \int d\Omega_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E_1 \to E_3)dE_3 \right)$$

$$+ \int d\Omega_4 \int dE_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})\delta(E_4 - E)$$

$$\times \int d\Omega_5 \int (\tau_{\text{trans}} + \tau_{\text{surf}})\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4)\delta(E_5 - E_4)dE_5.$$

$$(29c)$$

Evaluating integrals with Dirac delta functions on the energy variables of integration, E_i,

$$Q_{\Upsilon}(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \int d\Omega_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_1 - \hat{\boldsymbol{\Omega}})$$

$$\times \left(\int d\Omega_2 (\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x}_1, E)\delta(\hat{\boldsymbol{\Omega}}_2 - \hat{\boldsymbol{\Omega}}_1) \right.$$

$$\left. + \int d\Omega_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}}_1 \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)dE_3 \right)$$

$$+ \int d\Omega_4 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) \delta(\hat{\boldsymbol{\Omega}}_4 - \hat{\boldsymbol{\Omega}})$$

$$\times \int d\Omega_5 (\tau_{\text{trans}} + \tau_{\text{surf}})\delta(\hat{\boldsymbol{\Omega}}_5 - \hat{\boldsymbol{\Omega}}_4).$$

$$(29d)$$

Evaluating integrals with Dirac delta functions on the direction variables of integration, $\hat{\boldsymbol{\Omega}}_i$, yields the simplified result,

$$Q_\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int dx_1 \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_1\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left((\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x}_1, E)\right.$$

$$+ \int d\Omega_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x}_1, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)dE_3\Bigg) \tag{29e}$$

$$+ \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)(\tau_{\text{trans}} + \tau_{\text{surf}}).$$

Again defining $\boldsymbol{x}_1 = \boldsymbol{x} + a\hat{\boldsymbol{\Omega}}$ and a_s to be the distance along $\hat{\boldsymbol{\Omega}}$ to the boundary of Γ, equal to $\|\boldsymbol{x} - \boldsymbol{x}_s\|$, yields

$$Q_\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}-a\hat{\boldsymbol{\Omega}}\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left((\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right.$$

$$+ \int d\Omega_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)dE_3\Bigg) da \tag{29f}$$

$$+ \exp\left(-\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_s\|} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)(\tau_{\text{trans}} + \tau_{\text{surf}}).$$

Simplifying the integral bounds of the exponents,

$$Q_\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left((\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right.$$

$$+ \int d\Omega_3 \int (\tau_{\text{trans}} + \tau_{\text{col},S})\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}_3, E \to E_3)dE_3\Bigg) da \tag{30}$$

$$+ \exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)(\tau_{\text{trans}} + \tau_{\text{surf}}).$$

The integral FTE may now be formed in characteristic coordinates by combining Eqs. 28 and 30 and changing notation from phase space with a specific subscript, X_i, to phase space of integration, X',

$$\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)$$

$$\times \int d\Omega' \int dE' \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)da$$

$$+ \exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)$$

$$+ \int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left((\tau_{\text{trans}} + \tau_{\text{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right. \tag{31}$$

$$+ (\tau_{\text{trans}} + \tau_{\text{col},S})\int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')dE'\Bigg) da$$

$$+ (\tau_{\text{trans}} + \tau_{\text{surf}})\exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right).$$

Rearranging terms,

$$\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left((\tau_{\mathrm{trans}} + \tau_{\mathrm{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right.$$

$$+ \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\left(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},S} + \Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)\right)dE'\bigg)da$$

$$+ \left(\tau_{\mathrm{trans}} + \tau_{\mathrm{surf}} + \Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)\right)\exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right). \tag{32}$$

The above is a valid form of the FTE, however, further simplification may be applied by recognizing the following,

$$(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)$$

$$+ \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\left(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},S} + \Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)\right)dE'$$

is equivalent to

$$(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)$$

$$+ \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\int d\Omega' \int P(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\left(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},S} + \Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)\right)dE'$$

by Eq. 6. Because $P(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')$ is a PDF it integrates to unity, so the above may be written as

$$(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E) + \tau_{\mathrm{trans}}\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E) + \tau_{\mathrm{col},S}\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)$$

$$+ \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\int d\Omega' \int P(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'.$$

A factor of the total cross section may then be multiplied and divided across the time terms,

$$\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\mathrm{trans}}\left(\frac{\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)} + \frac{\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}\right)\right.$$

$$+ \tau_{\mathrm{col},A}\frac{\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)} + \tau_{\mathrm{col},S}\frac{\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}\bigg)$$

$$+ \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\int d\Omega' \int P(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'.$$

From Eq. 4 it is apparent that

$$\frac{\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)} + \frac{\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)} = 1 \tag{33}$$

and the following cross section weighted collision event processing time term,

$$\tau_{\mathrm{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E) = \tau_{\mathrm{col},A}\frac{\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)} + \tau_{\mathrm{col},S}\frac{\Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}{\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)}, \tag{34}$$

is defined so that

$$(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},A})\Sigma_a(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)$$

$$+ \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\left(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},S} + \Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)\right)dE' =$$

$$\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\mathrm{trans}} + \tau_{\mathrm{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right)$$

$$+ \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\int d\Omega' \int P(\boldsymbol{x}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'. \tag{35}$$

Inserting Eq. 35 into Eq. 32 results in

$$\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left(\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\text{trans}} + \tau_{\text{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right)\right.$$

$$+ \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'\right)da \qquad (36)$$

$$+ \left(\tau_{\text{trans}} + \tau_{\text{surf}} + \Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)\right)\exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right).$$

This form may be further simplified by defining the following function,

$$\Upsilon_b(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) = \tau_{\text{trans}} + \tau_{\text{surf}} + \Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w). \qquad (37)$$

Note that $\Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)$ in Eq. 37 arises from the surface-crossing operator $\mathcal{S}(\boldsymbol{p}, \boldsymbol{p}')$ operating on $\Upsilon(\boldsymbol{p}')$, as shown in the derivation of Eq. 28. This means that, although not explicitly given by the phase space, $\Upsilon(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)$ represents the expected future time on the outside of $\delta\Gamma$, i.e., the expected future time before the surface-crossing event required to enter the current cell is accounted for. The following subscript is introduced to make this distinction evident,

$$\Upsilon_b(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) = \tau_{\text{trans}} + \tau_{\text{surf}} + \Upsilon_{\text{outside}}(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w), \qquad (38a)$$

For consistency with the definition of the surface-crossing operator and Eq. 12b the following is also defined,

$$\Upsilon_{\text{outside}}(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = 0, \boldsymbol{x} \in \{\boldsymbol{x}_{\text{Boundary Surfaces}}\}. \qquad (38b)$$

The simplified form of the integral FTE in characteristic coordinates is then

$$\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left(\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\text{trans}} + \tau_{\text{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right)\right.$$

$$+ \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'\right)da$$

$$+ \Upsilon_b(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)\exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right),$$

where,

a_s is the distance along $\hat{\boldsymbol{\Omega}}$ from $\boldsymbol{x}$ to $\delta\Gamma$,

$\Upsilon_b(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) = \tau_{\text{trans}} + \tau_{\text{surf}} + \Upsilon_{\text{outside}}(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w)$, and

$\Upsilon_{\text{outside}}(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = 0, \boldsymbol{x} \in \{\boldsymbol{x}_{\text{Boundary Surfaces}}\}.$

$$(39)$$

2.4.2 Transformation from Integral to Integro-differential Form

With the integral FTE in the simplified, characteristic-coordinates form given by Eq. 39, it may be converted into the integro-differential form. The conversion begins by moving the boundary term to the left-hand side,

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) - \Upsilon_b(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) \exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) =
$$

$$
\int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left(\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\text{trans}} + \tau_{\text{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right)\right.
$$

$$
\left. + \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'\right)da. \tag{40}
$$

First, observe from Eq. 40 that

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \Upsilon_b(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w), \ a_s = 0, \tag{41}
$$

which may be equivalently stated as

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) = \Upsilon_b(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w), \ \boldsymbol{x} \in \delta\Gamma, \ \hat{\boldsymbol{\Omega}} \cdot \boldsymbol{n} > 0, \tag{42}
$$

where $\boldsymbol{n}$ is the outward-directed normal vector of $\delta\Gamma$, i.e., at the boundary of the cell the expected future time is equivalent to the boundary function Υ_b. Next, recognize that the left-hand side of Eq. 40 is equivalent to an integral over a along $\hat{\boldsymbol{\Omega}}$ from zero to a_s of the negative derivative with respect to a of the expected future time multiplied by an integrating factor,

$$
\Upsilon(\boldsymbol{x}, \hat{\boldsymbol{\Omega}}, E, w) - \Upsilon_b(\boldsymbol{x} + a_s\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) \exp\left(-\int_0^{a_s} \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right) =
$$

$$
\int_{a_s}^0 \frac{\partial}{\partial a}\left[\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\right]da =
$$

$$
-\int_0^{a_s} \frac{\partial}{\partial a}\left[\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\right]da. \tag{43a}
$$

Inserting Eq. 43a into Eq. 40,

$$
-\int_0^{a_s} \frac{\partial}{\partial a}\left[\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\right]da =
$$

$$
\int_0^{a_s} \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left(\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\text{trans}} + \tau_{\text{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right)\right.
$$

$$
\left. + \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'\right)da. \tag{43b}
$$

Because a_s in Eq. 43b is arbitrary, the integrands must be equal as well,

$$
-\frac{\partial}{\partial a}\left[\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}, E, w) \exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\right] =
$$

$$
\exp\left(-\int_0^a \Sigma_t(\boldsymbol{x} + \ell\hat{\boldsymbol{\Omega}}, E)d\ell\right)\left(\Sigma_t(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\left(\tau_{\text{trans}} + \tau_{\text{col},W}(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, E)\right)\right.
$$

$$
\left. + \int d\Omega' \int \Sigma_s(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}} \to \hat{\boldsymbol{\Omega}}', E \to E')\Upsilon(\boldsymbol{x} + a\hat{\boldsymbol{\Omega}}, \hat{\boldsymbol{\Omega}}', E', w)dE'\right). \tag{43c}
$$

The derivative term may be expanded using the chain rule,

$$
-\frac{\partial}{\partial a}\Upsilon(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}},E,w)\exp\left(-\int_0^a\Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}},E)d\ell\right)
$$

$$
+\Sigma_t(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},E)\Upsilon(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}},E,w)\exp\left(-\int_0^a\Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}},E)d\ell\right)=
$$

$$
\exp\left(-\int_0^a\Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}},E)d\ell\right)\left(\Sigma_t(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},E)\left(\tau_{\text{trans}}+\tau_{\text{col},W}(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},E)\right)\right.
$$

$$
\left.+\int d\Omega'\int\Sigma_s(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}}\to\hat{\boldsymbol{\Omega}}',E\to E')\Upsilon(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}}',E',w)dE'\right). \quad (43\text{d})
$$

Dividing out the integrating factor $\exp\left(-\int_0^a\Sigma_t(\boldsymbol{x}+\ell\hat{\boldsymbol{\Omega}},E)d\ell\right)$ results in,

$$
-\frac{\partial}{\partial a}\Upsilon(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}},E,w)+\Sigma_t(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},E)\Upsilon(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}},E,w)=
$$

$$
\int d\Omega'\int\Sigma_s(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}}\to\hat{\boldsymbol{\Omega}}',E\to E')\Upsilon(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},\hat{\boldsymbol{\Omega}}',E',w)dE'
$$

$$
+\Sigma_t(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},E)\left(\tau_{\text{trans}}+\tau_{\text{col},W}(\boldsymbol{x}+a\hat{\boldsymbol{\Omega}},E)\right). \quad (43\text{e})
$$

To transform back to Cartesian coordinates, note that

$$
\frac{\partial}{\partial a}\Upsilon=\frac{\partial x}{\partial a}\frac{\partial}{\partial x}\Upsilon+\frac{\partial y}{\partial a}\frac{\partial}{\partial y}\Upsilon+\frac{\partial z}{\partial a}\frac{\partial}{\partial z}\Upsilon \quad (44\text{a})
$$

and

$$
\left(\frac{\partial x}{\partial a},\frac{\partial y}{\partial a},\frac{\partial z}{\partial a}\right)=\hat{\boldsymbol{\Omega}}, \quad (44\text{b})
$$

so

$$
\frac{\partial}{\partial a}\Upsilon=\hat{\boldsymbol{\Omega}}\cdot\nabla\Upsilon. \quad (44\text{c})
$$

Using the above relation, redefining $\boldsymbol{x}+a\hat{\boldsymbol{\Omega}}$ as simply $\boldsymbol{x}$, and recalling Eq. 42, the integro-differential form of the FTE is then found to be

$$
-\hat{\boldsymbol{\Omega}}\cdot\nabla\Upsilon(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,w)+\Sigma_t(\boldsymbol{x},E)\Upsilon(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,w)=\int d\Omega'\int\Sigma_s(\boldsymbol{x},\hat{\boldsymbol{\Omega}}\to\hat{\boldsymbol{\Omega}}',E\to E')\Upsilon(\boldsymbol{x},\hat{\boldsymbol{\Omega}}',E',w)dE'
$$

$$
+\Sigma_t(\boldsymbol{x},E)(\tau_{\text{trans}}+\tau_{\text{col},W}(\boldsymbol{x},E))
$$

$$
\text{where,}
$$

$$
\Upsilon(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,w)=\tau_{\text{trans}}+\tau_{\text{surf}}+\Upsilon_{\text{outside}}(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,w),\ \boldsymbol{x}\in\delta\Gamma,\ \hat{\boldsymbol{\Omega}}\cdot\boldsymbol{n}>0,
$$

$$
\text{and}
$$

$$
\Upsilon_{\text{outside}}(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,w)=0,\ \boldsymbol{x}\in\{\boldsymbol{x}_{\text{Boundary Surfaces}}\}.
$$

$$
(45)
$$

Because computational particles mirror physical particles in analog Monte Carlo simulations, Eq. 45 resembles the adjoint neutron transport equation with specific source terms. The inhomogeneous source term of Eq. 45,

$$
\Sigma_t(\boldsymbol{x},E)(\tau_{\text{trans}}+\tau_{\text{col},W}(\boldsymbol{x},E)),
$$

represents the computational time required to process particles transitioning to and undergoing collisions. The boundary source term of Eq. 45,

$$
\tau_{\text{trans}}+\tau_{\text{surf}},
$$

represents the computational time required required to process particles transitioning to and crossing surfaces. Note that the statistical weight w is included in Eq. 45 for consistency, but is not necessary to solve the equation because an analog Monte Carlo simulation was assumed.

19

Conclusion

A detailed derivation of the Future Time Equation (FTE) in integro-differential form for analog Monte Carlo simulation in non-multiplying media is presented in this report. The derivation begins with an event-based description of Monte Carlo particle transport, forms the Future Time Probability Density Function (FTPDF) in integral form, computes the FTE in integral form as the first time moment of the FTPDF, and converts the FTE to the integro-differential form given in Eq. 45. Solving the FTE yields the expected computational time required to simulate a particle from a point in phase space through a Monte Carlo history. It is hoped that both the integro-differential form and detailed derivation shown in this work assists future researchers in the field.

References

1. J. A. Kulesza, C. J. Solomon, and B. C. Kiedrowski, "Discrete Ordinates Analysis of the Forced-Flight Variance Reduction Technique in Monte Carlo Neutral Particle Transport Simulations," *J. Comput. Phys.*, vol. 429, 2021. [Online]. Available: https://doi.org/10.1016/j.jcp.2020.109997

2. R. J. Juzaitis, "Minimizing the Cost of Splitting in Monte Carlo Radiation Transport Simulation," Ph.D. Thesis, University of Virginia, Oct. 1980, LA-8546-T. [Online]. Available: https://doi.org/10.2172/6753224

3. J. A. Kulesza, "Cost-optimized Automated Variance Reduction for Highly Angle-dependent Radiation Transport Analyses," Ph.D. Thesis, University of Michigan, 2018. [Online]. Available: http://hdl.handle.net/2027.42/147541

4. C. J. Solomon, "Discrete-Ordinates Cost Optimization of Weight-Dependent Variance Reduction Techniques for Monte Carlo Neutral Particle Transport," Ph.D. Thesis, Kansas State University, Dec. 2010. [Online]. Available: http://hdl.handle.net/2097/7014

5. B. C. Kiedrowski, J. A. Kulesza, C. J. Solomon, "Discrete Ordinates Prediction of the Forced-Collision Variance Reduction Technique in Slab Geometry," in *Proc. 2019 ANS Math. and Comp. Div.*, Aug. 2019.

6. E. S. Gonzalez *et al.*, "Hammer: An Educational and Research Platform for Neutral Particle Transport Code Development," *Trans. Am. Nucl. Soc.*, vol. 121, no. 1, pp. 245–248, Nov. 2019. [Online]. Available: https://doi.org/10.13182/T31322

7. E. J. Pearson, J. A. Kulesza, and B. C. Kiedrowski, "Discrete Ordinate Prediction of Analog Monte Carlo Computational Time with Embedded Timer Estimators," *Trans. Am. Nucl. Soc.*, 2021, submitted.