

# 1. THE MOMENT-BASED LOW-ORDER EQUATIONS

## 1.1 Forming the Low-Order System

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

$$\langle \cdot \rangle_{L,i} = \frac{2}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)(\cdot) dx, \quad (1.1)$$

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  $b_{R,i}(x) = (x - x_{i-1/2})/h_i$ . It is noted in this notation  $\langle \phi \rangle_{L,i}$  and  $\langle \phi \rangle_{R,i}$  represent spatial moments of the intensity over cell  $i$ , opposed to  $\phi_{L,i}$  and  $\phi_{R,i}$ , which represent the interior value of the linear representation of  $\phi(x)$  at  $x_{i-1/2}$  and  $x_{i+1/2}$  within the cell. 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  $\phi^+(x) = \int_0^1 I(x, \mu) d\mu$  and  $\phi^-(x) = \int_{-1}^0 I(x, \mu) d\mu$ , respectively. Thus, in terms of half-range quantities,  $\phi(x) = \phi^-(x) + \phi^+(x)$ .

### 1.1.1 Radiation Energy Equations

Pairwise application of the  $L$  and  $R$  basis moments with the  $+$  and  $-$  half-range integrals to Eq. (??) ultimately yields four moment equations per cell. As in [28], algebraic manipulation is performed to form intensity-weighted averages of  $\mu$ , which we denote as consistency terms. As an example, the equation resulting from

application of the  $L$  moment and positive half-range integral is

$$\begin{aligned}
& -2\mu_{i-1/2}^{n+1,+} \phi_{i-1/2}^{n+1,+} + \{\mu\}_{L,i}^{n+1,+} \langle \phi \rangle_{L,i}^{n+1,+} + \{\mu\}_{R,i}^{n+1,+} \langle \phi \rangle_{R,i}^{n+1,+} + \left( \sigma_{t,i}^{n+1} + \frac{1}{c\Delta t} \right) h_i \langle \phi \rangle_{L,i}^{n+1,+} \\
& - \frac{\sigma_{s,i} h_i}{2} (\langle \phi \rangle_{L,i}^{n+1,+} + \langle \phi \rangle_{L,i}^{n+1,-}) = \frac{h_i}{2} \langle \sigma_a^{n+1} ac T^{n+1,4} \rangle_{L,i} + \frac{h_i}{c\Delta t} \langle \phi \rangle_{L,i}^{n,+}, \quad (1.2)
\end{aligned}$$

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.,

$$\{\mu\}_{L,i}^{n+1,+} \equiv \frac{\langle \mu I^{n+1} \rangle_{L,i}^+}{\langle I^{n+1} \rangle_{L,i}^+} = \frac{\frac{2}{h_i} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu b_{L,i}(x) I^{n+1}(x, \mu) dx d\mu}{\frac{2}{h_i} \int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) I^{n+1}(x, \mu) dx d\mu}. \quad (1.3)$$

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

### 1.1.2 Material Energy Equations

To derive the LO material energy equations,  $T(x)$  is represented spatially in the LDFE trial space, i.e.,  $T(x) \simeq T_{L,i} b_{L,i}(x) + T_{R,i} b_{R,i}(x)$ ,  $x \in (x_{i-1/2}, x_{i+1/2})$ . 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 equations; the LDFE representations for  $T(x)$  and  $\sigma_a ac T^4(x)$  are used to simplify the spatial integrals. For example, the final LO material energy equation resulting from application of the  $L$  moment is

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

$$= \sigma_{a,i}^{n+1} ac \left( \frac{2}{3} T_{L,i}^4 + \frac{1}{3} T_{R,i}^4 \right)^{n+1}. \quad (1.4)$$

Cross sections have been assumed constant over each element, evaluated at the average temperature within the element, i.e.,  $\sigma_{a,i}^{n+1} = \sigma_{a,i}([T_{L,i}^{n+1} + T_{R,i}^{n+1}]/2)$ . Because the material energy balance only contains angularly integrated quantities, there is no need to take angular moments of the above equation.

## 1.2 Closing the System with Information from the HO solution

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 four radiation and two material energy equations define a system of equations for the six DOF, coupled to other cells via upwinding in the streaming term. The relation between the volume and face averaged quantities and the angular consistency parameters (e.g., Eq. (1.3)) are not known a priori. 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. (1.3)) using the latest HO solution  $\tilde{I}^{n+1,k+1/2}$  as an approximation for  $I^{n+1}(x, \mu)$ . To close the LO system spatially, a linear-discontinuous (LD) spatial closure with the usual upwinding approximation is used. For example, for positive flow (e.g., Eq. (1.2)) 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.,  $\phi_{i+1/2}^+ = 2\langle \phi \rangle_R^+ - \langle \phi \rangle_L^+$ . Because there are no derivatives of  $T$  in Eq. (??), there is no need to define  $T$  on the faces; the temperature has been assumed linear within a cell to relate  $T$  and  $T^4$ .

The choice of a LD spatial closure should preserve the equilibrium diffusion limit.

In this limit, the MC HO solution will estimate angular consistency terms associated with an isotropic intensity, based on a spatially LD emission source. The isotropic-intensity consistency terms will produce LO equations that are equivalent to  $S_2$  equations, with quadrature points of  $\pm 1/2$ . Because the spatial closure produces equations that are equivalent to an LDFE solution to these equations, we expect the equations to preserve the equilibrium diffusion limit [18, 4].

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 negative values of intensity 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; negative values 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) [18]. 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 average within a cell, but the relation between the moments and the outflow is modified. For example, for positive  $\mu$ , 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 negative intensities occur.

### 1.2.1 Newton's Method for LO Equations

Adding the equations for each cell together forms a global system of coupled equations. The equations are nonlinear due to the Planckian emission source. We have used Newton's method to solve the nonlinear system, based on a typical linearization

of the Planckian source with cross sections evaluated at temperatures from the previous iteration, as described in [18]. 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  $t^* \in [t^n, t^{n+1}]$ , gives

$$\sigma_a^{n+1} ac T^{4,n+1} \simeq \sigma_a^* ac [T^{*4} + (T^{n+1} - T^*) 4T^{*3}] \quad (1.5)$$

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

$$\rho c_v \left( \frac{T^{n+1} - T^n}{\Delta t} \right) = \sigma_a^* \phi^{n+1} - \sigma_a^* ac [T^{*4} + (T^{n+1} - T^*) 4T^{*3}]. \quad (1.6)$$

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

$$T^{n+1} = \frac{1}{\rho c_v} f \sigma_a^* \Delta t (\phi^{n+1} - ca T^{*4}) + f T^n + (1 - f) T^*. \quad (1.7)$$

where  $f^* = [1 + \sigma_a^* c \Delta t 4a T^{*3} / (\rho c_v)]^{-1}$  is often referred to as the Fleck factor [8]. The expression for  $T^{n+1}$  can be substituted back into Eq. (1.5) to form an explicit approximation for the emission source at  $t_{n+1}$  as

$$\sigma_a ac T^{4,n+1} \simeq \sigma_a^* (1 - f^*) \phi^{n+1} + f^* \sigma_a^* ac T^{4,n} + \rho c_v \frac{1 - f^*}{\Delta t} (T^n - T^*) \quad (1.8)$$

where  $f^* = (1 + \sigma_a^* c \Delta t \beta^*)^{-1}$  is the usual Fleck factor [8] with

$$\beta^* = \frac{4aT^{*3}}{\rho c_v} \quad (1.9)$$

The material temperature is updated at the end of the time step using Eq. 1.7. If  $T^* = T^n$ , then this is equivalent to the standard IMC linearization.

Next, the above equation must be spatially discretized. Taking the left spatial moment yields

$$\langle \sigma_a^* a c T^{4,n+1} \rangle_L = \frac{2}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} b_L(x) [\sigma_a^* (1 - f^*) \phi^{n+1} + f^* \sigma_a^* a c T^{4,n}] \mathfrak{X}. \quad (1.10)$$

To keep the derivation general, we look at the two terms on the right side separately:  $f^* \sigma_a^* a c T^{4,n}$  can be evaluated explicitly because the spatial dependence over a cell of  $T^{4,n}$  is already assumed LD. For simplicity,  $f^*$  is assumed constant over a cell, i.e.,  $f_i^* \equiv \sigma_a(T_i^*)$  ( $\sigma_a^*$  has already been assumed constant over a cell). Any error introduced by this approximation goes away as the non-linearity is converged and  $T^* \rightarrow T^{n+1}$ . The equation then becomes

$$\langle \sigma_a^* a c T^{4,n+1} \rangle_L = \sigma_a^* (1 - f^*) \langle \phi^{n+1} \rangle_L + f^* \sigma_a^* \langle a c T^{4,n} \rangle_L \quad (1.11)$$

A similar expression can be derived for  $\langle \sigma_{a,i} a c T^4 \rangle_R$ . Based on an estimate for  $T^*$ , the above equation gives an expression for the Planckian emission source on the right hand side of Eq. (1.2) with an additional effective scattering source. This allows for four linear equations for the four remaining radiation unknowns to be fully defined. The final equation for the left basis moment and positive flow is

$$\begin{aligned}
& -2\mu_{i-1/2}^{n+1,+} \phi_{i-1/2}^{n+1,+} + \langle \mu \rangle_{L,i}^{n+1,+} \langle \phi \rangle_{L,i}^{n+1,+} + \langle \mu \rangle_{R,i}^{n+1,+} \langle \phi \rangle_{R,i}^{n+1,+} + \left( \sigma_t^* + \frac{1}{c\Delta t} \right) h_i \langle \phi \rangle_{L,i}^{n+1,+} \\
& - \frac{h_i}{2} (\sigma_s^* + \sigma_a^* (1 - f^*)) (\langle \phi \rangle_{L,i}^{n+1,+} + \langle \phi \rangle_{L,i}^{n+1,-}) = \\
& \frac{1}{2} h_i \sigma_a^* a c f^* \left( \frac{2}{3} T_{L,i}^{4,n} + \frac{1}{3} T_{R,i}^{4,n} \right) + \frac{h_i}{c\Delta t} \langle \phi \rangle_{L,i}^{n,+} \quad (1.12)
\end{aligned}$$

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Once these linear equations have been solved for  $\phi^{n+1}$ , a new estimate of  $T^{n+1}$  can be determined. To conserve energy, the same linearization used to solve the radiation equation must be used in the material energy equation. Substitution of Eq. (1.11) into the material energy equation yields

$$\rho c_v \frac{T^{n+1} - T^n}{\Delta t} = \sigma_a^* \phi^{n+1} - (\sigma_a^* (1 - f) \phi^{n+1} + f \sigma_a^* a c T^{4,n}), \quad (1.13)$$

which gives a temperature at the end of the time step as

$$T^{n+1} = \frac{f^* \sigma_a^* \Delta t}{\rho c_v} (\phi^{n+1} - c a T^{n4}) + T^n, \quad (1.14)$$

This is how the IMC method estimates the temperature at the end of the time step, following the MC solve. Here, the LO radiation equations have taken the place of the Monte Carlo solve. To account for spatial dependence, the above equation can simply be evaluated using  $\phi_L^{n+1}$  and  $T_L^*$  to get  $T_L^{n+1}$ .

Based on these equations, the algorithm for solving the LO system with constant  $f^*$  and cross sections over a cell is defined as

1. Guess  $T_L^*$  and  $T_R^*$ , typically using  $T^n$ .
2. Build the LO system based on the effective scattering  $(1 - f^*)$  and emission terms (i.e., evaluation of Eq. (1.12)).

3. Solve the linearized LO system to produce an estimate for  $\phi^{n+1}$ .
4. Evaluate a new estimate of the  $T_{L,i}$  and  $T_{R,i}$  at the end of the time step  $\tilde{T}^{n+1}$  using Eq. (1.14).
5.  $T^* \leftarrow \tilde{T}^{n+1}$ .
6. Repeat 2-5 until  $\tilde{T}^{n+1}$  and  $\phi^{n+1}$  are converged.

Because of the chosen linearization, the convergence primarily takes place in the lagged material properties and factor  $f$ .

Isotropic scattering, including effective scattering terms from the linearization, are included in the system matrix. The system matrix is an asymmetric, banded matrix with 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. Convergence is calculated using the spatial  $L_2$  norm of the change in  $\phi^{n+1}(x)$  and  $T^{n+1}(x)$ , relative to the norm of each solution. The lumping-equivalent discretization discussed above is used for cells where the solution for  $\phi^{n+1}$  becomes negative. When negative values for  $\phi^{n+1,\pm}(x)$  are detected, the lumping-equivalent discretization is used within those cells and that Newton step is repeated.



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## APPENDIX A

### FIRST APPENDIX

Text for the Appendix follows.



Figure A.1: TAMU figure

## APPENDIX B

### SECOND APPENDIX WITH A LONGER TITLE - MUCH LONGER IN FACT

Text for the Appendix follows.



Figure B.1: TAMU figure

#### B.1 Appendix Section