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 [**?**]

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

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

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 [14] is a standard computational method in the field of radiation transport. The implicit Monte Carlo (IMC) method [5] 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 ad-

vance 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. 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.

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 [6, 3]. Also, the approximate linearization of the system is not iterated on for greater accuracy due to the high computational cost of the MC transport, for each time step; this imposes a limit on the time step size to produce physically accurate results [20]. The unphysical behavior is a violation of the discrete maximum principle, caused by the emission source not being truly implicit in time. In problems where the maximum principle is violated, the material energy becomes artificially larger than the radiation temperature, greater in magnitude than the boundary conditions and sources should physically allow. The work in [**?**] produces an implicit system which prevents this from happening, but has very poor convergence in diffusive problems.

PICTURE OF STANDARD MC SOLUTION AND MAXIMUM PRINCIPLE VIOLATION?

WHAT IS UP WITH THE WEIRD DIFFUSION LIMIT

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" [8]. 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 reconstruction is also necessary to preserve the equilibrium diffusion limit [**?**]. Preserving the equilibrium diffusion limit is an important aspect of a numerical method for TRT problems. In this limit, the material and radiation energy fields approach equilibrium, and the radiation solution becomes isotropics. Spatial discretizations which do not preserve the EDL can produce highly-inaccurate solutions in relatively smooth regions of the problem, where the inaccuracies are not described by standard truncation error [9].

1.3 Previous work on related methods

An alternative MC approach to the TRT equations is moment-based hybrid Monte Carlo (MC) methods. Recent work has focused on so-called high-order low-order (HOLO) methods [18, 10, 19, 1]. These methods involved 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 [18, 10]. The high-order (HO) transport problem is defined by Eq. (1), with sources estimated from the previous LO solution. These sources have a truly implicit time-discretization, preserving the maximum principle. The HO equation can be 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. The HO system does not directly estimate a new material temperature, eliminating stability issues that would require linearization of the emission source in Eq. (1). 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. Too much statistical variance can contaminate the LO solution.

Another key area of related research to the proposed research here is application of residual Monte Carlo. This is also referred to as the difference formulation. The work in [19] used residual MC as a HO solver to significantly reduce 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 RMC algorithm uses a piecewise constant trial space representation for the intensity in x and μ. An approach similar to IMC is the symbolic IMC method (SIMC), which as been performed in conjunction with the difference formulation.. SIMC forms a standard FE solution to the material energy balance equation, and uses symoblic weights in the MC transport to solve for expansion coefficents. This has added complexity of solving for a mix of expansion coefficients and physical particle weights. The SIMC has also been applied with what is known as a difference formulation, which is similar to teh RMC in [19]. The formulation of the residual in both [19, **?**] can produce minimal statistical noise in slowly varying problems where the behavior of the system is near equilibrium. You are just solving for the deviation from equilibrium, which can limit MC statistical noise. This is only really true in regions of minimal variation. The SIMC method has been applied to the case of a piece-wise linear FE representation of the emission source. The SIMC work made some attempts as higher-accuracy time treatment, but with little investigation into a second order treatment.

1.4 Proposed algorithm

The research proposed herein provides a new HOLO approach for radiative transfer. In this work, we demonstrate the utility of an S_2-like LO operator [21] in conjunction with an exponentially-convergent MC (ECMC) method [11] for the HO solver. Our LO system and approach to enforcing consistency contrast greatly from the typical formulation in [19, 18, 10]. Exponentially-convergent Monte Carlo (ECMC)[11, 1] provides an 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. Additionally, no particle histories are required in regions where the radiation and material energy field are in equilibrium. 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 particle histories have less computational cost than the often slow, scattering-dominated IMC histories. We have derived the LO operator directly from the transport equation, using a linear-discontinuous (LD) finite-element (FE) spatial discretization. The method contains many of the desired qualities, such as preserving the equilibrium diffusion limit, prserving the maximum principle, and in particular, providing high-fidelity MC solution to the TRT equations in an efficient manner.

2 Proposed Research

2.1 Overview of the HOLO Algorithm

For simplicity, the HOLO method is described with a backwards Euler discretization in time, as well as constant specific heats and cell-wise constant cross sections. An alternative time discretization is discussed in Sec. 5. The time-discretized equations are

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

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

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 $T(x)$ at 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 [21], 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 (similar to coarse-mesh finite difference methods [**?**]) used by other HOLO methods [19, 10, 18]. In DNA methods an artificial term is added to the equations and estimated using a previous HO solution to enforce consistency. In our method we have simply manipulated space-angle moments of equations, which will ideally 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 [11]. 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 temperature at the end of the time step; it is only used to estimate the angular consistency parameters for the LO equations, which eliminates typical operator splitting stability issues that require linearization of the emission source.

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 $T^{n+1,0}(x)$ and $\phi^{n+1,0}(x)$, based on consistency terms estimated with $\tilde{I}^n$.
2. Solve the HO system for $\tilde{I}^{n+1,k+1/2}(x,\mu)$ with ECMC, based on the current LO estimate of the emission and scattering sources.
3. Compute LO consistency parameters with $\tilde{I}^{n+1,k+1/2}$.
4. Solve the LO system with HO consistency parameters to produce a new estimate of $\phi^{n+1,k+1}$ and $T^{n+1,k+1}$.
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.

where the superscript k denotes the outer HOLO iteration. 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 Forming the Low-Order System

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 [21], 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

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

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.,

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

The $\mu_{i-1/2}^{n+1,+}$ 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 $T^4(x) \simeq T_{L,i}^4 b_{L,i}(x) + T_{R,i}^4 b_{R,i}(x)$. The L and R spatial moments are taken of the material energy equation, using these definitions for $T(x)$ and $\sigma_a acT^4(x)$ to simplify moments. For example, the final LO material energy equation resulting from application of the L moment

is

$$\frac{\rho_i c_{v,i}}{\Delta t}\left[\left(\frac{2}{3}T_{L,i}+\frac{1}{3}T_{R,i}\right)^{n+1}-\left(\frac{2}{3}T_{L,i}+\frac{1}{3}T_{R,i}\right)^{n}\right]+\sigma_{a,i}^{n+1}\left(\langle\phi\rangle_{L,i}^{+}+\langle\phi\rangle_{L,i}^{-}\right)^{n+1}$$
$$=\sigma_{a,i}^{n+1}ac\left(\frac{2}{3}T_{L,i}^{4}+\frac{1}{3}T_{R,i}^{4}\right)^{n+1}. \quad (8)$$

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

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 usual upwinding approximation 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 previous HO solve is used to estimate the angular consistency parameters. In the HOLO algorithm, the equations for LO unknowns at iteration $k+1$ use consistency parameters computed (via relations, e.g., Eq. (7)) using the latest HO solution $\tilde{I}^{n+1,k+1/2}$ as an approximation for $I^{n+1}(x,\mu)$.

2.4 Solution of the LO equations and Diffusion Synthetic Accleration

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 temperatures of the previous iteration, as described in [9]. Once the system is linearized, a discrete matrix equation is formed. Scattering can be included in the system matrix, producing a banded-matrix which can be efficiently inverted directly. However, an S_2 like system cannot be efficiently inverted directly in higher dimensions. Thus, we will also investigate the use of a

standard source iteration scheme with a nearly-consistent DSA method to accelerate source iterations [17].

It is improtance for the effectiveness of acceleration methods to A true LDFE discretization for DSA results in equations that cannot be efficiently solved. T The diffusion synthetic accleration method solves for the error in a current sourc eiteration (in this case the residual is from the scattering source,w here the scattering source includes an effective scattering source resulting from the lineraization of the planckian emission osurce [9]. This effective scattering source becomes dominant in . In such problems,

Newton iterations are repeated until $\phi^{n+1}(x)$ and $T^{n+1}(x)$ are converged to a desired relative tolerance.

3 The ECMC High Order Solver

The transport equation to be solved by the HO solver is

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

where the superscript k represents the outer HOLO iteration index. Material property indices will be suppressed from now on. Here, $k+1/2$ denotes the ECMC solution within outer HOLO iteration k, whereas k and $k+1$ represent successive LO solves. The sources at k in Eq. (9) are estimated by the previous LO solution. The LDFE representation of the emission source mitigates teleportation error and preserves the EDL. As all sources on the right side of the equation are known, this defines a fixed-source, pure absorber transport problem.

In operator notation, the previous equation can be written as

$$\mathbf{L}^k I^{n+1,k+1/2}=q^k \quad (10)$$

where $I^{n+1,k+1/2}$ is the transport solution of the angular intensity based on the k-th LO

estimate of q^k. The linear operator $\mathbf{L}^k$ 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 $r^{(m)} = q - \mathbf{L}^k \tilde{I}^{n+1,(m)}$. 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 transport codes, but the source will now contain positive and negative weight particles. The space-angle moments of the error computed in $\tilde{\epsilon}^{(m)}$ 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. 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 the 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 [14], 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 [11, 1]. 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. Once error stagnation has occurred (and mesh refinement has reached a maximum level), additional histories can be performed with a fixed residual source to reduce the statistical variances in of the estimate of the remaining error in the current solution. Although the remaining error will converge statistically at a standard $1/\sqrt{N}$ convergence rate, the remaining error will be much smaller than for a standard MC simulation, producing a much more efficient solution method overall.

We can 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 sufficient number of histories in less probable regions to prevent large statistical noise. However, there is no need to sample histories in regions in equilibrium. The residual gives a good indication of where histories are most likely to contribute to the error, particularly in optically thick cells where particles do not transport long distances. This is perofrmed using a modified systematic sampling method [14] For cells that are significant, but have a predetermined number of histories below some preset minimum histories to be sampled. Particle weights are adjusted to prevent biasing.

4 Issues in Optically THick Cellsm

The linear-discontinuous (LD) closure with upwinding is not strictly positive. In particular, for optically thick cells with a steep intensity gradient, the solution becomes negative. These negativities 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. 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. Thus, an alternative spatial closure is used that is equivalent to the standard FE lumping procedure. The L and R moments are defined the same as before, preserving the same average within a cell, but the relation between the moments and the outflow is modified. For example, for positive μ, the outflow is now defined as $\phi^+_{i+1/2} = \langle\phi\rangle^+_R$. Because the basis function $b_{R,i}(x)$ is strictly positive, the outflow is positive. This closure is only used in cells where negativities

occur.

For the HO solver, in cells near the radiation wave front, the LDFE trial space results in negativities in $\tilde{I}^{n+1}(x,\mu)$, similar to the LO solver. Because the residual formulation in ECMC allows for negative weight particles to occur, currently we do not treat these cells specially. We detect if the consistency terms lie in the appropriate half space at the end of the HO solve, an indication that the intensity was negative within that cell. If the terms are non-physical, then they are replaced with the corresponding S_2-equivalent value. In general, in such cells where the trial space cannot accurately represent the solution, error stagnation will rapidly occur. In strongly absorbing regions, the linear discontinuous spatial representation can lead to unphysical negative solutions in certain cells In the LO system, we set a strict floor value and preserve energy conservation to determine the cell average. For the HO system, we rotate $\tilde{I}(x,\mu)$ to be strictly positive after each batch. However, $\tilde{I}_{\text{rotated}}(x,\mu)$ doesn't satisfy the original residual equation, so the ECMC convergence quickly stagnates. Thus, we add an artifical source $\tilde{\delta}(x,\mu)$, which is estimated iteratively as

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

where $\mathbf{L}$ is the continuous streaming plus removal operator. The solution will now converge towards the strictly positive projection $\tilde{I}^{n+1}_{\text{rotated}}$. We also allow the outflow from the cell to be discontinuous, allowing for greater angular accuracy on faces

5 Alternative time discretization

6 COMPUTATIONAL RESULTS

We will compare results of the HOLO method to IMC with a source tilting algorithm for two test problems [16]. Also, we briefly compare performance in Section **??**. Finally, we will demonstrate the efficiency advantage of ECMC in our HOLO algorithm by comparing the results to the same HOLO algorithm if the ECMC algorithm is replaced with a standard

Monte Carlo (SMC) simulation. Results are also given for the case of a single ECMC batch, which is similar to a RMC method.

7 CONCLUSIONS

Unlike IMC, our method requires no effective scattering events to be included in the MC simulation, which limits the run time of particle tracking, while adding the cost of a LO newton solver. Average LO iteration counts did not significantly increase as the time step size was increased. The LDFE spatial representation mitigates issues with teleportation error, producing results with spatial accuracy comparable to IMC with source tilting. 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 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.

The primary difficulty to overcome in the ECMC algorithm is when the solution cannot be accurately represented by the trial space, e.g., in optically thick cells where the solution is driven negative. We are currently developing an approach to allow the ECMC iterations to continue converging globally when there are such regions present. It is necessary to ensure the closure in the LO system is consistent with the HO representation for the solution in such regions. The ability to represent the solution accurately in rapidly varying regions of the problem will be key for generalization of this method to higher dimensions. A formulization of the ECMC method that allows for time-continuous MC transport (similar to IMC) is also currently being investigated. This may reduce some of the loss of accuracy in optically thin regions due to the time discretization of the transport equation in the HO solver. However, greater time accuracy is not of primary concern as this method is intended for use in problems dominated by large absorption opacities, where the absorption-reemission physics make the LO acceleration is critical.

Future work will also explore the accuracy of the HOLO method, in particular, analyzing the optimal number of batches and the benefit of adaptive refinement. This will likely require the use of manufactured solutions. The sensitivity of the method to mesh sizes and time step sizes will be investigated more thoroughly. For TRT problems, it is important that the LO spatial discretization satisfies the equilibirium diffusion limit. To extend to higher dimensions, our LDFE representation may require the use of a higher-degree spatial representation for the LO system to achieve the diffusion limit. Further asymptotic analysis on the method will be applied before implementation. It may be necessary to use a different LO system (e.g., the non-linear diffusion acceleration approach in [19]), if the S_2-like equations become too inefficient or difficult to implement in higher dimensions. Alternatively, a variable Eddington Tensor approach may provide more stability in rapidly variable regions of the problem while still allowing for a consistent, LDFE solution that is efficiently solvable.

The remaining research to be performed is summarized below:

1. To finish implementation of the time-continuous treatment for the ECMC algorithm, and a consistent LO algorithm. Once implemented, this will be investigated on optically thin problem and compared to IMC for accuracy in wave-fronts.

2. Investigate the maximum principle violation, and demonstrate, with sufficient convergence of Newton iterations, that our method will preserve the maximum value principle.

3. Numerically demonstrate the ability of this method to accurately preserve the equilibrium diffusion-limit compared to a step discretization which will not.

4. Diffusion synthetic acceleration of scattering source iterations in the LO system. Demonstrating the ability to accelerate the iterations in diffusive, optically thick problems.

5. Test this method. In particular, difficult 1D test problems, such as 1D Marshak waves, featuring a mix of optically thick and optically thin problems, with material-dependent problems. Compare the benefits of ECMC in this algorithm, as well as

comparing to the accuracy of e

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