A HIGH-ORDER LOW-ORDER ALGORITHM WITH EXPONENTIALLY-CONVERGENT MONTE CARLO FOR THERMAL RADIATIVE TRANSFER PROBLEMS

A Dissertation

by

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ABSTRACT

We have implemented a new high-order low-order (HOLO) algorithm for solving thermal radiative transfer problems. The low-order (LO) system is based on spatial and angular moments of the transport equation and a linear-discontinuous finite-element spatial representation, producing equations similar to the standard S_2 equations. The LO solver is fully implicit in time and efficiently resolves the non-linear temperature dependence at each time step. The HO solver utilizes exponentially-convergent Monte Carlo (ECMC) to give a globally accurate solution for the angular intensity to a fixed-source, pure absorber transport problem. This global solution is used to compute consistency terms, which require the HO and LO solutions to converge towards the same solution. The use of ECMC allows for the efficient reduction of statistical noise in the MC solution, reducing inaccuracies introduced through the LO consistency terms. We compare results with an implicit Monte Carlo (IMC) code for one-dimensional, gray test problems and demonstrate the efficiency of ECMC over standard Monte Carlo in this HOLO algorithm.

1. THE EXPONENTIALLY-CONVERGENT MONTE CARLO HIGH-ORDER SOLVER

The time-discretized transport equation to be solved by the HO solver is

$$\mu\frac{\partial I^{n+1,k+1/2}}{\partial x}+\left(\sigma_t^k+\frac{1}{c\Delta t}\right)I^{n+1,k+1/2}=\frac{\sigma_s}{2}\phi^{n+1,k}+\frac{1}{2}\left(\sigma_a^k acT^4\right)^{n+1,k}+\frac{\tilde{I}^n}{c\Delta t} \quad (1.1)$$

where the superscript k represents the outer HOLO iteration index. Here, $k+1/2$ denotes the HO solve within outer HOLO iteration k, whereas k and $k+1$ represent successive LO solves. The sources at k in Eq. (1.1) are estimated by the previous LO solution. Temperature-dependent cross sections are evaluated at $T^{n+1,k}$. As all sources on the right side of the equation are known, this defines a fixed-source, pure absorber transport problem. The above transport equation has the same form as a steady-state neutronics problem. We will solve this transport problem using the ECMC method.

In the remainder of this chapter, an overview of the ECMC solution method applied in this work is given. First, the LDFE trial space used by the ECMC algorithm is detailed. Then, the ECMC algorithm is developed, followed by more specific sampling and tracking details.

1.1 Implementation of LDFE $x-\mu$ Trial Space

To form the algorithm, a trial-space representation for the intensity is necessary. The ECMC solver uses a finite element representation in space and angle. On the interior of the cell with the i-th spatial index and j-th angular index, the linear

representation is defined as

$$\tilde{I}(x,\mu) = I_{a,ij} + \frac{2}{h_i} I_{x,ij}\,(x - x_i) + \frac{2}{h_j} I_{\mu,ij}\,(\mu - \mu_j)\,, \qquad (x,\mu) \in \mathcal{D}_{ij}, \tag{1.2}$$

where $\mathcal{D}_{ij} : x_{i-1/2} \le x \le x_{i+1/2} \times \mu_{j-1/2} \le \mu \le \mu_{j+1/2}$ is a rectangular cell in space and angle. The spatial cell width is h_i, the angular width is h_j, the center of the cell is (x_i, μ_j), and

$$I_{a,ij} = \frac{1}{h_i h_j} \iint\limits_{\mathcal{D}_{ij}} I(x,\mu)\,\mathrm{d}x\mathrm{d}\mu \tag{1.3}$$

$$I_{x,ij} = \frac{6}{h_i h_j} \iint\limits_{\mathcal{D}_{ij}} \left(\frac{x - x_i}{h_i}\right) I(x,\mu)\,\mathrm{d}x\mathrm{d}\mu \tag{1.4}$$

$$I_{\mu,ij} = \frac{6}{h_i h_j} \iint\limits_{\mathcal{D}_{ij}} \left(\frac{\mu - \mu_j}{h_j}\right) I(x,\mu)\,\mathrm{d}x\mathrm{d}\mu, \tag{1.5}$$

where I_a is the cell-averaged intensity, and I_μ and I_x define the the first moment in μ and x of the intensity, respectively. The streaming term requires definition of $I(x,\mu)$ on faces. Standard upwinding in space is used to define $I(\mu)$ on incoming faces, e.g., for an unrefined mesh,

$$\tilde{I}_{ij}(x_{i-1/2},\mu) = \begin{cases} I_{a,i-1,j} + I_{x,i-1,j} + \frac{2}{h_j} I_{\mu,i-1,j}\,(\mu - \mu_j) & 0 \le \mu_{j-1/2} \le \mu \le \mu_{j+1/2} \\ I_{a,ij} - I_{x,ij} + \frac{2}{h_j} I_{\mu,ij}\,(\mu - \mu_j) & \mu_{j-1/2} \le \mu \le \mu_{j+1/2} \le 0 \end{cases} \tag{1.6}$$

and

$$\tilde{I}_{ij}(x_{i+1/2},\mu) = \begin{cases} I_{a,ij} + I_{x,ij} + \frac{2}{h_j} I_{\mu,ij}\,(\mu - \mu_j) & 0 \le \mu_{j-1/2} \le \mu \le \mu_{j+1/2} \\ I_{a,i+1,j} - I_{x,i+1,j} + \frac{2}{h_j} I_{\mu,i+1,j}\,(\mu - \mu_j) & \mu_{j-1/2} \le \mu \le \mu_{j+1/2} \le 0 \end{cases}, \tag{1.7}$$

for all i and j on the interior of the domain; specified boundary conditions for $I(x,\mu)$ are upwinded at boundaries.

1.2 The ECMC Algorithm

The ECMC method is an iterative residual MC method. In operator notation, Eq. (1.1) can be written as

$$\mathbf{L}^k I^{n+1,k+1/2} = q^k \tag{1.8}$$

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 *continuous* streaming plus removal operator, given by the left-hand side of Eq. (1.1), i.e.,

$$\mathbf{L}^k(\cdot) = \left[\mu\frac{\partial}{\partial x} + \left(\sigma_t^k + \frac{1}{c\Delta t}\right)\right](\cdot) \tag{1.9}$$

We will use superscript (m) to indicated the m-th inner HO iteration. The LDFE representation of the m-th approximate solution to Eq. (1.8) is denoted $\tilde{I}^{n+1,(m)}(x,\mu)$. The associated residual is defined as $r^{(m)} = q - \mathbf{L}^k\tilde{I}^{n+1,(m)}$. Explicitly, the residual at iteration m is

$$\begin{aligned} r^{(m),k+1/2} = \frac{\sigma_s}{2}\phi^{n+1,k} + \frac{1}{2}\left(\sigma_a acT^4\right)^{n+1,k} + \frac{\tilde{I}^n}{c\Delta t} \\ - \left(\mu\frac{\partial\tilde{I}^{n+1,k+1/2}}{\partial x} + \left(\sigma_t^k + \frac{1}{c\Delta t}\right)\tilde{I}^{n+1,k+1/2}\right)^{(m)} \end{aligned} \tag{1.10}$$

where the k terms have a LDFE representation in space on the coarsest mesh and are not recalculated at any point during the HO solve. The functional form of $\tilde{I}^n$ is defined from the final HO solution of the previous time step. The HOLO iteration indices are suppressed for the remainder of this chapter because the LO-estimated q^k and $\mathbf{L}^k$ *remain constant for the entire HO solve.*

Addition of $\mathbf{L}I^{n+1} - q = 0$ to the Eq. (1.10), i.e., the residual equation, and manipulation of the result yields the error equation

$$\mathbf{L}(I^{n+1} - \tilde{I}^{n+1,(m)}) = \mathbf{L}\epsilon^{(m)} = r^{(m)} \tag{1.11}$$

where I^{n+1} is the exact solution[1] to the problem defined by Eq. (1.1) and $\epsilon^{(m)}$ is the true error in the approximate solution $\tilde{I}^{n+1,(m)}$. The $\mathbf{L}$ operator in the above equation is inverted with the MC method, which statistically estimates an LDFE projection of the error in $\tilde{I}^{n+1,(m)}$, i.e.,

$$\tilde{\epsilon}^{(m)} = \mathbf{L}^{-1} r^{(m)} \tag{1.12}$$

where $\mathbf{L}^{-1}$ is the Monte Carlo inversion of the streaming and removal operator. This inversion is strictly a standard Monte Carlo simulation; particle histories are tracked and the mean behavior estimated as in standard solutions to a Boltzmann transport equation [8, 11], although the source is complicated and produces both positive and negative statistical weights; sampling of the source is detailed in Sec. 1.3. It is noted that the exact error in $\tilde{I}^{n+1,(m)}$ (with respect to Eq. (1.1)) is being estimated with MC; tallies produce an integral projection of the error onto a LDFE space-angle trial space. Volumetric flux tallies over each space-angle element are required to estimate $\tilde{\epsilon}^{(m)}$, as detailed in Sec. 1.4. The space-angle moments of the error, preserved with the representation $\tilde{\epsilon}^{(m)}$, can be added to the moments of $\tilde{I}^{n+1}(m)$ to produce a more accurate solution.

The ECMC algorithm iterates on this process as follows:

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

[1]For clarity, in this chapter the exact solution is the exact solution to the transport problem defined by Eq. (1.1), not to the continuous equations that are trying to be solved.

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.

Exponential convergence is obtained if the error ϵ is reduced each batch. 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 at each iteration m, relative to the solution I^{n+1}. 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.

1.2.1 Projection and Statistical Accuracy of ECMC

Here, we emphasize the solution $\tilde{I}^{n+1,(m)}$ represents the LDFE projection of the exact Monte Carlo solution to the transport problem defined by Eq. (1.1). The discretization error is in q, i.e., the LD spatial representation of the emission and scattering source and the LDFE space-angle projection $\tilde{I}^n(x, \mu)$. The projection of the intensity is in general far more accurate than a standard finite element solution, e.g., a S_N collocation method in angle. In typical IMC calculations, the average energy deposition within a cell is a projection that is computed with a standard path-length volumetric flux tally; the zeroth moment of the LDFE projection of ϵ is computed using an equivalent tally, preserving the zeroth moment of the true error.

To see why the true error is being estimated, it is important to note that $\mathbf{L}$ in Eq. (1.11) is the continuous operator. The MC inverse $\mathbf{L}^{-1}$ is a statistical solution

method for an integral equation. The solution to this integral equation can be shown to provide the analytic inverse of the operator $\mathbf{L}$ [8, 9]. Applying L^{-1} to Eq (1.11) and adding the result to the previous solution yields the desired moments of the exact solution:

$$\tilde{I}^{n+1,(m+1)} = \tilde{I}^{n+1,(m)} + \tilde{\epsilon}^{(m)} \tag{1.13}$$

$$\simeq \tilde{I}^{n+1,(m)} + \mathbf{L}^{-1}\left(q - \mathbf{L}\tilde{I}^{n+1,(m)}\right) \tag{1.14}$$

$$\simeq \mathbf{L}^{-1}q \tag{1.15}$$

where the above expression is equal in the limit of an infinite number of histories, within a single batch.

A MC batch provide a standard MC transport estimate of moments of the error. Each batch estimate of the moments of ϵ has a statistical uncertainty that, with sufficient sampling, is governed by the standard $1/\sqrt{N}$ convergence rate [8], 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. It is noted that there is statistical correlation across batches because $I^{n+1,(m+1)}$ and $\epsilon^{(m)}$ are correlated through $I^{n+1,(m)}$ and the MC source $r^{(m)}$. A general proof of exponential convergence for related adaptive MC transport methods is depicted in [4].

Because the intensity is saved between time steps, there is correlation that can not be easily measured. However, within a batch, the statistical uncertainty in moments of $\epsilon^{(m)}$ can be estimated with the sample variance of histories, using the standard sample-variance of MC mean estimators [8]. This provides a statistical estimate of moments of the solution estimated in that batch that asymptotically obey the central limit theorem [8], conditioned on the previous solution $I^{n+1,(m)}$. However,

care must be taken with these statistical estimates, as they do not have the usual MC interpretation of confidence intervals because of correlations. Explicitly, if a particular simulation is repeated with independent sets of random numbers, the sample means will not (on average) correctly reproduce the confidence interval that the sample variance from the original simulation estimated. Additionally, the number of histories within each batch are likely too low for the central limit theorem to truly apply, as they do not sample the full solution space sufficiently [11].

1.2.2 Adaptive Mesh Refinement

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 [7, 1]. For TRT problems where absorption-reemission physics dominate, the diffusive and slowly varying regions of the problem require a less refined angular mesh to capture the solution than typical neutronics problems. However, greater spatial resolution is needed due to steep spatial gradients. Once error stagnation has occurred (and mesh refinement has reached a maximum level), additional histories can be performed with a fixed residual source to estimate 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.

Detailed equations for performing projections between meshes and computing the residual source on the refined meshes can be found in [7]. At the end of the ECMC batch, refinement is performed in space-angle cells based on a jump indicator. The

jump indicator is the magnitude of the different between $I(x,\mu)$ in adjacent cells, averaged over each edge. The value of the largest jump, out of the four edges within a cell, is used as the indicator for that cell; alternatively, the error could directly be used as an indicator. Based on this indicator, a preset fraction of cells are refined based on the indicator. The refinement of a cell is chosen to be symmetric, with each space-angle cell divided into four equal-sized cells and only one refinement level difference between adjacent cells is allowed, except for cells that share an edge across $\mu = 0$. The solution for $\tilde{I}^{n+1}(x,\mu)$ of the batch is projected onto the finer mesh for the next batch. Because the dimensionality of the sample space has increased, we increase the number of histories per batch such that the ratio of the number of histories to total cells is approximately constant for all meshes. At the end of the last HO solve in a time step, $\tilde{I}^{n+1}$ is projected back onto the original, coarsest mesh and stored as $\tilde{I}^{n}$ for the next time step.

1.3 Systematic Sampling Algorithm for Residual Source

The LDFE representation given by Eqs. (1.2), (1.6), and (1.7) is substituted into Eq. (1.10) and evaluated to produce the residual source for each ECMC batch. The MC source $r^{(m)}(x,\mu)$ in Eq. (1.12) consists of volumetric sources and face sources that are sampled. The face sources result from the spatial derivative applied to the discontinuities in the trial space. The source can also produce positive and negative weight particles. The probability distribution function (PDF) for sampling particle coordinates is formed by dividing $r^{(m)}(x,\mu)$ by $\|r^{(m)}(x,\mu)\|_1$, i.e., the L_1 norm over space and angle of the residual. Particle coordinates (in x and μ) are sampled from the strictly positive PDF; then, if the residual is negative at the sampled coordinates, the weight of the particle history is negative. With the statistical weights of each particles normalized to unity, then the tallies must be multiplied by $\|r^{(m)}\|_1$ to pro-

duce the correct magnitude for moments of error. More details on specific equations for evaluating integrals of the residual for steady-state neutronics problems can be found in [7].

As a method to improve statistical efficiency within a batch, a modified version of the systematic sampling method [8] (a form of stratified sampling) was implemented for determining the number of histories sampled from each space-angle cell. In the systematic sampling algorithm, the number of particle histories sampled in each space-angle cell is predetermined and proportional to the integral of the PDF over that cell. The goal is to effectively distribute particle histories to regions of importance, but to sample a preset, minimum number of histories $N_{\min}$ in less probable regions; this is to limit bad statistics in low probability cells (this is primarily important for adaptively refined meshes). However, there is no need to sample histories from regions in thermal equilibrium, where the probability of a particle being born is on the order of roundoff. In most of the simulations performed for this work $N_{\min} = 1$; this choice is made to keep the total number of histories per time step constant throughout the simulation for comparison to IMC.

The unmodified probability of a particle being born in cell ij is

$$p_{ij} = \frac{\|r^{(m)}\|_{1,ij}}{\|r^{(m)}\|_1} \tag{1.16}$$

where $\|r\|_{1,ij}$ is the L_1 norm over cell ij, including the upwind face and interior volumetric source. Thus, the number of particles in cell ij is

$$N_{ij} = \begin{cases} \lfloor (N_b p_{ij}) \rceil & N_b p_{ij} > N_{\min} \\ 0 & p_{ij} < O(\epsilon_{prec}) \\ N_{\min} & \text{else} \end{cases} \tag{1.17}$$

where $N_{\min}$ is the minimum number of histories in significant cells, N_b is the total number of histories sampled that batch, and ϵ_{prec} is on the order of double precision. Particle weights must be adjusted to account for the difference between the number sampled from a particular cell and the original probability of that element being sampled. This rounding requires some additional histories needing to be sampled, or removed, to reach a specific number of histories. These modifications are made to the most probable cell

The algorithm for sampling each of the N_{ij} starting histories, from each ij element, is

1. Sample random number $\eta \sim U(0,1)$
   (a) If $\eta < \|r^{(m)}_{\text{face}}\|_{1,ij} / \|r^{(m)}\|_{1,ij}$:
      - Sample (x, μ) from $\overline{r}_{ij,\text{face}}$ face source with rejection sampling
   (b) Else:
      - Sample (x, μ) from $\overline{r}_{ij,\text{int}}$ volumetric source using rejection sampling
2. Set particle weight to $p_{ij} N_b / N_{ij}$

where $\overline{r}_{i,\text{face}}$ and $\overline{r}_{i,\text{int}}$ are the upwind face and interior residual in cell ij.

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. Systematic sampling is a variance reduction technique that reduces the variance of the function, i.e., the residual, being sampled [8]. Thus, we expect variance to be reduced by more efficiently sampling the residual in optically thick cells. In thin cells, where particles transport farther, this sampling procedure does not guarantee less variance overall.

1.4 Continuous Weight Deposition Tallies

During a MC batch, moments of the error are tallied. The necessary moments of the error are defined analogously to Eq.'s (1.3)–(1.5). The tallies are evaluated by weighting the particle density with the appropriate basis function and integrating along the history path through the cell. The LDFE representation results in local tallies where only particles entering a particular cell contribute to that cell's estimators. For the cell average, the n-th particle that enters the cell ij makes the contribution, or *score*,

$$\epsilon^n_{a,ij} = \frac{1}{h_i h_j} \int_{s^n_o}^{s^n_f} w^n(x,\mu) \mathrm{d}s, \tag{1.18}$$

where s^n_o and s^n_f are the beginning and end of the n-th particle track in the cell and $w(x,\mu)$ is the weight of the error particle in the MC simulation.

As in [6], 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. Histories are allowed to stream in this manner for 6 mean free paths (mfp) before switching to analog path length sampling; this limits the tracking of very small weight histories. The choice of 6 mfp allows particles to continuously deposit weight until they reach 0.25% of their original weight. Path lengths are tracked in terms of mfp, so there is no need to resample at material interfaces.

Weight is attenuated exponentially, i.e., $w(x,\mu) \propto \exp(-\sigma_t^{\text{eff}}|x/\mu|)$, where for the time-discretized equations $\sigma_t^{\text{eff}} = \sigma_t + 1/(c\Delta t)$. Substitution of the weight represen-

tation into Eq. (1.18) produces the result

$$\epsilon^n_{a,ij} = \frac{w(x_0,\mu)}{\sigma_t^{\text{eff}} h_i h_j}\left(1 - e^{-\sigma_t^{\text{eff}} s^n}\right). \tag{1.19}$$

Here, $w(x_0,\mu)$ is statistical weight of the particle at the start of the path and s^n is the length of the track. The contribution of a particle track to ϵ_x is given by

$$\epsilon^n_{x,ij} = \frac{w(x_0,\mu)}{h_i^2 h_j \sigma_t^{\text{eff}}}\left[x_0 - x_f e^{-\sigma_t^{\text{eff}} s^n} + \left(\frac{\mu}{\sigma_t^{\text{eff}}} - x_i\right)\left(1 - e^{-\sigma_t^{\text{eff}} s^n}\right),\right] \tag{1.20}$$

where x_0 and x_f are the beginning and ending x coordinates of the n-th path. The contribution to the first moment in μ is

$$\epsilon^n_{\mu,ij} = \frac{w(x_0,\mu)}{h_j^2 h_i \sigma_t^{\text{eff}}}\left(\mu - \mu_j\right)\left(1 - e^{-\sigma_t^{\text{eff}} s^n}\right), \tag{1.21}$$

where the particle x-direction cosine μ does not change because it is a pure-absorber simulation. The unbiased estimators for the moments of the error, e.g., $\hat{\epsilon}_{a,ij}$, are simply the average score from all histories:

$$\hat{\epsilon}^{(m)}_{a,ij} = \frac{1}{N_b}\sum_{n=1}^{N_b} \epsilon^n_{a,ij} \tag{1.22}$$

where N_b is the number of particle histories performed within that batch.

1.4.1 Face Tallies and correction near $\mu = 0$

Face-averaged estimators of $\epsilon(x,\mu)$ are required to compute the outflow for estimating the spatial closure discussed in Sec. **??**. The standard face-based tallies [8, 2] are used. Tallies are weighted by the appropriate basis functions to compute a linear FE projection in μ at each face. The tally score, for the angular-averaged error $\epsilon_{a,i}$

is defined as

$$\hat{\epsilon}_{a,i\pm1/2,j} = \frac{1}{N} \sum_{m=1}^{N_{i\pm1/2,j}} \frac{w_m(x_{i\pm1/2},\mu)}{h_\mu|\mu|}, \tag{1.23}$$

where N is the number of histories performed and $N_{i\pm1/2,j}$ is the number of histories that crossed the surface $i \pm 1/2$, in the j angular element. For the first moment, the tally is

$$\hat{\epsilon}_{\mu,i\pm1/2,j} = \frac{1}{N} \sum_{m=1}^{N_{i+1/2,j}} 6\left(\frac{\mu-\mu_j}{h_\mu}\right) \frac{w_m(x_{i\pm1/2},\mu)}{|\mu|h_\mu}. \tag{1.24}$$

For positive and negative directions, solutions are only tallied on the $x_{i+1/2}$ and $x_{i-1/2}$ faces, respectively. Particles are only tallied after leaving a cell, and, as discussed in Section 1.5, particles born on a surface do not contribute to the tally of that surface.

Near $\mu = 0$, particles can contribute large scores to the zeroth angular moment that lead to large and unbounded variances [2]. To avoid large variances, we have applied the standard fixup [11, 2]. For $|\mu|$ below some small value μ_{cut}, particles contribute the expected score over the range $(0, |\mu_{cut}|)$ for an approximate isotropic particle density. Thus, scores in this range have no variance, but are biased for non-isotropic intensities. For all results in this work $\mu_{cut} = 0.01$. Assuming an isotropic particle density I_0, the average of $1/\mu$, for positive μ, is

$$\overline{1/\mu} = \frac{\int_0^{\mu_{cut}} \frac{1}{\mu} I_0 \, \mathrm{d}\mu}{\int_0^{\mu_{cut}} I_0 \, \mathrm{d}\mu} = \frac{2}{\mu_{cut}}. \tag{1.25}$$

For negative μ, $\overline{1/\mu} = -2/\mu_{cut}$. All particles in the range $(0, |\mu_{cut}|)$ contribute the expected score by evaluating the appropriate estimator at $\pm\mu = \pm 2/\mu_{cut}$. It is noted that the first angular moment would be well behaved, but it is inconsistent to only modify the zeroth moment in the I_μ estimators. Additionally, assuming an isotropic intensity near $\mu = 0$ helps to limit the first μ moment, where the LD trial space often

cannot resolve the solution anyways.

1.5 MC solution for Linear Doubly-Discontinuous trial space

The inclusion of the outflow discontinuity has a minimal effect on the treatment of the residual source. The residual source and process of estimating moments of the error on the interior of a space-angle cell is unchanged. The process of estimating the solution on the outgoing face requires tallying the solution when particles leave a cell. The tallying process is discussed later in Section 1.4.1.

Applying L to the LDD trial space, as shown in Fig. **??**, results in two δ functions at each interior face. For positive flow, at a face $x_{i+1/2}$, the face portion of the residual is defined as

$$r_{\text{face}}(x_{i+1/2}) = -\mu \frac{\partial \tilde{I}^{(m)}}{\partial x}\Big|_{x_{i+1/2}} \tag{1.26}$$

$$= r_{\text{face}}(x^-_{i+1/2})\delta^-(x - x_{i+1/2}) + r_{\text{face}}(x^+_{i+1/2})\delta^+(x - x_{i+1/2}) \tag{1.27}$$

where

$$r_{\text{face}}(x^-_{i+1/2}) = -\mu \left(\tilde{I}^{(m)}(x_{i+1/2}, \mu) - \tilde{I}^{(m)}(x^-_{i+1/2}, \mu) \right) \tag{1.28}$$

$$r_{\text{face}}(x^+_{i+1/2}) = -\mu \left(\tilde{I}^{(m)}(x^+_{i+1/2}, \mu) - \tilde{I}^{(m)}(x_{i+1/2}, \mu) \right). \tag{1.29}$$

Here, $I^{(m)}(x^+_{i+1/2})$ and $I^{(m)}(x^-_{i+1/2})$ are the LD solution extrapolated to $x_{i+1/2}$ from the x cell $i+1$ and cell i, respectively. Particles sampled from the two δ-functions have the same starting location. The only difference is, for positive μ, particles sampled from $r_{\text{face}}(x^-_{i+1/2})$ will contribute to the face tally at $x_{i+1/2}$; the opposite is true for negative μ.

To reduce variance, we do not sample the two δ functions independently. Instead,

we combine the two δ-functions into a single face source, do not score particles at the face from which they are sampled. To account for the untallied error, we add the analytic contribution to the error from the face source to the corresponding face at the end of a batch. It is noted the combination of the two δ-functions produces the same residual source as the original LD residual.

Define the additional error contribution from the face sources at $x_{i+1/2}$ as $\delta\epsilon^{(m)}$. This additional error is tallied everywhere by MC, except for at $x_{i+1/2}$. The transport equation satisfied by $\delta\epsilon^{(m)}$, for positive μ, with effective total cross section $\hat{\sigma}_t$, is

$$\mu\frac{\partial\delta\epsilon^{(m)}}{\partial x}+\hat{\sigma}_t\delta\epsilon^{(m)}=r_{\text{face}}(x^-_{i+1/2})\delta^-(x-x_{i+1/2})+r_{\text{face}}(x^+_{i+1/2})\delta^+(x-x_{i+1/2}) \quad (1.30)$$

This equation is integrated from $x_{i+1/2}-\alpha$ to $x_{i+1/2}$ to produce

$$\begin{aligned}\mu\delta\epsilon^{(m)}(x_{i+1/2},\mu)-\mu\delta\epsilon^{(m)}(x_{i+1/2}-\alpha,\mu)+&\int_{x_{i+1/2}-\alpha}^{0}\hat{\sigma}_t\delta\epsilon^{(m)}\mathrm{d}x\\ &=r_{\text{face}}(x^-_{i+1/2})+\int_{x_{i+1/2}-\alpha}^{0}r_{\text{face}}(x^+_{i+1/2})\delta^+(x-x_{i+1/2})\mathrm{d}x. \quad (1.31)\end{aligned}$$

The integral on the right side of the equation is zero because $\delta^+(x-x_{i+1/2})$ is zero for $(-\infty,x_{i+1/2}]$. The limit of the above equation is taken as $\alpha\to 0$, i.e.,

$$\lim_{\alpha\to 0}\left(\mu\delta\epsilon^{(m)}(x_{i+1/2},\mu)-\mu\delta\epsilon^{(m)}(x_{i+1/2}-\alpha,\mu)+\int_{x_{i+1/2}-\alpha}^{0}\hat{\sigma}_t\delta\epsilon^{(m)}\mathrm{d}x\right)=\lim_{\alpha\to 0}r_{\text{face}}(x^-_{i+1/2}) \quad (1.32)$$

The integral goes to zero because $\delta\epsilon^{(m)}$ is smooth on the interior of the cell, and $\mu\delta\epsilon^{(m)}(x_{i+1/2}-\alpha,\mu)$ goes to zero because there is no source upstream of $x^-_{i+1/2}$.

Thus, the final solution is

$$\delta\epsilon^{(m)}(x_{i+1/2},\mu) = \frac{r_{\text{face}}(x^{-}_{i+1/2})}{\mu} = \tilde{I}^{(m)}(x^{-}_{i+1/2},\mu) - \tilde{I}^{(m)}(x_{i+1/2},\mu). \tag{1.33}$$

The update for $I(x_{i+1/2},\mu)$ is

$$\tilde{I}^{(m+1)}(x_{i+1/2},\mu) = \tilde{I}^{(m)}(x_{i+1/2},\mu) + \epsilon^{(m)}(x_{i+1/2},\mu) + \delta\epsilon^{(m)}(x_{i+1/2},\mu) \tag{1.34}$$

$$= \tilde{I}^{(m)}(x^{-}_{i+1/2},\mu) + \epsilon^{(m)}(x_{i+1/2},\mu). \tag{1.35}$$

This result has the serendipitous effect that the estimation of the solution on a face depends only on the interior solution $\tilde{I}^{(m)}(x^{-}_{i+1/2},\mu)$ and not the previous face value $\tilde{I}^{(m)}(x_{i+1/2},\mu)$. This adds a benefit that the face values can be estimated in particular cells, at any chosen batch.

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APPENDIX A

DERIVATIONS AND EQUATIONS FOR THE LO SYSTEM

A.1 Useful Moment Relations for LO Equations

There are several relations between various moment definitions that are useful in derivation and manipulation of the LO equations. The following are derived for $\phi(x)$, but can be applied to general moments of functions. The volumetric average terms can be eliminated in terms of the L and R moments from the relation $b_{L,i}(x) + b_{R,i}(x) = 1$.

$$\phi_i = \frac{1}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} 1 \, \phi(x) \mathrm{d}x \tag{A.1}$$

$$= \frac{1}{h_i} \left(\int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)\phi(x)\mathrm{d}x + \int_{x_{i-1/2}}^{x_{i+1/2}} b_{R,i}(x)\phi(x)\mathrm{d}x \right) \tag{A.2}$$

$$= \frac{1}{2} \left(\langle \phi \rangle_{L,i} + \langle \phi \rangle_{R,i} \right) \tag{A.3}$$

A similar relation can be derived for the first moment in space as

$$\phi_{x,i} = \frac{3}{2} \left(\langle \phi \rangle_{R,i} - \langle \phi \rangle_{L,i} \right) \tag{A.4}$$

The above relations can be inverted to derived a relation for the L and R moments in terms of the slope and average moments. These moment expressions are defined purely in terms of integrals, and are independent of the chosen spatial representation

Once a linear relation on the interior has been assumed, there are other useful closures that can be derived. The standard linear interpolatory expansion, for the

positive half-range, is restated here:

$$\phi^+(x) = \phi^+_{L,i} b_{L,i}(x) + \phi^+_{R,i} b_{R,i}(x) \tag{A.5}$$

Using this expansion, one can derive a relation between the outflow from a cell and the hat function moments that is equivalent to the standard LDFE Galerkin method:

$$\phi^+_{i,R} = 2\langle\phi\rangle^+_{R,i} - \langle\phi\rangle^+_{L,i}, \tag{A.6}$$

where for standard LD $\phi^+_{i+1/2} \equiv \phi_{i,R}$. The assumption of a linear relation on the interior of the cell defines the value for $\phi^+_{i,L}$:

$$\phi^+_{i,L} = 2\langle\phi\rangle^+_{L,i} - \langle\phi\rangle^+_{R,i}, \tag{A.7}$$

To eliminate the LO unknowns in a manner that produces the same moments as the LDFE Galerkin method, the following expression can be used for the outflow from a cell

$$\phi^+_{i+1/2} = \phi^+_i + \frac{\phi^+_{x,i}}{3}, \tag{A.8}$$

which in terms of the hat function moments is equivalent to $\phi^+_{i+1/2} = \langle\phi\rangle^+_{R,i}$. Inserting this expression into Eq. (**??**), and using the same definition for the linear representation over the interior of $\phi^+_{i+1/2}(x) = \phi_{L,i} b_{L,i}(x) + \phi_{R,i} b_{R,i}(x)$, will produce an equivalent set of unknowns as a linear discontinuous method with a lumped representation for the radiation. The temperature equation must be independently lumped. This relation preserves the average within a cell but modifies the first moment.

A similar expression produces a lumped-equivalent representation on the interior

of the cell:

$$\phi^+_{i,R} = \phi^+_i + \frac{\phi^+_x}{3}, \tag{A.9}$$

The moment equations are not modified by using this expression, however the interpretation of the moments as a linear representation over the cell has been altered. This allows for us to ensure a lumped representation on the interior while still using the HO solution to eliminate the outflow from the equations.

A.2 Newtons Method for the LO Equations

Because we have only considered problems with constant densities and heat capacities, the linearization described below is in terms of temperature T rather than material internal energy, for simplicity. However, the linearization can be formed in terms of internal energy to apply this method to a general equation of state.

To formulate the Newton iterations, the Planckian source is linearized in the material and radiation equations (Eq. (**??**) & Eq. (**??**)). Application of the first order Taylor expansion in time to the implicit emission source $B(T^{n+1})$, about some temperature T^* at some time $t^* \in [t^n, t^{n+1}]$, yields

$$\sigma_a^{n+1} acT^{4,n+1} \simeq \sigma_a^* ac \left[T^{*4} + (T^{n+1} - T^*)4T^{*3}\right] \tag{A.10}$$

where $\sigma_a^* \equiv \sigma_a(T^*)$. Substitution of this expression into Eq. (**??**) yields

$$\rho c_v \left(\frac{T^{n+1} - T^n}{\Delta t}\right) = \sigma_a^* \phi^{n+1} - \sigma_a^* ac \left[T^{*4} + (T^{n+1} - T^*)4T^{*3}\right]. \tag{A.11}$$

Algebraic manipulation of this equation yields an expression for $T^{n+1} - T^*$:

$$\left(T^{n+1} - T^*\right) = \frac{\frac{\sigma_a^* \Delta t}{\rho c_v}\left[\phi^{n+1} - acT^{*4}\right] + (T^n - T^*)}{1 + \sigma_a^* ac\Delta t \frac{4T^{*3}}{\rho c_v}}.$$

This expression is substituted back into Eq. (A.10) to form an explicit approximation for the emission source at t^{n+1} as

$$\sigma_a acT^{4,n+1} \simeq \sigma_a^*(1-f^*)\phi^{n+1} + f^*\sigma_a^* acT^{4,n} + \rho c_v \frac{1-f^*}{\Delta t}(T^n - T^*) \tag{A.12}$$

where $f^* = [1 + \sigma_a^* c\Delta t 4aT^{*3}/(\rho c_v)]^{-1}$ is often referred to as the Fleck factor [3].

Next, the above equation must be spatially discretized. Application of the L spatial moment yields

$$\langle \sigma_a^* acT^{4,n+1}\rangle_{L,i} = \sigma_{ai}^*(1-f_i^*)\langle\phi^{n+1}\rangle_{L,i} + f_i^*\sigma_{ai}^* ac\left(\frac{2}{3}T_{L,i}^{4,n} + \frac{1}{3}T_{R,i}^{4,n}\right) \\ \rho_i c_{vi}\frac{1-f_i^*}{\Delta t}\left[\frac{2}{3}\left(T_{L,i}^n - T_{L,i}^*\right) + \frac{1}{3}\left(T_{R,i}^n - T_{R,i}^*\right)\right], \tag{A.13}$$

where $T^{4,n}$ and T^n have been assumed LD and f^* is assumed constant over a cell, i.e., $f_i^* \equiv \sigma_a(T_i^*)$. The error introduced by a constant f^* approaches zero as the non-linearity is converged because T^* approaches T^{n+1}. Based on an estimate for T^*, Eq. (A.13) is an expression for the Planckian emission source in the radiation moment equations with an additional effective scattering source. A similar expression can be derived for $\langle\sigma_{a,i}acT^4\rangle_R$ and the right moment equations. The expressions for the emissions source is substituted into the radiation moment equations (Eq. (**??**)–(**??**)) to produce a linear system of equations for the new radiation intensity moments.

Once the linear equations have been solved for new radiation moments, new temperature unknowns can be estimated. To conserve energy, the same linearization and discretizations used to solve the radiation equation must be used in the material energy equation. Substitution of Eq. (A.13) into the material energy L moment equation ultimately yields

$$\frac{2}{3}T_{L,i}^{n+1} + \frac{1}{3}T_{R,i}^{n+1} = \frac{f_i^* \sigma_{ai}^* \Delta t}{\rho c_v}\left[\langle \phi^{n+1} \rangle_{L,i} - ac\left(\frac{2}{3}T_{L,i}^{4,n} + \frac{1}{3}T_{R,i}^{4,n}\right)\right] + (1 - f_i^*)\left(\frac{2}{3}T_{L,i}^{*} + \frac{1}{3}T_{R,i}^{*}\right) + f\left(\frac{2}{3}T_{L,i}^{n} + \frac{1}{3}T_{R,i}^{n}\right) \quad \text{(A.14)}$$

A similar expression is produced for the R moment equation. This produces a local matrix equation to solve for new T unknowns. If both the radiation and temperature unknowns are lumped, this matrix becomes diagonalized.

Based on these equations, the algorithm for solving the LO equations, with iteration index l, is defined as

1. Initialize T unknowns using T^n or the last estimate of T^{n+1} from previous LO solve
2. Build the LO system based on the effective scattering $(1 - f^l)$ and emission terms evaluated using T^l.
3. Solve the linearized LO system to produce an estimate for $\phi^{n+1,l}$.
4. Evaluate a new estimate of T^{n+1} unknowns using Eq. (A.14).
5. $T^* \leftarrow \tilde{T}^{n+1}$.
6. Repeat 2-5 until $(T^{n+1,k})^4$ and $\phi^{n+1,k}$ are converged.

Figure A.1: TAMU figure

A.3 Analytic Neutronics answer for Source fixup

In this section we model a fixed-source, pure-absorber neutronics calculation where we know the analytic answer to test our fixup. If we make the mesh thick enough, we can set the solution to be the equilibrium answer $\psi(x) = \frac{q(x)}{2\sigma_a}$. For a general isotropic source $Q(x)$, the 1D transport equation to be solved is

$$\mu \frac{\partial \psi}{\partial x} + \sigma_a \psi(x, \mu) = \frac{q(x)}{2} \tag{A.15}$$

with boundary condition $\psi(0, \mu) = \psi_{inc}$, $\mu > 0$ and $\psi(x_R, \mu) = \frac{q(x_R)}{2\sigma_a}$ for $\mu < 0$, where x_R is the right boundary. This first order differential equation is solved using

an integration factor. The solution to this equation for $\mu > 0$ is given by

$$\psi(x,\mu) = \psi_{inc} e^{\frac{-\sigma_a x}{\mu}} + \int_0^x \frac{q(x')}{2\mu} e^{\frac{-\sigma_a x'}{\mu}} \mathrm{d}x', \quad \mu > 0 \tag{A.16}$$

Integration of this result over the positive half range of μ gives

$$\phi^+(x) = \psi_{inc}\, \mathrm{E}_2(\sigma_a x) + \frac{1}{2}\int_0^x q(x')\, \mathrm{E}_1(\sigma_a x')\mathrm{d}x'. \tag{A.17}$$

In the simplification of a constant source, the integral reduces to

$$\phi^+(x) = \psi_{inc}\, \mathrm{E}_2(\sigma_a x) + \frac{q}{2\sigma_a}\left(1 - \mathrm{E}_2(\sigma_a x)\right). \tag{A.18}$$

Also, for a constant source the solution for the negative half range becomes a constant, i.e.,

$$\phi^-(x) = \frac{q}{\sigma_a} \tag{A.19}$$

Combination of the above two equations gives the solution for the scalar flux:

$$\phi(x) = \psi_{inc}\, \mathrm{E}_2(\sigma_a x) + \frac{q}{2\sigma_a}\left(1 - \mathrm{E}_2(\sigma_a x)\right) + \frac{q}{\sigma_a}. \tag{A.20}$$

APPENDIX B

DERIVATION OF THE WLA-DSA EQUATIONS

In this section, we derive the discretized diffusion equation and LD mapping equations that are used in the WLA-DSA equations. To simplify notation, we derive the equations from a generic transport equation (rather than the error equations) with isotropic scattering and source q_0, i.e.,

$$\mu\frac{\partial I}{\partial x} + \sigma_t I = \frac{\sigma_s}{2}\left(\phi(x) + q_0\right). \tag{B.1}$$

B.1 Forming a Continuous Diffusion Equation

First, a continuous spatial discretization of a diffusion equation is derived. The mean intensity ϕ will ultimately be assumed continuous at faces to produce a standard three-point finite-difference diffusion discretization. The zeroth and first μ moment of Eq. (B.1) produce the P_1 equations [5, 12], i.e.,

$$\frac{\partial J}{\partial x} + \sigma_a\phi = q_0 \tag{B.2}$$

$$\sigma_t J + \frac{1}{3}\frac{\partial \phi}{\partial x} = 0. \tag{B.3}$$

The spatial finite element moments (defined by Eq. (**??**) and (**??**)) are taken of the above equations. The mean intensity is assumed linear on the interior of the cell, i.e., $\phi(x) = \phi_L b_L(x) + \phi_R b_R(x)$, for $x \in (x_{i-1/2}, x_{i+1/2})$. Taking the left moment, evaluating integrals, and rearranging yields

$$J_i - J_{i-1/2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{L,i}\ , \tag{B.4}$$

where J_i is the average of the flux J over the cell. The moments of q are not simplified to be compatible with the error equations which are in terms of moments. For the R moment

$$J_{i+1/2} - J_i + \frac{\sigma_{a,i} h_i}{2} \left(\frac{2}{3} \phi_{L,i} + \frac{1}{3} \phi_{R,i} \right) = \frac{h_i}{2} \langle q \rangle_{R,i} \ . \tag{B.5}$$

The equation for the L moment is evaluated for cell $i+1$ and added to the R moment equation evaluated at i. The flux J is assumed continuous at $i + 1/2$ to eliminate the face fluxes from the equations. The sum of the two equations becomes

$$J_{i+1} - J_i + \frac{\sigma_{a,i+1} h_{i+1}}{2} \left(\frac{2}{3} \phi_{L,i+1} + \frac{1}{3} \phi_{R,i+1} \right) + \frac{\sigma_{a,i} h_i}{2} \left(\frac{1}{3} \phi_{L,i} + \frac{2}{3} \phi_{R,i} \right) = \frac{h}{2} \left(\langle q \rangle_{L,i+1} + \langle q \rangle_{R,i} \right) . \tag{B.6}$$

The mean intensity is approximated as continuous at each face, i.e., $\phi_{L,i+1} = \phi_{R,i} \equiv \phi_{i+1/2}$. Adding the L and R moments of Eq. (B.3) together, with the continuous approximation for $\phi_{i+1/2}$, produces a discrete Fick's law equation [10]

$$J_i = -D_i \frac{\phi_{i+1/2} - \phi_{i-1/2}}{h_i}, \tag{B.7}$$

where $D_i = 1/(3\sigma_{t,i})$. Substitution of Eq. (B.7) into Eq. (B.6) and rearranging yields the following discrete diffusion equation:

$$\left(\frac{\sigma_{a,i+1} h_{i+1}}{6} - \frac{D_{i+1}}{h_{i+1}} \right) \phi_{i+3/2} + \left(\frac{D_{i+1}}{h_{i+1}} + \frac{D_i}{h_i} + \frac{\sigma_{a,i+1} h_{i+1}}{3} + \frac{\sigma_{a,i} h_i}{3} \right) \phi_{i+1/2} + \left(\frac{\sigma_{a,i} h_i}{6} - \frac{D_i}{h_i} \right) \phi_{i-1/2} = \frac{h_{i+1}}{2} \langle q \rangle_{L,i+1} + \frac{h_i}{2} \langle q \rangle_{R,i} \ . \tag{B.8}$$

To allow for the use of lumped or standard LD in these equations, we introduce the factor θ, with $\theta = 1/3$ for standard LD, and $\theta = 1$ for lumped LD. The diffusion

equation becomes

$$\left(\frac{\sigma_{a,i+1}h_{i+1}}{4}(1-\theta)-\frac{D_{i+1}}{h_{i+1}}\right)\phi_{i+3/2}+\left(\frac{D_{i+1}}{h_{i+1}}+\frac{D_i}{h_i}+\left(\frac{1+\theta}{2}\right)\left[\frac{\sigma_{a,i+1}h_{i+1}}{2}+\frac{\sigma_{a,i}h_i}{2}\right]\right)\phi_{i+1/2}$$
$$+\left(\frac{\sigma_{a,i}h_i}{4}(1-\theta)-\frac{D_i}{h_i}\right)\phi_{i-1/2}=\frac{h_{i+1}}{2}\langle q\rangle_{L,i+1}+\frac{h_i}{2}\langle q\rangle_{R,i}\ . \quad \text{(B.9)}$$

Summation over all cells forms a system of equations for ϕ at each face.

B.1.1 Diffusion Boundary Conditions

The upwinding in the LO system exactly satisfies the inflow boundary conditions, therefore a vacuum boundary condition is applied to the diffusion error equations. The equation for the left moment at the first cell is given by

$$J_1-J_{1/2}+\frac{\sigma_{a,i}h_i}{2}\left(\frac{1+\theta}{2}\phi_{L,i}+\frac{1-\theta}{2}\phi_{R,i}\right)=\frac{h_i}{2}\langle q\rangle_{L,i}\ , \quad \text{(B.10)}$$

The Marshak boundary condition for the vacuum inflow at face $x_{1/2}$ is given as

$$J^+_{1/2}=0=\frac{\phi_{1/2}}{4}+\frac{J_{1/2}}{2}, \quad \text{(B.11)}$$

which can be solved for $J_{1/2}$. Substitution of the above equation and Eq. (B.7) into Eq. (B.10) gives

$$\left(\frac{1}{2}+\sigma_{a,1}h_1\frac{1+\theta}{4}-\frac{D_1}{h_1}\right)\phi_{1/2}+\left(\sigma_{a,1}h_1\frac{1-\theta}{4}-\frac{D_1}{h_1}\right)\phi_{3/2}=\frac{h_i}{2}\langle q\rangle_{L,1} \quad \text{(B.12)}$$

A similar expression can be derived for the right-most cell.

B.2 Mapping Solution onto LD Unknowns

Solution of the continuous diffusion equation will provide an approximation to ϕ on faces, denoted as $\phi^C_{i+1/2}$. We now need to map the face solution onto the LD

representation of ϕ. To do this, first we take the L and R finite element moments of the P_1 equations. A LDFE dependence is assumed on the interior of the cell for J and ϕ. Taking moments of Eq. (B.2) and simplifying yields

$$J_{i+1/2} - \frac{J_{L,i} + J_{R,i}}{2} + \frac{\sigma_{a,i} h_i}{2} \left(\frac{1}{3}\phi_{L,i} + \frac{2}{3}\phi_{R,i} \right) = \frac{h_i}{2} \langle q \rangle_{R,i} \tag{B.13}$$

$$\frac{J_{L,i} + J_{R,i}}{2} - J_{i-1/2} + \frac{\sigma_{a,i} h_i}{2} \left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i} \right) = \frac{h_i}{2} \langle q \rangle_{L,i} \tag{B.14}$$

The moment equations for Eq. (B.3) are

$$\frac{1}{3} \left(\phi_{i+1/2} - \frac{\phi_{i,L} + \phi_{i,R}}{2} \right) + \frac{\sigma_{t,i} h_i}{2} \left(\frac{1}{3} J_{L,i} + \frac{2}{3} J_{R,i} \right) = 0 \tag{B.15}$$

$$\frac{1}{3} \left(\frac{\phi_{i,L} + \phi_{i,R}}{2} - \phi_{i-1/2} \right) + \frac{\sigma_{t,i} h_i}{2} \left(\frac{2}{3} J_{L,i} + \frac{1}{3} J_{R,i} \right) = 0 \tag{B.16}$$

The face terms $J_{i\pm1/2}$ and $\phi_{i\pm1/2}$ need to be eliminated from the system. First, the scalar intensity is assumed to be the value provided by the continuous diffusion solution at each face, i.e., $\phi_{i\pm1/2} = \phi^C_{i\pm1/2}$. Then, the fluxes are decomposed into half-range values to decouple the equations between cells. At $x_{i+1/2}$, the flux is composed as $J_{i+1/2} = J^+_{i+1/2} + J^-_{i+1/2}$, noting that in this notation the half-range fluxes are $J^\pm_{i+1/2} = \pm \int_0^\pm \mu I(x_{i+1/2}, \mu) \mathrm{d}\mu$[1]. We approximate the incoming fluxes, e.g., $J^-_{i+1/2}$, based on $\phi^C_{i+1/2}$ and a P_1 approximation. The P_1 approximation provides the following relation [12]

$$\phi = 2(J^+ - J^-). \tag{B.17}$$

At $x_{i+1/2}$, the above expression is solved for the incoming current $J^-_{i+1/2}$. The total

[1]Typically, the half-range fluxes are defined with integrals weighted with $|\mu|$, but this notation would not be consistent with our definition of the half-range consistency terms

current becomes

$$J_{i+1/2} = J^+_{i+1/2} - J^-_{i+1/2} = 2J^+_{i+1/2} - \frac{\phi^C_{i+1/2}}{2}, \tag{B.18}$$

In the positive direction, at the right face, the values of ϕ and J are based on the LD representation within the cell at that face, i.e., $\phi_{R,i}$ and $J_{R,i}$. The standard P_1 approximation for the half-range fluxes is used[10], i.e.,

$$J^\pm = \frac{\gamma\phi}{2} \pm \frac{J}{2}, \tag{B.19}$$

where γ accounts for the difference between the LO parameters and the true P_1 approximation. Thus, for the right face and positive half-range,

$$J^+_{i+1/2} = \frac{\gamma}{2}\phi_{i,R} + \frac{J_{i,R}}{2} \tag{B.20}$$

A similar expression can be derived for $x_{i-1/2}$. The total fluxes at each face are thus

$$J_{i+1/2} = \gamma\phi_{i,R} + J_{i,R} - \frac{\phi^C_{i+1/2}}{2} \tag{B.21}$$

$$J_{i-1/2} = \frac{\phi^C_{i-1/2}}{2} - \gamma\phi_{i,L} + J_{i,L} \tag{B.22}$$

Substitution of these results back into the LD balance equations and introduction of the lumping notation yields the final equations

$$\left(\gamma\phi_{i,R} + J_{i,R} - \frac{\phi^C_{i+1/2}}{2}\right) - \frac{J_{L,i} + J_{R,i}}{2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{(1-\theta)}{2}\phi_{L,i} + \frac{(1+\theta)}{2}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{R,i} \tag{B.23}$$

$$\frac{J_{L,i}+J_{R,i}}{2}-\left(\frac{\phi^C_{i-1/2}}{2}-\gamma\phi_{i,L}+J_{i,L}\right)+\frac{\sigma_{a,i}h_i}{2}\left(\frac{(1+\theta)}{2}\phi_{L,i}+\frac{(1-\theta)}{2}\phi_{R,i}\right)=\frac{h_i}{2}\langle q\rangle_{L,i} \tag{B.24}$$

$$\frac{1}{3}\left(\phi^C_{i+1/2}-\frac{\phi_{i,L}+\phi_{i,R}}{2}\right)+\frac{\sigma_{t,i}h_i}{2}\left(\frac{(1-\theta)}{2}J_{L,i}+\frac{(1+\theta)}{2}J_{R,i}\right)=0 \tag{B.25}$$

$$\frac{1}{3}\left(\frac{\phi_{i,L}+\phi_{i,R}}{2}-\phi^C_{i-1/2}\right)+\frac{\sigma_{t,i}h_i}{2}\left(\frac{(1+\theta)}{2}J_{L,i}+\frac{(1-\theta)}{2}J_{R,i}\right)=0. \tag{B.26}$$

The above equations are completely local to each cell and fully defined, including for boundary cells. For simplicity, we just take $\gamma = 1/2$. The system can be solved for the desired unknowns $\phi_{i,L}$, $\phi_{i,R}$, $J_{i,L}$, and $J_{i,R}$, which represent the mapping of $\phi^C_{i+1/2}$ onto the LD representation for $\phi^{\pm}(x)$.