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Residual Monte Carlo Transport in Time with Consistent Low-Order Acceleration for 1D Thermal Radiative Transfer

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Abstract - *We have extended a high-order low-order (HOLO) algorithm for thermal radiative transfer problems to include Monte Carlo (MC) integration of the time variable. Within each discrete time step, fixed-point iterations are performed between a high-order (HO) exponentially-convergent Monte Carlo (ECMC) solver and a low-order (LO) system of equations. The ECMC algorithm integrates the angular intensity over a time step, and the low-order (LO) radiation equations are closed consistently in the time variable. The time closure increases accuracy in optically-thin problems compared to a backward Euler discretization. The LO system is based on spatial and angular moments of the transport equation and a linear-discontinuous finite-element (LDFE) spatial representation, producing equations similar to the standard S_2 equations. The emission source is fully implicit in time, and Newton iterations efficiently resolve the non-linear temperature dependence of the LO equations at each time step. The HO solver provides a globally accurate solution for the angular intensity to a fixed-source, pure absorber transport problem. The HO solver computes angular and temporal consistency terms that preserve the accuracy of the MC integration in the LO equations. We have implemented the ECMC algorithm for two different temporal trial spaces and compared results to an implicit Monte Carlo (IMC) code. One-dimensional, gray test problems were tested for a range of optical thicknesses. For certain problems, the algorithm is more efficient than IMC with sufficient mesh resolution.*

I. INTRODUCTION

Accurate solutions to the thermal radiative transfer (TRT) equations are important for simulations in the high-energy, high-density physics regime, e.g., for inertial confinement fusion and astrophysics. Computational modeling of TRT problems features coupling between a photon radiation field and a high-temperature material, where energy is exchanged through absorption and emission of photons by the material. Typical applications often require solution in a mix of streaming and diffusive regions due to absorption-emission physics and cross sections that are a function of material temperature. In this work, we improve on the time-integration accuracy of a high-order low-order (HOLO) method in optically thin regions where particles stream without undergoing many interactions, while preserving the computational efficiency of a residual MC HO solver in optically thick regions.

Moment-based hybrid Monte Carlo (MC) methods have demonstrated great potential for accelerated solutions to TRT problems [1, 2, 3]. These nonlinear acceleration methods iterate between a high-order (HO) transport equation and a low-order (LO) system formulated with angular moments and a fixed spatial discretization. Physics operators that are expensive for the HO solver to resolve directly in tightly coupled problems, e.g., photon absorption and emission, are moved to the LO system. The lower-rank LO equations can be solved with Newton methods to allow for non-linearities in the LO equations to be efficiently resolved [4, 2]. The high-order (HO) problem is defined by the radiation transport equation with isotropic sources computed with the previous LO solution. A MC transport solution to the HO problem is used to construct consistency terms that appear in the LO equations. These consistency terms preserve the accuracy of the HO solution in the next LO solve, as the two solutions iteratively converge.

Previously, residual MC methods have been used to provide efficient solution to the HO transport problem [1, 2]; high-fidelity solutions, with minimal statistical noise, have been achieved for problems with optically-thick, diffusive regions that lead to slowly varying solutions. However, the algorithms in previous work have used a backward Euler (BE) discretization for the time variable. The BE discretization can inaccurately disperse radiation wavefronts in optically thin problems, leading to inaccuracies.

We have extended the algorithm in [2] to include higher-accuracy MC treatment of the time variable for the radiation unknowns. The exponentially-convergent Monte Carlo (ECMC) algorithm was modified to include integration of the time variable; this includes the introduction of a step, doubly-discontinuous (SDD) trial space representation in time. We have also investigated a LDFE projection in time, which requires a modified sampling approach that should be useful for extending the ECMC algorithm to higher spatial dimensions. A new parametric closure of the LO equations, introducing additional time-closure consistency terms, was derived to capture the time accuracy of the HO ECMC simulations. The LO equations can preserve the accuracy of the ECMC radiation transport treatment in time, with the same numerical expense as Backward Euler (BE) time-discretized S_2 equations. We have derived the LO equations directly from the transport equation such that, neglecting spatial discretization differences, the HO and LO solutions are consistent upon convergence, preserving space-angle-time moments. Herein we briefly describe the algorithm, and we present results for one-dimensional (1D), grey test problems. We compare our method to the implicit MC (IMC) method [5] for accuracy and statistical efficiency for several representative problems.

1. Thermal Radiative Transfer Background and IMC

The continuous 1D, grey TRT equations consist of the radiation and material energy rate equations, i.e.,

$$\frac{1}{c}\frac{\partial I(x,\mu,t)}{\partial t} + \mu\frac{\partial I(x,\mu,t)}{\partial x} + \sigma_a I(x,\mu,t) = \frac{1}{2}\sigma_a acT^4(x,t) \quad (1)$$

$$\rho c_v \frac{\partial T(x,t)}{\partial t} = \sigma_a \phi(x,t) - \sigma_a acT^4(x,t), \quad (2)$$

with appropriate initial and boundary conditions specified. In the above equations, x is the position, t is the time, μ is the x-direction cosine of the angular intensity $I(x,\mu,t)$, σ_a is the macroscopic absorption cross section (cm^{-1}), and a, c, ρ, and c_v are the radiation constant, speed of light, mass density, and specific heat, respectively. Physical scattering could be included in Eq. (1), but it is omitted for brevity and simplicity. The desired transient unknowns are the material temperature $T(x,t)$ and the mean radiation intensity $\phi(x,t) = \int_{-1}^{1} I(x,\mu,t)\,\mathrm{d}\mu$. The mean intensity is related to the radiation energy density E_r by the relation $E_r = \phi/c$. The equations can be strongly coupled through the gray Planckian emission source $\sigma_a acT^4$, which is a nonlinear function of temperature, and the absorption term $\sigma_a\phi$. In optically thin problems, with small σ_a, the solution becomes increasingly linear as the emission source becomes negligible.

We will compare results in this work to the implicit Monte Carlo (IMC) method. The IMC method [5] is the standard approach for solution of the TRT equations with Monte Carlo particle transport [6]. The IMC method partially linearizes the system of equations over a discrete time step, with material properties evaluated at the previous-time-step temperature. The linearized system produces a transport equation with an approximate emission source and an effective scattering cross section representing absorption and re-emission of photons over a time step [5]. This transport equation is advanced over a time step via a MC simulation. The MC transport simulation tallies energy absorption over a discretized spatial mesh, which can be used to directly estimate a spatially discretized representation of the end of time step material temperature.

For this work, we are primarily interested in comparing to the time discretization of IMC. The material temperature and emission source are discretized with an implicit time discretization, i.e., a BE discretization. However, because the linearization is approximate, the system is not truly implicit, and there is a limit on the time step size to produce physically accurate results in problems that are tightly coupled and strongly non-linear [7]. The linearized equations are integrated over the n-th time step defined for $t \in [t^{n-1/2}, t^{n+1/2}]$, with width $\Delta t = t^{n+1/2} - t^{n-1/2}$ and center $t^n = t^{n-1/2} + \Delta t/2$. The radiation equation is solved via MC simulation of particle histories, with the time-averaged energy deposition tallied over the spatial mesh. The time-integrated radiation equation, in nonlinear form, is

$$I^{n+1/2}(x,\mu) - I^{n-1/2}(x, \ldots$$
$$\Delta t\left[\sigma_a^{n-1/2}\overline{I}(x,\mu) + \frac{1}{2}\sigma_a ac\left(T^{n+1/2}\right)^4(x)\right]. \quad (3)$$

The end-of-time-step intensity $I^{n+1/2}(x,\mu) \equiv I(x,\mu,t^{n+1/2})$ is stored as "census" particles that have reached $t^{n+1/2}$,, representing a continuous sample of the phase space at that particular time [5], to be used in the next time step. In strongly diffusive regions, the accuracy will be limited to first order by the time discretization of the temperature terms. However, in optically-thin regions, higher-accuracy for the radiation terms is achieved. It is noted that the time-averaged effective scattering source resulting from linearization of the emission source in IMC is treated approximately in the time variable to allow the MC simulation to simulate the isotropic scattering events [6, 5].

2. The High-Order Low-Order Algorithm

Previously, we have developed a HOLO algorithm for 1D TRT problems, based on BE time-discretized HO and LO equations [2]. In the time-discrete HOLO algorithm, the LO solver resolves the material temperature spatial distribution $T(x)^{n+1}$ over each time step, whereas the HO solver computes weighted angular integrals of the the intensity. The HOLO formulation has several desirable properties. In particular, the LO solver can efficiently converge non-linearities in diffusive systems, without the need to solve the nonlinear equations with MC simulation. Because the non-linearities are converged, the temperature and emission source have a truly implicit discretization, preserving the discrete maximum principle [8]. Additionally, by using the ECMC HO solver, solutions with minimal statistical noise can be achieved efficiently, preventing instability issues that may be introduced through noise in the consistency terms.

To achieve temporal accuracy similar to IMC, we compute weighted temporal integrals of the intensity with the HO solver, resulting in additional consistency terms. We must assume a time discretization for the temperature field to produce a linear HO transport problem with closable LO equations. As in the IMC method, a BE time discretization is applied to emission source throughout, but the radiation variables are left in terms of time-averaged and end-of-time-step unknowns. Currently, our residual formulation requires a space-angle LDFE projection of the solution in order to estimate $I(x,\mu,t^{n+1})$, rather than the continuous sample represented by the census in IMC. This projection can be inaccurate with insufficient mesh resolution in near-void problems. However, the LDFE projection of the solution, estimated with MC inversion of the linear transport operator, will greatly increase the accuracy over a standard finite-difference discretization of the radiation equation. The HOLO algorithm should still demonstrate improvement over IMC in efficiency and accuracy in problems with intermediate and large optical thickness.

The fully-discrete LO equations are based on space-time-angle moments of the TRT equations, formed over a spatial finite-element (FE) mesh. Angularly, the LO radiation equations are similar to S_2 equations, with element-averaged consistency parameters that are time-averaged, intensity-weighted averages of μ. The angular treatment is analogous to the hybrid method in [9]. A linear-discontinuous finite element (LDFE) spatial discretization (e.g., see [10]) is used to close the system spatially. Additional consistency parameters must be introduced to the LO equations to eliminate the auxiliary time-unknowns from the LO radiation equations. The additional time consistency terms are based on parametric modifications to a standard time discretization. Once closed, a system of equations is formed for the primary moment unknowns. If the angular and time consistency parameters were exact, then the LO equations would produce the exact moments of the solution, neglecting spatial discretization differences between the two systems. The HO consistency parameters are lagged in each LO solve. The LO equations always conserve energy, independent of the accuracy of the consistency terms.

The solution to the LO system is used to construct a spatially LDFE, and temporally constant, representation of the emission source on the right hand side of Eq. (1). This defines a fixed-source, pure absorber transport problem for the HO operator. This HO transport problem is solved with the ECMC algorithm. The HO transport problem can be viewed as a characteristic method, where we are using ECMC to invert the continuous streaming, time-derivative, and removal operators [2]. The ECMC algorithm is an iterative residual MC method that uses batches of MC histories to estimate the error in the current trial-space estimate of $I(x,\mu,t)$. It is noted that because we are not using mesh adaptation in this work, exponential convergence in iterations cannot generally be maintained, but reduced variance overall can still be achieved. The initial guess for each solve is based on the solution from the previous time step, which allows for efficient reduction of statistical noise in problems with minimal change over the time step. The output from ECMC is a projection $\tilde{I}(x,\mu,t)$ of the intensity onto the chosen finite-element trial space, i.e., the functional representation of the intensity. Once computed, $\tilde{I}(x,\mu)$ is used to directly evaluate the necessary LO angular and time-closure consistency parameters. The HO solution is not used to directly estimate a new temperature at the end of the time step, which eliminates the need to linearize the emission source for stability.

Iterations between the HO and LO solves can increase accuracy in strongly nonlinear problems. However, for the problems tested here, only a single HO solve is performed during each time step. Thus, the HOLO algorithm, for the n'th time step, is

1. Perform a LO solve to produce an initial guess for $T_{LO}^{n+1/2}(x)$ and $\phi_{LO}^{n+1/2}(x)$, based on angular consistency terms estimated with $\tilde{I}^{n-1/2}(x,\mu)$ and a BE time discretization.

2. Solve the HO system for $\tilde{I}_{HO}(x,\mu,t)$ using ECMC, based on the current LO estimate of the emission source.

3. Compute LO angular and time-closure consistency parameters with $\tilde{I}_{HO}(x,\mu,t)$.

4. Solve the LO system using HO consistency parameters to produce a new estimate of $\phi_{LO}^{n+1/2}$ and $T_{LO}^{n+1/2}$.

5. Store $\tilde{I}^{n+1/2}(x,\mu) \rightarrow \tilde{I}^{n-1/2}(x,\mu)$, and move to the next time step.

II. THE LO SYSTEM

We will define the LO equations and closure before detailing the HO solver that is used to compute consistency terms present in the LO equations. To derive the LO equations, we reduce the dimensionality of Eq. (1) and Eq. (2) by taking spatial, angular, and temporal integrals. We will then introduce approximations to close the system, while being as consistent with the HO solver as possible.

The spatial domain is divided into N_c uniform spatial cells. The spatial moments are taken over each spatial cell i: $x \in [x_{i-1/2}, x_{i+1/2}]$, weighted with the standard linear FE basis functions. For example, the left moment operator is defined by

$$\langle \cdot \rangle_{L,i} = \frac{2}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)(\cdot)\mathrm{d}x, \tag{4}$$

where $h_i = x_{i+1/2} - x_{i-1/2}$ is the width of the spatial element and $b_{L,i}(x) = (x_{i+1/2} - x)/h_i$ is the basis function corresponding to position $x_{i-1/2}$. The right moment is defined with basis function $b_{R,i}(x) = (x - x_{i-1/2})/h_i$. Angularly, the equations are integrated over the positive and negative half ranges. The angular integrals of the intensity are defined as $\phi^{\pm}(x) = \pm 2\pi \int_0^{\pm 1} I(x,\mu)\mathrm{d}\mu$. Finally, the equations are integrated over the n'th time step defined for $t \in [t^{n-1/2}, t^{n+1/2}]$ with width $\Delta t = t^{n+1/2} - t^{n-1/2}$ and center t^n.

The L and R moments and + and − half-range integrals are applied in pair-wise combination to Eq. (1), followed by integration over the time step. After algebraic manipulation, this ultimately produces 4 moment equations per spatial element. The streaming terms in the resulting equations are manipulated to form averages of μ, weighted with basis functions and the time-averaged intensity, analogous to previous work [2, 9]. The emission source and temperature-dependent cross sections are approximated with a BE discretization to help close the system. For example, application of the $\langle \cdot \rangle_{L,i}$ moment with the positive half-range integral to Eq. (1) ultimately yields

$$\begin{aligned}\frac{\langle \phi \rangle_{L,i}^{+,n+1/2} - \langle \phi \rangle_{L,i}^{+,n-1/2}}{c\Delta t} - 2\overline{\mu}_{i-1/2}^{+}\overline{\phi}_{i-1/2}^{+} + \overline{\{\mu\}}_{L,i}^{+}\langle\overline{\phi}\rangle_{L,i}^{+} + \overline{\{\mu\}}_{R,i}^{+}\langle\overline{\phi}\rangle_{R,i}^{+} \\ + \sigma_{a,i}^{n+1/2} h_i \langle\overline{\phi}\rangle_{L,i}^{n+1/2,+} = \frac{h_i}{2}\langle \sigma_a^{n+1/2} acT^{n+1/2,4}\rangle_{L,i},\end{aligned} \tag{5}$$

where over-barred quantities represent the exact averaging over the time step. A more thorough derivation and definitions for all of the moment equations can be found in [11].

At this point, the only approximation has been the BE time-discretization of the emission source. The face- and volume-averaged angular consistency terms, e.g., $\overline{\mu}_{i-1.2}^{+}$, were formed only through algebraic manipulation. They are approximated with angular intensity from the previous HO solve. For example, the L and + time-averaged consistency term is

$$\overline{\{\mu\}}_{L,i,HO}^{+} \simeq \frac{\dfrac{2}{h_i \Delta t} \displaystyle\int_{t^{n-1/2}}^{t^{n+1/2}} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu\, b_{L,i}(x) \tilde{I}_{HO}(x,\mu,t)\mathrm{d}x\mathrm{d}\mu\mathrm{d}t}{\dfrac{2}{h_i \Delta t} \displaystyle\int_{t^{n-1/2}}^{t^{n+1/2}} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) \tilde{I}_{HO}(x,\mu,t)\mathrm{d}x\mathrm{d}\mu\mathrm{d}t}, \tag{6}$$

where $\tilde{I}_{HO}(x,\mu,t)$ is a space-angle-time finite element projection of the HO intensity, to be later defined. For simplicity, the face terms $\phi^{\pm}_{i\pm 1/2}$ are eliminated from the system using a lumped LDFE spatial approximation, with standard upwinding [2]. The emission source is also represented with a lumped LDFE interpolant. There is some inconsistency introduced in this approximation, but it has proven stable for problems tested and demonstrates preservation of the equilibrium diffusion limit [11]. Boundary conditions are incorporated through upwinding and the face term resulting from integration of the streaming operator.

The material energy equations are similarly integrated in space and time. The lumped LDFE approximation is introduce for $T(x)$ and $T^4(x)$ to close the equation spatially, along with the BE time discretization for the emission source. The L moment temperature equation is

$$\frac{\rho_i c_{v,i}}{\Delta t}\left[T^{n+1/2}_{L,i} - T^{n-1/2}_{L,i}\right] + \sigma^{n+1/2}_{a,i}\left(\langle\overline{\phi}\rangle^{+}_{L,i} + \langle\overline{\phi}\rangle^{-}_{L,i}\right) = \sigma^{n+1/2}_{a,i} ac\left(T^{n+1/2}_{L,i}\right)^4, \quad (7)$$

where cross sections have been evaluated at $t^{n+1/2}$ and $T_{L,i}$ and $T_{R,i}$ are the LD edge values of the temperature, e.g., $T(x) = b_{L,i}(x)T_{L,i} + b_{R,i}(x)T_{R,i}$ for $x \in (x_{i-1/2}, x_{i+1/2})$.

1. Parametric Time Closure with HO information

At this point, there is still too many unknowns in the LO equations. Quantities at $t^{n-1/2}$ are known from the previous time step or an initial condition, but a a relation is needed between the time-averaged radiation quantities and their corresponding values at $t^{n+1/2}$. The closure of each LO equation must account for inconsistencies in the time-discretization of the two solvers. Previous work, applied to radiation-hydrodynamics problems, has enforced consistency in time by adding a local artificial source to the time-discretized LO equations in each cell [3]. This source was based HO estimate of the difference in the integral treatments of the time derivative between the HO and LO systems. The advantage of this form is that the LO solver exclusively deals in time-averaged unknowns for the radiation terms in the equations. Alternatively, we will use a local, parametric closure to directly eliminate the auxiliary temporal radiation unknowns, introducing additional consistency terms.

Equation (5) will only contain time-averaged radiation unknowns if $\langle\phi\rangle^{n+1/2}_{L,i}$ is eliminated from the system. The simplest closure is a weighted average

$$\langle\phi\rangle^{+,n+1/2}_{L,i} = \gamma^{+}_{L,i,HO}\langle\overline{\phi}\rangle^{+}_{L,i}, \quad (8)$$

where $\gamma^{+}_{L,i,HO}$ is a time-closure consistency parameter. The consistency parameter can be determined from Eq. (8) by using moments of $\overline{I}_{HO}(x,\mu)$ and $I^{n+1/2}_{HO}(x,\mu)$, i.e.,

$$\gamma^{+}_{L,i,HO} = \frac{\langle\phi_{HO}\rangle^{+,n+1/2}_{L,i}}{\overline{\phi}^{+}_{L,i,HO}}. \quad (9)$$

Because the time-closures account for the different spatial moment equations, there is four per spatial cell.

The unknowns of interest are $\langle\overline{\phi}\rangle^{\pm}_{L,i}$, $\langle\overline{\phi}\rangle^{+}_{R,i}$, $T^{n+1/2}_{L,i}$, and $T^{n+1/2}_{R,i}$. The four radiation moment equations per cell with the LDFE spatial closure, the HO approximation of the angular consistency terms, the two temperature moment equations, and the parametric time closures produce (e.g., Eqs. (5), (6), (7), and (8)) provide sufficient equations to solve for these unknowns. Summation of the moment equations over all cells and application of boundary conditions defines a global, nonlinear LO system of equations. This discrete system of equations is solved using a hybrid Newton-Picard method, as in previous work [2]. The linearized equations produce scattering terms that couple the two directions together, which can be directly inverted in 1D. The LO system is fully converged within each solve. Once time-averaged unknowns have been calculated, the local time closures provide $\phi^{n+1/2}_{LO}(x)$ for the next time step.

For the initial LO solve, within a time step, the angular parameters are calculated based on the $\tilde{I}^{n-1/2}_{HO}(x,\mu)$ and all γ values are set to unity, producing a BE discretization. Other closures, e.g., a modified Crank-Nicolson, have been explored. In optically thin problems, the problem is nearly linear, and the choice of this closure has minimal effect on results because all other auxiliary unknowns have been consistently eliminated from the system with HO information (with the exception of the spatial closure). However, for optically thick problems with high statistical noise, the Crank-Nicolson introduced some instabilities.

III. THE RESIDUAL MC HIGH ORDER SOLVER

1. Trial Space Representation

To apply the ECMC algorithm [12, 2], it is necessary to have a functional representation of the intensity for all phase space variables, so a residual can be evaluated. A finite element representation is formed in x, μ, and t. The domain is divided into a uniform grid, where the element with the i-th spatial, j-th angular, and n-th temporal indices spans the domain $\mathcal{D}_{ijn} : x_{i-1/2} < x < x_{i+1/2} \times \mu_{j-1/2} \le \mu \le \mu_{j+1/2} \times t^{n-1/2} < t \le t^{n+1/2}$. We have implemented two different trial space representations for the intensity in t. However, in x and μ, the intensity is always represented with an LDFE projection, which we will denote $\tilde{I}(x,\mu)$. The LDFE projection preserves the zeroth and first moments in x and μ of the intensity. Standard upwinding is used to define the solution on faces for evaluating terms resulting from the spatial derivative in the streaming term [10]. In time, values at $t^{n-1/2}$ are upwinded from the previous time step for both trial spaces.

The first time space is a step, doubly-discontinuous (SDD) trial space. The SDD trial space representation for $I(x,\mu,t)$ is

$$\tilde{I}(x,\mu,t) = \begin{cases} \tilde{I}^{n-1/2}(x,\mu) & t = t^{n-1/2} \\ \tilde{I}^{n}(x,\mu) & t \in (t^{n-1/2}, t^{n+1/2}) \\ \tilde{I}^{n+1/2}(x,\mu) & t = t^{n+1/2} \end{cases} \quad (10)$$

where we have used $\tilde{I}^n$ to denote the time-averaged LDFE projection in x and μ of the intensity over the interior of the time step; the LDFE projections at $t^{n-1/2}$ and $t^{n+1/2}$ are denoted $\tilde{I}^{n-1/2}$ and $\tilde{I}^{n+1/2}$, respectively. The SDD trial space provides a projection for all the desired unknowns that result from time integration of the transport equation; it provides sufficient information to close the LO equations and evaluate the temporal consistency terms. Another benefit of this trial space is it allows for the residual sampling infrastructure from the time-discrete formulation of this algorithm to be used with minor modifications.

The second trial space is an LDFE trial space in x, μ, and t. For a particular space-angle-time element, this trial space is defined as

$$\tilde{I}(x,\mu,t) = \begin{cases} \tilde{I}^n_{ij}(x,\mu) + \frac{2}{\Delta t} I^n_{t,ij}\,(t - t^n)\,, & t \in (t^{n-1/2}, t^{n+1/2}], \\ \tilde{I}^{n-1/2}(x,\mu) & t = t^{n-1/2} \end{cases} \tag{11}$$

where $\tilde{I}^n_{ij}(x,\mu)$ is the time-averaged LDFE projection in x and μ over $\mathcal{D}_{ijn}$ and $I^n_{t,ij}$ is the finite-element slope of $I(x,\mu,t)$ averaged over $\mathcal{D}_{ijn}$, i.e.,

$$I^n_{ij} = \frac{6}{\Delta t} \iiint\limits_{\mathcal{D}_{ijn}} \left(\frac{t - t^n}{\Delta t}\right) I(x,\mu,t)\mathrm{d}x\mathrm{d}\mu\mathrm{d}t. \tag{12}$$

Thus, there is a unique time slope for each element. To compute consistency terms and advance to the next time step, $\tilde{I}(x,\mu,t)$ is evaluated at t^{n+1}, extrapolating to the end of the time step, which introduces an additional projection error.

2. The Algorithm

The transport equation to be solved by ECMC is given by Eq. (1), but with a fixed LDFE Planckian emission source that is estimated by the previous LO solve. We write the equation in operator notation as

$$\mathbf{L}I(x,\mu,t) = q_{LO}(x) \tag{13}$$

where $q_{LO} = \sigma_a ac \left(T^{n+1/2}\right)^4_{LO}/2$ denotes the latest estimate of the emission source, and remains constant for the entire HO solve. The *continuous* linear transport operator $\mathbf{L}$ is

$$\mathbf{L}I(x,\mu,t) \equiv \left[\frac{1}{c}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x} + \sigma_a\right] I(x,\mu,t). \tag{14}$$

The m'th approximate solution to Eq. (13) is $\tilde{I}^{(m)}(x,\mu,t)$, where m identifies the MC batch. The m'th residual is

$$r^{(m)} = q - \mathbf{L}\tilde{I}^{(m)}. \tag{15}$$

Addition of the residual equation to Eq. (13) gives the error equation

$$\mathbf{L}(I - \tilde{I}^{(m)}) = \mathbf{L}\epsilon^{(m)} = r^{(m)}, \tag{16}$$

where I is the exact solution to Eq. (13) (which contains approximation error from the representation of $\tilde{I}^{n-1/2}(x,\mu)$ and q_{LO}), and $\epsilon^{(m)}$ is the error in $\tilde{I}^{(m)}$.

The inverse of $\mathbf{L}$ in Eq. (16) is estimated via MC simulation without discretization error. This is a standard MC simulation, where particle histories are tracked in space, angle, and time, e.g., in IMC [5, 6, 11]. Particle histories are sampled from the source $r^{(m)}(x,\mu,t)$, as explained below. Tallies of the error particles estimate moments of $\epsilon^{(m)}$, which is added to the moments used to produce the LDFE projection $\tilde{I}^{(m)}$. In operator notation, we denote this as $\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1}r^{(m)}$. The LDFE projections of the error $\overline{\epsilon}$ and $\epsilon^{n+1/2}$ are computed using generalizations of volumetric path-length and particle density estimators. The estimators are weighted by appropriate basis functions over each element. For the algorithm with the SDD trial space, particles are allowed to stream without interaction, and the tallies are adjusted accordingly [2]. The details of the tallies specific to this work are given in Sec. 5..

The ECMC algorithm is

1. Initialize $\tilde{I}^{(0)}(x,\mu,t)$ with $\tilde{I}^{n-1/2}(x,\mu)$.
2. Compute $r^{(m)}$.
3. Estimate $\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1}r^{(m)}$ with N Monte Carlo histories.
4. Compute $\tilde{I}^{(m+1)} = \tilde{I}^{(m)} + \tilde{\epsilon}^{(m)}$
5. Optionally repeat 2 – 4 for desired number of batches.

The use of $\tilde{I}^{(0)}(x,\mu,t)$ as the initial guess greatly increases statistical efficiency in regions of the problem where the solution is slowly varying. If the error is sufficiently estimated each batch, both statistically and with the trial-space representation, then the overall error in the solution can converge at an exponential rate. However, eventually the error is not sufficiently estimated and adaptive refinement would be necessary to continue convergence. Thus, we are primarily only gaining the residual benefit for the algorithm in this work, although in some cases multiple batches can improve overall efficiency over a single batch. A drawback of this HO algorithm is that a truncation error occurs by keeping only the LDFE projection of the intensity between time steps, which is not present in IMC. Adaptive mesh refinement is likely necessary to efficiently capture rapidly-varying solutions, but this was not done here for simplicity. Adaptive refinement could be included in the iterative algorithm in future work, which has been demonstrated for the time-discrete algorithm previously in [2].

3. Sampling from the Residual

A. The SDD Trial Space

Computing and sampling from the residual defined by Eq. (15) is similar to the sampling algorithms for a steady-state transport equation [13, 2]. The discontinuities in Eq. (10) introduce δ-function sources at $t^{n-1/2}$ and $t^{n+1/2}$ because of the time derivative. Additionally, the residual has a spatial δ-function source on the upwind face of each element (resulting from the spatial derivative in the streaming term), and a 2D linear interior volumetric source. The contribution from the δ-function source at $t^{n+1/2}$ can be analytically determined because all particles born immediately reach census [11]. Thus, it is never sampled, and the contribution is added in at the end of the simulation.

Because the residual can be negative, particles can be sampled with both negative and positive weights. The particles are sampled from $|r(x,\mu,t)|$ using rejection sampling over each element. The weights are modified to be negative if $r(x,\mu,t) < 0$

for the sampled phase-space position. Starting particle weights are normalized to have a magnitude of unity. The final tallies are then multiplied by $\|r(x,\mu,t)\|_1$, the L_1 norm of the residual over the entire sampling domain. Because of the choice of the SDD trial space, the most complex L_1 integral is the two-dimensional integral of a linear function. Thus, the L_1 norm over all sampling space can be analytically evaluated, as in previous work [13]. To reduce variance in optically thick regions, systematic sampling [14] is performed, with particles placed proportional to the magnitude of the residual over each element, as in [2]. Then the choice of a volumetric or either δ-function source within the element is discretely sampled, and the corresponding probability distribution function (PDF) sampled with rejection. Although excluded from the results in this work, a minimum number could be placed on each sampled cell to ensure sufficient sampling of the phase space.

B. The LD Trial Space

Sec. 5. provides a definition of the residual for the LD trial space. Unlike the SDD trial space, we can not evaluate the L_1 norm of the residual exactly. Additionally, the higher-dimensional residual terms will generally be less efficient to sample with rejection, at least for certain elements. Alternatively, we can use importance sampling [14] with unnormalized particle weights to estimate the magnitude of the residual. Previous work on higher-dimensional residual MC has applied a similar approach for a continuous global polynomial expansion trial space [15]. Because the solution is continuous, except for at the boundary, a uniform sampling can be performed over the entire domain and boundary, with weights that correct for the bias and estimate the magnitude of the residual. Because our finite element space contains spatial and temporal discontinuities for each element, particles should be distributed more closely to the true residual. Additionally, because $\tilde{I}^{n-1}(x,\mu,t)$ is typically a good approximation to $I(x,\mu,t^{n+1})$, uniform sampling of the domain is very inefficient for thermal radiative transfer problems.

To apply the importance sampling algorithm, we sample from a simpler PDF that represents a decent approximation to the residual. For each element, the new PDF to be sampled from is a piece-wise constant function, spanning the same domain as the true residual, i.e., including the two δ functions with their corresponding subsection of the domain and the full domain $\mathcal{D}_{ijn}$ (for the interior source). The probability of sampling a particular constant source is proportional to an approximation of the L_1 norm of the residual over that element. The L_1 norm is approximated with product 2-point Gaussian quadratures over each piece of the residual domain. Thus, the PDF for the element with domain $\mathcal{D}_{ijn}$ is

$$p(x,\mu,t) = \begin{cases} \frac{\|r\|^n_{1,i\pm1/2j}}{\|r\|_1\Delta t\Delta\mu}\delta^{\mp}\left(x-(x_i\pm\frac{h_i}{2})\right), & (\mu,t)\in\mathcal{D}_{ijn} \\ \frac{\|r\|^{n-1/2}_{1,ij}}{\|r\|_1\Delta x\Delta\mu}\delta^{+}(t-t^{n-1/2}), & (x,\mu)\in\mathcal{D}_{ijn} \\ \frac{\|r\|^n_{1,ij}}{\|r\|_1\Delta t\Delta\mu\Delta x}, & (x,\mu,t)\in\mathcal{D}_{ijn}, \end{cases} \tag{17}$$

where $\|r\|_1$ is the L_1 norm over the entire domain, $\|r\|^n_{1,i\pm1/2j}$ is the norm of the spatial δ-function portion of the element residual (where the sign of the δ-function corresponds to the direction of μ for the element), $\|r\|^{n-1/2}_{1,ij}$ is the norm of the temporal δ-function portion of the residual, and $\|r\|^n_{1,ij}$ is the norm of the residual over the interior of the element domain; all of these norms are approximated with quadrature. Particles are trivially sampled from $p(x,\mu,t)$ and particle weights are initialized as

$$w(x,\mu,t) = \frac{r(x,\mu,t)}{p(x,\mu,t)}. \tag{18}$$

Although the quadrature approximation may be poor in regions of the domain where zero-crossings of the residual occur, the overall sampling algorithm is unbiased. We expect that for reasonably fine meshes the particle origins are proportional to the magnitude of the residual. It is noted that low-variance samples of the source do not guarantee low variance in the tallies overall, particularly in thin regions. High relative variance in weights of particles can also lead to large variances in the tallies [14]. However, the slope tallies should produce less noise than the census tallies of the SDD trial space overall. As before, we stratify based on $p(x,\mu,t)$ to place particles proportional to the total probability of sampling from each element and adjust the weights to account for sampling of integer number of histories.

APPENDIX

The Residual for the LDFE Trial Space

The LDFE representation for the element with center (x_i,μ_j,t^n), spanning the interior of the domain $\mathcal{D}_{ijn}$, is

$$\tilde{I}(x,\mu,t) = I^n_{a,ij}+\frac{2}{h_i}I^n_{x,ij}(x-x_i)+\frac{2}{\Delta\mu}I^n_{\mu,ij}\left(\mu-\mu_j\right)+\frac{2}{\Delta t}I^n_{t,ij}(t-t^n) \tag{A.1}$$

where $\Delta\mu = \mu_{j+1/2}-\mu_{j-1/2}$ and $I^n_{a,ij}$, $I^n_{x,ij}$, $I^n_{\mu,ij}$, and $I^n_{t,ij}$ are the average, x slope, μ slope, and t slope moments, respectively [11]. We substitute Eq. (A.1) into Eq. (15) and analytically apply the continuous transport operator to determine the residual. For each cell, the residual is the sum of three components. The first is the interior volumetric source:

$$r^n_{ij}(x,\mu,t) = r^n_{a,ij}+\frac{2}{h_i}r^n_{x,ij}(x-x_i)+\frac{2}{\Delta\mu}r^n_{\mu,ij}\left(\mu-\mu_j\right)+\frac{2}{\Delta t}r^n_{t,ij}(t-t^n) \tag{A.2}$$

where

$$r^n_{a,ij} = q_{a,i}-\sigma_{a,i}I^n_{a,ij}-\frac{2}{c\Delta t}I^n_{t,ij}-\mu_j\frac{2}{\Delta\mu}I^n_{x,ij}, \tag{A.3}$$

$$r^n_{x,ij} = q_{x,i}-\sigma_{a,i}I^n_{x,ij}, \tag{A.4}$$

$$r^n_{\mu,ij} = -\sigma_{a,i}I^n_{\mu,ij}-\frac{\Delta\mu}{h_i}I^n_{x,ij}, \tag{A.5}$$

$$r^n_{t,ij} = -\sigma_{a,i}I^n_{t,ij} \tag{A.6}$$

where $q_{a,i}$ and $q_{x,i}$ are the zeroth and first moments of the LO LDFE emission source over the i-th spatial element ($q_{LO}(x)$ does not have a first moment in μ or t). The spatial derivative produces a δ-function source due to the discontinuities in the trial space. Upwinding is used to define the intensity on the inflowing face. The face source component, for $\mu > 0$, becomes

$$r^n_{i-1/2j} = \delta^+(x-x_{i-1/2})\mu\left[r^{n,f}_{a,ij} + \frac{2}{\Delta\mu}r^{n,f}_{\mu,ij}\left(\mu-\mu_j\right)+\frac{2}{\Delta t}r^{n,f}_{t,ij}(t-t^n)\right] \tag{A.7}$$

where

$$r^{n,f}_{a,ij} = \left(I^n_{a,i-1,j} + I^n_{x,i-1,j}\right) - \left(I^n_{a,ij} - I^n_{x,ij}\right) \tag{A.8}$$
$$r^{n,f}_{\mu,ij} = I^n_{\mu,i-1,j} - I^n_{\mu,ij}, \tag{A.9}$$
$$r^{n,f}_{t,ij} = I^n_{t,i-1,j} - I^n_{t,ij}. \tag{A.10}$$

The face sources for elements with $\mu < 0$ are similarly defined. Finally, the time-derivative source component is

$$r^{n-1/2}_{ij} = \delta^+(t - t^{n-1/2})\frac{1}{c}\left[r^{n-1/2}_{a,ij} + \frac{2}{h_i} r^{n-1/2}_{x,ij}(x - x_i) + \frac{2}{\Delta\mu} r^{n-1/2}_{\mu,ij}\left(\mu - \mu_j\right)\right] \tag{A.11}$$

where

$$r^{n-1/2}_{a,ij} = I^{n-1/2}_{a,ij} - \left(I^n_{a,ij} - I^n_{t,ij}\right), \tag{A.12}$$
$$r^{n-1/2}_{x,ij} = I^{n-1/2}_{x,ij} - I^n_{x,ij}, \tag{A.13}$$
$$r^{n-1/2}_{\mu,ij} = I^{n-1/2}_{\mu,ij} - I^n_{\mu,ij}. \tag{A.14}$$

Tallies for the Error

Tallies compute weighted moments of the error, averaged over the phase-space volume of each element. For both trial spaces, the time-averaged LDFE projection $\tilde{I}^n(x,\mu)$ is computed. This requires tallies for the average, x, and μ moments of the error. The tally for analog path-length sampling and the x moment of the error is

$$\hat{\epsilon}^n_{x,ij} = \frac{1}{N}\frac{6}{\Delta t h_i}\sum_{m=1}^{N_{score}} \frac{s_m}{h_i \Delta\mu} w_m \left(x^m_c - x_i\right), \tag{A.15}$$

where x^m_c is the center x-coordinate of the path length for the m-th particle history with length s_m and constant weight w_m, and N_{score} is the number of particles that have traversed the domain $\mathcal{D}_{ijn}$.. There are similar definitions for the average and μ moment. The tallies are derived by integrating the differential contribution of a path length, to the moment of interest, over the entire path length [11]. As in previous work, these tallies can be modified to allow for particles that stream without absorption and have exponentially attenuated weights [2].

For the SDD trial space, moments of $\epsilon(x,\mu,t^{n+1/2})$ must be estimated to produce a projection of the intensity at the end of the time step. For example, the x moment of the error at the end of time step is

$$\epsilon^{n+1/2}_{x,ij} = \frac{6}{h_i \Delta\mu \Delta t}\iint_{\mathcal{D}_{ij}} \left(\frac{x - x_i}{h_i}\right)\epsilon(x,\mu,t^{n+1/2})\mathrm{d}x\mathrm{d}\mu \tag{A.16}$$

The estimators for these moments are a generalization of the census tallies used in IMC [6, 5]. The census estimator for the x moment is

$$\hat{\epsilon}^{n+1/2}_{x,ij} = \frac{1}{N}\frac{6}{\Delta\mu h_i^2}\sum_{n=1}^{N_{score}} c w_m \left(x_m - x_i\right), \tag{A.17}$$

where x_m is the coordinate of the m-th particle that has reached the end of the time step. Similar tallies are defined for the other space-angle moments. These tallies can be exceptionally noisy in optically thick cells because only particles that reach the end of the time step contribute.

For the LDFE time space, it is necessary to tally the slope of the intensity in t over each element, i.e., estimate Eq. (12). The estimator, for analog path-length sampling, is

$$\hat{\epsilon}^n_{t,ij} = \frac{1}{N}\frac{6}{h_i \Delta\mu \Delta t}\sum_{m=1}^{N_{score}} \left(\frac{t^m_c - t^n}{\Delta t}\right) w_m s_m \tag{A.18}$$

where t^m_c is the time of the particle at the center of the path length.

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