CHAPMAN-ENSKOG ANALYSIS OF DISCRETIZED TRANSPORT EQUATIONS

Bertrand Laubsch
Dept. of Physics
Oregon St. University
301 Weniger Hall
Corvallis, OR 97331
laubschb@ucs.orst.edu

Todd S. Palmer
Dept. of Nuclear Engineering
Oregon St. University
116 Radiation Center
Corvallis, OR 97331
palmerts@engr.orst.edu

ABSTRACT

Chapman-Enskog (CE) theory can be used to derive discretized diffusion equations from discretized transport equations. This method has previously been applied to derive analytic diffusion theories from analytic transport equations. This work demonstrates that both isotropic diffusion theory (IDT) discretizations and flux limited diffusion theory (FLDT) discretizations can be obtained directly from discretized transport equations. Specifically, we illustrate this new procedure by applying it to the Simple Corner Balance (SCB) transport equations in one-dimensional slab geometry for photons, without boundary conditions. The IDT result is a three point diffusion equation, which matches equations found from a traditional asymptotic analyses. We find that FLDT analysis predicts that the values for cell edge energy density are not guaranteed to be continuous; therefore twice as many (six) unknowns are involved in each cell's discrete FLDT diffusion equation. A numerical scheme for solving the derived FLDT equations is left for future work.

INTRODUCTION

Flux-limited diffusion theory (FLDT) is a commonly used model for obtaining numerical solutions to radiation transport problems. Typically, the particular form of the flux-limiter is derived by considering properties of the *analytic* transport operator that should be preserved by the *analytic* diffusion operator, generally forcing the parabolic diffusion operator to become a hyperbolic operator where streaming is a dominant physical process. For years researchers have obtained solutions to numerical FLDT problems in this way:

- choose a grid to impose on the physical space (typically a structured grid);
- discretize the diffusion operator (independent of the flux-limiter used);
- discretize the flux-limiter, attempting to "fit" its spatial representation to the discretized diffusion equations.

The process as described has some limitations. First, there are few documented successes involving unstructured grids. Perhaps more importantly, this process is not mathematically rigorous; i.e. the discretization of the FLDT system is not derived directly from a discretized transport equation. Often times ad hoc "averaging" procedures are needed to assure that radiation will not be trapped at the interface between hot and cold zones. Deriving *discretized* FLDT diffusion equations directly from well-behaved discretized transport equations may provide insight into the nature of these averaging schemes, or suggest more accurate or robust FLDT schemes.

One standard technique of obtaining diffusion equations from transport equations is an asymptotic analysis. In the past, this has been a valuable tool for ensuring that numerical transport schemes were accurate and well-behaved in optically thick, diffusive regions. An asymptotic analysis alone, though, provides no connection between transport and flux-limited diffusion.

The goal of our research is to apply Chapman-Enskog (CE) theory, a technique used to derive FLDT from analytic transport equations, to discretized transport equations. We begin by reviewing the CE method applied to analytic transport equations. We then show that the CE method can be applied to obtain discretized isotropic diffusion equations from discretized transport equations. These results match those from traditional asymptotic analysis, excluding boundary effects. Next, we apply the CE method to obtain FLDT equations; we first review the analytic derivation and later show a derivation for the discrete system. We will see that the FLDT results differ from the IDT results by allowing discontinuities in the energy density at the edges, thus increasing the number of unknowns per cell. Future work will include finding a numerical method for handling the additional unknowns in the FLDT equations.

THE CHAPMAN-ENSKOG TECHNIQUE

We briefly outline the application of the Chapman-Enskog (CE) method to the analytic transport equation since only an unpublished version of such work may exist; for the full details of this method the reader should refer to the internal paper by C. D. Levermore [1].

The procedure consists of four steps: 1) obtaining a functional differential equation from the transport equation, 2) scaling the functional equation so that the zeroth order solution is solvable and describes a desired limit, 3) asymptotically expanding the intensity in the scaling parameter, and 4) recursively solving the equations to a desired order, then substituting these results into the balance equation to obtain a diffusion equation.

We begin with the analytic radiation transport equation:

$$\frac{1}{c}\frac{\partial}{\partial t}I + \hat{\Omega}\cdot\nabla I + \sigma_T I = \frac{c}{4\pi}\left(\sigma_A B + \sigma_S U\right), \tag{1}$$

and obtain a balance equation by integrating the above over all angles,

$$\frac{\partial}{\partial t}U + \nabla\cdot\vec{F} + c\sigma_A(U - B) = 0, \tag{2}$$

where the flux $\vec{F}$ is the first angular moment of I $\left(\vec{F} = \int_{4\pi}\hat{\Omega} I d\Omega\right)$, U is the energy density $\left(U = \frac{1}{c}\int_{4\pi} I\, d\Omega\right)$, and $\sigma_T = \sigma_A + \sigma_S$.

The intensity $I(\hat{\Omega}, \vec{x}, t)$ is now expressed as a functional, $I[U]$, of the energy density $U(\vec{x}, t)$. It is then possible to write derivatives of the intensity in terms of derivatives of the energy density using (2):

$$\frac{\partial}{\partial t} I = \frac{\delta I}{\delta U} \frac{\partial}{\partial t} U = \frac{\delta I}{\delta U} \left[-\nabla F - c\sigma_A (U - B) \right].$$

The functional derivative $\frac{\delta I}{\delta U}$ is an operator acting on the bracketed quantity, above. Thus, the first step in the CE procedure is to rewrite the transport equation (1) as a functional differential equation by substituting the above time derivative into (1). After some manipulation the transport equation may be written:

$$\sigma_T \left(I - \frac{c}{4\pi} U \right) = \frac{\delta I}{\delta U} \left[\frac{1}{c} \nabla \cdot \vec{F} + \sigma_A (U - B) \right] - \hat{\Omega} \cdot \nabla I - \frac{c}{4\pi} \sigma_A (U - B). \quad (3)$$

The next step is to expand the functional solution $I[U]$ in orders of a parameter ϵ:

$$I \equiv \sum_{k=0}^{\infty} \epsilon^k I^{(k)}. \quad (4)$$

Likewise, other functions of I such as the flux, $F(I)$, are expanded in terms of corresponding orders $F^{(k)} = F(I^{(k)})$. Terms in the functional 'transport' equation (3) are then carefully scaled by the formal parameter ϵ so that two conditions are satisfied: 1) the zero-th order of the solution becomes solvable, 2) the zero-th angular moment of the 'transport' equation (3) yields an equality for any order of ϵ. The second point must be satisfied exactly, since (3) was written from (1) via the zero-th angular moment of (1). One of the simplest examples satisfying the above two points is the scaling for isotropic diffusion theory (IDT):

$$\sigma_T \left(I - \frac{c}{4\pi} U \right) = \epsilon \frac{\delta I}{\delta U} \left[\frac{1}{c} \nabla \cdot \vec{F} + \sigma_A (U - B) \right] - \epsilon \, \vec{\Omega} \cdot \nabla I - \epsilon \frac{c}{4\pi} \sigma_A (U - B). \quad (5)$$

The final step in the CE method, is to find the zero-th order solution, $I^{(0)}[U]$, and iteratively solve to a desired order. We quickly find that the zero-th order intensity is isotropic,

$$I_0 = \frac{c}{4\pi} U, \quad (6)$$

which implies

$$\vec{F}_0 = 0, \tag{7}$$

$$\frac{\partial I_0}{\partial U} = 0, \tag{8}$$

$$\frac{\partial \vec{F}_0}{\partial U} = 0. \tag{9}$$

The leading order results can then be used to calculate the order ϵ^1 intensity:

$$I_1 = -\frac{c}{4\pi}\frac{1}{\sigma_T}\hat{\Omega}\cdot\nabla U, \tag{10}$$

which implies

$$\vec{F}_1 = -\frac{c}{3\sigma_T}\nabla U, \tag{11}$$

$$\frac{\partial I_1}{\partial U} = -\frac{c}{4\pi}\frac{1}{\sigma_T}\hat{\Omega}\cdot\nabla, \tag{12}$$

$$\frac{\partial \vec{F}_1}{\partial U} = -\frac{c}{3\sigma_T}\nabla. \tag{13}$$

In practice, the solution is truncated after only a few orders, so that the approximation is only applicable when the quantities affected by ϵ, above, are relatively small. The solution to $I[U]$ now gives a diffusion equation for U, by substituting $F(I)$ into the balance equation (2),

$$\frac{\partial U}{\partial t} - \nabla\cdot\left(\frac{c}{3\sigma_T}\nabla U\right) + c\sigma_A\left(U - B\right) = 0. \tag{14}$$

IDT RESULTS FOR DISCRETIZED TRANSPORT EQUATIONS

The CE method has been successfully applied to one set of spatially discretized slab-geometry transport equations, namely the Simple Corner Balance [2] (SCB) equations. We chose this transport method because it is known to exhibit robust behavior for optically thick, diffusive problems. We apply the Chapman-Enskog procedure to this system of equations in the way demonstrated in the previous section. The SCB transport equations are

$$\frac{\Delta x_j}{2c}\frac{\partial I_{j,L}}{\partial t} + \mu\left[\frac{I_{j,L}+I_{j,R}}{2} - I_{j-1/2}\right] + \sigma_{T,j}\frac{\Delta x_j}{2} I_{j,L} = \frac{c}{2}\frac{\Delta x_j}{2}\left(\sigma_{A,j}B_{j,L} + \sigma_{S,j}U_{j,L}\right),$$

$$\frac{\Delta x_j}{2c}\frac{\partial I_{j,R}}{\partial t} + \mu\left[I_{j+1/2} - \frac{I_{j,L}+I_{j,R}}{2}\right] + \sigma_{T,j}\frac{\Delta x_j}{2} I_{j,R} = \frac{c}{2}\frac{\Delta x_j}{2}\left(\sigma_{A,j}B_{j,R} + \sigma_{S,j}U_{j,R}\right), \tag{15}$$

with upstream closure relationships for the edge fluxes:

$$I_{j-1/2} = \begin{cases} I_{j-1,R}, & \mu > 0, \\ I_{j,L}, & \mu < 0. \end{cases} \tag{16}$$

Here the index of the spatial grid cell is j, the subscripts L and R refer to left and right half-cell averaged values, and the angular variable μ is $\mu = cos(\theta) = \hat{\Omega}\cdot\hat{e}_x$. We have left the time derivative in its analytic form, as we will eliminate it when we form the functional derivative of the intensity.

Now we form the functional derivative of I, substitute in for the time derivative of the energy density U, and scale terms in a way consistent with IDT, and expand the corner intensities $I_{j,L}$ and $I_{j,R}$ in terms of the small parameter ϵ. We find that the leading order intensity is isotropic and continuous across the cell edges:

$$I^0_{j,R} = I^0_{j+1/2} = I^0_{j+1,L}, \tag{17}$$

$$I^0(\mu, x_{j+1/2}, t) = I^0_{j+1/2} = \frac{c}{2}U_{j+1/2}(x,t). \tag{18}$$

Furthermore, U satisfies the following diffusion equation:

$$\frac{1}{c}\frac{\partial U_{j+1/2}}{\partial t} - \frac{2}{\Delta x_j + \Delta x_{j+1}}\left[\frac{U_{j+3/2}-U_{j+1/2}}{3\sigma_{T,j+1}\,\Delta x_{j+1}} - \frac{U_{j+1/2}-U_{j-1/2}}{3\sigma_{T,j}\,\Delta x_j}\right]$$

$$+\left(\frac{\sigma_{A,j}\Delta x_j + \sigma_{A,j+1}\Delta x_{j+1}}{\Delta x_j + \Delta x_{j+1}}\right) U_{j+1/2} = \frac{\sigma_{A,j}\Delta x_j B_{j,R} + \sigma_{A,j+1}\Delta x_{j+1}B_{j+1,L}}{\Delta x_j + \Delta x_{j+1}}. \tag{19}$$

This diffusion equation is consistent with previous results obtained from a traditional asymptotic analysis [2,3]. These IDT results also suggest that, using a different scaling, the CE method for spatially discretized transport may yield results for FLDT and a better (discrete) flux-limited diffusion system might be derived when starting from discretized transport equations. We will demonstrate the application of CE to derive FLDT in the next section.

CHAPMAN ENSKOG METHOD FOR FLUX LIMITING

The isotropic solution for the flux $F = -D\frac{d}{dx}U$ has a fixed diffusion coefficient D; for steep gradients $\frac{d}{dx}U$ it will have unphysically large fluxes and violate the flux inequality:

$$\tfrac{1}{c}|F| \leq U. \tag{20}$$

Flux limited diffusion theories (FLDT) obtain expressions for the flux with variable diffusion coefficients D which limit the flux to be consistent with (20). For this reason, Levermore's Chapman-Enskog FLDT starts with the following definition,

$$\tfrac{1}{c}I(x,t,\mu) \equiv U(x,t)\,\phi(x,t,\mu), \tag{21}$$

where ϕ is a normalized angular distribution,

$$\int_{-1}^{+1} \phi \, d\mu = 1. \tag{22}$$

Now the flux is guaranteed to be consistent with (20):

$$F = \int_{-1}^{+1} \mu\, I \, d\mu = U \int_{-1}^{+1} \mu\,\phi\, d\mu \equiv c\,U\,f, \tag{23}$$

where f, defined above, is the normalized flux.

The CE method can be applied to solve for ϕ as an expression in U. As in the isotropic analysis, the intensity is thought of as a functional of U:

$$I[U] \;=\; c\,U\,\phi[U]\,.$$

The functional derivative will be useful for writing derivatives of I in terms of derivatives in U. Using the product rule for differentiation, we can write:

$$\tfrac{1}{c}\left(\frac{\delta I}{\delta U}\right) = \left(\frac{\delta}{\delta U}\,U\phi\right) = \phi + U\,(\tfrac{\delta\phi}{\delta U}). \qquad (24)$$

Now we are ready to write the differential transport equation as a functional transport equation. The transport equation (1) can now be written:

$$\left(\frac{\delta I}{\delta U}\right)\left(\frac{1}{c}\frac{\partial U}{\partial t} + \mu\frac{\partial U}{\partial x}\right) + \sigma_T\, I = \tfrac{c}{2}\,(\sigma_A B + \sigma_S U)\,.$$

After the balance equation (2) is substituted and (24) is used, we get:

$$\left(\phi + U\,\tfrac{\delta\phi}{\delta U}\right)\left(\mu\tfrac{\partial}{\partial x}U - \tfrac{\partial}{\partial x}\,(U\,f) - \sigma_A(U-B)\right) + \sigma_T\,U\,\phi = \tfrac{1}{2}\,(\sigma_A B + \sigma_S U)\,.$$

After some algebra the above can be written as:

$$\begin{aligned}(\mu - f)\,\phi\,\tfrac{\partial}{\partial x}U \quad &+ \quad (\phi - \tfrac{1}{2})(\sigma_A B + \sigma_S U) \\ &= \quad U\phi\,\tfrac{\partial f}{\partial x} - U\tfrac{\delta\phi}{\partial U}\left((\mu - f)\,\tfrac{\partial U}{\partial x} + \sigma_A(B-U) - U\tfrac{\partial f}{\partial x}\right).\end{aligned}$$

Levermore defines a normalized gradient X,

$$X \equiv -\frac{\tfrac{\partial}{\partial x}U}{\sigma_T\,U}, \qquad (25)$$

and an albedo ω,

$$\omega \equiv \frac{\sigma_A B + \sigma_S U}{\sigma_T U}\ . \qquad (26)$$

The functional transport equation, above, can be written:

$$\begin{aligned}&\phi\,(f-\mu)\sigma_T X + (\phi - \tfrac{1}{2})\sigma_T\omega \\ = \quad &\tfrac{\partial f}{\partial x} - \tfrac{\delta\phi}{\delta U}\left((\mu - f)\tfrac{\partial U}{\partial x} + \sigma_A(B-U) - U\,\tfrac{\partial f}{\partial x}\right).\end{aligned}$$

It is important to notice that when the left hand side of (27) is integrated over the angular variable μ, we get zero. This allows suppression of the difficult terms on the right hand side. In terms of

$$R \equiv \frac{X}{\omega} \quad , \tag{27}$$

the functional equation above can thus be scaled:

$$\phi\,(f-\mu)R + (\phi - \tfrac{1}{2}) = \epsilon \cdot \frac{\frac{\partial f}{\partial x} - \frac{\delta\phi}{\delta U}\left((\mu - f)\frac{\partial U}{\partial x} + \sigma_A(B-U) - U\,\frac{\partial f}{\partial x}\right),}{\omega\sigma_T} \tag{28}$$

where the scaling parameter ϵ allows us to expand the solution $\phi[U]$ as a polynomial in ϵ

$$\phi \equiv \Sigma_{i=0}^{\infty}\, \epsilon^i \phi^{(i)}.$$

The scaling (28) also yields easily solvable zeroth order solutions. The order ϵ^0 terms in (28) produce the equation:

$$\phi^{(0)}\left[1 \,+\, (f^{(0)} - \mu)R\right] = \frac{1}{2}.$$

So the angular form, to zeroth order, has the following solution:

$$\phi^{(0)} = \frac{\frac{1}{2}}{1 \,+\, (f^{(0)} - \mu)R}. \tag{29}$$

The easiest way to solve for the flux $f^{(0)}$ is to use the condition that $\phi^{(0)}$, like ϕ, is normalized:

$$\int_{-1}^{+1} \phi^{(0)}\, d\mu = \int_{-1}^{+1} \frac{\frac{1}{2}\, d\mu}{1 \,+\, (f^{(0)} - \mu)R} \;=\; 1.$$

So after evaluating the integral one finds the flux:

$$f^{(0)} \;=\; \coth(R) - \frac{1}{R}. \tag{30}$$

Thus one finds the variable diffusion coefficient D in Fick's law $F = -D\frac{\partial U}{\partial x}$:

$$D = \frac{\lambda(R)}{\omega\sigma_T} \quad \text{where} \quad \lambda(R) = \frac{f^{(0)}(R)}{R} \;=\; \frac{1}{R}\left(\coth(R) - \frac{1}{R}\right). \tag{31}$$

This diffusion coefficient is bell shaped in R, peaking at the isotropic limit $1/3$ for small gradients (i.e., small R) and vanishing for large gradients (i.e., large R).

FLUX LIMITING FOR DISCRETE TRANSPORT EQUATIONS

As in our isotropic analysis we will start with the SCB transport equations. The transport equations in the left and right cells (denoted by the subscripts L and R), are given by

$$\frac{\Delta x_j}{2c}\frac{\partial I_{j,L}}{\partial t} + \mu\left[I_j - I_{j-1/2}\right] + \sigma_{Tj}\tfrac{\Delta x_j}{2} I_{j,L} = \tfrac{c}{2}\tfrac{\Delta x_j}{2}\left(\sigma_{Aj}B_{j,L} - \sigma_{Sj}U_{j,L}\right),$$
$$\frac{\Delta x_j}{2c}\frac{\partial I_{j,R}}{\partial t} + \mu\left[I_{j+1/2} - I_j\right] + \sigma_{Tj}\tfrac{\Delta x_j}{2} I_{j,R} = \tfrac{c}{2}\tfrac{\Delta x_j}{2}\left(\sigma_{Aj}B_{j,R} - \sigma_{Sj}U_{j,R}\right), \tag{32}$$

where the cell edge intensity $I_{j+1/2}$ is defined by the upstream closure relation (16), and where the cell center intensity I_j is:

$$I_j = \frac{I_{j,L} + I_{j,R}}{2}. \tag{33}$$

As in the analytic FLDT, the intensity is separated into a magnitude and an angular distribution:

$$\tfrac{1}{c} I_{j,L} = U_{j,L}\phi_{j,L} \quad \text{and} \quad \tfrac{1}{c} I_{j,R} = U_{j,R}\phi_{j,R}, \tag{34}$$

where the distributions $\phi_{j,L}$ and $\phi_{j,R}$ are normalized: $\int_{-1}^{+1} \phi \, d\mu = 1$.

The goal is to find expressions for $\phi_{j,L}$ and $\phi_{j,R}$ in terms of the energy density U. For brevity, let us demonstrate this for the right half-cell only. The time derivative $\frac{\partial I_{j,R}}{\partial t}$ is rewritten in terms of the functional derivative:

$$\frac{1}{c}\left(\frac{\delta I_{j,R}}{\delta U_{j,R}}\right) = \phi_{j,R} + U_{j,R}\,(\tfrac{\delta \phi}{\delta U})_{j,R}.$$

Thus the time derivative term is:

$$\frac{1}{c}\frac{\partial I_{j,R}}{\partial t} = \frac{1}{c}\left(\frac{\delta I}{\delta U}\right)_{j,R}\frac{\partial U_{j,R}}{\partial t} = \left(\phi_{j,R} + U_{j,R}\,(\tfrac{\delta \phi}{\delta U})_{j,R}\right)\frac{\partial U_{j,R}}{\partial t}. \tag{35}$$

To eliminate explicit time dependence in the functional differential equation, the balance equation below is $\frac{\partial U}{\partial t}$:

$$\frac{\partial}{\partial t} U_{j,R} + \frac{2}{\Delta x_j} \left(F_{j+1/2} - F_j \right) = c\sigma_{Aj} \left(B_{j,R} - U_{j,R} \right). \tag{36}$$

Applying the above steps to the transport equation (32) we now have a functional equation.

$$\begin{aligned} &\mu \left[I_{j+1/2} - I_j \right] + \sigma_{Tj} \tfrac{\Delta x_j}{2} I_{j,R} - \tfrac{c}{2} \tfrac{\Delta x_j}{2} \left(\sigma_{Aj} B_{j,R} - \sigma_{Sj} U_{j,R} \right) \\ &= \left(\phi_{j,R} + U_{j,R} \left(\tfrac{\delta \phi}{\delta U} \right)_{j,R} \right) \left(\left(F_{j+1/2} - F_j \right) + c \tfrac{\Delta x_j}{2} \sigma_{Aj} \left(U - B \right)_{j,R} . \right) \end{aligned}$$

Next we substitute our definitions (34), $\frac{1}{c} I_{j,R} = U_{j,R} \phi_{j,R}$, into the above. We can also define a normalized $\phi_{j+1/2}$ such that $\frac{1}{c} I_{j+1/2} = U_{j+1/2} \phi_{j+1/2}$ satisfies the upstream closure definition (16); and we can define a ϕ_j such that $\frac{1}{c} I_j = U_j \phi_j = \frac{I_{j,L} + I_{j,R}}{2}$, and show that ϕ_j is normalized when $\phi_{j,L}$ and $\phi_{j,R}$ are normalized. After these substitutions we write the above expression as:

$$\begin{aligned} &\mu \left[\phi_{j+1/2} U_{j+1/2} - \phi_j U_j \right] + \sigma_{Tj} \tfrac{\Delta x_j}{2} \phi_{j,R} U_{j,R} - \tfrac{1}{2} \tfrac{\Delta x_j}{2} \left(\sigma_{Aj} B_{j,R} - \sigma_{Sj} U_{j,R} \right) \\ &= \left(\phi_{j,R} + U_{j,R} \left(\tfrac{\delta \phi}{\delta U} \right)_{j,R} \right) \left(\left[f_{j+1/2} U_{j+1/2} - f_j U_j \right] + \tfrac{\Delta x_j}{2} \sigma_{Aj} \left(U - B \right)_{j,R} \right). \end{aligned} \tag{37}$$

The quantities in the square brackets above are problematic, because they involve solutions to ϕ_j and $\phi_{j+1/2}$. In order to be in a position to suppress these difficult terms we work on the quantity below:

$$\begin{aligned} &\mu \left[\phi_{j+1/2} U_{j+1/2} - \phi_j U_j \right] - \phi_{j,R} \left[f_{j+1/2} U_{j+1/2} - f_j U_j \right] \\ &= 2\mu \left(\frac{\phi_{j+1/2} - \phi_j}{2} \frac{U_{j+1/2} + U_j}{2} + \frac{\phi_{j+1/2} + \phi_j}{2} \frac{U_{j+1/2} - U_j}{2} \right) \\ &- 2\phi_{j,R} \left(\frac{f_{j+1/2} - f_j}{2} \frac{U_{j+1/2} + U_j}{2} + \frac{f_{j+1/2} + f_j}{2} \frac{U_{j+1/2} - U_j}{2} \right). \end{aligned}$$

Let us define the quantities:

$$\begin{aligned} \Delta \phi_{j,R} &= \frac{\phi_{j+1/2} + \phi_j}{2} - \phi_{j,R}, \\ \Delta f_{j,R} &= \frac{f_{j+1/2} + f_j}{2} - f_{j,R} = \int_{-1}^{+1} \mu \, \Delta \phi_{j,R} \, d\mu. \end{aligned} \tag{38}$$

With the use of these definitions and some algebra, we can write:

$$\begin{aligned}
& \mu\left[\phi_{j+1/2}U_{j+1/2}-\phi_j U_j\right]-\phi_{j,R}\left[f_{j+1/2}U_{j+1/2}-f_jU_j\right] \\
= \quad & (U_{j+1/2}-U_j)\,\phi_{j,R}\,(\mu-f_{j,R}) \\
+ \quad & (U_{j+1/2}-U_j)\,\left[\mu\,\Delta\phi_{j,R}-\phi_{j,R}\,\Delta f_{j,R}\right] \\
+ \quad & \tfrac{1}{2}(U_{j+1/2}+U_j)\left[\mu(\phi_{j+1/2}-\phi_j)-\phi_{j,R}(f_{j+1/2}-f_j)\right].
\end{aligned} \tag{39}$$

All three terms above will vanish when integrated over μ, which is what one expects as well for the left hand side. In the scaled auxiliary equation, we will suppress the last two terms; in effect we say:

$$\begin{aligned}
& \mu\left[\phi_{j+1/2}U_{j+1/2}-\phi_jU_j\right]-\phi_{j,R}\left[f_{j+1/2}U_{j+1/2}-f_jU_j\right] \\
= \quad & (U_{j+1/2}-U_j)\,\phi_{j,R}\,(\mu-f_{j,R})\,+\epsilon\cdot\Big\{\,(U_{j+1/2}-U_j)\,\left[\mu\,\Delta\phi_{j,R}-\phi_{j,R}\,\Delta f_{j,R}\right] \\
& \qquad + \;\tfrac{1}{2}(U_{j+1/2}+U_j)\left[\mu(\phi_{j+1/2}-\phi_j)-\phi_{j,R}(f_{j+1/2}-f_j)\right]\Big\}.
\end{aligned}$$

We can produce a scaled functional equation from (37) that is analagous to the analytic scaling. The only difference is that there are more terms suppressed in the discrete case; call these terms Υ.

$$\begin{aligned}
\Upsilon_{j,R} \equiv\; & U_{j,R}(\tfrac{\delta\phi}{\delta U})_{j,R}\left(\tfrac{1}{c}(F_{j+1/2}-F_j)+\tfrac{\Delta x_j}{2}\sigma_{Aj}(U-B)_{j,R}\right) \\
& -\tfrac{1}{2}\,(U_{j+1/2}+U_j)[\mu(\phi_{j+1/2}-\phi_j)-\phi_{j,R}(f_{j+1/2}-f_j)] \\
& -(U_{j+1/2}-U_j)\,[\mu\,\Delta\phi_{j,R}-\phi_{j,R}\Delta f_{j,R}].
\end{aligned} \tag{40}$$

Then the scaled functional equation is:

$$\left(\phi_{j,R}-\tfrac{1}{2}\right)(\sigma_{Sj}U_{j,R}+\sigma_{Aj}B_{j,R})+(\mu-f_{j,R})\,\phi_{j,R}(U_{j+1/2}-U_j)=\epsilon\Upsilon_{j,R}. \tag{41}$$

We define $X_{j,R}$, $\omega_{j,R}$, and $R_{j,R}$ analogous to (25), (26), and (27). Similarily, this is done for the left half-cell:

$$X_{j,R}=\frac{-(U_{j+1/2}-U_j)}{\frac{\Delta x_j}{2}\sigma_{Tj}U_{j,R}} \quad \text{and} \quad X_{j,L}=\frac{-(U_j-U_{j-1/2})}{\frac{\Delta x_j}{2}\sigma_{Tj}U_{j,L}}, \tag{42}$$

$$\omega_{j,R}=\frac{\sigma_{Sj}U_{j,R}+\sigma_{Aj}B_{j,R}}{\sigma_{Tj}U_{j,L}} \quad \text{and} \quad \omega_{j,L}=\frac{\sigma_{Sj}U_{j,L}+\sigma_{Aj}B_{j,L}}{\sigma_{Tj}U_{j,L}}, \tag{43}$$

$$R_{j,R}=\frac{X_{j,R}}{\omega_{j,R}} \quad \text{and} \quad R_{j,L}=\frac{X_{j,L}}{\omega_{j,L}}. \tag{44}$$

An R in each half-cell is an important difference between this formulation and standard discretizations of the FLDT equations.

The leading order solution is analogous to (29)

$$\phi^{(0)}_{j,R} = \frac{\frac{1}{2}}{1 + (\mu - f^{(0)})R_{j,R}}, \tag{45}$$

and has a flux:

$$\tfrac{1}{c}F^{(0)}_{j,R} = -\frac{\lambda(R_{j,R})}{\omega_{j,R}} \frac{U_{j+1/2} - U_j}{\Delta x_j/2}, \tag{46}$$

where $\lambda(R)$ is given by (31).

The cell-center flux is an average of the left and right half-cell fluxes:

$$\tfrac{1}{c}F^{(0)}_j = -\tfrac{\lambda(R_{j,L})}{\omega_{j,L}\Delta x_j} \left(U_j - U_{j-1/2}\right) - \tfrac{\lambda(R_{j,R})}{\omega_{j,R}\Delta x_j} \left(U_{j+1/2} - U_j\right). \tag{47}$$

Likewise, the center scalar intensity is the average, $U_j = \frac{U_{j,L}+U_{j,R}}{2}$, while the edge intensity $U_{j+1/2}$ is obtained by integrating $\mu I_{j+1/2}$ with the upstream closure relation (16). The flux (47) involves $U_{j+1/2}$ given below.

$$U_{j+1/2} = \frac{U_{j,L} + U_{j,R}}{2} - \frac{U_{j+1,L}\,\rho(R_{j+1,L}) - U_{j,R}\,\rho(R_{j,R})}{2} + O(\epsilon), \tag{48}$$

where $\rho(R) = \log(\cosh R)/R$.

Let us write down the balance equations for both half cells around an edge $x = x_{j+1/2}$:

$$\begin{aligned} \tfrac{\Delta x_j}{2}\frac{\partial U_{j,R}}{\partial t} + \left(F_{j+1/2} - F_j\right) + c\sigma_{Aj}\tfrac{\Delta x_j}{2}(U_{j,R} - B_{j,R}) &= 0, \\ \tfrac{\Delta x_{j+1}}{2}\frac{\partial U_{j+1,L}}{\partial t} + \left(F_{j+1} - F_{j+1/2}\right) + c\sigma_{Aj+1}\tfrac{\Delta x_{j+1}}{2}(U_{j+1,L} - B_{j+1,L}) &= 0. \end{aligned} \tag{49}$$

The flux F_j above is taken to be the leading order expression, i.e., $O(\epsilon^0)$, for the flux given by (47). When the above diffusion equations are added together, we can obtain a diffusion equation in terms of the average edge quantities $\frac{1}{2}(U_{j+1,L} + U_{j,R})$ and edge discontinuities $(U_{j+1,L} - U_{j,R})$. The dependence on the discontinuities can not be removed; thus, the number of unknowns per cell is twice the unknowns found for the IDT equations. This is the primary result of our Chapman Enskog analysis. These discontinuous FLDT equations are more difficult to solve, in general. We are interested in relating these equations to typical FLDT formulations, and in finding a solution technique.

We are currently working on a method to handle these additional unknowns. Currently we are pursuing the following solution strategy:

- Assume that the discontinuities in the energy density are zero;
- Solve the three point *continuous* discretized diffusion equations;
- Now, write the *discontinuous* discretized diffusion equations and solve for the two energy densities around each edge ($U_{j,R}$ and $U_{j+1,L}$) using data from the continuous solve for all other data;
- Iterate this process to convergence.

We are just beginning this work and have no numerical results for this technique at this time.

CONCLUSION

Chapman-Enskog theory can be successfully applied to discrete transport equations to directly yield discrete diffusion equations. This method has been applied for IDT scaling, as well as FLDT scaling. For IDT we find that the edge values of the scalar intensity U are continuous. The edge centered diffusion equation for IDT becomes a three-point difference equation for U. In contrast, for FLDT we find the edge values are, in general, discontinuous. If we assume these discontinuities to be zero, the FLDT results would also reduce to an equation with a three point edge-centered stencil. Finding a method to solve for these discontinuities could improve numerical results of Levermore's FLDT. The diffusion solution should also reflect characteristics of the underlying (in our case, SCB) discretized transport equations. We are currently working on finding and testing a numerical FLDT method that involves the discontinuities suggested from the CE analysis.

References

1. C. D. Levermore, "A Chapman-Enskog Approach to Flux-Limited Diffusion Theory", Lawrence Livermore Laboratory, *document:* UCID-18229, July 1979.

2. M.L. Adams "A New Transport Discretization Scheme for Arbitrary Spatial Meshes in XY Geometry," *Proceedings of the International Topical Meeting of the American Nuclear Society–Advances in Mathematics, Computations and Reactor Physics*, **3**, 13.2 2-1 to 13.2 2-9, Pittsburg, PA, 1991.

3. E.W. Larsen and J.E. Morel, "Asymptotic Solutions of Numerical Transport Problems in Optically Thick, Diffusive Regimes II," *J. Comput. Phys.*, **83**, 212 (1989); see also "Corrigendum," *J. Comput. Phys.*, **91**, 249, (1990).

4. R.H. Szilard and G.C. Pomraning, "Numerical Transport and Diffusion Methods in Radiative Transfer," *Nucl. Sci. Eng.*, **112**, 256, (1992).