A High-Order Low-Order Algorithm with Exponentially-Convergent Monte Carlo for Thermal Radiative Transfer Problems

Dissertation Proposal
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1 Introduction

1.1 Thermal radiative transfer background

Thermal radiative transfer (TRT) physics describe the time-dependent energy distributions of a photon radiation field and a high-temperature material. The material and radiation exchange energy through absorption and emission of photons by the material. Accurate modeling of TRT physics becomes relevant in the high-energy, high-density physics regime. Typical computational applications of TRT include simulation of inertial confinement fusion and astrophysics phenomena. The transport of photons through a material is characterized by particle position, direction, and frequency. The material energy distribution is described by the material internal energy (often described by material temperature) as a function of position. The high-dimensional space results in a difficult, nonlinear transport problem.

This research will focus on a simplified one spatial dimension and frequency-integrated (grey) TRT model. The governing equations for this simplified model are the radiation and

material energy balance equations

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

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

In the above equations the fundamental unknowns are the material temperature $T(x,t)$ and the angular intensity $I(x,\mu,t)$ of radiation, where x is the position, t is the time, μ is the x-direction cosine of the photon direction of travel, and a, c, ρ, and c_v are the radiation constant, speed of light, material mass density, and material specific heat; σ_a, σ_s, and σ_t are the absorption, scattering, and total cross sections (cm^{-1}), respectively. The scalar radiation intensity $\phi(x,t) = \int_{-1}^{1} I(x,\mu,t)\text{d}\mu$ is related to the radiation energy density E (with typical units Jks cm^{-3} sh^{-1}) by the relation $E = \phi/c$. The equations are strongly coupled through the gray Planckian emission source $\sigma_a acT^4$, which is a nonlinear function of temperature, and the radiation absorption term $\sigma_a\phi$. In general, the material properties are a function of T. The temperature dependent material properties and absorption-reemission physics lead to systems that require accurate modeling of photon transport through a mix of streaming and optically-thick, diffusive regions. Although in most physical applications material motion is present, it is not the focus of this research and will not be considered. The purpose of the proposed research is to demonstrate the ability of of a new algorithm to provide highly-accurate and efficient solutions to Eq. (1) and Eq. (2).

1.2 The implicit Monte Carlo method

The Monte Carlo (MC) method [1] is a standard computational method in the field of radiation transport. The implicit Monte Carlo (IMC) method [2] is the most common approach for applying the MC method to TRT problems. The IMC method linearizes Eq. (1) & Eq. (2) over a discrete time step to produce a linear transport equation, which can be solved with MC simulation. The linear transport equation contains an approximate emission source and effective scattering cross section that represent absorption and reemission of photons over a time step. The transport equation is solved with MC simulation to advance

the distribution of radiation to the end of the time step and determine the energy absorbed by the material over the time step. The energy absorption by the material is tallied over a discrete spatial mesh, computed with cell-averaged quantities. The energy absorption in each mesh cell is used to directly estimate a new end of time step material temperature based on the linearized material energy balance equation. Integration of the time-variable is treated continuously over the time step via MC sampling, but the linearized Planckian source in the transport equation is based on a time-discrete approximation.

The IMC method has some limitations. In optically thick regions, or for large time steps, the effective scattering dominates interactions. In these diffusive regions IMC becomes computationally expensive. Acceleration methods typically attempt to improve efficiency by allowing particles to take discrete steps through optically-thick regions based on a spatially-discretized diffusion approximation [3, 4]. Another issue occurs due to the approximate linearization of the system which can not be iteratively improved due to the high computational cost of the MC transport. For some problems, the linearization can yield non-physical results that violate the discrete maximum principle if the time step size is too large or the cell size is too small [5]. The violation of the maximum principle results in the material temperature being artificially higher than the boundary conditions and sources should physically allow. The violation is caused by the temperature in the emission source not being fully implicit in time due to the necessary linearization. The work in [6] uses less-expensive MC iterations to produce an implicit system which prevents this from happening, but has very slow iterative convergence in diffusive problems. In IMC, temperature-dependent material properties, in particular cross sections, are evaluated at the previous-time step temperature. These lagged cross sections can produce inaccurate solutions but do not cause stability issues.

For TRT simulations, inaccurate spatial representation of the emission source over a cell can result in energy propagating through the domain artificially fast, yielding non-physical results referred to as "teleportation error" [7]. The IMC method uses a fixup known as source tilting to mitigate this problem. Source tilting reconstructs a more accurate linear-discontinuous representation of the emission source within a cell based on the cell-averaged

material temperatures in adjacent cells. This linear reconstruction is also necessary to preserve the asymptotic equilibrium diffusion limit (EDL), at least for a more general time step size and class of problems than for a piece-wise constant representation [8]. Preserving the equilibrium diffusion limit is an important aspect of a numerical method for TRT problems. In this limit, cells are optically thick and diffusive, and the material and radiation energy fields approach equilibrium. Spatial discretizations which do not preserve the EDL can produce inaccurate solutions, even though the mesh size should accurately capture the behavior of the solution [9].

1.3 Previous work on moment-based acceleration methods

An alternative application of MC to the TRT equations is moment-based hybrid MC methods. Recent work has focused on so-called high-order low-order (HOLO) methods [10, 11, 12, 13]. These methods involve fixed-point iterations between high-order (HO) MC solution of a transport equation and a deterministic LO system. The low-order (LO) operator is based on angular moments of the transport equation, formulated over a fixed spatial mesh. Physics operators that are time consuming for MC to resolve, e.g., absorption-reemission physics, are moved to the LO system. The reduced angular dimensionality of the system and Newton methods allow for non-linearities in the LO equations to be fully resolved efficiently [10, 11]. The high-order (HO) transport problem is defined by Eq. (1), with sources estimated from the previous LO solution. The high-order (HO) transport equation is solved via MC to produce a high-fidelity solution for the angular intensity. The MC estimate of the angular intensity is used to estimate consistency terms, present in the LO equations, that require the LO system to preserve the angular accuracy of the MC solution. These consistency terms are present in all spatial-regions of the problem, requiring statistical variance to be reduced sufficiently throughout the entire domain of the problem.

Another area of related research is application of residual Monte Carlo. The residual MC method is also referred to as the difference formulation of the transport equation, with some minor differences in implementation. The goal of these methods is to modify the transport equation, by subtracting equilibrium terms, such that the MC simulation solves

for unknowns representing only the change in the intensity over a time step. This has the potential to limit statistical noise significantly in regions where the solution is near equilibrium. The work in [12] used residual MC as a HO solver for 1D grey problems. The residual MC demonstrated impressive reduction in statistical variance. However, a piecewise constant representation was used for the space-angle representation of the intensity, which does not preserve the EDL and can be inaccurate in angularly complex regions of the problem. The difference formulation has also been applied to another algorithm known as the symbolic IMC method (SIMC), for the case of 1D multi-frequency problems [14]. SIMC forms a standard FE solution to the material energy balance equation, and uses symbolic weights in the MC transport to solve for expansion coefficents. The difference formulation was also applied to a linear-discontinuous FE spatial representation of the emission source, demonstrating accuracy in the EDL [15]. Both [14] and [12] produced minimal statistical noise in slowly varying problems where the behavior of the system is near equilibrium.

1.4 Proposed algorithm

The research proposed herein provides a new HOLO algorithm for radiative transfer. In this work, we propose an S_2-like LO operator [16] in conjunction with an exponentially-convergent MC (ECMC) method [17] for the HO solver. Our LO system and approach to enforcing consistency contrast greatly from the typical formulation in [12, 10, 11]. We have derived the LO operator directly from the transport equation, using a linear-discontinuous finite-element (LDFE) spatial discretization. Exponentially-convergent Monte Carlo (ECMC)[17, 13] provides an iterative algorithm that can efficiently reduce statistical noise to the same order as the HOLO iteration error with significantly less particle histories than standard MC. In particular, ECMC is exceptionally efficient in time-dependent TRT problems because information about the intensity from the previous time step can be used as an accurate initial guess for the new end of time step intensity. However, implementation of ECMC is non-trivial, requiring a finite-element representation of the solution in all phase-space variables that are being sampled with MC. The method contains many of the desired qualities, such as preserving the equilibrium diffusion limit, preserving the maximum principle,

and in particular, providing high-fidelity MC solution to the TRT equations in an efficient manner.

Herein an overview of our algorithm and the research performed thus far is detailed. Then, the remaining areas to be investigated are proposed. Finally, a summary of the research and outline of research to be performed are given.

2 Description of Research

2.1 Overview of the HOLO Algorithm

For simplicity, our HOLO method uses a backwards Euler discretization in time, as well as constant specific heats and cell-wise constant cross sections. The time-discretized equations are

$$\mu \frac{\partial I^{n+1}}{\partial x} + \left(\sigma_t^{n+1} + \frac{1}{c\Delta t} \right) I^{n+1} = \frac{\sigma_s}{2} \phi^{n+1} + \frac{1}{2} \left(\sigma_a a c T^4 \right)^{n+1} + \frac{I^n}{c\Delta t} \tag{3}$$

$$\rho c_v \frac{T^{n+1} - T^n}{\Delta t} = \sigma_a^{n+1} \phi^{n+1} - \sigma_a a c (T^4)^{n+1}, \tag{4}$$

where Δt is the uniform time step size, the superscript n is used to indicate the n-th time step. Cross sections are evaluated at the end of time step temperature, i.e., $\sigma_a^{n+1} \equiv \sigma_a(T^{n+1})$.

In the HOLO context, the LO solver models the physical scattering and resolves the material temperature spatial distribution $T^{n+1}(x)$, for each time step. The LO equations are formed via half-range angular and spatial moments of Eq. (3) and Eq. (4). The spatial moments are formed over a finite-element mesh and a linear-discontinuous spatial closure with upwinding is used to close the system. The angular treatment in the LO equations has the same form as those used in the hybrid-S_2 method in [16], with consistency parameters that represent angularly-weighted averages of the intensity. If the angular consistency parameters were estimated exactly, then the LO equations preserve the exact angular-averaged solution, with respect to the chosen spatial discretization. These consistency parameters are lagged

in each LO solve, estimated from the previous HO solution for the intensity, or from a previous time step. The discrete LO equations always conserve total energy, independent of the accuracy of the consistency terms. It is noted that our LO operator is different from the nonlinear diffusion acceleration (NDA) methods used by other HOLO methods [12, 11, 10]. In NDA methods, an artificial term is added to the LO equations to enforce consistency and estimated using a previous HO solution. In our method we have simply algebraically manipulated space-angle moment equations to produce our consistency terms, which will hopefully produce more stability in optically-thick regions where NDA methods demonstrate stability issues.

The solution to the LO system is used to construct a LDFE spatial representation of the scattering and emission sources on the right hand side of Eq. (3). This HO transport problem represents a characteristic method that uses MC to invert the continuous streaming plus removal operator with an LDFE representation of sources. We will solve this transport problem using ECMC [17]. The output from ECMC is $\tilde{I}^{n+1}(x,\mu)$, a space-angle LDFE projection of the exact solution for $I^{n+1}(x,\mu)$. Once computed, $\tilde{I}^{n+1}(x,\mu)$ is used to directly evaluate the necessary consistency parameters for the next LO solve. The HO solution is not used to directly estimate a new material temperature, which eliminates typical operator splitting stability issues that require linearization of the emission source in Eq. (1).

The process of performing subsequential HO and LO solves, within a single time step, can be repeated to obtain an increasingly accurate solution for $\phi^{n+1}(x)$ and $T^{n+1}(x)$. Thus, the HOLO algorithm, for the n-th time step, is

1. Perform a LO solve to produce an initial guess for $T^{n+1}(x)$ and $\phi^{n+1}(x)$, based on consistency terms estimated with $\tilde{I}^{n}$.

2. Solve the HO system with ECMC for $\tilde{I}^{n+1}(x,\mu)$, based on the current LO estimate of emission and scattering sources.

3. Compute new LO consistency parameters with $\tilde{I}^{n+1}$.

4. Solve the LO system with HO consistency parameters to produce a new estimate of ϕ^{n+1} and T^{n+1}.

5. Optionally repeat 2 – 4 until desired convergence is achieved.

6. Store $\tilde{I}^n \leftarrow \tilde{I}^{n+1}$, and move to the next time step.

The consistency terms force the HO and LO solutions for $\phi^{n+1}(x)$ to be consistent to the order of the current HOLO iteration error, as long as the LDFE spatial representation can accurately represent $\phi(x)$ and $T(x)$.

2.2 The Low-Order Equations

This section contain explicit details of the LO operator. To form the LO system of equations, spatial moments are taken over each spatial cell i: $x \in [x_{i-1/2}, x_{i+1/2}]$, weighted with the standard linear finite element (FE) interpolatory basis functions. For example, the L moment operator is defined by

$$\langle\cdot\rangle_{L,i} = \frac{2}{h_i}\int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)(\cdot)\mathrm{d}x, \tag{5}$$

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 FE basis function, for cell i, corresponding to position $x_{i-1/2}$. The right moment $\langle\cdot\rangle_{R,i}$ is defined with weight function $b_{R,i}(x) = (x - x_{i-1/2})/h_i$. To reduce the angular dimensionality, positive and negative half-range integrals of the angular intensity are taken. The half-range averages of I are defined as $\phi^+(x) = \int_0^1 I(x,\mu)\mathrm{d}\mu$ and $\phi^-(x) = \int_{-1}^0 I(x,\mu)\mathrm{d}\mu$, respectively. Thus, in terms of half-range quantities, $\phi(x) = \phi^-(x) + \phi^+(x)$.

Pairwise application of the L and R basis moments with the $+$ and $-$ half-range integrals to Eq. (3) ultimately yields four moment equations per cell. As in [16], algebraic manipulation is performed to form intensity-weighted averages of μ, which we denote consistency terms. As an example, the equation resulting from application of the L moment and positive half-range integral is

$$\begin{aligned} -2\mu_{i-1/2}^{n+1,+}\phi_{i-1/2}^{n+1,+} + \{\mu\}_{L,i}^{n+1,+}\langle\phi\rangle_{L,i}^{n+1,+} + \{\mu\}_{R,i}^{n+1,+}\langle\phi\rangle_{R,i}^{n+1,+} + \left(\sigma_{t,i}^{n+1} + \frac{1}{c\Delta t}\right)h_i\langle\phi\rangle_{L,i}^{n+1,+} \\ - \frac{\sigma_{s,i}h_i}{2}\left(\langle\phi\rangle_{L,i}^{n+1,+} + \langle\phi\rangle_{L,i}^{n+1,-}\right) = \frac{h_i}{2}\langle\sigma_a^{n+1}acT^{n+1,4}\rangle_{L,i} + \frac{h_i}{c\Delta t}\langle\phi\rangle_{L,i}^{n,+}, \end{aligned} \tag{6}$$

where the $\phi^+_{i-1/2}$ and $\mu^+_{i-1/2}$ terms represent face-averaged quantities at $x_{i-1/2}$. The negative direction and R moment equations are derived analogously. The element-averaged angular consistency terms are defined in terms of half-range integrals, e.g.,

$$\{\mu\}^{n+1,+}_{L,i} \equiv \frac{\langle \mu I^{n+1}\rangle^+_{L,i}}{\langle I^{n+1}\rangle^+_{L,i}} = \frac{\frac{2}{h_i}\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu\, b_{L,i}(x) I^{n+1}(x,\mu)\mathrm{d}x\mathrm{d}\mu}{\frac{2}{h_i}\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) I^{n+1}(x,\mu)\mathrm{d}x\mathrm{d}\mu}. \tag{7}$$

The $\mu^{n+1,+}_{i-1/2}$ term is defined analogously and represents an angular average on the face at $x_{i-1/2}$.

To derive the LO material energy equations, $T(x)$ is represented spatially in the LDFE trial space, i.e., $T(x) \simeq T_{L,i} b_{L,i}(x) + T_{R,i} b_{R,i}(x), \quad x \in (x_{i-1/2}, x_{i+1/2})$. Similarly, the emission term is represented in the material and radiation equations with the LDFE interpolant $T^4(x) \simeq T^4_{L,i} b_{L,i}(x) + T^4_{R,i} b_{R,i}(x)$. The L and R spatial moments are taken of the material energy equation, using these definitions for $T(x)$ and $\sigma_a a c T^4(x)$ to simplify moments. For example, the final LO material energy equation resulting from application of the L moment is

$$\frac{\rho_i c_{v,i}}{\Delta t}\left[\left(\frac{2}{3}T_{L,i} + \frac{1}{3}T_{R,i}\right)^{n+1} - \left(\frac{2}{3}T_{L,i} + \frac{1}{3}T_{R,i}\right)^{n}\right] + \sigma^{n+1}_{a,i}\left(\langle\phi\rangle^+_{L,i} + \langle\phi\rangle^-_{L,i}\right)^{n+1} = \sigma^{n+1}_{a,i} a c \left(\frac{2}{3}T^4_{L,i} + \frac{1}{3}T^4_{R,i}\right)^{n+1}. \tag{8}$$

Cross sections have been assumed constant over each element, evaluated at the average temperature within the element, i.e., $\sigma^{n+1}_{a,i} = \sigma_{a,i}([T^{n+1}_{L,i} + T^{n+1}_{R,i}]/2)$.

2.3 Closing the LO equations

The six degrees of freedom (DOF) over each cell i are the four moments $\langle\phi\rangle^+_{L,i}$, $\langle\phi\rangle^+_{R,i}$, $\langle\phi\rangle^-_{L,i}$, and $\langle\phi\rangle^-_{R,i}$ and the two spatial edge values $T_{L,i}$ and $T_{R,i}$. The relation between the volume and face averaged quantities and the angular consistency parameters (e.g., Eq. (7)) are not known a priori. To close the LO system spatially, the standard LDFE approximation

with upwinding is used. For example, for positive flow (e.g., Eq. (6)) the face terms $\mu_{i-1/2}$ and $\phi_{i-1/2}$ are upwinded from the previous cell $i-1$ or from a boundary condition; the terms at $x_{i+1/2}$ are linearly extrapolated, computed using the L and R basis moments, e.g., $\phi^+_{i+1/2} = 2\langle\phi\rangle^+_R - \langle\phi\rangle^+_L$. A lagged estimate of I^{n+1} from the latest HO solve is used to estimate the angular consistency parameters.

2.4 Solution of the LO equations and Diffusion Synthetic Acceleration

Newton's method is used to solve the global system of coupled LO equations, based on a typical linearization of the Planckian source with cross sections evaluated at lagged temperatures. This procedure is described in [9]. Once the system is linearized, a discrete matrix equation is formed. Scattering (including the effective scattering resulting from the linearization of the Planckian source) can be included in the system matrix, producing an asymmetric, banded-matrix. The matrix has a band width of seven and is inverted directly. Newton iterations are repeated until $\phi^{n+1}(x)$ and $T^{n+1}(x)$ are converged to a desired relative tolerance.

2.5 The ECMC High Order Solver

The transport equation to be solved by the HO solver is

$$\mu\frac{\partial I^{n+1}}{\partial x} + \left(\sigma_t + \frac{1}{c\Delta t}\right) I^{n+1} = \frac{\sigma_s}{2}\phi^{n+1}_{LO} + \frac{1}{2}\left(\sigma_a acT^4_{LO}\right)^{n+1} + \frac{\tilde{I}^n}{c\Delta t}, \tag{9}$$

where the emission and scattering sources are known from the previous LO solution and $\tilde{I}^n$ is the LDFE projection of $I(x,\mu)$ from the previous time step. This defines a fixed-source, pure absorber transport problem that must be solved for each HO solve. In operator notation, Eq. (9) can be written as

$$\mathbf{L}I^{n+1} = q \tag{10}$$

where I^{n+1} is the exact transport solution for the end-of-time-step intensity. The linear operator $\mathbf{L}$ is the streaming plus removal operator defined by the left hand side of Eq. (3).

The m-th approximate LDFE solution to Eq. (10) (m is the index of inner HO batches) is represented as $\tilde{I}^{n+1,(m)}$. The m-th residual is defined as $r^{(m)} = q - \mathbf{L}\tilde{I}^{n+1,(m)}$. Addition of $\mathbf{L}I^{n+1} - q = 0$ to the residual equation and manipulation of the result yields the error equation

$$\mathbf{L}(I^{n+1} - \tilde{I}^{n+1,(m)}) = \mathbf{L}\epsilon^{(m)} = r^{(m)} \tag{11}$$

where I^{n+1} is the exact solution and $\epsilon^{(m)}$ is the error in $\tilde{I}^{n+1,(m)}$. We have suppressed the HOLO iteration indices because the LO estimated q^k and $\mathbf{L}^k$ remain constant over the entire HO solve. The $\mathbf{L}$ operator in the above equation is inverted yielding the Monte Carlo LDFE projection of the error in $\tilde{I}^{n+1,(m)}$, i.e.,

$$\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1} r^{(m)} \tag{12}$$

where $\mathbf{L}^{-1}$ is the inversion of the streaming and removal operator via MC simulation. The fundamental transport of particles is the same as standard MC particle transport codes, but the LDFE source will now contain positive and negative weight particles. The space-angle moments of the computed error $\tilde{\epsilon}^{(m)}$ can be added to the moments of $\tilde{I}^{n+1,(m)}$ to produce a more accurate solution.

Here, we emphasize the solution $\tilde{I}^{n+1,(m)}$ represents the projection of the exact Monte Carlo solution onto the LDFE trial space. This is in general far more accurate than a standard finite element solution, particularly in the angular variable. For example, in typical IMC calculations the average energy deposition within a cell is computed using a standard path-length volumetric flux tally; the zeroth moment of the LDFE projection of $\tilde{\epsilon}$ is computed using an equivalent tally. The primary truncation error is in the LD spatial representation of the source term q. Volumetric flux tallies over each space-angle element are required to represent $\tilde{\epsilon}^{(m)}$.

The ECMC algorithm is

1. Initialize guess for $\tilde{I}^{n+1,(0)}$ to $\tilde{I}^n$ or the projection of $\tilde{I}^{n+1}$ from the latest HO solve
2. Compute $r^{(m)}$.

3. Perform a MC simulation to obtain $\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1} r^{(m)}$

4. Compute a new estimate of the intensity $\tilde{I}^{n+1,(m+1)} = \tilde{I}^{n+1,(m)} + \tilde{\epsilon}^{(m)}$

5. Repeat steps 2 – 4 until desired convergence criteria is achieved.

The initial guess for the angular intensity $I^{n+1,(0)}$ is computed based on the previous solution for $\tilde{I}^{n}$. This is a critical step in the algorithm; it significantly reduces the required number of particles per time step because the intensity does not change drastically between time steps in optically thick regions. Exponential convergence is obtained because with each batch a better estimate of the solution is being used to compute the new residual, decreasing the magnitude of the MC residual source each iteration m, relative to the solution I^{n+1}. Each MC estimate of the moments of ϵ still has a statistical uncertainty that is governed by the standard $1/\sqrt{N}$ convergence rate [1], for a particular source $r^{(m)}$, where N is the number of histories performed. If the statistical estimate of the projection $\tilde{\epsilon}$ is not sufficiently accurate, then the iterations would diverge.

Because the exact angular intensity does not in general lie within the LDFE trial space, the iterative estimate of the error will eventually stagnate once the error cannot be sufficiently represented by a given FE mesh. An adaptive $h-$refinement algorithm has been implemented that can be used to allow the system to continue converging towards the exact solution [17, 13]. In general, for TRT problems, optically thick and slowly varying regions of the problem do not require as refined of a mesh as neutronics calculation to accurately capture the solution because there is less variation in the angular dependence of the solution. It is noted the adaptive refinement is only applied to the HO mesh; the LO spatial mesh is fixed.

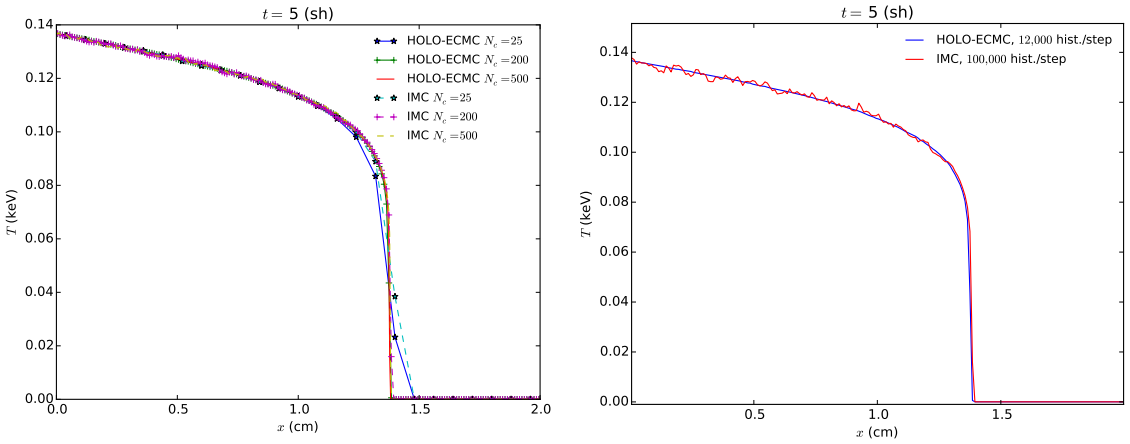
We apply some simple and common variance reduction techniques. Because we are solving a pure absorber problem with Monte Carlo, we will allow particles to stream without absorption to reduce statistical variance in the tallies. The weight of particles is reduced deterministically along the path as they stream, with no need to sample a path length. Another aspect of variance reduction is biased source sampling locations. The goal is to effectively distribute particle histories to regions of importance, but to sample a minimum

number of histories in less probable regions to prevent large statistical noise. However, there is no need to sample histories where the solution is in equilibrium. The importance sampling is performed using a modified systematic sampling method [1].

2.6 Computational Results

To demonstrate the efficacy of our algorithm, we provide results of our HOLO algorithm for two Marshak wave test problems. Marshak wave problems provide a standard test for computational methods in radiative transfer. For the first problem, the radiation and material energies are initially in equilibrium at a cold temperature. A large, isotropic incident intensity is applied at $x = 0$. The absorption cross section varies as $\sigma(T) = 0.001\ \rho\ T^{-3}$ (cm^{-1}). The simulation is advanced until $t = 5$ sh (1 sh $\equiv 10^{-8}$ s) with a fixed time step size of 0.001 sh. We have performed no mesh refinement, only performed one HOLO iteration per time step, and used a fixed 3 HO batches with equal number of histories per batch. Radiation energy distributions are plotted as an equivalent temperature given by $T_r = (\phi/(ac))^{0.25}$. Cell-averaged quantities are plotted.

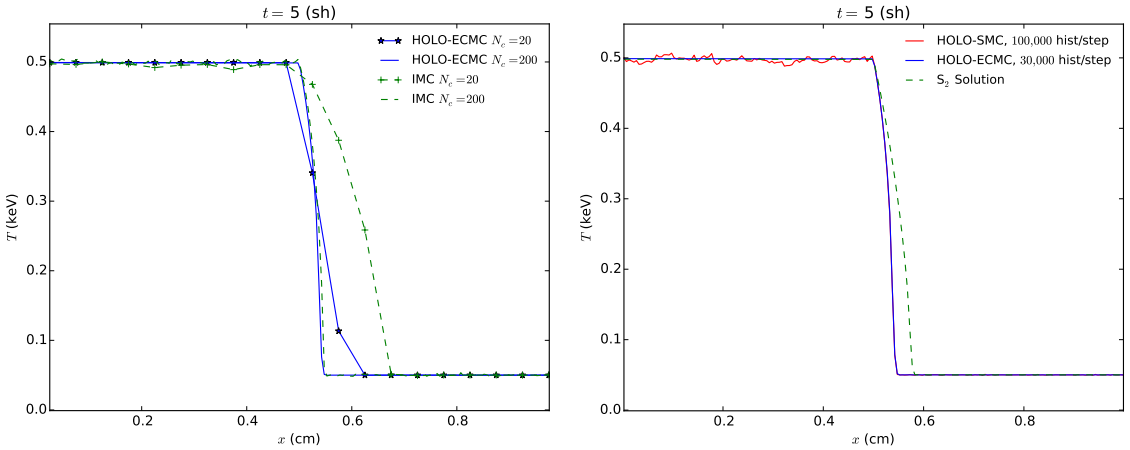
Fig. 1a compares the cell-averaged radiation temperatures for IMC with source tilting and the HOLO method with ECMC, for various number of spatial mesh cells N_c; we have used HOLO-ECMC to denote our algorithm because later results will use different HO solvers. The IMC and HOLO solutions agree as the mesh is converged. Fig. 1b compares solutions for the case of 200 cells. The HOLO method demonstrates significantly less statistical noise, even though it used fewer histories per time step.



(a) Spatial convergence of IMC and HOLO. **(b)** Comparison of solutions for 200 spatial cells.

Figure 1: Comparison of radiation temperatures for Marshak wave problem at t = 5 sh.

The second problem has similar behavior to the first problem, however the geometry consists of an optically thin (left) and an optically thick (right) material region, with temperature-independent cross sections. Fig. 2a compares the HOLO and IMC radiation temperatures at the end of the simulation. The IMC and HOLO results show good agreement over the finer mesh. On the coarse mesh ($N_c = 20$), the LDFE representation of T^4 in the HOLO method predicts the location of the wave front more accurately than the source tilting of the IMC method. Fig. 2b demonstrates the benefit of ECMC as a HO solver compared to standard MC. The HOLO algorithm with the ECMC HO solver (HOLO-ECMC) results are for running 3 batches of 10,000 histories, per time step. The solution for the HOLO method with a standard MC solver as the HO solver (HOLO-SMC) with standard source sampling uses 10^5 histories per time step. The HOLO-SMC solution demonstrates significant statistical noise. This noise is introduced into the LO solver by poor statistics in the MC computed consistency terms. Also plotted is an S_2 solution obtained with consistency terms that are equivalent to S_2 and no HO correction. The S_2 solution results in an artificially fast wave front, as expected, demonstrating the necessity of HO correction in this problem.



(a) Comparison of IMC and HOLO-ECMC. **(b)** Comparison of SMC and ECMC HO solvers.

Figure 2: Comparison of radiation temperatures for two material problem.

3 Proposed Research

3.1 Diffusion Synthetic Acceleration of the LO Equations

As described in Sec. 2.4, the fully-discretized LO equations can include the scattering term in the system matrix. This allows for the system to be directly inverted. However, an S_2 like system cannot be efficiently inverted directly in higher spatial dimensions. To demonstrate a possible path forward in higher dimensions, we will investigate the use of a standard source iteration scheme to solve the LO equations. As material properties become more diffusive (e.g., c_v is small and σ_a is large), the effective scattering source becomes large. This results in a spectral radius of the source iterations that approaches unity [9]. These regimes are typical in TRT simulations, so an acceleration method is necessary. We will accelerate the source iterations with a nearly-consistent diffusion synthetic acceleration (DSA) method [18, 19].

We can perform standard source iterations by lagging the scattering source in the LO equations, which uncouples unknowns between the two half-ranges. This produces a lower-triangular system where the spatial unknowns can be determined sequentially along the two

directions of flow via a standard sweeping procedure [20, 9]. The newly computed half-range intensities can be used to compute the scattering source for the next iteration. This process is repeated until convergence. A form of DSA referred to as the WLA method is used to accelerate the source iterations [18]. Between each source iteration, a residual equation is formed that provides the error in the current scattering iteration. The DSA method uses an approximate, lower-order operator to estimate the error in the zeroth angular moment of the intensity. The DSA equations can be more efficiently solved than the S_2-like sweeps that are being accelerated, but will accurately resolve the slowly converging diffusive error modes. It is important for the spatial discretization of the DSA equations to be closely related to the discretization of the LO equations for the acceleration to be effective. The WLA method first solves a spatially-continuous discretization of the diffusion equation for the iterative error on faces. The error on the faces is then mapped onto the volumetric moment unknowns via a LD discretization of diffusion equation [18]. The LD mapping resolves issues that would occur in optically-thick cells, while the continuous diffusion equation is accurate in the EDL where acceleration is important. It is noted that in higher dimensions, it would likely be necessary to recast the DSA as a preconditioner to a Krylov method for the acceleration to be effective [9].

3.2 Resolving Issues in Optically Thick Cells

The linear-discontinuous (LD) closure with upwinding is not strictly positive. In particular, for optically thick cells with a steep intensity gradient, the intensity becomes negative. In typical TRT problems (e.g., the Marshak wave problems above), this negativity occurs at the wave-front of the radiation intensity in thick materials. These negativities are not physical and can propagate to adjacent cells. In thick regions of TRT problems, reasonably fine spatial cells can still be on the order of millions of mean free paths; negativities with an LD representation are unavoidable in practice for such cells, and mesh refinement is of minimal use. We will explore several methods for resolving negativities.

Typically, for a standard LDFE method, the equations are lumped to produce a strictly positive solution (for 1D) [9]. However, standard FE lumping procedures would introduce

difficulties in computing the consistency terms from the HO solution. Also, lumping does not guarantee positivity for the space-angle LDFE representation for the HO intensity. For the LO equations, a modified spatial closure can be used that is equivalent to the standard FE lumping procedure by modifying the relation between the spatial moments and the outflow. This lumping-equivalent closure, in conjunction with S_2 equivalent consistency terms, has been used to preserve positivity. However, this approach is not extendable to higher-dimensions and will not work in general problems. Alternatively, the equations within a cell can be modified to ensure the outflow is not below the floor value (the initial temperature of the problem), and energy balance is conserved. The LD shape is reconstructed by extrapolating from the outflow back through the average. This closure is more promising for extendability into higher dimensions and being consistent with the HO solver.

For the HO solver, after an ECMC batch, we detect cells that produced a negative intensity. In these cells, we rotated the linear intensity (in x and μ) to be greater than the floor value. This rotation process is underdefined, so there is not a unique way to enforce positivity. The rotation procedure is not an emphasis of the research, so we choose the simple approach of scaling the slopes such that the ratio of the slope in x and μ is unchanged. The rotated intensity will not satisfy the original residual equation accurately because we have modified the first moments. Thus, the ECMC error estimates will rapidly stagnate, and produce relatively inaccurate solutions. This rotation can also lead to negativities in unexpected down-stream cells. To mitigate stagnation and improve accuracy, we will add an artifical source $\tilde{\delta}^{m+1}(x,\mu)$ to the HO equation. This source is estimated iteratively as

$$\tilde{\delta}(x,\mu)^{(m+1)} = \mathbf{L}(\tilde{I}^{n+1,(m)} - \tilde{I}^{n+1,(m)}_{\text{rot}}),$$

where $\tilde{I}^{n+1}_{rot}$ is the modified positive solution. Essentially, this source is modifying the first moments of the transport equation (but not the zeroth moment) to ensure a positive solution within the negative cells. Neglecting statistical noise, the solution will converge towards the strictly positive projection $\tilde{I}^{n+1}_{\text{rotated}}$ in the next batch. We can estimate the necessary source again in the next batch. The source $\tilde{\delta}$ lies in the same functional space as the residual, and thus can use the existing code for computing the residual and will be straight forward to

extend to higher dimensions.

We will also explore the possibility of a doubly discontinuous trial space, allowing the outflow from the cell to be discontinuous in space for difficult cells. This should produce greater angular accuracy on faces, and limit observed issues with the spatial slope being artificially high to account for the discrepancy in angular shape between the internal and face solution. In application, the outflow would be computed using a face-based tally of the MC solution. However, for simple proof of concept, we choose the outflow to be isotropic at the floor temperature in fixed-up cells. We know that in 1D test problems the true outflow at these locations is isotropic at the floor temperature (the dominant source of particles at the outgoing face in optically thick, cold cells will be from the floor-temperature emission source at that point). It may become necessary to include face tallies to compute the outflow from these cells, particularly if statistics results in activation of the fixup in cells that are not near the wave-front. However, it is expected these face tallies will have very poor statistics due to undersampling.

It will be necessary to investigate the accuracy and robustness of the added source method, and whether it should be applied in every batch or only when cells go negative again. It will also be necessary to ensure consistency with the LO solution, particularly in the case of adaptively refined meshes and the doubly-discontinuous trial space. Statistical noise may lead to the doubly-discontinuous trial space being inaccurate in cells where the projected outflow should not physically be negative.

4 Summary

A new HOLO algorithm has been implemented, and results have demonstrated the ability to reproduce IMC solutions accurately for two difficult Marshak wave test problems. The ECMC approach, with initial guesses based on the previous radiation intensity, results in efficient reduction of statistical error and allows for particles to be distributed to largely varying regions of the problem. The LO solver resolves the non-linearities in the equations resulting in a fully implicit time discretization. Overall, the LO solver can accurately and

efficiently resolve the solution in diffusive regions, while the HO transport solver provides the accuracy of a full transport treatment where necessary.

We have proposed extensions of our method in 1D to demonstrate the efficacy of our method. The ability to overcome rapid stagnation in the ECMC algorithm when the solution cannot be accurately represented by the trial space, e.g., negativities in optically thick cells, will be key for generalization of this method to higher dimensions. The goal of our proposed fixup is to allow the the ECMC iterations to continue converging globally when there are such regions present. Ideally, the added source will reduce the error to the point that the stagnation is on the order of the global stagnation that occurs due to the solution lieing outside the mesh. It is important to investigate difficulties that may arise in consistency between the LO and HO solutions in such regions. We also need to demonstrate the ability of DSA to accelerate our LO equations. Thus, we propose the following work:

1. The source iteration method with DSA for the LO solver will be implemented and applied to test problems to ensure a significant reduction in total scattering iterations in diffusive problems. Problems that provide a mix of optically thick and thin regions will be investigated.

2. Problems where IMC violates the maximum principle will be simulated with our method. We will demonstrate that our implicit equations preserve the maximum principle, and that our method can produce higher accuracy due to implicit cross section treatment. Such problems will likely require implementation of damping in the Newton iterations.

3. We will numerically demonstrate the ability of our method to preserve the equilibrium diffusion limit. The HOLO method will also be tested with a step discretization to demonstrate inaccuracy in the EDL.

4. The negativity fix-ups discussed in Sec. 3.2 will be investigated for robustness and accuracy. An analytic neutronics problem or refined deterministic TRT solution will be used to test for accuracy. The ability of ECMC to reduce noise in the fixup regions will also be investigated.

5. We will investigate the sensitivity of ECMC and the LO equations to variable parameters, e.g., initial mesh-sizes, adaptive refinement, time step size, history counts, and batch sizes. The computational cost of the HOLO method, in particular particle tracking times, as compared to IMC will be briefly explored.

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