

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 (LDFFE) 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 LDFFE 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.,

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

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

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 scalar radiation intensity $\phi(x, t) = \int_{-1}^1 I(x, \mu, t) d\mu$. The scalar 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 $\sigma_a a c T^4$, 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

$$I^{n+1/2}(x, \mu) - I^{n-1/2}(x, \mu) = \Delta t \left[\sigma_a^{n-1/2} \bar{I}(x, \mu) - \mu \frac{\partial \bar{I}(x, \mu)}{\partial x} + \frac{1}{2} \sigma_a a c (T^{n+1/2})^4(x) \right]. \quad (3)$$

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 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 LDPE, 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

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

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 $\phi^\pm(x) = \pm 2\pi \int_0^{\pm 1} I(x, \mu) d\mu$. 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

$$\frac{\langle \phi \rangle_{L,i}^{+,n+1/2} - \langle \phi \rangle_{L,i}^{+,n-1/2}}{c\Delta t} - 2\bar{\mu}_{i-1/2}^+ \bar{\phi}_{i-1/2}^+ + \{\bar{\mu}\}_{L,i}^+ \langle \bar{\phi} \rangle_{L,i}^+ + \{\bar{\mu}\}_{R,i}^+ \langle \bar{\phi} \rangle_{R,i}^+ + \sigma_{a,i}^{n+1/2} h_i \langle \bar{\phi} \rangle_{L,i}^{n+1/2,+} = \frac{h_i}{2} \langle \sigma_a^{n+1/2} acT^{n+1/2,4} \rangle_{L,i}, \quad (5)$$

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 in both governing equations. The face- and volume-averaged angular consistency terms, e.g., $\bar{\mu}_{i-1/2}^+$, 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

$$\{\bar{\mu}\}_{L,i,HO}^+ \approx \frac{\frac{2}{h_i \Delta t} \int_{t^{n-1/2}}^{t^{n+1/2}} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu b_{L,i}(x) \tilde{I}_{HO}(x, \mu, t) dx d\mu dt}{\frac{2}{h_i \Delta t} \int_{t^{n-1/2}}^{t^{n+1/2}} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) \tilde{I}_{HO}(x, \mu, t) dx d\mu dt}, \quad (6)$$

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 $\phi_{i\pm 1/2}^\pm$ 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 the lumped LDFE spatial approximations. Assuming iterative convergence of consistency terms, the LO solution and projection of the HO solution may differ for any given spatial mesh, but the two solutions will converge as the mesh is refined. This approximation 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 introduced 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

$$\frac{\rho_i c_{v,i}}{\Delta t} [T_{L,i}^{n+1/2} - T_{L,i}^{n-1/2}] + \sigma_{a,i}^{n+1/2} (\langle \bar{\phi} \rangle_{L,i}^+ + \langle \bar{\phi} \rangle_{L,i}^-) = \sigma_{a,i}^{n+1/2} ac (T_{L,i}^{n+1/2})^4, \quad (7)$$

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 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 $\langle \phi \rangle_{L,i}^{n+1/2}$ is eliminated from the system. The simplest closure is a weighted average

$$\langle \phi \rangle_{L,i}^{+,n+1/2} \approx \gamma_{L,i,HO}^+ \langle \bar{\phi} \rangle_{L,i}^+, \quad (8)$$

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

$$\gamma_{L,i,HO}^+ = \frac{\langle \phi_{HO} \rangle_{L,i}^{+,n+1/2}}{\langle \bar{\phi} \rangle_{L,i,HO}^+}. \quad (9)$$

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

The unknowns of interest are $\langle \bar{\phi} \rangle_{L,i}^\pm$, $\langle \bar{\phi} \rangle_{R,i}^+$, $T_{L,i}^{n+1/2}$, and $T_{R,i}^{n+1/2}$. 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 $\phi_{LO}^{n+1/2}(x)$ for the next time step.

For the initial LO solve, within a time step, the angular parameters are calculated based on the $\tilde{I}_{HO}^{n-1/2}(x, \mu)$ 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 $\mathcal{D}_{ijn} : x_{i-1/2} < x < x_{i+1/2} \times \mu_{j-1/2} \leq \mu \leq \mu_{j+1/2} \times t^{n-1/2} < t \leq t^{n+1/2}$. 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 [10, 2] is used to define the solution on faces for evaluating terms resulting from the spatial derivative in the streaming term. The LDFE projection is not guaranteed to be positive. Before computing consistency terms, any detected negative values for $\tilde{I}^{n+1/2}(x, \mu)$ or $\tilde{I}^n(x, \mu)$ are made positive by uniformly decreasing the slopes or setting the average to the floor temperature in some cases (see [11] for more details).

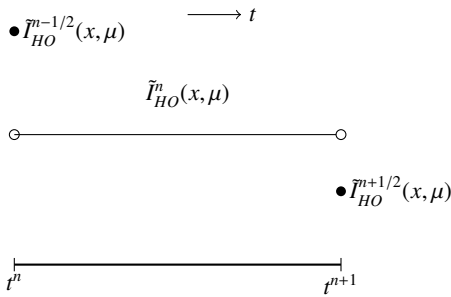
In time, values at $t^{n-1/2}$ are upwinded from the previous time step for both trial spaces.

The first time space is a step, doubly-discontinuous (SDD) trial space, with the time variable illustrated in Fig. ???. The

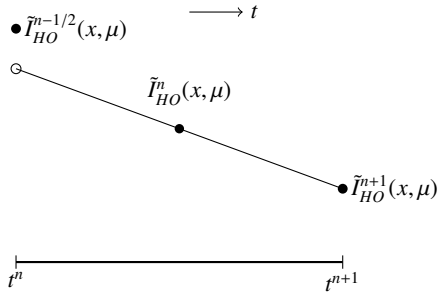
SDD trial space representation for $I(x, \mu, t)$ is

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

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.



(a) SDD trial space



(b) LDFE trial space

Fig. 1: Illustration of the time variable for $\tilde{I}_{HO}(x, \mu, t)$ with two unique trial spaces.

The second trial space is an LDFE trial space in x, μ , and t , as illustrated in Fig. 1b. For a particular space-angle-time element, this trial space is defined as

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

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

$$I_{ij}^n = \frac{6}{\Delta t} \iiint_{\mathcal{D}_{ijn}} \left(\frac{t - t^n}{\Delta t} \right) I(x, \mu, t) dx d\mu dt. \quad (12)$$

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

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

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

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

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

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

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

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

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 $\tilde{\epsilon}$ 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. VI.

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 $\tilde{I}^{n-1/2}(x, \mu)$ as the initial guess greatly increases statistical efficiency in regions of the problem where the solution is slowly varying. For the LDD trial space, we also initialize the time slopes with the values of the previous time step. If the error is sufficiently estimated each batch, both statistically and with the projected trial-space representation, then the overall error in the solution can converge at an exponential rate. However, eventually the estimated projection of the error is not sufficiently accurate 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. It is also not clear what the best approach to adapt the solution in time is, or if it is practical. Adaptive refinement in space and angle could be included in the iterative algorithm in future work, which has been demonstrated for the time-discrete algorithm previously in [2]. This would also help minimize memory requirements for keeping the projected solution between time steps.

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 [12, 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 [12]. 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. VI. 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 an element becomes

$$p_{ij}^n(x, \mu, t) = \frac{\|r\|_{1,i\pm 1/2j}^n}{\|r\|_1 \Delta t \Delta \mu} \delta^\mp \left(x - (x_i \pm \frac{h_i}{2}) \right) + \frac{\|r\|_{1,ij}^{n-1/2}}{\|r\|_1 \Delta x \Delta \mu} \delta^+ \left(t - t^{n-1/2} \right) + \frac{\|r\|_{1,ij}^n}{\|r\|_1 \Delta t \Delta \mu \Delta x}, \quad (x, \mu, t) \in \mathcal{D}_{ijn}, \quad (17)$$

where $\|r\|_1$ is the L_1 norm of $r(x, \mu, t)$ over the entire domain, $\|r\|_{1,i\pm 1/2j}^n$ is the norm of the spatial δ -function portion of the element residual (where the \pm sign corresponds to the direction of μ for the element), $\|r\|_{1,ij}^{n-1/2}$ is the norm of the temporal δ -function portion of the residual, and $\|r\|_{1,ij}^n$ 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

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

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.

IV. RESULTS AND ANALYSIS

We have simulated three 1D, grey test problems to demonstrate the efficacy of our HOLO algorithm: a near-void problem, an optically thin problem, and a standard Marshak wave problem. We will compare sample statistics and accuracy of solutions to an IMC code with source tilting [16] and the HOLO algorithm with BE time-discretized equations [?]. Throughout this section, results that use the BE time discretization are indicated with HOLO-BE and results with the MC-based time closure are indicated with HOLO-LD, HOLO-LDD, or HOLO-SDD, corresponding to the chosen trial space. All plotted results depict the LO solution from the HOLO algorithm. Some figures depict an effective radiation temperature defined as $T_r(x) = (\phi(x)/ac)^{1/4}$.

To provide a quantitative measure, a spatially integrated measure of variance in cell-averaged radiation energy densities $E_{r,i}^{n+1/2}$ was computed, based on the solution at the simulation end time. To form sample estimates of the variance in quantities, twenty independent simulations for each particular result and method were performed using unique random number generator seeds. The sample variance for a particular cell-averaged $E_{r,i}^{n+1/2}$ is

$$S_i^2 = \frac{20}{20-1} \sum_{l=1}^{20} \left(E_i^{n+1/2} - E_{r,i}^{n+1/2,(l)} \right)^2, \quad (19)$$

where $E_i^{n+1/2,(l)}$ is the cell-averaged scalar intensity for cell i from the l -th of 20 independent simulations and $E_i^{n+1/2}$ is the corresponding sample mean, from the 20 simulations. To provide a normalized, spatially-integrated result, we form a norm over cells as

$$\|s\| = \left(\frac{\sum_{i=1}^{N_c} S_i^2}{\sum_{i=1}^{N_c} E_{r,i}^2} \right)^{1/2}, \quad (20)$$

where N_c is the number of spatial elements.

We will also form a figure of merit (FOM) to demonstrate how statistical accuracy scales with the number of histories performed. Our FOM is defined as

$$\text{FOM} = \frac{1}{N_{\text{tot}} \|s\|^2} \quad (21)$$

where N_{tot} is the total number of histories performed during a particular simulation. A larger value of the FOM indicates

that the method produced less variance in the solution, per history performed, for a given problem. This form of the FOM is typically chosen because the variance is expected to reduce inversely proportional to N_{tot} , so for standard MC simulations the FOM becomes, on average, independent of N_{tot} [14]. The FOM is not necessarily expected to be independent of N_{tot} for the HOLO method because of correlations in the ECMC solver. It is difficult to compare computational times with the IMC method because they are implemented in different code infrastructures. Additionally, the HOLO algorithm is converging nonlinearities, whereas the IMC method is only taking a single linearized step, for each time step. Thus, we only focus on the reduction in overall variance, per particle history, as a measure of efficiency.

1. Near-Void Problem

For the first problem, the material properties are uniform throughout a 2.0 cm wide domain with $\rho c_v = 0.01374 \text{ GJ cm}^{-3} \text{ keV}^{-1}$, $\sigma_a = 10^{-6} \text{ cm}^{-1}$. The near-void cross section essentially uncouples the material and radiation. The material and radiation are initially in equilibrium at a temperature of 0.01 keV. An isotropic incident intensity with $T_r = 0.150 \text{ keV}$ is applied at $x = 0$ for $t > 0$; the incident intensity on the right boundary is 0.01 keV. The simulation end time is $t = 0.003 \text{ sh}$. This problem represents a limiting case where IMC will be very efficient because particles are simply streaming, only the space of the initial source needs to be sampled. By taking large time steps, we also strain the consistency terms.

A comparison of the cell-averaged radiation energy densities E_r for IMC and the HOLO method with the HO time closure for the LDD and SDD trial spaces are depicted in Fig. 2a, both for the time-averaged solutions and end-of time step values, from the final time step. The end of time step value for the HOLO method with a BE discretization is also depicted. For the HOLO results, three ECMC batches were performed with a total of 3×10^6 histories per time step and the IMC results were generated with 12×10^6 histories per time step; all IMC results in this section used $\Delta t = 0.001 \text{ sh}$. The minimum number of histories for any sampled space-angle cell, N_{min} in Eq. (??), is 20 for all HOLO simulations. The spatial meshes had 100 spatial cells and both HOLO results used 20μ cells. The MC treatment of the time variable and the closure of the LO equations allow the LO results to correctly reconstruct the wave-front location of IMC, whereas the BE discretization artificially propagates energy. Although not plotted, the results were visually equivalent for either the diamond-like or implicit-like closures in this problem. This is because the problem is nearly linear due to the small cross sections, so the HO moments are reproduced accurately, independent of the chosen closure equation.

A comparison of the same results depicted as radiation temperatures is given in Fig. 2b. By plotting proportional to the fourth-root of the radiation energy density, the noise at low magnitudes past the wave-front are more apparent in the 3 batches and $\Delta t = 0.001$ case. This noise is small relative to the scale of E_r , but it demonstrates a deficiency of the trial space. The step representation over the time step leads to particles sampled near the wave-front with a time near t^n that travel

into the equilibrium region. This is not a bias but rather an under-sampling of the phase space; if sufficient histories were performed there would be negative particles that canceled out this error. The ECMC iterations can lead to negative averages in the HO solution out front of the wave front. In such cells, the average was set to the floor value and slopes to zero. This effect is significantly reduced when a smaller time step is taken, although the mesh imprinting error is increased. Fig. 2c illustrates the convergence of the mesh-imprinting error in angle.

For the case of a single batch, there is less noise past the wavefront because the choice of $I^n(x, \mu)$ as an initial guess for $I^{n+1}(x, \mu)$ prevents most particles from traveling past what the physical transport should allow. The discrepancy between the IMC and the single batch HOLO solution near the foot of the wave is a result of the spatial discrepancy between the LD FE HO projection and the lumped LD LO equations; this dispersion is not present in the HO solution. This discrepancy can also lead to some negativities in the LD edge values of $\phi^{n+1}(x)$, which are set to the floor value for the next time step. Figure. 2c compares radiation energy densities for various numbers of μ cells. At coarser mesh sizes, the imprinting of the mesh is visible in the location of the wave-front. This is a result of the projection onto the space-angle mesh between time steps. As the mesh is refined, the solution converges towards the IMC solution. Smaller time step sizes can increase the mesh imprinting because the projection onto the trial space happens more often. However, it is important to note that this problem is a limiting case; the mesh imprinting will be reduced as σ_a is increased and absorption-emission events smooth the angular intensity across each time step.

2. Optically-Thin Problem

We modify the near-void problem by increasing the absorption cross section to 0.2 cm^{-1} ; all other problem parameters are the same. Radiation temperatures at the end of the last time step are compared for IMC, HOLO-TC, and HOLO-BE in Fig. 3. The HOLO-TC and HOLO-BE results were generated with 30μ cells, and all spatial meshes used 100 cells. All results used 3×10^6 histories per time step. At smaller time step sizes, the effects of mesh imprinting are visually apparent in the HOLO-TC results, leading to more dispersion near the wave-front. There is good agreement between the HOLO-TC results and IMC, except some dispersion near the wavefront. As in the previous problem, the HOLO-BE results are very inaccurate at capturing the wavefront location. IMC demonstrates substantial statistical noise in the equilibrium region.

The accuracy of the HOLO-TC and IMC method were compared against a reference IMC solution. Because the material is loosely coupled in this problem we expect IMC to be accurate with sufficient particle histories. The reference solution is the average of 20 IMC simulations of 20×10^6 histories, each with $\Delta t = 10^{-4}$ sh. The estimated value of $\|s\|$ for the reference solution is 0.025%. The discrete norm of the error in cell-averaged mean intensities $\|e\|_{a,rel}$ is computed using Eq. (??) for ϕ^{n+1} from the last time step, averaged over 20 simulations. Sample statistics for cell-averaged ϕ^{n+1} were

also computed using the FOM from Eq. (??).

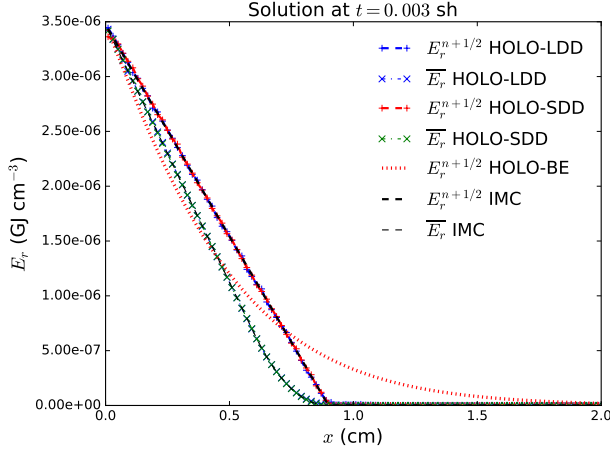
Table. ?? compares computed values of $\|e\|_{a,rel}$ and FOM for the census radiation energy densities, for the case of $\Delta t = 0.0005$ sh. HOLO results were generated for the case of 1 and 2 batches, with the same total number of histories per time step, where the number of batches is indicated in parenthesis. The standard deviation of each estimate of $\|e\|_{a,rel}$ follows each value in parenthesis. At low particle counts, the HOLO-TC method demonstrates substantial noise. A plot of the inaccuracies for the case of 30,000 histories and a single batch is given in Fig. ???. As demonstrated, statistical noise in the estimate of \tilde{I}^{n+1} introduce instabilities into the LO result. This is due to the trial space representation of the census particles at the end of the time step being poorly estimated. For the 2 batch case, there is less error in the estimate of $\tilde{I}^{n+1}(x, \mu)$ because only the deviation from the first batch estimate of

$\tilde{I}(x, \mu)$ is estimated with MC. At higher history counts there is an increase in efficiency, however the IMC method is more accurate overall due to the projection error between time steps. For reference, statistics were measured for the HOLO-BE method with two batches of 150,000 histories per time step, producing $\|e\|_{a,rel} = 10.5\%$ and FOM = 3100, demonstrating substantial inaccuracy but improved efficiency.

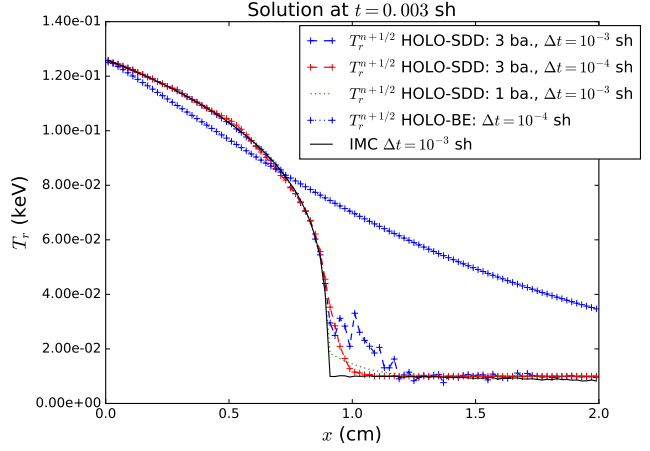
Table I compares results for $\Delta t = 0.0001$ sh. The results were generated for two different mesh sizes, but $\|e\|_{a,rel}$ is computed using the same 100 spatial cell reference solution in both cases. All FOM values are relative to IMC with 100 x cells and 30,000 histories. At the coarser mesh size, the HOLO-TC method has a factor of 95 higher FOM, indicating much-improved statistical efficiency. However, the projection error limits accuracy to around 1.5%. At the finer mesh size, the HOLO-TC method remains more efficient (as long as the batch size is sufficient) and produces higher accuracy than the IMC results. For reference, statistics were measured for the HOLO-BE method with two batches of 150,000 histories per time step. The HOLO-BE results produced $\|e\|_{a,rel} = 3.7\%$ and FOM = 4700 for the coarse mesh, and $\|e\|_{a,rel} = 3.6$ and FOM = 9600 for the fine mesh. The accuracy of the HOLO-BE method is limited by the time integration accuracy.

TABLE I: Comparison of accuracy and FOM for the end of time step radiation energy densities, of the last time step, for the optically thin problem and $\Delta t = 1 \times 10^{-4}$ sh. The reference IMC result has 100 x cells. Simulation end time is $t = 0.003$ sh. Fractional error in all results < 0.05

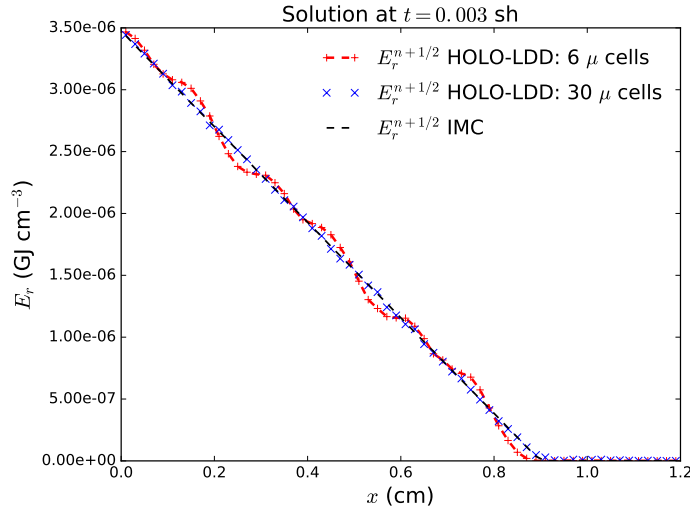
$\ e\ _{a,rel}$			
hists./step	IMC	HOLO-SDD (1)	HOLO-LDD (1)
30,000	2.93%	14.00%	%
300,000	0.99%	0.37%	%
1,000,000	0.49%	0.18%	%
FOM			
hists./step	IMC	HOLO-SDD (1)	HOLO-LDD (1)
30,000	1	0.11	0.10
300,000	0.90	14.24	8.61
1,000,000	1.01	81.71	71.36



(a) Radiation energy densities $E_{r,i}$ with $\Delta t = 0.001$ sh.



(b) Radiation temperatures $T_{r,i}$ for different time step sizes and numbers of batches.



(c) Census radiation energy densities $E_{r,i}^{n+1/2}$ for the HOLO-LDD method with different numbers of μ cells and $\Delta t = 0.001$ sh.

Fig. 2: Comparisons between IMC and the HOLO method with different time discretizations and settings.

3. Marshak Wave Problem

It is important to demonstrate that the time closures are stable in a mix of optically thick and optically thin regions, and that the ECMC method is still efficient for such problems. This problem has the same material properties as the optically thin problem except $\sigma_a(T) = 0.001T^{-3}$ and the initial temperature is 2.5×10^{-5} keV. The time step size is linearly increased from 0.001 sh to a maximum step of 0.01 sh over the first 10 time steps. It was found for this problem that it was necessary to use more than one batch for the HOLO-TC algorithm to stably converge. This is because few particles reach t^{n+1} in optically thick regions.

This slowly-evolving problem can be accurately modeled with the BE time discretization, but the MC time closure demonstrates stability, with sufficient histories, in the mix of

optically thick and thin regions that occurs as the material heats. Table II compares FOM values for IMC and the HOLO method with MC time treatment and for a BE discretization. The HOLO-TC is not as statistically efficient as HOLO-BE for this problem, but is more efficient than IMC with sufficient histories.

The time step size is linearly increased from 0.001 sh to a maximum step of 0.01 sh over the first 10 time steps; the last time step is adjusted to reach the desired simulation end time. It was found for this problem that it was necessary to use more than one batch for the HOLO-SDD method to stably converge as it is difficult for particles to reach the end of the time step.

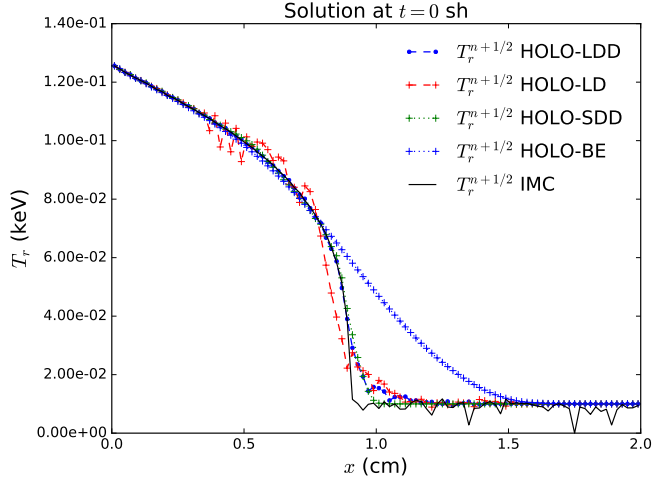


Fig. 3: Comparison of radiation temperatures of IMC and the HOLO method for different time step sizes and numbers of batches, for optically thin problem.

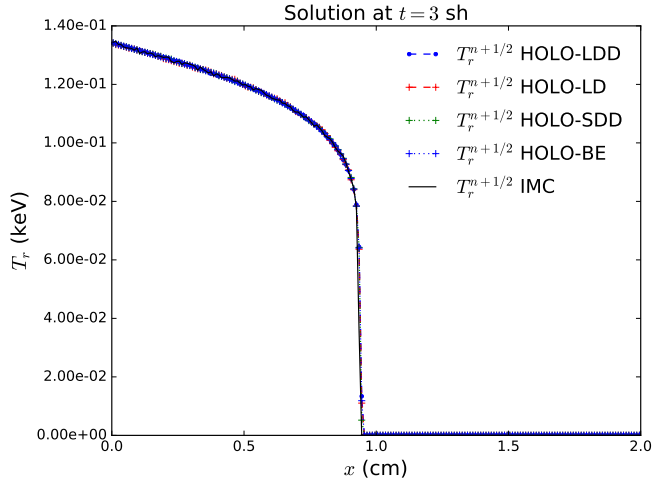


Fig. 4: Comparison of HOLO-TC, HOLO-BE, and IMC methods for the Marshak Wave problem, with 10^6 histories per time step.

The doubly-discontinuous trial spaces were found to be exceptionally noisy for this problem, requiring 10^6 histories per time step to remove visible noise, although they were still more efficient than standard IMC.

Figure 4 compares the accuracy of IMC and the various HOLO methods, showing agreement between the solutions. The values of t_{ted} at $t = 3$ sh, with 10^6 histories per time step for all simulations. As demonstrated, there is good agreement among the results, with the plots overlaying each other. This problem can be accurately modeled with the Backward Euler time discretization, but the MC time closure is stable for this problem with a mix of optically thick and thin regions. Table II compares sample statistics for IMC, the HOLO-LD, HOLO-SDD, and the HOLO-BE method. The HOLO-BE method is significantly more efficient for comparable accuracy in this problem with a very optically thick region. The HOLO-LD

method is much more efficient than the HOLO-SDD method in this problem because particles do not need to transport the thick region to reach the end of the time step. There were some convergence issues for multiple batches for the HOLO-LD method..

TABLE II: Comparison of FOM for the Marshak wave problem. Simulation end time is $t = 3.0$ sh.

hists./step	FOM			
	IMC	HOLO-SDD (2)	HOLO-LD (2)	HOLO-BE (2)
50,000	0.92	—	96.2	1708
300,000	1.00	0.43	200	2050
1,000,000	0.94	15.95	201	1806

V. CONCLUSIONS

Our HOLO method has been extended to include a residual MC treatment of the time variable. Results demonstrate that residual MC methods can be extended to include the time variable, increasing accuracy in optically thin regions compared to a BE discretization. Our ECMC algorithm can be more statistically efficient than IMC, with sufficient batch sizes, although sufficient mesh resolution is needed to limit projection error between time steps. We have demonstrated a new approach to closing the LO equations in time that produces accurate solutions. Long-term, an ideal solution would require no projection between time steps, which will likely require an operator split on the radiation time derivative. At this point, we believe that the SDD trial space in time suffers from inaccuracy because only histories that reach the end-of-time step contribute to $I^{n+1/2}$ and because of the flat interior representation. Alternatively, the LDFE trial space could include the time variable. Then, all particle tracks contribute to slopes over the interior of the time step. However, there is some additional truncation error as $\tilde{I}^{n+1/2}$ is an extrapolated quantity. This trial space requires substantial modifications to the residual sampling algorithm because of how the residual is currently sampled. An importance sampling methodology has been developed but remains to be implemented. Modifications to the sampling algorithm are necessary to extend to higher spatial dimensions, so determining if our approach is efficient will be beneficial to future work. We will include results for the LDFE time representation for the full paper.

VI. FUTURE WORK

Treatment of scattering, if time-averaged scattering is OK or if we need something more advanced.

Incorporating the LD temperature time dependence? But that would be real hard. How to split off census particles

Ideally operator split off the census, and ideally be able to map the particles and error back onto the error particles, but keeping both will be exceptionally memory intensive.

APPENDIX

The Residual for the LDFF Trial Space

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

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

where $\Delta\mu = \mu_{j+1/2} - \mu_{j-1/2}$ and $I_{a,ij}^n$, $I_{x,ij}^n$, $I_{\mu,ij}^n$, and $I_{t,ij}^n$ 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:

$$r_{ij}^n(x, \mu, t) = r_{a,ij}^n + \frac{2}{h_i} r_{x,ij}^n (x - x_i) + \frac{2}{\Delta\mu} r_{\mu,ij}^n (\mu - \mu_j) + \frac{2}{\Delta t} r_{t,ij}^n (t - t^n) \quad (\text{A.2})$$

where

$$r_{a,ij}^n = q_{a,i} - \sigma_{a,i} I_{a,ij}^n - \frac{2}{c\Delta t} I_{t,ij}^n - \mu_j \frac{2}{\Delta\mu} I_{x,ij}^n, \quad (\text{A.3})$$

$$r_{x,ij}^n = q_{x,i} - \sigma_{a,i} I_{x,ij}^n, \quad (\text{A.4})$$

$$r_{\mu,ij}^n = -\sigma_{a,i} I_{\mu,ij}^n - \frac{\Delta\mu}{h_i} I_{x,ij}^n, \quad (\text{A.5})$$

$$r_{t,ij}^n = -\sigma_{a,i} I_{t,ij}^n \quad (\text{A.6})$$

where $q_{a,i}$ and $q_{x,i}$ are the zeroth and first moments of the LO LDFF 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

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

where

$$r_{a,ij}^{n,f} = (I_{a,i-1,j}^n + I_{x,i-1,j}^n) - (I_{a,ij}^n - I_{x,ij}^n) \quad (\text{A.8})$$

$$r_{\mu,ij}^{n,f} = I_{\mu,i-1,j}^n - I_{\mu,ij}^n, \quad (\text{A.9})$$

$$r_{t,ij}^{n,f} = I_{t,i-1,j}^n - I_{t,ij}^n. \quad (\text{A.10})$$

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

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

where

$$r_{a,ij}^{n-1/2} = I_{a,ij}^{n-1/2} - (I_{a,ij}^n - I_{t,ij}^n), \quad (\text{A.12})$$

$$r_{x,ij}^{n-1/2} = I_{x,ij}^{n-1/2} - I_{x,ij}^n, \quad (\text{A.13})$$

$$r_{\mu,ij}^{n-1/2} = I_{\mu,ij}^{n-1/2} - I_{\mu,ij}^n. \quad (\text{A.14})$$

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 LDFF 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

$$\hat{\epsilon}_{x,ij}^n = \frac{1}{N} \frac{6}{\Delta t h_i} \sum_{m=1}^{N_{score}} \frac{s_m}{h_i \Delta\mu} w_m (x_c^m - x_i), \quad (\text{A.15})$$

where x_c^m 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 contribution of a differential 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

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

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

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

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 LDFF 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

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

where t_c^m is the time of the particle at the center of the path length.

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