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Todd S. Palmer

Spatially discretized diffusion approximation equations are derived directly from spatially discretized radiation transport equations in 1-D slab geometry. Derivations for isotropic diffusion theory (IDT) and Levermore-Pomraning's flux-limited diffusion theory (FLDT) are applied to lumped linear discontinuous (LLD) transport equations. We find that the (energy density) solution is continuous across the edge for IDT. For FLDT, we find that the intensity may be discontinuous across a cell edge; this doubles the number of points that traditionally need to be solved for in a diffusion approximation. The FLDT derivation produces unique discretized flux-limited diffusion equations. We produced a numerical scheme for these FLDT equations that includes a new iteration on the flux-limiting parameter and a local iteration on the edge discontinuities. Numerical results indicate that this approach is an improvement over standard numerical FLDT discretization schemes.

Flux-Limited Diffusion Theory for Spatially Discretized Equations: A Discretized Derivation of Levermore-Pomraning FLDT

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1. INTRODUCTION

1.1. Photon transport and its applications

The photon transport equation describes the flow of radiative energy carried by photons. The solution of the equation is the intensity as a function of position, time, direction (or angle), and the photon frequency. Intensity is the power per unit area, which is proportional to the number of photons flowing through the unit area. These photons flow through and interact with the matter, which may emit, scatter, and absorb photons. Material properties determine these interactions: the temperature determines the rate of blackbody emission, and optical opacities give the probability of scattering or absorption per unit length.

Radiative transfer problems can be numerically solved in the following three ways. One can solve discretized transport equations directly. Secondly, since the interactions of photons are probabilistic, the Monte-Carlo method can be used to simulate the photons. Lastly, one can also solve diffusion approximations to the transport problem; these approximations are usually obtained by assuming an approximate angular distribution for the intensity. Since the angular information is not computed in these approximations, the computational and storage requirements can be reduced greatly. Much numerical computation is usually required when solving problems with the Monte-Carlo method, which needs many samples to obtain good accuracy; these computations can be parallelized greatly, yet they currently

still take a long time to run while requiring large clusters of computers. Diffusion approximations can usually provide the quickest way of computing radiative transfer problems. Flux-limited diffusion theories (FLDT) provide improvements on earlier diffusion approximations and can thus make the diffusion approximation successfully applicable to more problems.

To convince the reader of the importance of photon transport problems and their numerical evaluation, let us give some examples of such applications. For instance, the pulse oximeter is a small medical device that clips on to a persons finger or earlobe and measures the level of oxygen saturation of the blood. A diode emits light into the finger, a sensor measures the light that is scattered back out, and the device computes the oxygen content of the blood and the heart pulse rate. In order to design such a device, it is necessary to understand how the light absorbs and scatters in living tissue.

Radiative transfer is most important in the field of nuclear engineering. A good example of a nuclear engineering application of is the ignition of the deuterium target for the inertial confinement fusion (ICF) project. The goal is to synchronize a number of radiation wave fronts to form single very radially symmetric wave front of radiation which converges on a cryogenic target of heavy hydrogen; hopefully, this spherical wave front will deliver energy evenly to the shell of the target, so that the outer layer of the small, cold, round target is heated rapidly, expands evenly, and implodes the core by creating a tremendous pressure. To achieve this pressure, the radiation must hit the target with very precise radial symmetry. In this example the wave fronts arrive at a very precise short time; i.e., the wave fronts are very sharp in space and time (imagine a wave front like a step function). On the other hand, simple diffusion approximations such as IDT would predict much smoother wave fronts.

Diffusion approximations suffer from a leakage of photons ahead of the actual wave front and will predict an early arrival of a significant number of photons. In fact, near a sharp wave front, where the spatial gradient is very steep, the IDT

approximation overestimates the flux to such an extent that the conservation of particles is violated. Successful FLDT approximations fix this unphysical condition, yet they will still predict some leakage ahead of the actual wave front; the significance of the effect of this 'leakage' of photons on the deuterium target would determine whether the FLDT approximation is valid and applicable. The ICF example also shows that it can be very important for the diffusion equations to approximate well in regions of steep gradients, so that wave fronts may accurately maintain their steep shape as the solution evolves in time.

Problems involving radiative transfer are also common in astrophysics, and FLDT diffusion approximations can often be used to help simulate events in the lifetime of stars. When a star implodes, either through a gravitational collapse or by an unusual pressure caused by fusion reactions in the outer shell of star, a tremendous amount of energy is produced in the core. Almost all of the energy released in a supernova is carried off by neutrinos, a massless (or near massless) fermion that interacts with matter very weakly. In contrast, it is very difficult for photons to escape the very dense, optically impenetrable star. The amount of energy released in neutrinos in such an event, called a supernova, is on the order of one tenth the solar mass of the inner part of the star, or on the order of a thousand times the amount of visible light that the star has emitted over its lifetime. FLDT radiation transport approximations have been used to model the neutrino transport in supernova.

1.2. A review of the FLDT effort

In this section we review the various diffusion theories for radiative transfer and the effort to improve these photon transport approximations with flux-limiters.

Isotropic Diffusion Theory (IDT) provides the simplest approximation to photon transport. The theory approximates photon transport in the limit of no angular (directional) dependence in the intensity. The assumption for such an isotropic

angular distribution becomes valid when working with relaxed solutions for the photon intensity in optically thick, isotropically scattering material. IDT provides the quickest way to approximate the solution. The fixed diffusion coefficient $D = 1/3$ is independent in the solution U and the flux is the linear expression: $F = -\frac{D}{\sigma}\nabla U$. The most serious problem with the approximation is for large gradients in the photon energy density U; in this case, the flux is overestimated, and the diffusion equation can then make the unphysical statement that the photons are streaming in the direction of the flux at a rate faster than all the photons inside a differential volume could possibly exit.

Near regions of large gradients, such as near a sharp wave front, an unrealistic amount of photons leaks ahead, and the poorly approximated solution for the energy density quickly looses its realistic sharp shape. To more accurately express the flux near large gradients in U, variable diffusion coefficients are needed. These variable diffusion coefficients, or "flux-limiters" are generally functions of the solution U and its gradients. Unlike IDT these variable coefficients lead to nonlinear diffusion equations.

Asymptotic diffusion theory (ADT) is a nonlinear diffusion approximation with a variable diffusion coefficient which only depends on the albedo (the ratio of in-going to out-going radiation). ADT can also violate the flux inequality for large gradients. One of the first flux limiters is the Winslow flux limiter which improves ADT [1]. Winslow cites unpublished work of Wilson, from 1964, for the idea of flux-limiting.

Other earlier flux-limiters are by Wilson, the simplest of which takes the form $D = \frac{1}{\omega(3+|R|)}$ where R is a unitless 'normalized' gradient of the solution, which we will here refer to as the flux limiting parameter. In the limit of large gradients (or R) the coefficient correctly vanishes.

Pomraning [5] compares many flux-limiter and notes that although the early flux-limiters above are valid for both isotropic (flat angular intensity distribution) and streaming (angular distribution which is completely polarized in the direction

of the gradient) limits, they can still show strange qualitative behavior, or violate an inequality relating the Eddington factor with the flux. (The Eddington factor is the second moment of the angular intensity distribution, which, in slab geometry, is equivalent to the normalized radiation pressure.) For example, the Eddington factor, or (normalized) radiation pressure p, is expected to be a monotonically increasing function of the (normalized) flux f. However, some flux limiters (Wilson Sum and Wilson Fit flux-limiters) predict a radiation pressure p that is not a monotonic function of f; one can conjecture that the flux f is underestimated around such 'dips' in $p(f)$. In contrast, the Wilson Max flux-limiter allows an unphysical and excessive radiation pressure $p(f) = 1/3 + f^2 > 1$. Since $p(f)$ is higher than is reasonable, one can conjecture that the flux is overestimated in regions where $p(f) > 1$. The Winslow flux-limiter also has a larger than allowable Eddington factor, which is a sign of an overestimated flux, or too little flux-limiting.

In comparing flux-limiters, Pomraning finds five flux-limiters with satisfying qualitative behavior. These flux-limiters share two common traits. Firstly, most of these flux-limiters were derived from mathematical or sound physical reasoning, instead of being produced *ad hoc* to fit the streaming and isotropic limits. They also share the same form:

$$D = \frac{\lambda(R)}{\omega}$$

where ω is the albedo and R is the unitless gradient, or flux-limiting parameter.

Let us review these five successful flux-limiter. Kershaw[1] looked at the inequalities that the higher moments of the intensity must satisfy and suggested a somewhat *ad hoc* Eddington factor that would fit these inequalities [6]. In evaluating flux-limiters, Pomraning [5] was testing very similar or equivalent conditions as Kershaw's inequalities, and not surprisingly, found that Kershaw's flux-limiter had all the desired qualities.

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[1]D.S. Kershaw, "Flux Limiting Nature's Own way", Lawrence Livermore National Laboratory, Livermore, CA, UCRL-78378, (1976)

The other four flux-limiters are derived by Levermore and Minerbo, who each give one physically motivated flux-limiter, and one derived more from mathematical reasons. Minerbo's Maximum Entropy flux-limiter is derived by computing the most likely angular distribution of the intensity by using statistical mechanics.[2] Levermore's uses relativistic physics to derive his Levermore-Lorentz flux-limiter. In the case of an isotropic intensity the radiation pressure (or Eddington factor) is given by $p = 1/3$. In a frame moving at the speed βc the radiation pressure can be found as a function of β (see [6] for details). Likewise, the flux can also be found as a function of β so that $p(f)$ is found, and the flux-limiter is found (see [5] for details).

Levermore also obtained a flux-limiter by applying the Chapman-Enskog (CE) method. The CE method is a mathematical method originally used by CE for work in statistical physics. This method will later be discussed in detail since we choose to use Levermore's CE derivation applied to spatially discretized transport equations.

FLDT diffusion equations are generally meant for numerical evaluation. This means that the analytic FLDT equations produced by the above flux-limiters need to be discretized. How are the discrete quantities such as the diffusion coefficient D and the flux-limiting parameter R to be constructed; and where are the gradients of the solution defined? Usually these quantities are constructed *ad hoc* and can lead to problems unless these quantities are defined with care. Szilard and Pomraning mention the problem of radiation trapping under certain thermal settings and suggest some (*ad hoc*) choices of R that allow the radiation to more realistically penetrate the cold slab. Other problems are choices of iteration on the nonlinear FLDT equations which can fail to converge or produce unphysical shocks or oscillations in the solution; averaging the radiation pressure p can help reduce such oscillations [9]. The reason that such fixes are required is that the discretization of FLDT equations

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[2]G. N. Minerbo, JQSRT, 20, 541 (1978)

is unclear and may remain an *ad hoc* process until some sound methods are found to produce discrete FLDT equations from analytic ones. This is the motivating reason for our work to obtain discretized FLDT equations directly from discretized transport equations.

1.3. Outline

The goal of this work is to investigate whether it is advantageous to derive discrete diffusion equations directly from discrete transport equations. We pick a discrete transport scheme that displays robust and stable behavior, and will derive a corresponding discrete diffusion approximation. The robustness of the scheme means that the solution does not assume unphysical negative intensities and is free of large unphysical oscillations. We pick simple corner balance (SCB) transport equations, which, in 1-D slab geometry, are equivalent to lumped linear discontinuous (LLD) equations. We would like to see that the robust and stable properties of the LLD transport scheme will be preserved in the derived diffusion approximation.

The next two chapters (2. and 3.) will give some background theory to the reader. In the second chapter we present the analytic transport equation (for grey,[3] elastic, isotropic scattering), the analytic diffusion equations, and the flux and Eddington factor inequalities that flux-limiters should satisfy. The third chapter will show how Levermore applied the Chapman-Enskog method to obtain Isotropic and flux-limited diffusion theories.

Chapters 4. and 5. present the new theoretical work obtained by applying the CE method to the discretized transport equations for the case of IDT and FLDT, respectively. For the IDT case we find that the edge energy density is continuous at the edges and we obtain a diffusion equation that is consistent with other stable IDT

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[3]'Grey' refers to working with photons of a single frequency.

discretizations. For the case of FLDT we find that the energy density is generally not continuous at the edges.

The fifth chapter should be read as two parts. The first part is the CE derivation with its FLDT results. These preliminary results hide some meaning until they are coded up. The results must be used for a code that is implicit in the time step iteration, as well as implicit in the iteration of the flux-limiting parameter. When stiff terms are treated explicitly the iteration will not converge[4]; however, when these terms are treated implicitly they can contribute to the stability of the iteration. The the preliminary results from Chapter 5.'s Chapman-Enskog derivation we interpret these terms to provide stable iterations for the discontinuous FLDT equations. This interpretation includes a local iteration for the discontinuities of the solution at the edges, and to a new iteration on the flux-limiting parameter R based on the relation of R at the edges.

The sixth chapter shows the results of a numerical test of our FLDT. We apply the benchmark provided Su and Olson [8] which gives exact analytical transport solutions. The benchmark involves a source which is suddenly turned on and creates wave that moves outward, and thermal coupling to material of constant (in temperature) optical opacities. We compare the discontinuous FLDT diffusion equations with the traditional FLDT interpretation where continuity is forced at the edges.

In our final chapter, we draw conclusions from this research and describe areas for future work.

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[4]See a numerical textbook, for example: A. Iserles, *A First Course in the Numerical Analysis of Differential Equations*, Cambridge University Press (1996).

2. PHOTON TRANSPORT

2.1. The transport problem

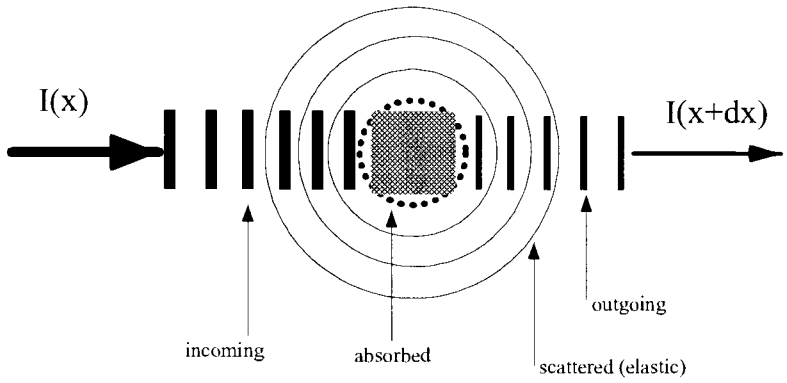

FIGURE 2.1. A depiction of the scattering terms: Isotropic elastic scattering is represented by the thin circular wavefronts. Absorption and reemission is also isotropic; the absorption is depicted by the thick dotted circle. The spatial change in the intensity is depicted by the difference in incoming and outgoing intensity. (Imagine a potato in a microwave oven.)

The intensity of light can be thought of as a function of space and angle. Photons vary in frequencies (energy), but let us think of photons of one energy group $h\nu$ solely, and describe their intensity by $I(\vec{x}, \vec{\Omega}, t)$. This quantity[1] describes how many photons are located at $\vec{x}$, with momentum $\frac{h\nu}{c}\vec{\Omega}$. The transport equation is an equation describing the conservation of these photons traveling through matter. For simplicity we only consider matter where the elastic scattering has no dependence on angle (isotropic); the elastic scattering is then described by $\sigma_S(\vec{x}, t)$. Since we are only dealing with one energy group, inelastic scattering counts as absorption, and is denoted by σ_A; if desired, re-emission into our energy group could be thrown into the blackbody source term $\sigma_A\, B$.

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[1]More exactly the quantity $\frac{I(\vec{x},\vec{\Omega},t)}{h\nu}$.

The conservation of photons is described by the radiation transport equation:

$$\frac{1}{c}\frac{\partial}{\partial t} I + \vec{\Omega} \cdot \nabla I + \sigma_T I = \frac{c}{4\pi} (\sigma_A B + \sigma_S U) \tag{2.1}$$

where $\sigma_T = \sigma_S + \sigma_A$, and the energy density U is:

$$U \equiv \frac{1}{c} \int_{4\pi} I \, d\vec{\Omega} \tag{2.2}$$

The transport equation (2.1) states that the time rate of change of the intensity plus the spatial change in intensity is equal to emissions from a source, plus isotropic outgoing scattering, minus photons lost due to absorption or (in-going) scattering. A drawing describing these terms is shown in Fig-2.1.

The equation for energy balance is obtained by integrating the transport equation (2.1) over all angles, and using the definition (2.2).

$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{F} = c\sigma_A(B - U) \tag{2.3}$$

where the flux $\vec{F}$ is defined:

$$\vec{F} \equiv \int_{4\pi} \vec{\Omega} \, I \, d\vec{\Omega} \tag{2.4}$$

One can already note that *if* the flux could be approximated well by a Fick's law $\frac{1}{c}\vec{F} = -\frac{D}{\sigma}\nabla U$, which states the flux is proportional to the gradient in concentration, then the balance equation is a diffusion equation. For 'thick' transport problems where there is much scattering, good approximations are possible. The goal when replacing the transport equation by the diffusion equation is to come up with a good physically consistent approximation of the flux, using a diffusion coefficient $D[U]$ that is an expression in $U(\vec{x})$ rather than $I(\vec{x}, \vec{\Omega})$.

2.2. Slab geometry transport equation

Our work deals with the transport equation in slab geometry. Imagine the transport equation in a two (or three) dimensional space, where the intensity field is only a function of one coordinate, say x: $I(x, y, z; \theta; t) = I(x; \theta; t)$. The angle θ

is the angle formed between the x-axis and the direction of photon and ranges from 0 to π; it is standard to use the direction cosine $\mu \equiv \cos\theta$ rather than the angle. The intensity field in slab geometry is written:

$$I(x, \mu, t) \quad \text{where} \quad -1 \leq \mu \leq +1$$

The photon transport equation in slab geometry is:

$$\frac{1}{c}\frac{\partial}{\partial t}I + \mu\frac{\partial}{\partial x}I + \sigma_T I = \frac{c}{2}(\sigma_A B + \sigma_S U) \tag{2.5}$$

The above is integrated over the angular variable μ to obtain the energy balance equation:

$$\frac{\partial}{\partial t}U + \frac{\partial}{\partial x}F = c\sigma_A(B - U) \tag{2.6}$$

where the flux is the first angular moment of I: $F = \int_{-1}^{+1} \mu I \, d\mu$.

The first moment of (2.5) gives a momentum balance equation:

$$\frac{1}{c}\frac{\partial}{\partial t}F + \frac{\partial}{\partial x}P + \sigma_T F = 0 \tag{2.7}$$

where the second moment of I is called the pressure P, which is defined as

$$P = \int_{-1}^{+1} \mu^2 I \, d\mu .$$

In three dimensions P becomes the pressure tensor, which can be approximated in terms of the Eddington factor, which is equivalent to $p = \frac{P}{cU}$.[2]

2.3. Diffusion approximations

One can show that the momentum balance equation can approximately give us a Fick's law $\frac{1}{c}\vec{F} = -\frac{D}{\sigma}\nabla U$. One starts out with the assumption that the flux F and pressure P can be written as

$$F = cf\,U \quad \text{and} \quad P = cp\,U$$

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[2]See Pomraning [3] for the Eddington approximation.

where f and p vary much more slowly in time and space than U, so that:

$$\frac{\partial}{\partial t}F \cong cf\frac{\partial U}{\partial t} \quad \text{and} \quad \frac{\partial}{\partial x}P \cong cp\frac{\partial U}{\partial x}$$

Using the above approximations with the balance equation (2.6), we can write the momentum balance equation (2.7) as:

$$\frac{1}{c}f\left[c\sigma_A(B-U) - cf\frac{\partial U}{\partial x}\right] + cp\frac{\partial U}{\partial x} + cf\sigma_T U \cong 0$$

$$f(\sigma_A B + \sigma_S U)) + \frac{\partial U}{\partial x}\left(p - f^2\right) \cong 0$$

We can define a normalized gradient $X \equiv \frac{-\frac{\partial U}{\partial x}}{\sigma_T U}$ and an albedo $\omega \equiv \frac{\sigma_A B + \sigma_S U}{\sigma_T U}$. Let us divide the above equation to get:

$$\omega f \cong X(p - f^2)$$

So the flux is:

$$F = Uf \cong \frac{XU}{\omega}(p - f^2) = -\frac{p - f^2}{\sigma_T \omega}\frac{\partial U}{\partial x} \equiv -\frac{D}{\sigma_T}\frac{\partial U}{\partial x} \tag{2.8}$$

As we limit to an isotropic solution, say $I = \frac{cU}{2}(1 + \mu\epsilon)$ as $\epsilon \to 0$, we have:

$$p = \int_{-1}^{+1} \frac{1 + \mu\epsilon}{2}\mu^2 d\mu = \frac{1}{3}$$

and,

$$f^2 = \left[\int_{-1}^{+1} \mu\frac{1 + \mu\epsilon}{2}\,d\mu\right]^2 = O(\epsilon^2)\,.$$

Therefore, in the isotropic limit the diffusion coefficient becomes:

$$D = \frac{1}{3}\frac{1}{\omega}$$

A streaming solution has all the intensity flowing at the same angle; i.e., the intensity has the form $I = cU\delta(\mu - \mu_0)$. In this case:

$$p = \int_{-1}^{+1} \mu^2\delta(\mu - \mu_0)\,d\mu = {\mu_0}^2$$

and,

$$f^2 = \left[\int_{-1}^{+1} \mu\delta(\mu - \mu_0)\,d\mu\right]^2 = {\mu_0}^2\,.$$

So the approximation (2.8) expects the diffusion coefficient to shrink near streaming regions, i.e., $D(x,t) \approx 0$ near streaming regions. Local approximations for the flux that only depend on values and derivatives of $U(x,t)$, rather than the actual intensity $I(\mu,x,t)$ will of course not always accurately represent the intensity. All well-known local approximations assume a family of angular forms of I, such that the second moment of the angular form ranges from the isotropic limit of $p = \frac{1}{3}$ to the extreme ($\mu_0 = \pm 1$) streaming limit of $p = 1$. Thus we have an example of how all local approximations inaccurately represent transport problems which have regions where $p < \frac{1}{3}$. To determine the suitability of the diffusion approximation to the transport problem we must compare how closely the first two angular moments of the true intensity $I(\mu,x,t)$ match those moments of the approximated intensity. In the section on flux limiters we present some of these approximations.

2.4. Flux problem

Fick's law defines the flux in terms of a variable diffusion coefficient D:

$$\frac{1}{c}F = -\frac{D}{\sigma_T}\frac{\partial U}{\partial x}$$

Since the intensity I is always a positive number, the magnitude of the flux must never exceed the energy density cU:

$$F \leq cU$$

The above conclusion is clear when one compares the integrands below:

$$|f| = \left|\frac{F}{cU}\right| = \left|\frac{\int_{-1}^{+1} \mu I d\mu}{\int_{-1}^{+1} I d\mu}\right| \leq 1$$

In other words:

$$|f| = |D\,X| \leq 1$$

where the normalized gradient X is defined as:

$$-\frac{1}{\sigma_T U}\frac{\partial U}{\partial x}$$

We recall from the previous section that in the isotropic limit an approximation for the flux was given from (2.8) which yielded the diffusion coefficient:

$$D = \frac{1}{3\omega} \quad \text{with } \omega \equiv \frac{\sigma_A B + \sigma_S U}{\sigma_T U}$$

Clearly there may be large enough gradients X such that:

$$|X| \leq \frac{1}{D} = 3\omega$$

is violated.

So the isotropic approximation produces unphysical behavior for large gradients in the solution.

2.5. Flux-limiters

A flux-limiter is an expression for the diffusion coefficient such that the flux inequality above is not violated.[3] Flux limiters should obey certain physical inequalities:

$$f^2 \leq p \leq 1 \quad \text{where } p \equiv \frac{\int_{-1}^{+1} \mu^2 I \, d\mu}{\int_{-1}^{+1} I \, d\mu}$$

and interpolate correctly between the isotropic limit with $p(f = 0, \omega) = \frac{1}{3}$ and streaming limit with $p(f = 1, \omega) = 1$. Pomraning [5] analyses a collection of thirteen flux limiters, five of which are found to be qualitatively correct. All[4] five correct flux limiters[5] are based on theory, while the rest were often simply unsuccessful *ad hoc* functions $D(f, \omega)$. All five of these flux limiters can be written as:

$$D = \frac{\lambda(R)}{\omega}$$

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[3]Or such that the flux inequality is violated 'less' than in IDT.

[4]One can argue that Kershaw's limiter does not entirely follow from theory, since he picked an *ad hoc* limiter to fit his theoretically derived conditions.

[5]1. Levermore (CE), 2. Kershaw, 3. Levermore (Lorentz), 4. Minerbo (Statistical), and 5. Minerbo (Linear).

Because of the similarity of these flux limiters, results for our analysis of Levermore CE flux limiter could also be applied to other successful flux limiters.

3. CHAPMAN-ENSKOG METHOD (CE)

This chapter reviews how Chapman-Enskog (CE) method can be used to approximate an analytic transport equation by an analytic diffusion equation, as is shown by Levermore [3]. This method can be used to derive IDT and Levermore's FLDT; we review these derivations in the following two sections. The reader should refer back to this chapter when reading the discrete derivations in Chapters 4. and 5., since the basic steps in the discrete and the analytical derivations are very similar.

The CE Method 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.

Let us begin with the CE derivation to obtain IDT.

3.1. Isotropic Diffusion Theory (IDT)

We begin with the analytic radiation transport equation:

$$\tfrac{1}{c}\tfrac{\partial}{\partial t} I + \hat{\Omega}\cdot\nabla I + \sigma_T I = \tfrac{c}{4\pi}\left(\sigma_A B + \sigma_S U\right), \tag{3.1}$$

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

$$\tfrac{\partial}{\partial t} U + \nabla\cdot\vec{F} + c\sigma_A(U-B) = 0, \tag{3.2}$$

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 (3.2):

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

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 (3.1) as a functional differential equation by substituting the above time derivative into (3.1). After some manipulation the transport equation may be written:

$$\sigma_T \left(I - \tfrac{c}{4\pi} U\right) = \tfrac{\delta I}{\delta U} \left[\tfrac{1}{c} \nabla \cdot \vec{F} + \sigma_A (U - B)\right] - \hat{\Omega} \cdot \nabla I - \tfrac{c}{4\pi} \sigma_A (U - B). \tag{3.3}$$

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

$$I \equiv \sum_{k=0}^{\infty} \epsilon^k I^{(k)}. \tag{3.4}$$

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 (3.3) 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 (3.3) yields an equality for any order of ϵ. The second point must be satisfied exactly, since (3.3) was written from (3.1) via the zero-th angular moment of (3.1). One of the simplest examples satisfying the above two points is the scaling for isotropic diffusion theory (IDT):

$$\sigma_T \left(I - \tfrac{c}{4\pi} U\right) = \epsilon \tfrac{\delta I}{\delta U} \left[\tfrac{1}{c} \nabla \cdot \vec{F} + \sigma_A (U - B)\right] - \epsilon \vec{\Omega} \cdot \nabla I - \epsilon \tfrac{c}{4\pi} \sigma_A (U - B). \tag{3.5}$$

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,

$$I_0 = \tfrac{c}{4\pi} U, \tag{3.6}$$

which implies

$$\vec{F}_0 = 0, \tag{3.7}$$

$$\tfrac{\partial I_0}{\partial U} = 0, \tag{3.8}$$

$$\frac{\partial \vec{F}_0}{\partial U} = 0. \tag{3.9}$$

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

$$I_1 = -\frac{c}{4\pi}\frac{1}{\sigma_T}\hat{\Omega}\cdot\nabla U, \tag{3.10}$$

which implies

$$\vec{F}_1 = -\frac{c}{3\sigma_T}\nabla U, \tag{3.11}$$

$$\frac{\partial I_1}{\partial U} = -\frac{c}{4\pi}\frac{1}{\sigma_T}\hat{\Omega}\cdot\nabla, \tag{3.12}$$

$$\frac{\partial \vec{F}_1}{\partial U} = -\frac{c}{3\sigma_T}\nabla. \tag{3.13}$$

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 (3.2),

$$\frac{\partial U}{\partial t} - \nabla\cdot\left(\frac{c}{3\sigma_T}\nabla U\right) + c\sigma_A\left(U - B\right) = 0. \tag{3.14}$$

3.2. Flux-Limited Diffusion Theory (FLDT)

Let us first give a description of flux limiting before we give a derivation of the FLDT equations. The term "flux limiting" refers to correcting a discrepancy between the flow (flux) out of a volume and the conservation of particles in that volume.

Let us consider an example first. In slab geometry the flow along the x-axis, at x, through a unit area cross section is

$$F(x) = \int_{-1}^{+1} \mu I(x,\mu)\, d\mu \quad \text{with} \quad I \geq 0 \quad \text{and} \quad -1 \leq \mu = \cos(\theta) \leq +1\ .$$

Thus clearly the flux should never exceed the scalar intensity:

$$U(x) = \frac{1}{c}\int_{-1}^{+1} I(x,\mu)\,d\mu \;\geq\; \tfrac{1}{c}\,|F| \quad .$$

However, expressions for the flux F are not exact; for example, consider the leading order flux from the isotropic diffusion theory; $F^{(1)} = \frac{-c}{3\sigma_T}\frac{dU}{dx}$. Thus, apparently the inequality

$$\tfrac{1}{c}\,|F| \leq U \tag{3.15}$$

may clearly be violated for large gradients in U in leading order isotropic diffusion theory. A flux limited solution will avoid such an unphysical behavior.

Let us now describe how Levermore's FLDT theory is set up. As in isotropic diffusion theory, the Chapman-Enskog (CE) method is used; the only difference is that the 'functional' transport equation (an equation derived by combining the transport equation with the balance equation[1]) is scaled differently. Levermore's scaling is set up so that the flux inequality (3.15) is inherently never violated.

For the purpose of flux limiting we separate $I(x,\mu)$ into a scalar function and a function that contains the 'form' of the angular distribution:

$$\frac{1}{c}I(x,\mu) \equiv U(x)\,\phi(x,\mu) \tag{3.16}$$

where ϕ is normalized over the angles,

$$1 \;=\; \int_{-1}^{1} \phi\,d\mu \tag{3.17}$$

and where $U(x)$ is the scalar intensity:

$$U(x) = \tfrac{1}{c}\int_{-1}^{1} I\,d\mu \tag{3.18}$$

The normalized flux is defined as:

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[1]The balance equation is the zeroth angular moment of the transport equation

$$f = \int_{-1}^{1} \mu\phi \, d\mu \tag{3.19}$$

or in terms of the flux, as:

$$\frac{1}{c}F = U\, f \tag{3.20}$$

The starting point is the analytic transport equation for one-dimensional slab geometry:

$$\frac{1}{c}\frac{\partial}{\partial t}I + \mu\frac{\partial}{\partial x}I + \sigma_T I = \frac{c}{2}\left(\sigma_A B + \sigma_S U\right) \tag{3.21}$$

When integrated over the angular variable, the above yields the balance equation:

$$\frac{\partial}{\partial t}U + \frac{\partial}{\partial x}F + c\sigma_A\left(U - B\right) = 0 \tag{3.22}$$

where F is the first angular moment of I, the energy density (scalar intensity) is $U = \frac{1}{c}\int_{-1}^{+1} I d\mu$, and $\sigma_T = \sigma_A + \sigma_S$.

The intensity is now thought of as a functional of energy density:

$$I\left[U(x,t)\right] = U\,\phi[U]$$

Using the product rule for differentiation, the functional derivative $\left(\frac{\delta I}{\delta U}\right)$ can be written as:

$$\frac{1}{c}\left(\frac{\delta I}{\delta U}\right) = \left(\frac{\delta}{\delta U}U\,\phi\right) = \left(\frac{\delta U}{\delta U}\right)\phi + U\left(\frac{\delta\phi}{\delta U}\right) = \phi + U\left(\frac{\delta\phi}{\delta U}\right) \tag{3.23}$$

The above linear operator is useful for rewriting derivatives of I in terms of derivatives in U:

$$\frac{\partial}{\partial t}I = \left(\frac{\delta I}{\delta U}\right)\frac{\partial U}{\partial t} = c\left(\phi + U\left(\frac{\delta\phi}{\delta U}\right)\right)\frac{\partial U}{\partial t}$$

Now, substituting the balance equation (3.22) for $\frac{\partial U}{\partial t}$ above, and inserting this into the transport equation (3.21) eliminates the time dependence; written in the notation of (3.16) we have:

$$\begin{aligned} -\tfrac{1}{c^2}\frac{\partial I}{\partial t} = \tfrac{1}{c}\left(\frac{\delta I}{\delta U}\right)\left(-\tfrac{1}{c}\frac{\partial U}{\partial t}\right) &= \left(\phi + U\left(\frac{\delta\phi}{\delta U}\right)\right)\left[\sigma_A(U - B) + \frac{\partial}{\partial x}(f\,U)\right] \\ &= \mu\frac{\partial}{\partial x}(\phi\,U) - \tfrac{1}{2}\left(\sigma_A\,B + \sigma_S\,U\right) + \sigma_T(\phi\,U) \end{aligned}$$

Let us rearrange some terms:

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

Let us rearrange terms again, putting the difficult derivative terms to the left hand side:

$$\phi\frac{\partial f}{\partial x}\,U + U\left(\frac{\delta\phi}{\delta U}\right)\left[\sigma_A(U-B) + \frac{\partial}{\partial x}(f\,U)\right] - \mu\frac{\partial\phi}{\partial x}\,U$$
$$= -\tfrac{1}{2}\left(\sigma_S U + \sigma_A B\right) + \left(\left(\sigma_S\,U + \sigma_A B\right) + \left(\mu - f\right)\frac{\partial}{\partial x}\,U\right)\,\phi \qquad (3.24)$$

The above equation is the transport equation written as a functional differential equation. It contains an operator $\left(\frac{\delta\phi}{\delta U}\right)$ called a "functional derivative" which acts on the square-bracketed quantity. The terms on the right hand side make this a difficult equation to solve. However, suppose that these terms turned out to be numerically very small; then an approximate solution would be easy. This is the idea of the procedure that follows. We will scale the right hand side by a variable ϵ, as is shown below in equation (3.26). We can solve the problem (3.26) when $\epsilon = 0$. To solve this problem, note that only the first term in the expansion (3.25) that is shown below is needed. The other limit is to set $\epsilon = 1$ to solve the full problem, where all the terms in the expansion (3.26) are required and weighted equally by $1 = \epsilon^i$.

First note that the terms in (3.24) have been arranged such that the right hand side integrates to zero.[2] This condition allows us to expand the solution into orders, that is:

$$\phi = \sum_{i=0}^{\infty} \epsilon^i\,\phi^{(i)} \qquad (3.25)$$

Likewise the flux f is expanded as a series $\sum_{i=0}^{\infty}\,\epsilon^i\,f^{(i)}$ containing orders of f:

$$f^{(i)} \equiv \int_{-1}^{+1} \mu\,\phi^{(0)}\,d\mu$$

---

[2]Recall the normalization condition of ϕ, (3.17), and note that $\int_{-1}^{+1}\,\frac{1}{2}\,d\mu = 1$.

We now suppress the left hand side of (3.24) by a factor of ϵ so that the first term of the solution, $\phi^{(0)}$, is solvable. The scaled 'transport' equation for FLDT now becomes:

$$\begin{aligned} &\epsilon \left(\phi \frac{\partial f}{\partial x} U - \mu \frac{\partial \phi}{\partial x} U \right) + \epsilon U \left(\frac{\delta \phi}{\delta U} \right) \left(\sigma_A (U - B) + \frac{\partial}{\partial x} (f U) \right) \\ &= \left((\sigma_S U + \sigma_A B) + (\mu - f) \frac{\partial}{\partial x} U \right) \phi - \tfrac{1}{2} (\sigma_S U + \sigma_A B) \end{aligned} \tag{3.26}$$

Collecting order ϵ^0 terms we get the following equation:

$$\left((\sigma_S U + \sigma_A B) + (\mu - f^{(0)}) \frac{\partial}{\partial x} U \right) \phi^{(0)} = \tfrac{1}{2} (\sigma_S U + \sigma_A B) \tag{3.27}$$

The zeroth order solution can now be read off easily:

$$\phi^{(0)} = \frac{\frac{1}{2} (\sigma_S U + \sigma_A B)}{(\sigma_S U + \sigma_A B) + (\mu - f^{(0)}) \frac{\partial}{\partial x} U}$$

This solution is written in terms of the dimensionless variables as:

$$\phi^{(0)} = \frac{\frac{1}{2}}{1 + (f^{(0)} - \mu) R} \tag{3.28}$$

where the dimensionless quantity $R = X/\omega$, the dimensionless gradient X, and the albedo ω are defined:

$$X \equiv \frac{-\frac{\partial}{\partial x} U}{\sigma_T U} \quad \text{and} \quad \omega \equiv \frac{\sigma_A B + \sigma_S U}{\sigma_T U} \tag{3.29}$$

$$R \equiv \frac{X}{\omega} = -\frac{\frac{\partial}{\partial x} U}{\sigma_A B + \sigma_S U} \tag{3.30}$$

Leading order flux:

We would like to solve for $f^{(0)}$, the leading order normalized flux. Note that the solution (3.28) is written in terms of $f^{(0)}$, so we can use the normalization condition of $\phi^{(0)}$ which can be seen from integration (over μ) of order ($\epsilon^0 = 1$) terms in the scaled equation (3.26):

$$1 = \int_{-1}^{+1} \mu \, \phi^{(0)} \, d\mu = \int_{-1}^{+1} \mu \, \frac{\frac{1}{2}}{a\mu + b} = \tfrac{1}{2} a^{-1} \log \frac{+a + b}{-a + b}$$

where $a = -R$ and $b = 1 + f^0 R$.

We will solve the above for f^0:

$$-2\,R = \log \frac{(1+f^0 R)-R}{(1+f^0 R)+R}$$
$$e^{2\,R} = \frac{(1+f^0 R)+R}{(1+f^0 R)-R} = \frac{(f^0+1/R)+1}{(f^0+1/R)-1}$$

But we can compare the above equation to the fact:

$$e^{2\,R} = \frac{e^{+R}}{e^{-R}} = \frac{\cosh R + \sinh R}{\cosh R - \sinh R} = \frac{\coth R + 1}{\coth R - 1}$$

The implication is that $\coth(R) = f^0 + 1/R$, i.e., the zeroth order FLDT result is:

$$f^{(0)} = \coth(R) - \frac{1}{R} \tag{3.31}$$

We can substitute the result above into (3.28) in order to write the "angular form" $\phi^{(0)}$ fully in terms of R:

$$\phi^{(0)} = \frac{\frac{1}{2}}{(\coth R - \mu)\,R} \tag{3.32}$$

The leading order flux in FLDT is given by

$$F^{(0)} = c\,U\,f^{(0)} = c\,U\left(\coth R - \frac{1}{R}\right)$$

The flux is conventionally put in the form of a Fick's law, which expresses the flux as a gradient in concentration multiplied by a diffusion coefficient D:

$$\tfrac{1}{c}F = -D\,\frac{\partial U}{\partial x} \tag{3.33}$$

Using definitions (3.29) and (3.30) for R, ω, and X, let us write the flux in this conventional form, (3.33).

$$\begin{aligned} \tfrac{1}{c}F^{(0)} &= (UR)\,\frac{f^{(0)}(R)}{R} = \frac{UX}{\omega}\,\frac{f^{(0)}(R)}{R} \\ &= -\frac{\lambda(R)}{\omega\,\sigma_T}\,\frac{\partial U}{\partial x} \\ &= -D\,\frac{\partial U}{\partial x} \end{aligned} \tag{3.34}$$

Thus the flux is given by a Fick's Law (3.33) with a non-constant diffusion coefficient, which is defined as:

$$D \equiv \frac{\lambda(R)}{\omega\,\sigma_T} \tag{3.35}$$

where R is a function of U, $\frac{\partial U}{\partial x}$, σ, and B given in (3.30), and where:

$$\lambda(R) \equiv \frac{f^{(0)}(R)}{R} = \frac{1}{R}\left(\coth R - \frac{1}{R}\right) \tag{3.36}$$

The normalized flux $f^{(0)}(R)$ is a sigmoid-like function; it is like a smoothed sign function. It ranges from -1 at $R = -\infty$ to $+1$ at $R = +\infty$; for small R it is linear: $f^{(0)}(R) \approx \frac{1}{3}R$. Thus the function $\lambda(R)$ is bell shaped. It peaks at $R = 0$ with the 'isotropic' factor of $\frac{1}{3}$ and vanishes for large R.

The diffusion coefficient D is "flux-limited" by $\lambda(R)$. So, as the gradient $\frac{\partial U}{\partial x}$ in Fick's Law (3.33) gets large, $\lambda(R)$ gets small enough so that the flux never exceeds the scalar intensity: $\frac{1}{c}|F| \leq U$. Such an expression for the diffusion coefficient D is often referred to as a "flux-limiter".

Diffusion equation:

The flux-limited leading order flux (3.33) is simply substituted into the balance equation (3.22) to obtain the diffusion equation:

$$\frac{\partial}{\partial t}U + \frac{\partial}{\partial x}\left(-c\,D\,\frac{\partial U}{\partial x}\right) + c\sigma_A\,(U - B) = 0 \tag{3.37}$$

where

$$D = \frac{\lambda(R)}{\omega\,\sigma_T} \quad \text{and} \quad \lambda(R) = \frac{1}{R}\left(\coth R - \frac{1}{R}\right)$$

4. DISCRETIZED IDT DERIVATION

The goal of this chapter is to use the Chapman-Enskog method to derive a discrete IDT approximation starting from the discrete transport equations.

In this chapter we will first introduce the discretized transport equations in 1-D slab geometry. These equations are spatially discretized, and the reader may first need to familiarize himself with the the subscript conventions for the spatial grid in Figure 4.1; this notation will be used in the next three chapters. The Simple corner balance (SCB) transport equations will be introduced. In 1-D slab geometry the SCB equations are also equivalent to Lumped linear-discontinous (LLD) equations; these equations that are introduced below will be used for this chapter and also the next chapter, a FLDT derivation. After introducing the discretized transport equations we proceed with the IDT derivation.

4.1. Discretized transport equations

Let us first describe the spatial grid used for the SCB transport equations. Let us have a grid of $J+1$ edge points: $x_{1/2}, x_{3/2}, x_{J+1/2}$ where the spacing between two neighboring edge points, say $x_{j-1/2}$ and $x_{j+1/2}$, is given by $\Delta x_j \equiv x_{j+1/2} - x_{j-1/2}$. The $j-$th cell has a center point, $x_j \equiv \frac{x_{j+1/2}+x_{j-1/2}}{2}$, which divides the cell into a left half-cell (j,L) and right half-cell (j,R), as shown in Fig-4.1. Quantities are defined to exist on edge points; a quantity $Q(x_{j+1/2})$ is simply abbreviated as $Q_{j+1/2}$. Likewise, $Q_j \equiv Q(x_j)$. Averages of quantities are defined to exist in left and right half-cells, and would be written as $Q_{j,L}$ and $Q_{j,R}$.

Let us now describe and define the spatially discretized SCB transport equations. The SCB equations define the center intensities to be the average intensities of both half cells, and define the edge intensities by an upstream closure relation. This leads to very robust numerical equations; robustness means that the solution will always remain positive (negative intensities are unphysical) and that the solution is not expected to have large unphysical oscillations.

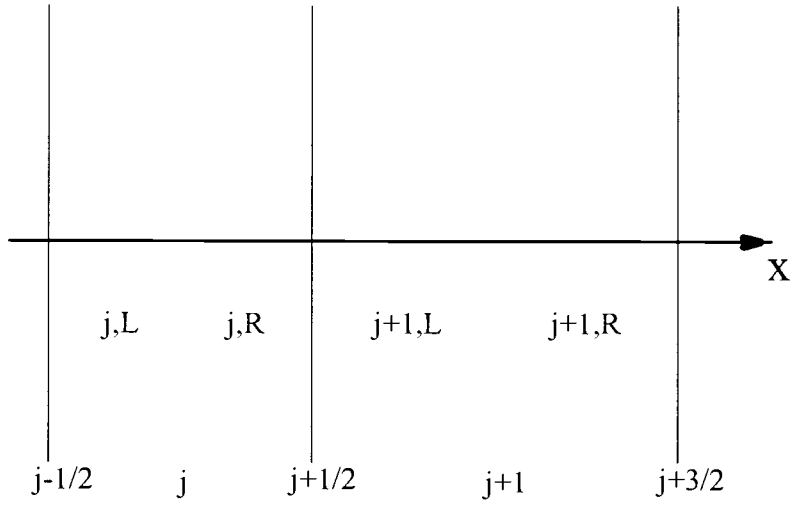

FIGURE 4.1. Notation for the spatial grid. The grid consists of edge points identified by half integers, and center points identified by integers. Each center point is surrounded by two half cells, referred to as the left (L) and right (R) half-cell at j. Both half cells have a width of $\frac{\Delta x_j}{2} = \frac{x_{j+1/2} - x_{j-1/2}}{2}$. Quantities that exist in the left and right half cell are subscripted with j, L and j, R, respectively.

The slab geometry Simple Corner Balance (SCB) transport equations are defined for our spatial grid described above. Let the spatial index range from $0 < j < J$. We have an equation for each half-cell:

$$\begin{aligned} \tfrac{c}{2}\left(\sigma_{Aj}B_{j,L} + \sigma_{Sj}U_{j,L}\right) &= \tfrac{1}{c}(\tfrac{\partial}{\partial t}I_{j,L}) + \mu\left(\tfrac{\Delta}{\Delta x}I\right)_{j,L} + \sigma_{Tj}I_{j,L} \\ \tfrac{c}{2}\left(\sigma_{Aj}B_{j,R} + \sigma_{Sj}U_{j,R}\right) &= \tfrac{1}{c}(\tfrac{\partial}{\partial t}I_{j,R}) + \mu\left(\tfrac{\Delta}{\Delta x}I\right)_{j,R} + \sigma_{Tj}I_{j,R} \end{aligned} \tag{4.1}$$

where the derivatives are defined[1] by:

$$\left(\tfrac{\Delta}{\Delta x}I\right)_{j,L} \equiv \frac{I_j - I_{j-1/2}}{\Delta x_j/2} \tag{4.2}$$

[1]General definition of spatial derivative: read I as some general quantity.

$$\left(\frac{\Delta}{\Delta x} I\right)_{j,R} \equiv \frac{I_{j+1/2} - I_j}{\Delta x_j / 2}$$

The intensity of the edges is given by the upstream relation:

$$I_{j+1/2} \equiv \begin{cases} I_{j,R} & \text{for } \mu > 0 \\ I_{j,L} & \text{for } \mu < 0 \end{cases} \tag{4.3}$$

The corresponding energy balance equations are obtained by integrating equations (4.1) and (4.2) over the angular variable.

$$\begin{aligned} \frac{\partial U_{j,L}}{\partial t} + \left(\frac{\Delta F}{\Delta x}\right)_{j,L} &= c\sigma_{Aj}\left(B_{j,L} - U_{j,L}\right) \\ \frac{\partial U_{j,R}}{\partial t} + \left(\frac{\Delta F}{\Delta x}\right)_{j,R} &= c\sigma_{Aj}\left(B_{j,R} - U_{j,R}\right) \end{aligned} \tag{4.4}$$

4.2. Applying the Chapman-Enskog method

The pair of Simple Corner Balance (SCB) transport equations are given as

$$\begin{aligned} \tfrac{c}{2}\left(\sigma_{Aj} B_{j,R} + \sigma_{Sj} U_{j,R}\right) &= \tfrac{1}{c}\left(\tfrac{\partial}{\partial t} I_{j,R}\right) + \mu\left(\tfrac{\Delta}{\Delta x} I\right)_{j,R} + \sigma_{Tj} I_{j,R} \\ \tfrac{c}{2}\left(\sigma_{Aj} B_{j,L} + \sigma_{Sj} U_{j,L}\right) &= \tfrac{1}{c}\left(\tfrac{\partial}{\partial t} I_{j,L}\right) + \mu\left(\tfrac{\Delta}{\Delta x} I\right)_{j,L} + \sigma_{Tj} I_{j,L} \end{aligned} \tag{4.5}$$

The terms on the left hand side above represent the quantity of photons emitted uniformly in all directions from the material, due to blackbody emission and outgoing isotropic scattering. On the right hand side the following terms are present: 1.) the change in intensity over time, 2.) the change in intensity over space written in terms of the directional derivative (in 1-D slab geometry), 3.) the quantity of photons with direction μ interacting with a unit 'volume' of the material by either absorption or in going scattering.

In the future, we will abbreviate pairs of equations like those above by writing just a single equation, with the right/left label (R/L) being replaced by a generic

label Γ; that is, we write the above pair of equations as:

$$0 = \tfrac{1}{c}(\tfrac{\partial}{\partial t} I_{j,\Gamma}) + \mu \left(\tfrac{\Delta}{\Delta x} I\right)_{j,\Gamma} + \sigma_{Tj} I_{j,\Gamma} - \tfrac{c}{2} \left(\sigma_{Aj} B_{j,\Gamma} + \sigma_{Sj} U_{j,\Gamma}\right)$$

where

$$\Gamma \equiv R \text{ or } L \tag{4.6}$$

In order to derive a conservation equation, we need to integrate the transport equation over angle. It helps to see the terms above integrated individually, so we write the above transport equation as:

$$0 = T_{\text{time}} + T_{\text{space}} + T_{\text{in}} + T_{\text{out}}$$

where

$$T_{\text{time}} = \tfrac{1}{c}(\tfrac{\partial}{\partial t} I_{j,\Gamma}) \quad , \qquad T_{\text{space}} = \mu \left(\frac{\Delta I}{\Delta x}\right)_{j,\Gamma}$$
$$T_{\text{in}} = \sigma_{Tj} I_{j,\Gamma} \text{ , and } \quad T_{\text{out}} = -\tfrac{c}{2} \left(\sigma_{Aj} B_{j,\Gamma} + \sigma_{Sj} U_{j,\Gamma}\right) .$$

The last of these terms is already μ independent, and will just pick up a factor of 2 upon integration. For the μ dependent terms, the definitions of the scalar intensity and the flux are used: $\frac{1}{c}\int_{-1}^{+1} d\mu\, I = U$ and $\int_{-1}^{+1} d\mu\, \mu I = F$. Integrated over the directional variable μ these terms become:

$$\int_{-1}^{+1} d\mu\, T_{\text{time}} = (\tfrac{\partial}{\partial t} U_{j,\Gamma})$$
$$\int_{-1}^{+1} d\mu\, T_{\text{space}} = \left(\frac{\Delta F}{\Delta x}\right)_{j,\Gamma}$$
$$\int_{-1}^{+1} d\mu\, T_{\text{in}} = c\sigma_{Tj} U_{j,\Gamma}$$
$$\int_{-1}^{+1} d\mu\, T_{\text{out}} = -c \left(\sigma_{Aj} B_{j,\Gamma} + \sigma_{Sj} U_{j,\Gamma}\right)$$

Thus we can write the conservation equation, or "balance equation".

$$\frac{\partial U_{j,\Gamma}}{\partial t} = -\left(\frac{\Delta F}{\Delta x}\right)_{j,\Gamma} - c\sigma_{Aj} \left(U_{j,\Gamma} - B_{j,\Gamma}\right) \tag{4.7}$$

The Chapman-Enskog method proposes the following. Assume that we have a solution $U = U(x,t)$ to the conservation equation (4.7)[2]. We think of the intensity

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[2]Assume the spatial grid taken to the continuous limit, i.e., $x_j \to x$.

as a functional of U

$$I(x,t,\mu) \equiv I[U] \equiv I\left(U(x,t),\mu\right)$$

The crucial point is that derivatives of I can now be written in terms of derivatives of U:

$$\frac{dI}{dx} = \left(\frac{\delta I}{\delta U}\right)\frac{\partial U}{\partial x} \tag{4.8}$$

Here $\left(\frac{\delta I}{\delta U}\right)$ is called a "functional derivative". In Levermore [3] its operation is defined as follows. $\left(\frac{\delta I}{\delta U}\right)$ acting on some displacement H in U is:

$$\left(\frac{\delta I}{\delta U}\right) H \equiv \frac{d}{ds} I\left(U+sH\right)|_{s=0} = \frac{\partial I}{\partial U} H \tag{4.9}$$

For the discrete case $U(x) \rightarrow U_{j,\Gamma}$ there may exist a reasonably good approximation for the functional derivative, which we will distinguish with square brackets:

$$\left(\frac{\delta I}{\delta U}\right) \rightarrow \left[\frac{\delta I}{\delta U}\right]_{U j,\Gamma}$$

We may at some point use the discrete functional derivative to express or approximate the derivatives $\frac{\Delta}{\Delta x} I$ and $\frac{\Delta}{\Delta x} F$ in terms of $\frac{\Delta}{\Delta x} U$. In this section, we are not forced to use it, at least for the lower order expressions of $I[U]$.

In the transport equation (4.5) we have a term $(\frac{\partial}{\partial t} I)$ which is then expressed using a continuous functional derivative. Thus we can eliminate the time derivative in the transport equation by substituting (4.7) into (4.5).

$$\begin{aligned} 0 = \; & \frac{1}{c}\left(\frac{\delta I_{j,\Gamma}}{\delta U}\right)\left[\frac{\partial U_{j,\Gamma}}{\partial t} = c\sigma_{Aj}(B_{j,\Gamma} - U_{j,\Gamma}) - (\tfrac{\Delta}{\Delta x} F)_{j,\Gamma})\right] \\ & + \mu\left(\tfrac{\Delta}{\Delta x} I\right)_{j,\Gamma} + \sigma_{Tj}(\tfrac{\Delta x_j}{2}) I_{j,\Gamma} - \tfrac{c}{2}\left(\sigma_{Aj} B_{j,\Gamma} + \sigma_{Sj} U_{j,\Gamma}\right) \end{aligned} \tag{4.10}$$

Let us now simply rewrite this into a form which will later be convenient. We produce a common factor $\sigma_A(B-U)$ by adding:

$$0 = \tfrac{c}{2}\left((\sigma_A + \sigma_S)U - \sigma_T U\right)$$

We get the central equation in this section: [3]

$$0 = \frac{1}{c}\left(\frac{\delta I_{j,\Gamma}}{\delta U}\right)\left[c\sigma_{Aj}(B_{j,\Gamma} - U_{j,\Gamma}) - (\tfrac{\Delta}{\Delta x}F)_{j,\Gamma}\right] + \mu\left(\tfrac{\Delta}{\Delta x}I\right)_{j,\Gamma}$$
$$- \tfrac{c}{2}\sigma_{Aj}\left(B_{j,\Gamma} - U_{j,\Gamma}\right) + \sigma_{Tj}\left(I_{j,\Gamma} - \tfrac{c}{2}U_{j,\Gamma}\right) \qquad (4.11)$$

If we now write out intensity functional $I[U]$ as an expansion in orders, utilizing a scaling factor ϵ, then some sort of scaling will be introduced into the above equation. We define:

$$I \equiv I^{(0)} + \epsilon I^{(1)} + \epsilon^2 I^{(2)} + ...$$

If we insist that all the isotropic (μ-independent) information is contained in the lowest order of I and that higher orders do not contribute to the scalar flux U then we shall see that a particular scaling for the above equation is possible and consistent. Our requirement forces

$$U \equiv \tfrac{1}{c}\textstyle\int_{-1}^{+1} d\mu\, I \equiv \tfrac{1}{c}\int_{-1}^{+1} d\mu\, I^{(0)} = \tfrac{2}{c}I^{(0)} \quad .$$

Note in the limit of $\epsilon \to 0$ that I is completely isotropic $I = I^{(0)}$. To find the scaling of our main equation (4.11) we look at the last term:

$$\left(I_{j,\Gamma} - \tfrac{c}{2}U_{j,\Gamma}\right) = \left(I^{(0)} - \tfrac{c}{2}U_{j,\Gamma}\right) + \epsilon I^{(1)} + ... = \epsilon I^{(1)} + \epsilon^2 I^{(2)} + ...$$

Thus the simplest way to scale equation (4.11) would be to put an ϵ^1 on all but the last term. This is what is done in Levermore [3]. The IDT scaling suppresses all but the last term with ϵ's. It conveniently suppresses the functional derivatives and derivatives of I and F:

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[3] With discrete functional derivatives the corresponding equation to (4.11) would be:

$$0 \cong \left(\frac{\delta I_{j,\Gamma}}{\delta U}\right)\left[\sigma_{Aj}(B_{j,\Gamma} - U_{j,\Gamma}) - \tfrac{1}{c}\left[\frac{\delta F}{\delta U}\right]_{Uj,\Gamma}\left(\frac{\Delta U}{\Delta x}\right)_{j,\Gamma}\right] + \mu\left[\frac{\delta I}{\delta U}\right]_{Uj,\Gamma}\left(\frac{\Delta U}{\Delta x}\right)_{j,\Gamma}$$
$$- \tfrac{c}{2}\sigma_{Aj}\left(B_{j,\Gamma} - U_{j,\Gamma}\right) + \sigma_{Tj}\left(I_{j,\Gamma} - \tfrac{c}{2}U_{j,\Gamma}\right)$$

$$0 = \frac{1}{c}\left(\frac{\delta I_{j,\Gamma}}{\delta U}\right)\left[c\sigma_{Aj}(B_{j,\Gamma} - U_{j,\Gamma}) - (\frac{\Delta}{\Delta x}F)_{j,\Gamma})\right]\epsilon + \mu\left(\frac{\Delta}{\Delta x}I\right)_{j,\Gamma}\epsilon$$
$$- \frac{c}{2}\sigma_{Aj}\left(B_{j,\Gamma} - U_{j,\Gamma}\right)\epsilon + \sigma_{Tj}\left(I_{j,\Gamma} - \frac{c}{2}U_{j,\Gamma}\right) \tag{4.12}$$

The flux expansion is defined to correspond to the expansion of the intensity:

$$F^{(i)} = \int_{-1}^{+1} d\mu\ \mu\ I^{(i)}$$

We start solving for I by solving (4.12) in progressive orders of ϵ. The 0-th order is easy enough

$$I_{j,\Gamma}^{(0)} = \frac{c}{2}U_{j,\Gamma} \tag{4.13}$$

thus

$$F_{j,\Gamma}^{(0)} = 0$$

The last equation states that the left and right cell (L and R) values of the flux are zero. We now insist on a very reasonable condition: the edge values $\vec{F}_{1/2}$ are a function of the L and R values ($\vec{F}_{j,\Gamma}$), and that this function $\vec{F}_{1/2}$ is zero when $\vec{F}_{j,\Gamma}$ is zero: i.e., that $\vec{F}_{1/2}[\vec{0}] = \vec{0}$. Any linear function would for example satisfy this reasonable condition. In fact, any reasonable closure relation between the edge values and the cell values would satisfy this condition. From this argument it follows that we can say that that $F_{j+1/2}^{(0)} = 0$ also. In summary:

$$0 = F_{j,\Gamma}^{(0)} = F_{j+1/2}^{(0)} \quad \text{and} \quad \left(\frac{\Delta}{\Delta x}F^{(0)}\right)_{j,\Gamma} = 0 \tag{4.14}$$

The result $F_{j+1/2}^{(0)} = 0$ is important because it will tell us something about the edge values $U_{j+1/2}$. The argument is as follows:

$$0 = F_{j+1/2}^{(0)} \equiv \int_{-1}^{+1} d\mu\ \mu I_{j+1/2}^{(0)} = \int_{-1}^{0} d\mu\,\mu\left(\frac{c}{2}U_{j+1,L}\right) + \int_{0}^{1} d\mu\,\mu\left(\frac{c}{2}U_{j,R}\right)$$

Since U is not a function of μ and the two last integrals evaluate to

$$-1/2 = (0^2 - (-1)^2)/2 \text{ and } 1/2 = (1^2 - 0^2)/2$$

respectively, we come to the important conclusion that:

$$U_{j+1,L} = U_{j,R}$$

The closure relation for U is derived in a similar way as above, by looking at the definition of $U \equiv \int I d\mu/c$. But first we note that $U = \int I^{(0)} d\mu/c$ and thus higher order $I^{(i)}$ do not contribute to U. So,

$$U_{j+1/2} = \tfrac{1}{c}\left(\int_{-1}^{0} d\mu\, I^{(0)}_{j+1/2} + \int_{0}^{1} d\mu\, I^{(0)}_{j+1/2}\right) = \tfrac{1}{2}U_{j+1,L} + \tfrac{1}{2}U_{j,R}$$

We summarize:

$$U_{j+1,L} = U_{j+1/2} = U_{j,R} \quad \text{and} \quad U_{j+1/2} = \tfrac{1}{2}U_{j+1,L} + \tfrac{1}{2}U_{j,R} = \tfrac{2}{c} I^{(0)}_{j+1/2} \tag{4.15}$$

We have dissected the leading order equation with our basic definitions and come up with ground-laying results (4.13), (4.14) and (4.15). This allows us to substitute the following quantities into (4.12) and solve for the higher orders.

$$\left(\frac{\delta I^{(0)}_{j,\Gamma}}{\delta U}\right) = \frac{c}{2}, \quad \left(\tfrac{\Delta}{\Delta x} I^{(0)}\right)_{j,\Gamma} = \frac{c}{2}\left(\tfrac{\Delta}{\Delta x} U\right)_{j,\Gamma}, \text{ and } \quad \left(\tfrac{\Delta}{\Delta x} F^{(0)}\right)_{j,\Gamma} = 0$$

The $\epsilon^{(1)}$ order equation obtained by substituting our expansion into (4.12) is:

$$0 = \sigma_{T_j} I^{(1)}_{j,\Gamma} + \tfrac{c}{2}\,\mu \left(\frac{\Delta U}{\Delta x}\right)_{j,\Gamma}$$

The first order correction to the intensity is just linear in μ and so the corresponding flux is easily found by integration:

$$I^{(1)}_{j,\Gamma} = -\tfrac{c}{2}\frac{\mu}{\sigma_{Tj}}\left(\frac{\Delta U}{\Delta x}\right)_{j,\Gamma} \tag{4.16}$$

$$F^{(1)}_{j,\Gamma} = -\frac{c}{3\sigma_{Tj}}\left(\frac{\Delta U}{\Delta x}\right)_{j,\Gamma} \tag{4.17}$$

It can also be shown that the edge values of F are average values of the neighboring cell values. This is done by starting from the definition, $F^{(1)}_{j+1/2} \equiv \int_{-1}^{+1} d\mu\ \mu I^{(1)}_{j+1/2}(\mu)$, then splitting this integral in two parts, and looking at the two results. We would find:

$$F^{(1)}_{j+1/2} = \tfrac{1}{2}\, F^{(1)}_{j,R} + \tfrac{1}{2}\, F^{(1)}_{j+1,L} \tag{4.18}$$

We have now iterated enough so that $F[U]$ contains a (nonzero) leading order term; $F \cong F^{(1)}$. Now we can substitute this expression $F[U(x)]$ into the conservation equation (4.7), which produces our PDE for $U(x)$ to first order:

$$0 = \frac{1}{c}\frac{\partial U_{j,\Gamma}}{\partial t} + \sigma_{Aj}\left(U_{j,\Gamma} - B_{j,\Gamma}\right) + \frac{1}{c}\left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j,\Gamma} \tag{4.19}$$

We are interested in the two balance equations (to first order) across the edge $j + \frac{1}{2}$; we rewrite the above, making use of our continuity results:

$$\begin{aligned} 0 &= \frac{\partial U_{j+1/2}}{\partial t} + c\sigma_{Aj}\left(U_{j+1/2} - B_{j,R}\right) + \left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j,R} \\ 0 &= \frac{\partial U_{j+1/2}}{\partial t} + c\sigma_{Aj+1}\left(U_{j+1/2} - B_{j+1,L}\right) + \left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j+1,L} \end{aligned} \tag{4.20}$$

The last term in the above equations is a derivative in the flux which is more difficult to evaluate; we try it for the right cell:

$$\left(\tfrac{\Delta x_j}{2}\right)\left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j,R} = \left(F^{(1)}_{j+1/2} - F^{(1)}_{j}\right) = \left(\tfrac{1}{2}F^{(1)}_{j+1,L} - \tfrac{1}{2}F^{(1)}_{j,L}\right)$$

We do further work on the above, substituting $F^{(1)}[U]$, from (4.17); then

$$\left(\tfrac{\Delta x_j}{2}\right)\left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j,R} = -\frac{c}{6}\left[\frac{1}{\sigma_{Tj+1}}\left(\frac{\Delta U}{\Delta x}\right)_{j+1.L} - \frac{1}{\sigma_{Tj}}\left(\frac{\Delta U}{\Delta x}\right)_{j,L}\right]$$

And likewise:

$$\left(\tfrac{\Delta x_j}{2}\right)\left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j+1,L} = -\frac{c}{6}\left[\frac{1}{\sigma_{Tj+1}}\left(\frac{\Delta U}{\Delta x}\right)_{j+1,R} - \frac{1}{\sigma_{Tj}}\left(\frac{\Delta U}{\Delta x}\right)_{j,R}\right]$$

The last two equations add together nicely; that is they produce U_j—independent quantities. To see this, recall the derivatives are defined as

$$\begin{aligned} \left(\tfrac{\Delta}{\Delta x}U\right)_{j,L} &= \frac{1}{\left(\frac{\Delta x_j}{2}\right)}\left[\,U_j - U_{j-1/2}\right] \\ \left(\tfrac{\Delta}{\Delta x}U\right)_{j,R} &= \frac{1}{\left(\frac{\Delta x_j}{2}\right)}\left[-U_j + U_{j+1/2}\right] \end{aligned}$$

so that

$$\left(\tfrac{\Delta}{\Delta x}U\right)_{j,L} + \left(\tfrac{\Delta}{\Delta x}U\right)_{j,R} = \frac{1}{\left(\frac{\Delta x_j}{2}\right)}\left[\,U_{j+1/2} - U_{j-1/2}\right]$$

Thus the cell-width weighted sum of flux derivatives adds together nicely:

$$\begin{aligned} &\left(\tfrac{\Delta x_j}{2}\right)\left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j,R} + \left(\tfrac{x_{j+1}}{2}\right)\left(\frac{\Delta F^{(1)}}{\Delta x}\right)_{j+1,L} \\ &= -\frac{c}{6}\frac{1}{\sigma_{Tj+1}\left(\frac{x_{j+1}}{2}\right)}\left[U_{j+3/2} - U_{j+1/2}\right] + \frac{c}{6}\frac{1}{\sigma_{Tj}\left(\frac{\Delta x_j}{2}\right)}\left[U_{j+1/2} - U_{j-1/2}\right] \end{aligned}$$

We combine equations (4.21) using the above weighted addition:

$$\frac{\Delta x_j+\Delta x_{j+1}}{2}\frac{\partial U_{j+1/2}}{c\,\partial t}+\frac{\sigma_{Aj}\Delta x_j+\sigma_{Aj+1}\Delta x_{j+1}}{2}U_{j+1/2}-\frac{\sigma_{Aj}\Delta x_j B_{j,R}+\sigma_{Aj+1}\Delta x_{j+1}B_{j+1,L}}{2}$$
$$-\frac{1}{6}\left[\frac{U_{j+3/2}-U_{j+1/2}}{\sigma_{Tj+1}\frac{\Delta x_{j+1}}{2}}-\frac{U_{j+1/2}-U_{j-1/2}}{\sigma_{Tj}\frac{\Delta x_j}{2}}\right]=0$$

Thus SCB-Transport equations and Chapman-Enskog method in the isotropic limit produce the following leading order diffusion equation:

$$0=\frac{1}{c}\frac{\partial U_{j+1/2}}{\partial t}+\left(\frac{\sigma_{Aj}\Delta x_j+\sigma_{Aj+1}\Delta x_{j+1}}{\Delta x_j+\Delta x_{j+1}}U_{j+1/2}-\frac{\sigma_{Aj}\Delta x_j B_{j,R}+\sigma_{Aj+1}\Delta x_{j+1}B_{j+1,L}}{\Delta x_j+\Delta x_{j+1}}\right)$$
$$-\frac{1}{3}\frac{2}{\Delta x_j+\Delta x_{j+1}}\left[\frac{U_{j+3/2}-U_{j+1/2}}{\sigma_{Tj+1}\,\Delta x_{j+1}}-\frac{U_{j+1/2}-U_{j-1/2}}{\sigma_{Tj}\,\Delta x_j}\right] \quad (4.21)$$

The above diffusion equations match those previously shown through a standard asymptotic analysis, but were obtained through a novel derivation. Our derivation directly applied the Levermore's Chapman-Enskog method to discretized transport equations, rather than discretizing analytic IDT equations.

5. DISCRETIZED FLDT DERIVATION

This chapter shows that the Chapman-Enskog (CE) method can be applied to a set of discrete transport equations. We show how the CE method applied to a set of Simple Corner Balance (SCB) equations (a robust transport scheme for thick diffusive problems) yields a set of diffusion equations. Without approximations, we are unable to uncouple the set of diffusion equations to produce a desired[1] single edge-centered diffusion equation. We propose some possible approximations which allow an edge-centered diffusion equation to be written.

5.1. Applying the Chapman-Enskog method

In the previous section Levermore's flux limiting procedure was applied to the analytic transport equation. Our goal is to show that the same method can be applied on a set of discrete transport equations. The Simple Corner Balance (SCB) equations were chosen because they are known to exhibit robust behavior for optically thick, diffusive problems.

The SCB equations are defined for all spatial half-cells:

$$\frac{\Delta x}{2c}\frac{\partial I_{j,L}}{\partial t} + \mu\left[\frac{I_{j,L}+I_{j,R}}{2} - I_{j-\frac{1}{2}}\right] + \sigma_{Tj}\left(\tfrac{\Delta x_j}{2}\right) I_{j,L} = \tfrac{c}{2}\left(\tfrac{\Delta x_j}{2}\right)\left(\sigma_{Aj}B_{j,L} + \sigma_{Sj}U_{j,L}\right) \tag{5.1}$$

and

$$\frac{\Delta x}{2c}\frac{\partial I_{j,R}}{\partial t} + \mu\left[I_{j+\frac{1}{2}} - \frac{I_{j,L}+I_{j,R}}{2}\right] + \sigma_{Tj}\left(\tfrac{\Delta x_j}{2}\right) I_{j,R} = \tfrac{c}{2}\left(\tfrac{\Delta x_j}{2}\right)\left(\sigma_{Aj}B_{j,R} + \sigma_{Sj}U_{j,R}\right) \tag{5.2}$$

The edge intensity is defined by the upstream closure relationship:

$$I_{j+\frac{1}{2}} = \begin{cases} I_{j,R} & \mu > 0 \\ I_{j+1,L} & \mu < 0 \end{cases} \tag{5.3}$$

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[1] An example of an edge centered diffusion equation was found in the last chapter.

We also often will use I_j to identify the cell center intensity; let us define:

$$I_j = \frac{I_{j,L} + I_{j,R}}{2} \tag{5.4}$$

The derivative quantities in square brackets will also be abbreviated by $(\Delta\ )$ or $(\frac{\Delta}{\Delta x}\ )$. In the left half-cells we define:

$$(\Delta I)_{j,L} \equiv \left[\frac{I_{j,L} + I_{j,R}}{2} - I_{j-\frac{1}{2}}\right] \equiv \frac{\Delta x_j}{2}\left(\frac{\Delta I}{\Delta x}\right)_{j,L} \tag{5.5}$$

Likewise the same is defined for the right half-cell (j, R):

$$(\Delta I)_{j,R} \equiv \left[I_{j+\frac{1}{2}} - \frac{I_{j,L} + I_{j,R}}{2}\right] \equiv \frac{\Delta x_j}{2}\left(\frac{\Delta I}{\Delta x}\right)_{j,R} \tag{5.6}$$

The SCB transport equations (5.1) and (5.2) are integrated over the angular variable to produce balance equations:

$$\frac{\partial U_{j,\Gamma}}{\partial t} = -\left(\frac{\Delta F}{\Delta x}\right)_{j,\Gamma} - c\sigma_{Aj}\left(U_{j,\Gamma} - B_{j,\Gamma}\right) \tag{5.7}$$

where the generic index label j, Γ has been substituted to denote either the j-th left-half cell (j, L) quantity, or the j-th right-half cell (j, R) quantity.

We will now substitute Levermore's definitions (3.16)–(3.20) and transform the transport equations into 'functional' transport equations.

The intensity I is written in terms of a normalized angular 'form' ϕ:

$$\frac{1}{c} I_{j,\Gamma} \equiv U_{j,\Gamma}\, \phi_{j,\Gamma}(\mu) \tag{5.8}$$

where $\int_{-1}^{+1} \phi_{j,\Gamma} d\mu \equiv 1$ so that $U = \int_{-1}^{+1} I_{j,\Gamma} d\mu$.

The flux is still related by:

$$\tfrac{1}{c} F_{j,\Gamma} = U_{j,\Gamma}\, f_{j,\Gamma} \quad \text{where} \quad f_{j,\Gamma} = \int_{-1}^{+1} \mu\, \phi_{j,\Gamma} d\mu \tag{5.9}$$

The functional derivative

$$\frac{1}{c}\frac{\delta I_{j,\Gamma}}{\delta U} = \frac{\delta(U_{j,\Gamma}\,\phi_{j,\Gamma})}{\delta U} = \left(\phi_{j,\Gamma} + U_{j,\Gamma}\frac{\delta \phi_{j,\Gamma}}{\delta U}\right)$$

is used to eliminate the time derivatives in the transport equations by writing derivatives in I in terms of derivatives in U:

$$\frac{\partial I_{j,\Gamma}}{\partial t} = c\left(\phi_{j,\Gamma} + U_{j,\Gamma}\frac{\delta\phi_{j,\Gamma}}{\delta U}\right)\frac{\partial U_{j,\Gamma}}{\partial t}$$

which can be written without explicit time dependence via the balance equation (i.e., the zeroth moment of the transport equation):

$$\frac{\partial I_{j,\Gamma}}{\partial t} = -c\left(\phi_{j,\Gamma} + U_{j,\Gamma}\frac{\delta\phi_{j,\Gamma}}{\delta U}\right)\left[\left(\frac{\Delta F}{\Delta x}\right)_{j,\Gamma} c\sigma_{Aj}\left(U_{j,\Gamma} - B_{j,\Gamma}\right)\right]$$

Putting the right hand side of the above into the transport equation we obtain the 'functional' equations of the Chapman-Enskog method:

$$\begin{aligned} 0 = \left(\phi_{j,\Gamma} + U_{j,\Gamma}\frac{\delta\phi_{j,\Gamma}}{\delta U}\right)\left[\sigma_{Aj}(B_{j,\Gamma} - U_{j,\Gamma}) - \frac{\Delta fU}{\Delta x}_{j,\Gamma}\right] + \mu\left(\frac{\Delta U\phi}{\Delta x}\right)_{j,\Gamma} \\ -\tfrac{1}{2}\sigma_{Aj}(B_{j,\Gamma} - U_{j,\Gamma}) + \sigma_{Tj}\left(U_{j,\Gamma}\phi_{j,\Gamma} - \tfrac{1}{2}U_{j,\Gamma}\right) \end{aligned}$$

The last two terms above (lower line) reduce to

$$\phi_{j,\Gamma}(\sigma_{Tj}U_{j,\Gamma}) - \tfrac{1}{2}(\sigma_{Aj}B_{j,\Gamma} + \sigma_{Sj}U_{j,\Gamma})$$

Now the unscaled functional equations are more neatly written:

$$\begin{aligned} U_{j,\Gamma}\frac{\delta\phi_{j,\Gamma}}{\delta U}\left[\left(\frac{\Delta}{\Delta x}fU\right)_{j,\Gamma} + \sigma_{Aj}(U_{j,\Gamma} - B_{j,\Gamma})\right] = \mu\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,\Gamma} - \phi_{j,\Gamma}\left(\frac{\Delta}{\Delta x}fU\right)_{j,\Gamma} \\ + \left(\phi_{j,\Gamma} - \tfrac{1}{2}\right)\left(\sigma_{Sj}U_{j,\Gamma} + \sigma_{Aj}B_{j,\Gamma}\right) \end{aligned} \tag{5.10}$$

Notice that the first two terms of the RHS will vanish under integration over angles; this happens because $\mu\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,\Gamma} = \left(\frac{\Delta}{\Delta x}\mu U\phi\right)_{j,\Gamma}$. Also notice that the last term of the RHS will vanish under integration over angles since:

$$\int_{-1}^{+1}\left(\phi_{j,\Gamma} - \tfrac{1}{2}\right)d\mu = 0$$

Thus we see that we could produce a scaling that would be consistent under integration over angles, by suppressing the LHS of (5.10) with an ϵ. However, this would produce equations where even the zeroth order solution may be unsolvable.

One of the goals of the Chapman-Enskog method is to make the zeroth order solvable. We wish to suppress quantities that allow the first order to be solved. These quantities should be small, since any terms that we suppress will be corrected for in higher orders, which we usually in practice do not solve for or use.

The difficulty with (5.10) lies within the derivatives. For example consider:

$$\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,R} = \frac{2}{\Delta x}\left(U_{j+1/2}\phi_{j+1/2} - U_j\phi_j\right) \tag{5.11}$$

Then it is clear that (5.10) for $\Gamma = R$ contains solutions $\phi_{j,R}$, $\phi_{j+1/2}$, and ϕ_j.[2] The goal is to eliminate two of these by suppressing more terms. We will expand the derivative in the above equation using the "product rule" below:

$$(AB - ab) = \tfrac{1}{2}(A + a)(B - b) + \tfrac{1}{2}(B + b)(A - a) \tag{5.12}$$

We can apply the product rule to one of the terms of (5.10):

$$\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,R} = \tfrac{1}{2}(U_j + U_{j+1/2})\left(\frac{\Delta\phi}{\Delta x}\right)_{j,R} + \tfrac{1}{2}(\phi_j + \phi_{j+1/2})\left(\frac{\Delta U}{\Delta x}\right)_{j,R} \tag{5.13}$$

We define a function of μ:

$$g^{\phi}_{j,R}(\mu) \equiv \tfrac{1}{2}(\phi_j + \phi_{j+1/2}) - \phi_{j,R} \tag{5.14}$$

and also define:

$$g^{f}_{j,R} \equiv \int_{-1}^{+1} \mu\, g^{\phi}_{j,R}(\mu)\, d\mu \tag{5.15}$$

An important property of $g^{\phi}_{j,R}(\mu)$ is that it vanishes under integration over angles, i.e.,

$$0 = \int_{-1}^{+1} g^{\phi}_{j,R}(\mu)\, d\mu\ .$$

---

[2]The edge and center distributions can be related to different half-cell neighbors. For example $\phi_{j+1/2}$ is related by upstream closure to $U_{j,R}, \phi_{j,R}$, $U_{j+1,L}, \phi_{j+1,L}$, and $U_{j+1/2}$. The center distribution ϕ_j is simply given by the equation

$$\frac{1}{c}I_j = \frac{\phi_{j,L}U_{j,L} + \phi_{j,R}U_{j,R}}{2} = \phi_j\,\frac{U_{j,L} + U_{j,R}}{2}$$

and is clearly normalized for normalized half-cell distributions $\phi_{j,L}$ and $\phi_{j,R}$.

Now we can write an even lengthier version of the derivative (5.13):

$$\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,R} = \tfrac{1}{2}(U_j + U_{j+1/2})\left(\frac{\Delta\phi}{\Delta x}\right)_{j,R} + (\phi_{j,R} + g^{\phi}_{j,R})\left(\frac{\Delta U}{\Delta x}\right)_{j,R} \tag{5.16}$$

Thus the first two terms in (5.10) can be expressed as:

$$\begin{aligned}
& \mu\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,R} - \phi_{j,R}\left(\frac{\Delta}{\Delta x}fU\right)_{j,R} \\
= \;& \tfrac{1}{2}(U_j + U_{j+1/2})\,\mu\left(\frac{\Delta\phi}{\Delta x}\right)_{j,R} + (\mu\,\phi_{j,R} + \mu g^{\phi}_{j,R})\left(\frac{\Delta U}{\Delta x}\right)_{j,R} \\
& - \tfrac{1}{2}(U_j + U_{j+1/2})\,\phi_{j,R}\left(\frac{\Delta f}{\Delta x}\right)_{j,R} - \phi_{j,R}\,(f_{j,R} + g^{f}_{j,R})\left(\frac{\Delta U}{\Delta x}\right)_{j,R} \\
= \;& \tfrac{1}{2}(U_j + U_{j+1/2})\,\left[\,\mu\left(\frac{\Delta\phi}{\Delta x}\right)_{j,R} - \phi_{j,R}\left(\frac{\Delta f}{\Delta x}\right)_{j,R}\,\right] \\
& + \left(\frac{\Delta U}{\Delta x}\right)_{j,R}\left[\mu g^{\phi}_{j,R} - \phi_{j,R}\,g^{f}_{j,R}\right] \\
& + \left(\frac{\Delta U}{\Delta x}\right)_{j,R}(\mu - f_{j,R})\,\phi_{j,R}
\end{aligned} \tag{5.17}$$

In the analytic Chapman-Enskog method, the spatial derivatives of ϕ and f are expressed as functional derivatives and derivatives of U. In the analytic derivation, terms with functional derivatives are suppressed to order ϵ in order to make the zeroth order solvable. Likewise, in our discrete derivation, we will suppress the first term on the last RHS of the equation above.

Again, for the sake of solvability of the zeroth order, we also will suppress the second term involving $g^{\phi}_{j,R}(\mu)$. We do not expect this term to be large since

$$g^{\phi}_{j,R}(\mu) \equiv \tfrac{1}{2}(\phi_j + \phi_{j+1/2}) - \phi_{j,R}$$

should be small for fine enough grids.

Recall that the original term

$$\mu\left(\frac{\Delta}{\Delta x}U\phi\right)_{j,R} - \phi_{j,R}\left(\frac{\Delta}{\Delta x}fU\right)_{j,R}$$

vanishes after angular integration. For consistency, we need to verify that this property is maintained after scaling. Note that the angular part of the first two compound terms, denoted by square brackets in equation (5.17) above, clearly both

vanish after angular integration. Note that the remaining third term also vanishes after angular integration. Thus, suppressing the first two terms while leaving the third untouched is a valid scaling. The unscaled equation (5.10) is expanded into:

$$\begin{aligned} & U_{j,R}\frac{\delta\phi_{j,R}}{\delta U}\left(\left(\tfrac{\Delta}{\Delta x}fU\right)_{j,R}+\sigma_{Aj}(U_{j,R}-B_{j,R})\right) \\ & -\tfrac{1}{2}(U_j+U_{j+1/2})\left[\mu\left(\tfrac{\Delta}{\Delta x}\phi\right)_{j,R}-\phi_{j,R}\left(\tfrac{\Delta}{\Delta x}f\right)_{j,R}\right]-\left(\tfrac{\Delta}{\Delta x}U\right)_{j,R}\left[\mu g^{\phi}_{j,R}-\phi_{j,R}\,g^{f}_{j,R}\right] \\ & =\left(\tfrac{\Delta}{\Delta x}U\right)_{j,R}(\mu-f_{j,R})\,\phi_{j,R}+\left(\phi_{j,R}-\tfrac{1}{2}\right)(\sigma_{Sj}U_{j,R}+\sigma_{Aj}B_{j,R}) \end{aligned} \tag{5.18}$$

The scaled equation has the left hand side suppressed:

$$\begin{aligned} \epsilon\,\Upsilon_{j,R} = {} & \phi_{j,R}\left((\sigma_{Sj}U_{j,R}+\sigma_{Aj}B_{j,R})+(\mu-f_{j,R})\left(\tfrac{\Delta}{\Delta x}U\right)_{j,R}\right) \\ & -\frac{1}{2}(\sigma_{Sj}U_{j,R}+\sigma_{Aj}B_{j,R}) \end{aligned} \tag{5.19}$$

where

$$\begin{aligned} \Upsilon_{j,R}\equiv U_{j,R}\frac{\delta\phi_{j,R}}{\delta U}\left(\left(\tfrac{\Delta}{\Delta x}fU\right)_{j,R}+\sigma_{Aj}(U_{j,R}-B_{j,R})\right)-\left(\tfrac{\Delta}{\Delta x}U\right)_{j,R}\left[\mu g^{\phi}_{j,R}-\phi_{j,R}\,g^{f}_{j,R}\right] \\ -\tfrac{1}{2}(U_j+U_{j+1/2})\left[\mu\left(\tfrac{\Delta}{\Delta x}\phi\right)_{j,R}-\phi_{j,R}\left(\tfrac{\Delta}{\Delta x}f\right)_{j,R}\right] \end{aligned} \tag{5.20}$$

The scaled equation for the $\Gamma = L$ equation can also be derived as:

$$\epsilon\,\Upsilon_{j,L} = \phi_{j,L}\left((\sigma_{Sj}U_{j,L}+\sigma_{Aj}B_{j,L})+(\mu-f_{j,L})\left(\tfrac{\Delta}{\Delta x}U\right)_{j,L}\right)-\frac{1}{2}(\sigma_{Sj}U_{j,L}+\sigma_{Aj}B_{j,L}) \tag{5.21}$$

where

$$\begin{aligned} \Upsilon_{j,L}\equiv U_{j,L}\frac{\delta\phi_{j,L}}{\delta U}\left(\left(\tfrac{\Delta}{\Delta x}fU\right)_{j,L}+\sigma_{Aj}(U_{j,L}-B_{j,L})\right)-\left(\tfrac{\Delta}{\Delta x}U\right)_{j,L}\left[\mu g^{\phi}_{j,L}-\phi_{j,L}\,g^{f}_{j,L}\right] \\ -\tfrac{1}{2}(U_j+U_{j-1/2})\left[\mu\left(\tfrac{\Delta}{\Delta x}\phi\right)_{j,L}-\phi_{j,L}\left(\tfrac{\Delta}{\Delta x}f\right)_{j,L}\right] \end{aligned} \tag{5.22}$$

with definitions equivalent to (5.14) and (5.15): $g^{\phi}_{j,L}(\mu)\equiv\frac{1}{2}(\phi_j+\phi_{j-1/2})-\phi_{j,L}$ and $g^{f}_{j,L}\equiv\int_{-1}^{+1}\mu\,g^{\phi}_{j,R}(\mu)\,d\mu$.

The scaling of the equations become meaningful when we write our solutions $\phi_{j,\Gamma}$ as an expansions in orders $\phi^{(i)}$:

$$\phi_{j,\Gamma} = \sum_{i=0}^{\infty} \epsilon^i \, \phi_{j,\Gamma}^{(i)} \tag{5.23}$$

We also define the quantities derived from the solution in orders:

$$f_{j,\Gamma}^{(i)} = \int_{-1}^{+1} d\mu \, \phi_{j,\Gamma}^{(i)}$$

We can summarize equations (5.20) and(5.21):

$$\epsilon \, \Upsilon_{j,\Gamma} = \phi_{j,\Gamma} \left((\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}) + (\mu - f_{j,\Gamma}) \left(\tfrac{\Delta}{\Delta x} U \right)_{j,\Gamma} \right) - \frac{1}{2} (\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}) \tag{5.24}$$

where we have defined (5.20), (5.22), (5.14), and (5.15).

So the leading order FDT equations are analogous to those found by the analytic CE method:

$$\phi_{j,\Gamma}^{(0)} \left((\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}) + (\mu - f_{j,\Gamma}^{(0)}) \left(\tfrac{\Delta}{\Delta x} U \right)_{j,\Gamma} \right) = \frac{1}{2} (\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}) \tag{5.25}$$

5.2. Leading order solutions and flux

We can read the zeroth order solution of the angular distribution from (5.25); note that it is a function of U and its derivative and has an angular form $1/(C+\mu)$.

$$\phi_{j,\Gamma}^{(0)} = \frac{\frac{1}{2}}{1 + (\mu - f_{j,\Gamma}^{(0)}) \frac{\left(\frac{\Delta}{\Delta x} U \right)_{j,\Gamma}}{\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}}} \tag{5.26}$$

Let us define the following two rationalized derivatives, R and X, and the albedo ω:

$$R_{j,\Gamma} \equiv \frac{X_{j,\Gamma}}{\omega_{j,\Gamma}} \equiv \frac{-\left(\frac{\Delta}{\Delta x} U \right)_{j,\Gamma}}{\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}} \tag{5.27}$$

$$X_{j,\Gamma} \equiv \frac{\left(\frac{\Delta}{\Delta x} U \right)_{j,\Gamma}}{\sigma_{Tj} U_{j,\Gamma}} \tag{5.28}$$

$$\omega_{j,\Gamma} \equiv \frac{\sigma_{Sj} U_{j,\Gamma} + \sigma_{Aj} B_{j,\Gamma}}{\sigma_{Tj} U_{j,\Gamma}} \tag{5.29}$$

The easy[3] way to calculate $f^{(0)}_{j,\Gamma}$ is to use the normalization condition $1 = \int_{-1}^{+1} d\mu\, \phi^{(0)}_{j,\Gamma}$ to solve for f. The method and the integration are exactly repeated as in the analytic example, since the discrete zeroth order solution is exactly analogous to the analytic zeroth order solution. We only roughly summarize the steps here; the reader should refer to the steps in derivation of (3.31) for the details of integration and solution.

$$1 = \int_{-1}^{+1} d\mu \frac{\frac{1}{2}}{1 + f^{(0)}_{j,\Gamma} R_{j,\Gamma} - \mu R_{j,\Gamma}} = \log\left(\frac{(1 + f^{(0)}_{j,\Gamma} R_{j,\Gamma}) + R_{j,\Gamma}}{(1 + f^{(0)}_{j,\Gamma} R_{j,\Gamma}) - R_{j,\Gamma}}\right)$$

The above is solved for $f^{(0)}$:

$$f^{(0)}_{j,\Gamma} = \coth R_{j,\Gamma} - \frac{1}{R_{j,\Gamma}} \tag{5.30}$$

Let us verify that we can repeat the above result working from the definition of flux $f^{(0)}_{j,\Gamma} \equiv \int_{-1}^{+1} d\mu\, \mu \phi^{(0)}_{j,\Gamma}$:

$$f^{(0)}_{j,\Gamma} = \int_{-1}^{+1} d\mu \frac{\frac{1}{2}\mu}{1 + f^{(0)}_{j,\Gamma} R_{j,\Gamma} - \mu R_{j,\Gamma}} := \frac{1}{2} \int \frac{\mu d\mu}{a\mu + b} = \frac{1}{2} a^{-1} \left[\mu - \frac{b}{a} \log(a\mu + b)\right]_{-1}^{+1}$$

where $a = -R_{j,\Gamma}$ and $b = 1 + f^{(0)}_{j,\Gamma} R_{j,\Gamma}$. Let us continue to evaluate the above:

$$f^{(0)}_{j,\Gamma} = \frac{1}{a}\left(1 - \frac{1}{2}\frac{b}{a} \log\left[\frac{+a+b}{-a+b}\right]\right) = \frac{-1}{R_{j,\Gamma}}\left(1 + \frac{f^{(0)}_{j,\Gamma} + \frac{1}{R}}{2} \log\left[\frac{+1 + f^{(0)}_{j,\Gamma} + \frac{1}{R}}{-1 + f^{(0)}_{j,\Gamma} + \frac{1}{R}}\right]\right)$$

We will work on the right hand side above, by substituting the solution $f + 1/R = \coth R$ and using the result $2R = \log\left[\frac{e^R}{e^{-R}}\right] = \log\left[\frac{\coth R + 1}{\coth R - 1}\right]$:

$$f^{(0)}_{j,\Gamma} = \frac{-1}{R_{j,\Gamma}}\left(1 - \frac{\coth R_{j,\Gamma}}{2} 2R_{j,\Gamma}\right) = \coth R_{j,\Gamma} - \frac{1}{R_{j,\Gamma}}$$

which is consistent.

Now we can substitute the solution for f into the angular form (5.26) to fully solve for the normalized angular distribution function:

---

[3]Compared to calculating directly from the definition of the flux and solving an equation in f.

$$\phi^{(0)}_{j,\Gamma} = \frac{\frac{1}{2}\, R_{j,\Gamma}{}^{-1}}{\coth\left(R_{j,\Gamma}\right) - \mu} \tag{5.31}$$

The solutions (5.30) and (5.31) are written in terms of R which is defined in (5.27)–(5.29).

5.3. Edge quantities

We also enforce flux limiting for the edge quantities:

$$U_{j+\frac{1}{2}} = \int_{-1}^{+1} d\mu\, I^{(0)}_{j+\frac{1}{2}} = U_{j+1,L} \int_{-1}^{0} \phi^{(0)}_{j+1,L} d\mu \; + \; U_{j,R} \int_{0}^{1} \phi^{(0)}_{j,R} d\mu \tag{5.32}$$

The integrals above are simply $\frac{-1}{2R}\log[\coth R - \mu]$ evaluated at $\left[^{0}_{\mu=-1}\right.$ and $\left[^{1}_{\mu=0}\right.$, for $R = R_{j+1,L}$ and $R_{j,R}$, respectively. So, the integral over positive and negative angles is $\frac{-(\pm 1)}{2R}\log[\frac{\coth R - (\pm 1)}{\coth R}] = \frac{-(\pm 1)}{2R}\log[\frac{\cosh R - (\pm)\sinh R}{\cosh R}]$, respectively; or $\frac{-(\pm 1)}{2R}[-(\pm R) - \log(\cosh R)] = \frac{1}{2} \pm \frac{1}{2R}\log(\cosh R)$. Thus,

$$U_{j+\frac{1}{2}} = \frac{U_{j+1,L} + U_{j,R}}{2} \; + \; \frac{1}{2}\left[\frac{U_{j,R}}{R_{j,R}}\log(\cosh R_{j,R}) \; - \; \frac{U_{j+1,L}}{R_{j+1,L}}\log(\cosh R_{j+1,L})\right] \tag{5.33}$$

The last term represents a sort of derivative $-\left[\frac{U_{j,\Gamma}}{R_{j,\Gamma}}\log(\cosh R_{j,\Gamma})\right]^{j+1,L}_{j,\Gamma=j,R}$, which is somewhat qualitatively similar to a derivative in $-[Uf]$, because qualitatively $\log(\cosh R)/R \;\sim\; \cosh R - 1/R$. The edge scalar flux expression above is difficult to handle because it is a function of average U's across the edge and nonlinear terms in U and its derivatives. Hence some approximations may be needed when writing an edge-based diffusion (or balance) equation.

Edge fluxes do not show up in the edge balance equations, yet we also will show the result for the edge fluxes. These are calculated from the positive and negative angular integrals below.

$$\frac{\pm 1}{2R}\int_{0}^{\pm 1} \frac{\mu d\mu}{\coth R - \mu} = \frac{\pm 1}{2R}(-1)[\mu + \coth R \log(\coth R - \mu)]^{\pm 1}_{\mu=0}$$

We continue to evaluate the above integral:

$$
\begin{aligned}
&-\tfrac{\pm 1}{2R}\left[\pm 1+\coth R\,\log\left(\tfrac{\coth R-(\pm 1)}{\coth R}\right)\right] \\
&=-\tfrac{\pm 1}{2R}\left[\pm 1+\coth R\,\log\left(\tfrac{\cosh R-(\pm 1)\sinh R}{\cosh R}\right)\right] \\
&=-\tfrac{\pm 1}{2R}\left[\pm 1-(\pm R)\coth R\,-\coth R\,\log(\cosh R)\right] \\
&=\tfrac{1}{2}\left[-\tfrac{1}{R}+\coth R\,\pm\,\tfrac{1}{R}\coth R\,\log(\cosh R)\right] \\
&=\tfrac{1}{2}f^{(0)}(R)\;\pm\;\tfrac{1}{R}\,\coth R\,\log(\cosh R)
\end{aligned}
$$

Thus the edge fluxes are also averages of the neighboring fluxes plus a pair of difficult nonlinear terms; referring to (3.20) we can write:

$$
\begin{aligned}
F^{(0)}_{j+\frac{1}{2}} = \quad & \frac{F^{(0)}_{j,R}+F^{(0)}_{j+1,L}}{2} \\
&+\tfrac{c}{2}\tfrac{U_{j,R}}{R_{j,R}}\coth R_{j,R}\,\log(\cosh R_{j,R})\;-\;\tfrac{c}{2}\tfrac{U_{j+1,L}}{R_{j+1,L}}\coth R_{j+1,L}\,\log(\cosh R_{j+1,L})
\end{aligned}
\tag{5.34}
$$

5.4. Summary of preliminary results

It was shown that it is possible to produce scaled functional transport equations that yield zeroth order results that are exactly analogous to Levermore's analytic results. That is, we are lead to the results below:

To zeroth order, the fluxes are given in Fick's form as:

$$
\begin{aligned}
F_{j,R} = c\,U_{j,R}\,f(R_{j,R}) &= -\frac{c\,\lambda(R_{j,R})}{\omega_{j,R}\,\sigma_j}\,\frac{U_{j+1/2}-U_j}{\Delta x_j/2} \\
&\qquad\text{and} \\
F_{j,L} = c\,U_{j,L}\,f(R_{j,L}) &= -\frac{c\,\lambda(R_{j,L})}{\omega_{j,L}\,\sigma_j}\,\frac{U_j-U_{j-1/2}}{\Delta x_j/2}
\end{aligned}
\tag{5.35}
$$

with $\lambda(R)\equiv\frac{1}{R}\left(\coth R\,-\,\frac{1}{R}\right)$, and the following definitions of the albedo ω, R, and the dimensionless gradient X:

$$
\begin{aligned}
&\omega_{j,R}\equiv\frac{\sigma_{Sj}U_{j,R}+\sigma_{Aj}B_{j,R}}{\sigma_{Tj}U_{j,R}}\quad\text{and}\quad\omega_{j,L}\equiv\frac{\sigma_{Sj}U_{j,L}+\sigma_{Aj}B_{j,L}}{\sigma_{Tj}U_{j,L}}\,, \\
&R_{j,R}\equiv\frac{X_{j,R}}{\omega_{j,R}}\quad\text{and}\quad R_{j,L}\equiv\frac{X_{j,L}}{\omega_{j,L}}\,, \\
&X_{j,R}\equiv\frac{-\frac{2}{\Delta x_j}\left(U_{j+1/2}-U_j\right)}{\sigma_{Tj}U_{j,R}}\quad\text{and}\quad X_{j,L}\equiv\frac{-\frac{2}{\Delta x_j}\left(U_j-U_{j-1/2}\right)}{\sigma_{Tj}U_{j,L}}\,.
\end{aligned}
\tag{5.36}
$$

From (5.35) we can read off the center flux $F_j = \int_{-1}^{+1} \mu \frac{I_{j,L}+I_{j,R}}{2} d\mu$:

$$F_j = -\frac{c}{\sigma_j \Delta x_j}\left[(U_j - U_{j-1/2})\frac{\lambda(R_{j,L})}{\omega_{j,L}} + (U_{j+1/2} - U_j)\frac{\lambda(R_{j,R})}{\omega_{j,R}}\right] \tag{5.37}$$

Likewise the edge flux is found in (5.34). The flux is thus an average across the cell plus an additional 'difference' quantity which gives the edge flux more weight from the flux in the upstream half-cell. Edge scalar intensities are also an average of two half cells across the edge, plus another 'difference' quantity. This is shown in (5.33). The meaning of these two results was not clear at first, but they are discovered in the next chapter on the numerical algorithm. Surprisingly, for the latter result, the dependence of $U_{j+1/2}$ on R makes the expression for R dependent on R, through $U_{j+1/2}(R)$; this leads to a new way of iterating for R. For the former result, it will be shown that the extra edge flux terms can add stability to the local equation in the next chapter.

The most general result is that the diffusion equations derived from a discrete CE derivation do not need to be continuous across the edges; i.e., $U_{j,R} \neq U_{j-1,L}$. The balance equations (5.7), along with the flux equations (5.37) and (5.33), produce the FLDT equations:

$$\begin{aligned} \tfrac{\Delta x_j}{2}\frac{\partial U_{j,R}}{\partial t} + \left(F_{j+1/2} - F_{j+1}\right) + c\sigma_{Aj}\tfrac{\Delta x_j}{2}\left(U_{j,R} - B_{j,R}\right) &= 0 \\ \tfrac{\Delta x_{j+1}}{2}\frac{\partial U_{j+1,L}}{\partial t} + \left(F_{j+1} - F_{j+1/2}\right) + c\sigma_{Aj+1}\tfrac{\Delta x_{j+1}}{2}\left(U_{j+1,L} - B_{j+1,L}\right) &= 0 \end{aligned} \tag{5.38}$$

5.5. Discontinuous discretized FLDT equations

The flux-limited diffusion equations (5.38) are different from the IDT results because discontinuities of the solution across the edges are allowed. For FLDT there is one equation per half-cell, and thus a different method for the solution is required. There are probably several ways the diffusion equations can be solved. We suggest writing equations in terms of edge averages and differences (of energy

density U) around an edge at $x_{j+1/2}$. The equations for the edge averages of U will have three point stencils, like the IDT solution, and will lead to a matrix equation with a tridiagonal matrix. The equations for the edge differences of U can be solved locally.

5.6. Notation for discontinuous FLDT: edge averages and differences

In this section we will define some useful notation. Since we are dealing with averages and differences it makes sense to use the notation described below.

Suppose we have some half-cell quantities $Q_{j,R}$ and $Q_{j,L}$ for all j on our spatial grid. Let us abbreviate the average quantity of Q across the edge $x = x_{j+1/2}$, i.e., the average of the half cells (j,R) and (j+1,L) as:

$$\langle Q \rangle_{j+1/2} = \frac{Q_{j+1,L} + Q_{j,R}}{2} \tag{5.39}$$

We also make an analogous definition for the (half) difference across the edge:[4]

$$\{Q\}_{j+1/2} = \frac{Q_{j+1,L} - Q_{j,R}}{2} \tag{5.40}$$

Half-cell quantities can be thought of in terms of averages and differences:

$$Q_{j,R} = \langle Q \rangle_{j+1/2} - \{Q\}_{j+1/2}$$

and

$$Q_{j+1,L} = \langle Q \rangle_{j+1/2} + \{Q\}_{j+1/2}$$

The 'product' rule (5.12) can be stated easily below. The (half) difference between a product AB, or the "edge discontinuity" of AB is written as:

---

[4]If only centered values $K_j, K_{j+1}...$ of a quantity K are defined, and we invoke the above notation (eg. $\langle K \rangle_{j+1/2}$ or $\{K\}_{j+1/2}$) then it is understood that we have simply defined the half-cell quantities as $K_{j,L} := K_j =: K_{j,R}$.

$$\{AB\}_{j+1/2} = \frac{A_{j+1,L}B_{j+1,L} - A_{j,R}B_{j,R}}{2} \tag{5.41}$$

which equals

$$\{AB\}_{j+1/2} = \{A\}_{j+1/2}\langle B\rangle_{j+1/2} + \langle A\rangle_{j+1/2}\{B\}_{j+1/2} \tag{5.42}$$

Likewise the average between two edge neighboring quantities equals:

$$\langle AB\rangle_{j+1/2} = \langle A\rangle_{j+1/2}\langle B\rangle_{j+1/2} + \{A\}_{j+1/2}\{B\}_{j+1/2} \tag{5.43}$$

Some additional notation:

Since we will solve for the edge discontinuities separately with a local equation, it will be convenient to describe quantities with the the discontinuities "turned off".

Let us use primed variables to denote variables with discontinuities turned off, i.e., with $U_{j,R} = U_{j+1,L}$ for all j.

$$Q' = Q\big|_{U_{j,R}=U_{j+1,L}\,\forall j}$$

For example, referring to (5.34) and[5] defining $\tilde{f}(R) \equiv \frac{\coth R \log(\cosh R)}{R}$, consider $U_{j+1/2} = \langle U\rangle_{j+1/2} - \{U\tilde{f}\}_{j+1/2}$. Then,

$$U'_{j+1/2} = \langle U\rangle_{j+1/2} - \langle U\rangle_{j+1/2}\{\tilde{f}\}_{j+1/2}. \tag{5.44}$$

We have simply linearized the term $U_{j+1/2}$ in terms of $\langle U\rangle$'s. Likewise let us repeat this for U_j:

$$U'_j = \left(\frac{U_{j,L}}{2} + \frac{U_{j,R}}{2}\right)' = \frac{\langle U\rangle_{j-1/2}}{2} + \frac{\langle U\rangle_{j+1/2}}{2} \tag{5.45}$$

Let us now linearize the centered flux F_j with the above two results:

---

[5]We named $\tilde{f} = \tilde{f}(R)$ after the leading order normalized flux $f(R) = \coth(R) - \frac{1}{R}$. The tilde is not part of any special notation that we define.

$$\begin{aligned}\tfrac{1}{c}F'_j &= \frac{-1}{\sigma_{Tj}\Delta x_j}\left[\frac{\lambda_{j,L}}{\omega_{j,L}}\left(U_j - U_{j-1/2}\right) + \frac{\lambda_{j,R}}{\omega_{j,R}}\left(U_{j+1/2} - U_j\right)\right]' \\ &= \frac{-1}{\sigma_{Tj}\Delta x_j}\left[\frac{1}{2}\left(\frac{\lambda_{j,R}}{\omega_{j,R}} + \frac{\lambda_{j,L}}{\omega_{j,L}}\right)\left(\langle U\rangle_{j+1/2} - \langle U\rangle_{j-1/2}\right)\right. \\ &\quad \left. -\frac{\lambda_{j,R}}{\omega_{j,R}}\{\tilde{f}\}_{j+1/2}\langle U\rangle_{j+1/2} + \frac{\lambda_{j,L}}{\omega_{j,L}}\{\tilde{f}\}_{j-1/2}\langle U\rangle_{j-1/2}\right] \end{aligned} \tag{5.46}$$

Let us also define the discontinuous parts of a quantity Q as δQ, where:

$$\delta Q = Q - Q' = Q - Q|_{U_{j,R}=U_{j+1,L}\,\forall j} \tag{5.47}$$

These quantities usually will involve terms that are linear in $\{U\}_{j+1/2}$.

5.7. Edge centered diffusion equation

We obtain the edge average energy density by solving the equations produced by the sum of left and right the half-cell diffusion equations (5.38). Using (5.43) we get:

$$\begin{aligned}&\frac{\langle\Delta x\rangle_{j+1/2}}{c}\frac{\partial}{\partial t}\langle U\rangle_{j+1/2} + \frac{1}{c}\left(F_{j+1} - F_j\right) + \langle\Delta x\sigma_A\rangle_{j+1/2}\langle U - B\rangle_{j+1/2} \\ &= -\frac{\{\Delta x\}_{j+1/2}}{c}\frac{\partial}{\partial t}\{U\}_{j+1/2} - \{\Delta x\sigma_A\}_{j+1/2}\{U - B\}_{j+1/2}\end{aligned} \tag{5.48}$$

The final step is to discretize time, so that

$$\frac{\partial}{\partial t}\langle U\rangle_{j+1/2} = \frac{\langle U\rangle^{\tau}_{j+1/2} - \langle U\rangle^{\tau-1}_{j+1/2}}{\Delta t}$$

where the superscripts τ and $\tau - 1$ denote the current and previous time step, respectively.

The remaining terms in (5.48) should be evaluated at the current time step τ, since full implicitiness is needed for unconditional stability for all timesteps.

We move the terms in (5.48) that are independent of edge average energy densities $\langle U\rangle_{i+1/2}$ to the right hand side of the equation. We have

$$\begin{aligned}&\left[\frac{\langle\Delta x\rangle_{j+1/2}}{c\,\Delta T} + \langle\sigma_A\Delta x\rangle_{j+1/2}\right]\langle U\rangle^{\tau}_{j+1/2} + \frac{1}{c}\left[F_{j+1} - F_j\right]' \\ &= \frac{\langle\Delta x\rangle_{j+1/2}}{c\,\Delta T}\langle U\rangle^{\tau-1}_{j+1/2}\langle\sigma_A\Delta x\,B\rangle_{j+1/2} - \frac{1}{c}\left[\delta F_{j+1} - \delta F_j\right] \\ &\quad -\frac{\{\Delta x\}_{j+1/2}}{c}\left[\{U\}^{\tau}_{j+1/2} - \{U\}^{\tau-1}_{j+1/2}\right] - \{\sigma_A\Delta x\}_{j+1/2}\{U\}^{\tau}_{j+1/2}.\end{aligned} \tag{5.49}$$

The linear terms for F' are given by (5.46); discontinuous quantities such as δF_j can be either numerically evaluated[6] or explicitly entered into the code.

5.8. Local equation

We subtract the half-cell diffusion equations (5.38) and use (5.42) to get:

$$\frac{\langle \Delta x \rangle_{j+1/2}}{c} \left\{ \frac{\partial U}{\partial t} \right\}_{j+1/2} + \frac{\{\Delta x\}_{j+1/2}}{c} \left\langle \frac{\partial U}{\partial t} \right\rangle_{j+1/2} + \frac{1}{c} \left(F_{j+1} - 2F_{j+1/2} + F_j \right) = \{\sigma_A \Delta x (B - U)\}_{j+1/2} \qquad (5.50)$$

The goal now is to find all the linear terms in $\{U\}_{j+1/2}$. Then the local equation is easily solved, fully implicitly. However we must first go through some lengthy algebra in order to extract all the terms in (5.50) that depend on the unknown quantity $\{U\}_{j+1/2}$. Unfortunately, this algebra is unavoidable because the unknown quantities must be solved implicitly; an iteration on a local equation with explicit $\{U\}_{j+1/2}$-dependence will be unstable because of stiffness.

5.9. Terms for second derivative of flux

The flux terms in the local equation (5.50) are the only ones that have a nontrivial dependence on the unknown $\{U\}_{j+1/2}$.

The center flux is given simply by $F_j = \frac{F_{j,L} + F_{j,R}}{2}$ while the edge flux is:

$$\frac{F_{j,R} + F_{j+1,L}}{2} - c\{\tilde{p} U\}_{j+1/2}$$

where $\tilde{p}(R) \equiv \frac{\coth R \log(\cosh R)}{R}$.

Using the above expressions for the fluxes, let us write down the following components of $(F_{j+1} - 2F_{j+1/2} + F_j)$:

$$F_{j+1/2} - F_j = \frac{F_{j+1,L} - F_{j,L}}{2} - c\{\tilde{p} U\}_{j+1/2}$$

$$F_{j+1/2} - F_{j+1} = \frac{F_{j,R} - F_{j+1,R}}{2} - c\{\tilde{p} U\}_{j+1/2}$$

---

[6]The only drawback is that terms are lagged from the last iteration.

We may add the above two equations, and multiply by $-\frac{1}{c}$ to obtain the intermediate result:

$$\frac{F_{j+1} - 2F_{j+1/2} + F_j}{c} = \frac{F_{j+1,R} - (F_{j+1,L} + F_{j,R}) + F_{j,L}}{2\,c} + 2\,\{\tilde{p}\,U\}_{j+1/2} \qquad (5.51)$$

It is interesting to note that the terms in $\tilde{p}(R)$ will have a stabilizing effect in the local equation (5.50), since their values are positive, ranging from $\frac{1}{2}$ to 1 for small and large R, respectively.

Since we require the local equation to be solved implicitly it is very important that we collect all linear terms in $\{U\}_{j+1/2}$. Explicit dependence in $\{U\}_{j+1/2}$ will cause instability through stiffness.

Let us examine the term $\frac{1}{c}(-F_{j,R} + F_{j,L})$. Let us write $F_{j,R}$ in a form that is convenient:

$$\tfrac{1}{c}F_{j,R} = -\frac{U_{j+1/2} - U_j}{\sigma_{T_j}\frac{\Delta x_j}{2}(\omega/\lambda)_{j,R}} = -\frac{U_{j+1,L} + U_{j,R} - 2\{\tilde{f}\,U\}_{j+1/2} - U_{j,L} - U_{j,R}}{\sigma_{T_j}\,2\frac{\Delta x_j}{2}\,(\omega/\lambda)_{j,R}}$$

Below we underline the terms that are important for collecting linear terms in $\{U\}_{j-1/2} = (U_{j+1,L} - U_{j,R})/2$:

$$\begin{aligned}
\tfrac{1}{c}F_{j,R} &= \frac{-\lambda_{j,R}}{\sigma_{T_j}\Delta x_j\omega_{j,R}}\left[\underline{U_{j+1,L}} - U_{j,L} - \underline{2\{\tilde{f}\,U\}_{j+1/2}}\right] \\
\tfrac{1}{c}F_{j,L} &= \frac{-\lambda_{j,L}}{\sigma_{T_j}\Delta x_j\omega_{j,L}}\left[\underline{U_{j,R}} - U_{j-1,R} - 2\{\tilde{f}\,U\}_{j-1/2}\right]
\end{aligned}$$

Let us repeat this for the $(j+1)$-th cell:

$$\begin{aligned}
\tfrac{1}{c}F_{j+1,R} &= \frac{-\lambda_{j+1,R}}{\sigma_{T_{j+1}}\Delta x_{j+1}\omega_{j+1,R}}\left[U_{j+2,L} - \underline{U_{j+1,L}} - 2\{\tilde{f}\,U\}_{j+3/2}\right] \\
\tfrac{1}{c}F_{j+1,L} &= \frac{-\lambda_{j+1,L}}{\sigma_{T_{j+1}}\Delta x_{j+1}\omega_{j+1,L}}\left[U_{j+1,R} - \underline{U_{j,R}} - \underline{2\{\tilde{f}\,U\}_{j+1/2}}\right]
\end{aligned}$$

Only terms that will contribute to the linear factor in $\{U\}$ are shown below:

$$\begin{aligned}
&\frac{F_{j+1,R} - (F_{j+1,L} + F_{j,R}) + F_{j,L}}{2\,c} \\
&= \frac{U_{j+1,L}}{2}\left[\frac{\lambda_{j+1,R}}{\sigma_{T_{j+1}}\Delta x_{j+1}\omega_{j+1,R}} + \frac{\lambda_{j,R}}{\sigma_{T_j}\Delta x_j\omega_{j,R}}\right] \\
&- \frac{U_{j,R}}{2}\left[\frac{\lambda_{j+1,L}}{\sigma_{T_{j+1}}\Delta x_{j+1}\omega_{j+1,L}} + \frac{\lambda_{j,L}}{\sigma_{T_j}\Delta x_j\omega_{j,L}}\right] \\
&+ \{\tilde{f}\,U\}_{j+1/2}\left[\frac{\lambda_{j+1,L}}{\sigma_{T_{j+1}}\Delta x_{j+1}\omega_{j+1,L}} - \frac{\lambda_{j,R}}{\sigma_{T_j}\Delta x_j\omega_{j,R}}\right] + \ldots
\end{aligned}$$

Using some algebra similar to (5.42) and (5.40), we will write down the linear terms in $\{U\}$ for the flux term (5.51):

$$\frac{F_{j+1,R} - (F_{j+1,L} + F_{j,R}) + F_{j,L}}{2\,c} + 2\,\{\tilde{p}\,U\}_{j+1/2}$$
$$= \left[\frac{1}{2}\left(\frac{\lambda_{j+1,R}}{\sigma_{Tj+1}\Delta x_{j+1}\omega_{j+1,R}} + \frac{\lambda_{j+1,L}}{\sigma_{Tj+1}\Delta x_{j+1}\omega_{j+1,L}} + \frac{\lambda_{j,R}}{\sigma_{Tj}\Delta x_j\omega_{j,R}} + \frac{\lambda_{j,L}}{\sigma_{Tj}\Delta x_j\omega_{j,L}}\right)\right.$$
$$\left. + 2\,\langle\tilde{p}\rangle_{j+1/2} + \langle\tilde{f}\rangle_{j+1/2}\left(\frac{\lambda_{j+1,L}}{\sigma_{Tj+1}\Delta x_{j+1}\omega_{j+1,L}} - \frac{\lambda_{j,R}}{\sigma_{Tj}\Delta x_j\omega_{j,R}}\right)\right]\{U\}_{j+1/2} + \ldots$$

As in the previous equation, the dots above represent other terms that are not dependent on $\{U\}_{j+1/2}$.

Let us summarize the above result and explain how the second derivative flux term will be evaluated in the local equation. We define the factor that appears in the equation above as:

$$W_{j+1/2} \equiv 2\,\langle\tilde{p}\rangle_{j+1/2} + 2\,\langle\tilde{f}\rangle_{j+1/2}\left\{\frac{\lambda}{\sigma_T\Delta x\,\omega}\right\}_{j+1/2} \tag{5.52}$$
$$+\frac{1}{2}\left(\frac{\lambda_{j+1,R}}{\sigma_{Tj+1}\Delta x_{j+1}\omega_{j+1,R}} + \frac{\lambda_{j+1,L}}{\sigma_{Tj+1}\Delta x_{j+1}\omega_{j+1,L}} + \frac{\lambda_{j,R}}{\sigma_{Tj}\Delta x_j\omega_{j,R}} + \frac{\lambda_{j,L}}{\sigma_{Tj}\Delta x_j\omega_{j,L}}\right)$$

The above is more simply written using center averages, as

$$W_{j+1/2} = 2\,\langle\tilde{p}\rangle_{j+1/2} + 2\,\langle\tilde{f}\rangle_{j+1/2}\left\{\frac{\lambda}{\sigma_T\Delta x\,\omega}\right\}_{j+1/2} + \left\langle\frac{\lambda}{\sigma_T\Delta x\,\omega}\right\rangle_{j+1} + \left\langle\frac{\lambda}{\sigma_T\Delta x\,\omega}\right\rangle_{j}.$$

Let the current iteration on $R, \langle U\rangle$, and $\{U\}$ be denoted by the index κ; then we treat the flux term as shown on the right hand side below: [7]

$$\frac{F^{\kappa}_{j+1} - 2F^{\kappa}_{j+1/2} + F^{\kappa}_{j}}{c} \tag{5.53}$$
$$= \frac{F^{\kappa-1}_{j+1} - 2F^{\kappa-1}_{j+1/2} + F^{\kappa-1}_{j}}{c} - W_{j+1/2}\,\{U\}^{\kappa-1}_{j+1/2} + W_{j+1/2}\,\{U\}^{\kappa}_{j+1/2}$$

5.10. Local iteration

The local equation (5.50) is rewritten below, and can easily be solved for the unknown $\{U\}^{\tau,\kappa}_{j+1/2}$.

---

[7]The idea of subtracting away lagged terms which will be replaced by terms that are to be solved implicitly is the same idea that was suggested in treating terms in (5.49).

$$\frac{\langle\Delta x\rangle_{j+1/2}}{c\Delta t}\left[\{U\}^{\tau,\kappa}_{j+1/2}-\{U\}^{\tau-1}_{j+1/2}\right]+W_{j+1/2}\{U\}^{\tau,\kappa}_{j+1/2}+\langle\sigma_A\Delta x\rangle_{j+1/2}\{U\}^{\tau,\kappa}_{j+1/2}$$
$$=\{\sigma_A\Delta x\,B\}_{j+1/2}-\{\sigma_A\Delta x\}_{j+1/2}\langle U\rangle^{\tau}_{j+1/2}-\frac{1}{c}\left(F^{\kappa-1}_{j+1}-2F^{\kappa-1}_{j+1/2}+F^{\kappa-1}_{j}\right)$$
$$-\frac{\{\Delta x\}_{j+1/2}}{c\Delta t}\left[\langle U\rangle^{\tau}_{j+1/2}-\langle U\rangle^{\tau-1}_{j+1/2}\right]+W_{j+1/2}\{U\}^{\tau,\kappa-1}_{j+1/2} \tag{5.54}$$

where $W_{j+1/2}$ is given by (5.52), where τ is the index for the time step iteration, and where κ is the index for the iteration on R, $\langle U\rangle$, and $\{U\}$ within the τ-iteration.

5.11. Edge relation for R

An interesting and unique result comes from the CE analysis of the SCB Transport equations, from the upstream closure relation. We will obtain a relation between the two neighboring flux-limiting parameters R around an edge. $R_{j,R}$ and $R_{j+1,L}$ share an averaged component. The relation suggests an iteration on R that could also be applicable for other flux limited diffusion equations.

For flux limiters that are functions of R, the iteration on R is basically the following: 0) Make an initial guess for $\vec{R}$. A fair guess may be $\vec{R}=\vec{0}$. 1) Solve for $\vec{U}$. 2) Construct a new $\vec{R}$ from $\vec{U}$. 3) Converge the solution of $(\vec{R},\vec{U})$ by iterating steps 1 and 2.

The result (5.33) that came out of the Upstream closure relation states:

$$U_{j+1/2} \;=\; \langle U\rangle_{j+1/2}+\frac{U_{j,R}\tilde{f}_{j,R}-U_{j+1,L}\tilde{f}_{j+1,L}}{2} \tag{5.55}$$

where $\tilde{f}$ is defined as,

$$\tilde{f}(R) \;=\; \log(\cosh R)\;. \tag{5.56}$$

The above (5.55) is significant, because we now notice that the definition of R has explicit dependence on R through $U_{j+1/2}$:

$$R_{j,R} \;=\; -\frac{U_{j+1/2}-U_j}{\frac{\Delta x}{2}\left(\sigma_S U+\sigma_A B\right)_{j,R}}$$

Before we noticed this dependence, we observed an unstable iteration on R in our code. The culprit probably was the explicit dependence on R through an

approximately linear relation of $\tilde{f}(R)$ at small R. The goal now is to remove the linear dependence in R. We first define:

$$\tilde{\lambda}(R) \equiv \frac{\tilde{f}(R)}{R} \tag{5.57}$$

$$m_{j,R} \equiv \frac{1}{\Delta x_j \left(\sigma_S U + \sigma_A B\right)_{j,R}} \tag{5.58}$$

$$R^0_{j,R} \equiv -\frac{\langle U\rangle_{j+1/2} - U_j}{\frac{\Delta x_j}{2}\left(\sigma_S U + \sigma_A B\right)_{j,R}} \tag{5.59}$$

and make similar definitions for $R^0_{j+1,L}$ and $m_{j+1,L}$.

Working from:

$$R_{j,R} = -2m_{j,R}\left[\langle U\rangle_{j+1/2} - U_j\right] \quad \text{and} \quad R_{j+1,L} = -2m_{j+1,L}\left[U_{j+1} - \langle U\rangle_{j+1/2}\right]$$

we see the linear relation between the edge R's, below.

$$R_{j,R} = R^0_{j,R} - m_{j,R}\left[R_{j,R}\,\tilde{\lambda}_{j,R}U_{j,R} - R_{j+1,L}\,\tilde{\lambda}_{j+1,L}U_{j+1,L}\right] \tag{5.60}$$

$$R_{j+1,L} = R^0_{j+1,L} - m_{j+1,L}\left[R_{j+1,L}\,\tilde{\lambda}_{j+1,L}U_{j+1,L} - R_{j,R}\,\tilde{\lambda}_{j,R}U_{j,R}\right] \tag{5.61}$$

Using the shorthand $\ell = \tilde{\lambda}\,U$,

$$\ell \equiv U\,\tilde{\lambda}(R)\ , \tag{5.62}$$

let us rewrite the relation in R as a matrix equation:

$$\begin{pmatrix} R_{j,R} \\ R_{j+1,L} \end{pmatrix} + \begin{pmatrix} m_{j,R}\,\ell_{j,R} & -m_{j,R}\,\ell_{j+1,L} \\ -m_{j+1,L}\,\ell_{j,R} & m_{j+1,L}\,\ell_{j+1,L} \end{pmatrix} \begin{pmatrix} R_{j,R} \\ R_{j+1,L} \end{pmatrix} = \begin{pmatrix} R^0_{j,R} \\ R^0_{j+1,L} \end{pmatrix} \tag{5.63}$$

We invert the 2x2 matrix A:

$$\mathsf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad \Rightarrow \quad \mathsf{A}^{-1} = \frac{1}{\det|\mathsf{A}|}\begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

with

$$\begin{aligned} a_{11} &= 1 + m_{j,R}\ell_{j,R} \quad a_{12} = -m_{j,R}\ell_{j+1,L} \\ a_{21} &= -m_{j+1,L}\ell_{j,R} \quad a_{22} = 1 + m_{j+1,L}\ell_{j+1,L} \end{aligned} \ . \tag{5.64}$$

The determinant is always positive since $m > 0$ and $\ell > 0$, and:

$$\det|\mathsf{A}| \;=\; 1 + m_{j,R}\,\ell_{j,R} + m_{j+1,L}\,\ell_{j+1,L} \tag{5.65}$$

The result is the following relation between $R_{j,R}$ and $R_{j+1,L}$:

$$\begin{pmatrix} R_{j,R} \\ R_{j+1,L} \end{pmatrix} = \frac{1}{\det|\mathsf{A}|} \begin{pmatrix} 1 + m_{j+1,L}\,\ell_{j+1,L} & m_{j,R}\,\ell_{j+1,L} \\ m_{j+1,L}\,\ell_{j,R} & 1 + m_{j,R}\,\ell_{j,R} \end{pmatrix} \begin{pmatrix} R^0_{j,R} \\ R^0_{j+1,L} \end{pmatrix} \tag{5.66}$$

We can further simplify; define

$$(\Delta U)_{j,R} \;\equiv\; 2\left(\langle U\rangle_{j+1/2} - U_j\right) \;\text{ and }\; (\Delta U)_{j+1,L} \;\equiv\; 2\left(U_{j+1} - \langle U\rangle_{j+1/2}\right), \tag{5.67}$$

so that the R^0's can be written simply:

$$R^0_{j,R} \;=\; -m_{j,R}(\Delta U)_{j,R} \quad \text{and} \quad R^0_{j+1,L} \;=\; -m_{j+1,L}(\Delta U)_{j+1,L}$$

These steps of algebra then follow from (5.66):

$$\det|\mathsf{A}| \begin{pmatrix} R_{j,R} \\ R_{j+1,L} \end{pmatrix} = \begin{pmatrix} R^0_{j,R} \\ R^0_{j+1,L} \end{pmatrix} - \begin{pmatrix} m_{j+1,L}\,\ell_{j+1,L} & m_{j,R}\,\ell_{j+1,L} \\ m_{j+1,L}\,\ell_{j,R} & m_{j,R}\,\ell_{j,R} \end{pmatrix} \begin{pmatrix} m_{j,R}(\Delta U)_{j,R} \\ m_{j+1,L}(\Delta U)_{j+1,L} \end{pmatrix}$$

The second term on the right hand side is just the vector

$$-\begin{pmatrix} m_{j+1,L}m_{j,R}\,\ell_{j+1,L}\left((\Delta U)_{j,R} + (\Delta U)_{j+1,L}\right) \\ m_{j+1,L}m_{j,R}\,\ell_{j,R}\left((\Delta U)_{j,R} + (\Delta U)_{j+1,L}\right) \end{pmatrix},$$

while

$$\left((\Delta U)_{j,R} + (\Delta U)_{j+1,L}\right) \;=\; 2\left(\langle U\rangle_{j+1/2} - U_j \;+\; U_{j+1} - \langle U\rangle_{j+1/2}\right) \;=\; 2\left(U_{j+1} - U_j\right).$$

Thus (5.66) can be simplified to the result below:

$$\det|\mathsf{A}| \begin{pmatrix} R_{j,R} \\ R_{j+1,L} \end{pmatrix} = \begin{pmatrix} R^0_{j,R} \\ R^0_{j+1,L} \end{pmatrix} - 2m_{j+1,L}m_{j,R}(U_{j+1} - U_j) \begin{pmatrix} U_{j+1,L}\tilde{\lambda}_{j+1,L} \\ U_{j,R}\tilde{\lambda}_{j,R} \end{pmatrix} \tag{5.68}$$

where $\tilde{\lambda}$, m, and R^0 are given by (5.57), (5.58), and (5.59), and where:

$$\det|\mathsf{A}| \;=\; 1 + m_{j,R}\,U_{j,R}\tilde{\lambda}_{j,R} + m_{j+1,L}\,U_{j,+1,L}\tilde{\lambda}_{j+1,L}\;.$$

We first notice that the strength of the averaging grows with the factor

$$m\,\ell \;=\; \frac{1}{\Delta x\,\sigma_T}\,\frac{\tilde{\lambda}}{\omega}\quad .$$

We also notice the strange reversed indices in the vector composed of the factor $U\,\tilde{\lambda}$. The significance of the reversals of the indices in the averaging term in (5.68) can be seen in this interpretation:

The relative strength of the averaging term, as compared with the edge neighbor's, is increased when the flux-limiting in the neighboring half-cell is smaller (smaller R implies greater $\tilde{\lambda}$)[8], and also can be increased when the intensity U of the neighbor is larger.

[8]The function $\tilde{\lambda}(R)$, like $\lambda(R)$, is bell shaped and peaks at $R = 0$.

6. NUMERICAL TESTING FOR FLDT EQUATIONS

6.1. Benchmark problem

Olsen and Su [8] provide a benchmark for a time-dependent radiative transfer algorithms involving the propagation of a shock wave. A radiative source of unit width in $\sigma_T x$ is turned on; the absorbing matter has a temperature dependent heat capacity $c_V(T)$. The scattering cross-sections are constant.

Exact solutions to this problem were found by Olsen and Su, and evaluated numerically. The exact transport solutions and the exact diffusion solutions are given in [8]. Olsen Auer and Hall [9] use this benchmark to test various approximate transport methods, including the Levermore (CE) FLDT. We will use the setup of this benchmark to compare the traditional Levermore FLDT equations against the discontinuous FLDT equations.

The material energy density B has the physical temperature dependence:

$$B = \frac{a}{c} T^4$$

while the heat capacity is chosen as

$$c_V = \alpha T^3$$

to make the problem linear in B, as shown below.

The derivative of B can be related to c_V:

$$\frac{\partial B}{\partial T} = \frac{4a}{c} T^3 = \frac{4a}{\alpha c} c_V = \frac{\epsilon}{c} c_V$$

where the constant $\epsilon \equiv \frac{4a}{\alpha}$ depends on the material properties a and α.

The differential equation for the material temperature is:

$$\frac{1}{c^2} c_V \frac{\partial T}{\partial t} = \sigma_A (U - B)$$

We now substitute $\frac{\partial B}{\partial T}$ for c_V:

$$\frac{1}{c^2} \frac{c}{\epsilon} \frac{\partial B}{\partial T} = \sigma_A (U - B)$$

So the linear differential equation in B is produced:

$$\frac{1}{c\epsilon\,\sigma_A}\frac{\partial B}{\partial t} = U - B \tag{6.1}$$

The above heat equations will be solved implicitly in our code, so that:

$$\frac{1}{\epsilon\, c\Delta t\, \sigma_A}\left(B^{\tau} - B^{\tau-1}\right) = U^{\tau} - B^{\tau}$$

Thus B^{τ} becomes an expression in $B^{\tau-1}$ and U^{τ}, after some algebra.

$$B^{\tau} = \frac{B^{\tau-1}}{1 + \epsilon\, c\Delta t\, \sigma_A} + \frac{U^{\tau}}{1 + \frac{1}{\epsilon\, c\Delta t\, \sigma_A}} \tag{6.2}$$

By symmetry of the unit source, the problem only needs to be solved for the half space $x \geq 0$; a reflecting boundary condition is placed at the left side, at $x = 0$.

6.2. Benchmark observations

We compare the FLDT solution with discontinuous terms to the standard FLDT solution. When the spatial grid is rough enough, we can notice discontinuities and can observe differences in the solutions, such as those seen in Figure 6.1. At later times the solution will become smooth, and discontinuities will disappear. Thus, the discontinuous FLDT equations mostly distinguishes itself in cases where the solution changes rapidly over time and space.

We observe steepening at the wave front; for example, Figure 6.3 shows a 4% higher value for $\langle U\rangle_{j+1/2}$ at $x = 0.5 - \Delta x$ and 4% lower value in the front of the wave front, at $x = 0.5 + \Delta x$, where $\Delta x = \frac{1}{8}$ and $t = 0.1$. If we compare half-cell values, the results are even better; $U_{6,L} = 0.0046$ against a continuous FLDT value of $U_{5,R} = U_{6,L} = 0.011$. The flux limiting parameter R shows this improvement, too. At the half-cell to the right of the edge at $x = \frac{1}{2}$, $R_{5,L} = 30$, while continuous FLDT has $R_{5,L} = 12$.

Other improvements for discontinuous FLDT are that the flux limiting parameter R is smoother and larger at the wave front. It is smooth enough so that

it does not need to be averaged. Figure 6.7 shows that the radiation pressure is also a smooth function. Some FLDT methods will smooth the radiation pressure by applying averaging, in order to prevent unphysical oscillations in the solution. This does not appear necessary for discontinuous FLDT. Both $R(x)$ and the pressure $p(x)\,U(x)$ appear very reasonable.

Figure 6.3 shows improvement ahead of the wave front. Percentagewise these differences are significant; however, the actual values are small and will be dwarfed by the size of the solution at later times. Hence, after the discontinuities in the relaxed solution vanish, these improved values at smaller times will not help to noticeably contribute later on. At later times, the 'tail' ahead of the wave front will be virtually identical in regular and discontinuous FLDT. Noticeable improvements at intermediate times will mostly accumulate at the top of the wave, as seen in Fig. 6.5.

The way to improve the 'tail' ahead of the wave front is to use a finer grid. For both FLDT equations the 'tail' at larger times is identical, and will be smaller valued for smaller grids with smaller time steps. An important observation is that both FLDT equations will produce increasingly similar results as we use finer mesh spacing. We expect that both FLDT equations will converge to the (same) analytic FLDT solution as the grid spacing is taken to zero.

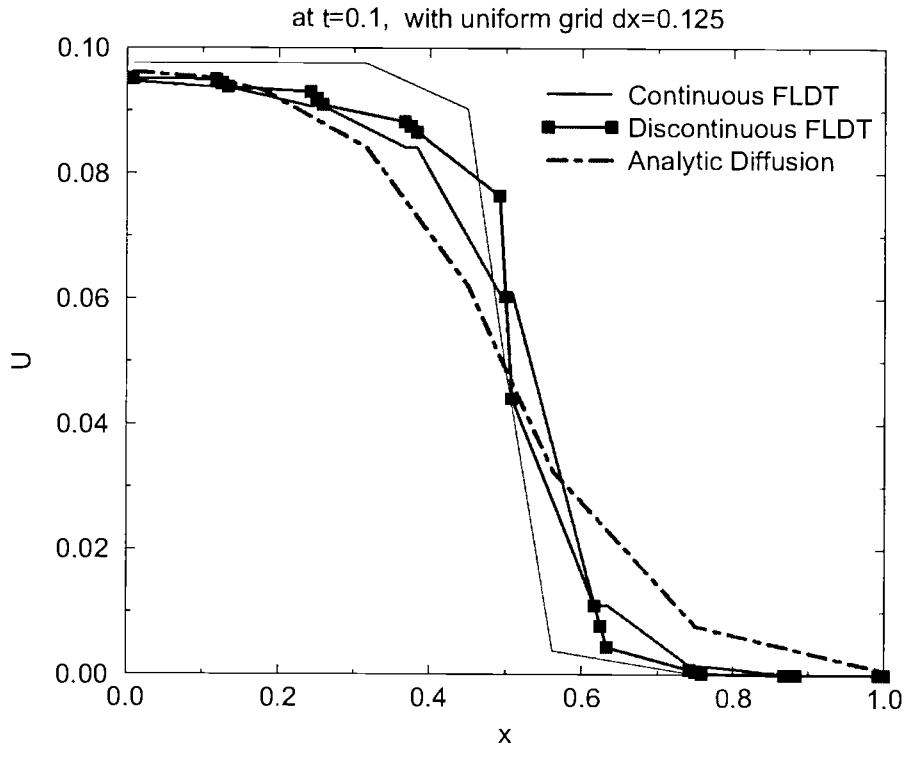

FIGURE 6.1. A rougher grid will let the discontinuities become significant, especially at smaller t.

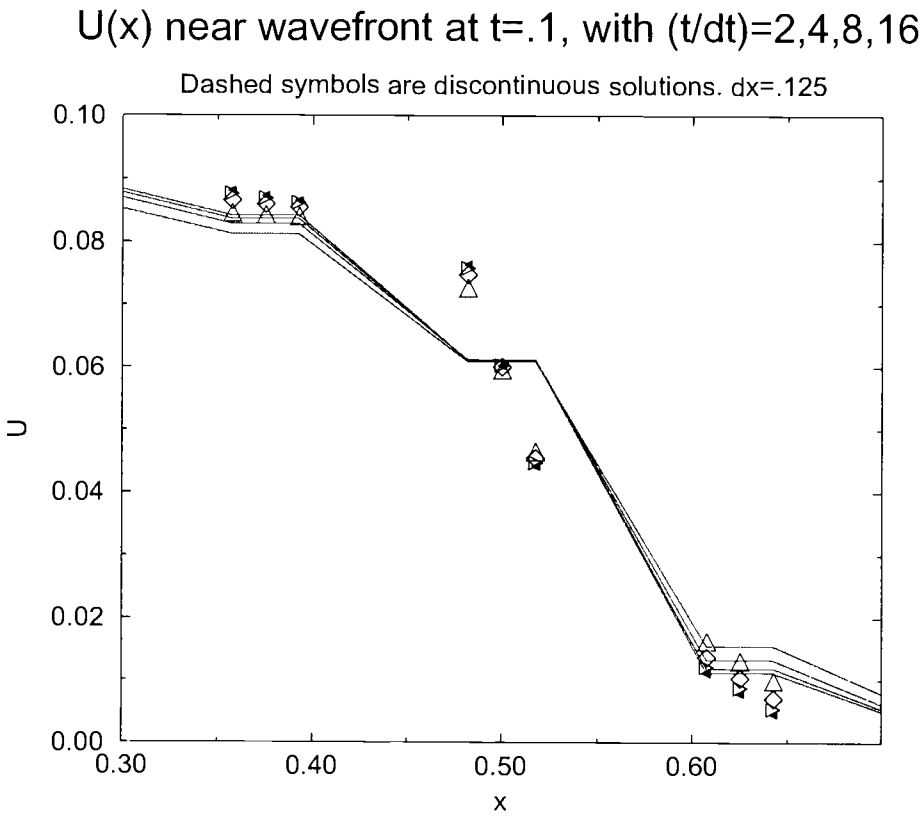

FIGURE 6.2. Above is a close-up view at the wave front. The solution is constructed with various smaller timesteps; we notice the solutions steepens as we move to smaller time steps; convergence is similar for both discontinuous and continuous FLDT solutions. Comparing edge average values around the edges neighboring the edge at $x = \frac{1}{2}$, discontinuous FLDT is a roughly four percent improvement. If we were to compare half-cell values, the improvements would be even better. At these values around the wave front, discontinuous FLDT with $dt = .025$ to 0.05 gives a similar result to regular FLDT with a finer time step of $dt = .00125$ to 0.00625.

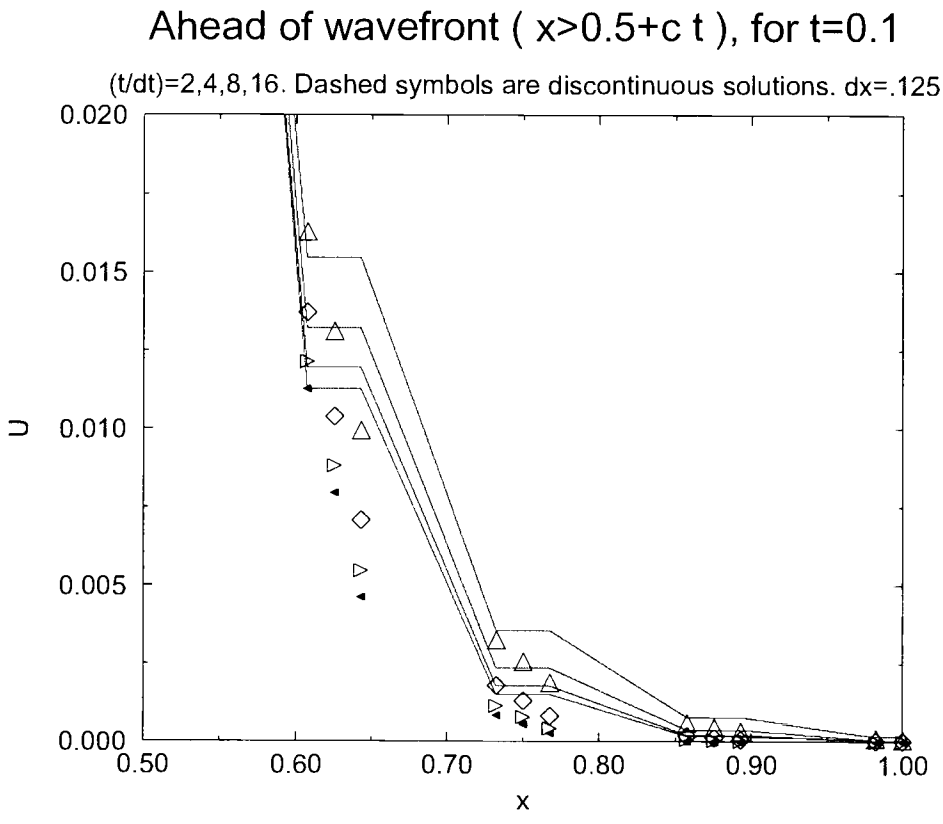

FIGURE 6.3. At small times, we see some improvement ahead of the wave front as well. Different solutions for different time step show convergence for smaller time steps.

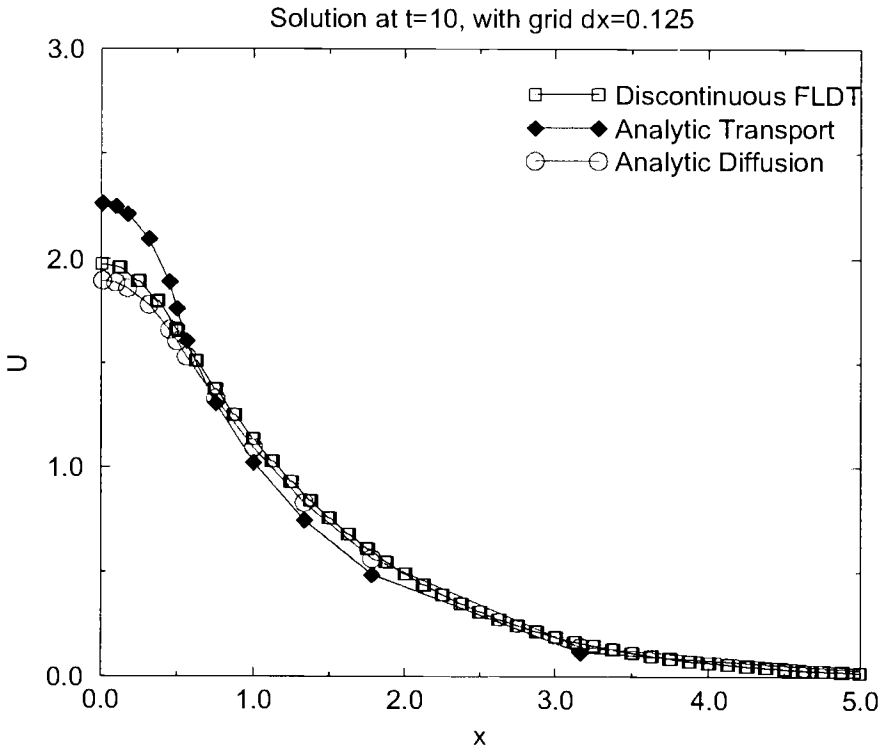

FIGURE 6.4. For larger times we observe the discontinuities become very small, as the solution smoothes; vanishing discontinuities with vanishing gradients are expected from our IDT derivation. After $t = 10$ the radiation source is turned off. For larger times gradients will become small, and the (IDT) diffusion approximation should dominate in the transport solution; the two analytic solutions should converge (Su, Olson).

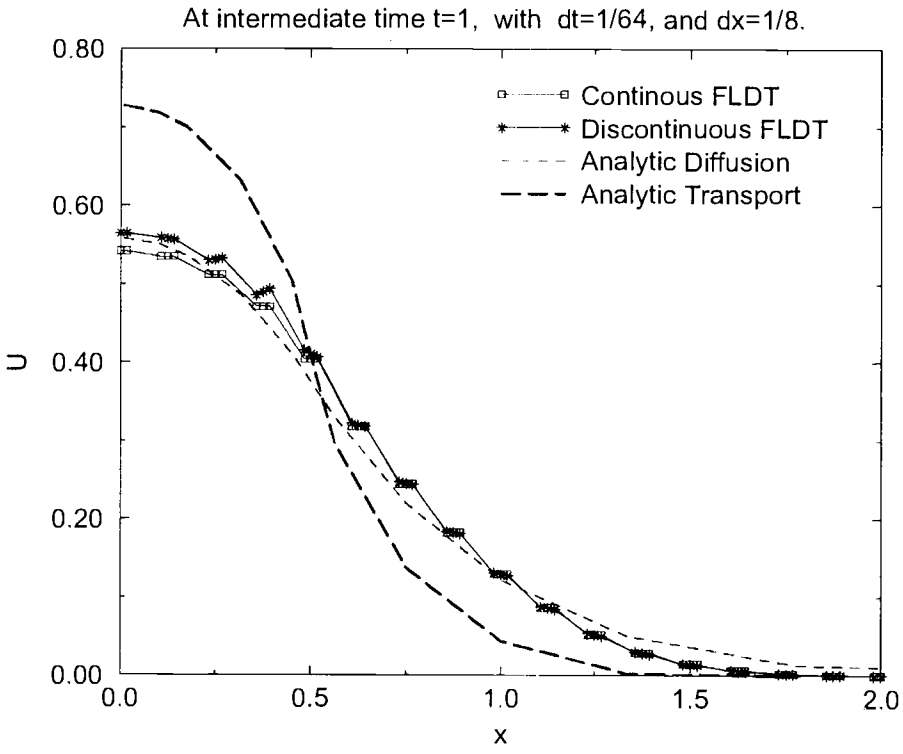

FIGURE 6.5. At intermediate times, benefits of discontinuous FLDT at earlier times are accumulated at the top of the wave. The improvement at the top is over 4 percent.

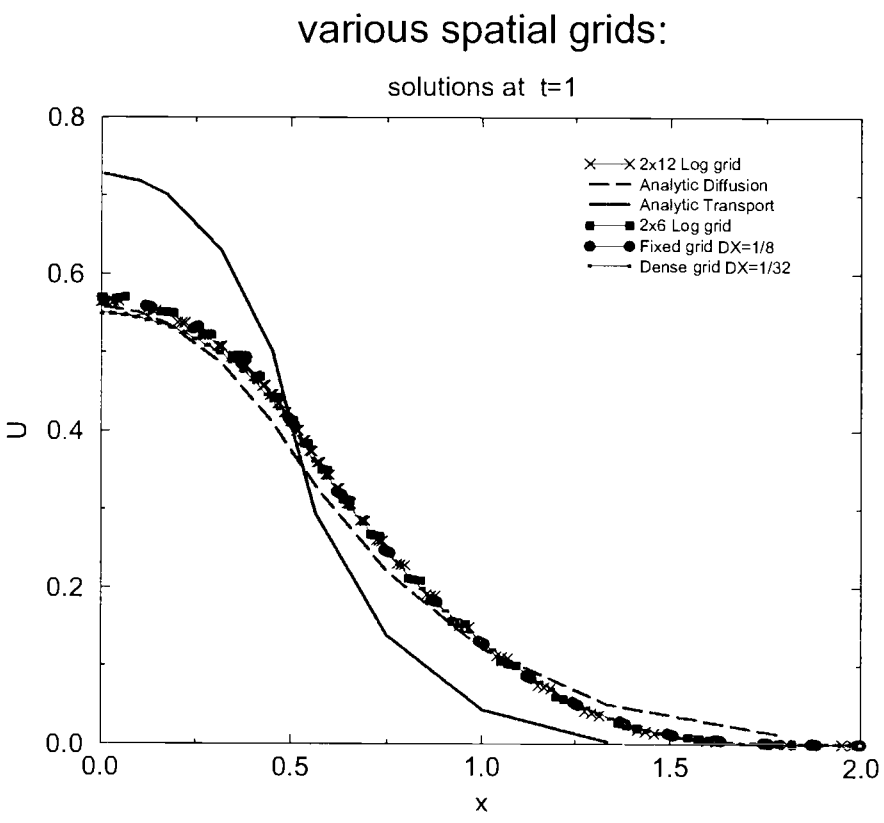

FIGURE 6.6. Various well chosen grids can perform better than a fine grid, such as $\sigma_T \, dx = \frac{1}{32}$. If we were to zoom in on the left and right end of the plot above, we would notice that thicker-grid solutions (for a well chosen grid) are noticeably better at the top, while being barely noticably worse in front of the wave front (around $x \geq 1.5$).

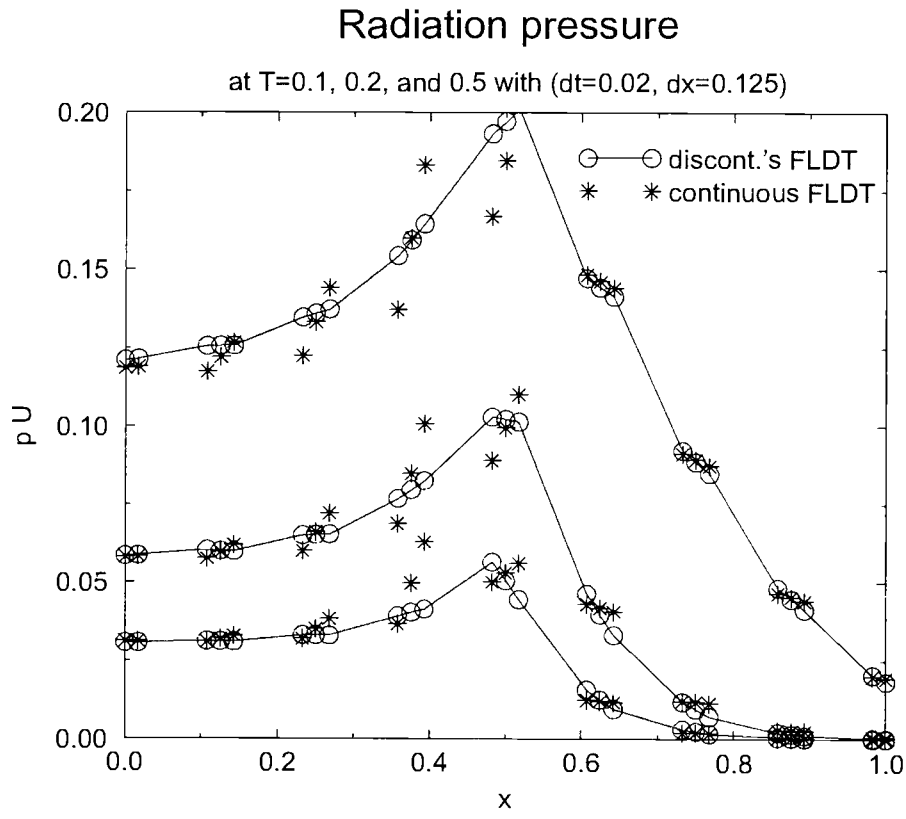

FIGURE 6.7. Radiation pressure comparison at various time steps. The comparison shows that the discontinuities help to smooth out the radiation pressure $P = cUp(R)$. When the edge energy density is forced to be continuous, we get a more erratic radiation pressure.

7. CONCLUSION

The derived discontinuous FLDT equations appear to have advantages that manifest themselves for solutions which vary rapidly in time and space, especially when coarser grids are chosen. Rapidly varying solutions such as very steep wavefronts can be better approximated with the discontinuous equations than with the traditional FLDT equations. For such solutions, we have numerically observed that edge discontinuities tend to become significant. However, when the solution is smooth and relaxed in space and time, or when a very fine grid is chosen, the the discontinuities become insignificant, and both the discontinuous FLDT and the traditional FLDT schemes appear to yield roughly the same results.

The discontinuous FLDT equations give better values for the flux-limiting parameter R compared to standard FLDT schemes. Numerical testing also indicates smooth values for the flux-limiting parameters R and the radiation pressure $U\,p(R)$. The iteration on R that follows from the upstream closure relation of the SCB transport method has variable averaging on R between edge neighbor half-cells. This method of iterating on R is unique, and it could be applied to other successful flux-limiters that may be superior to Levermore's CE FLDT; one should especially consider those flux-limiters derived from physical derivations, such as Levermore's Lorentz FLDT and Minerbo's statistical FLDT, that appeared to perform well in [5] or [9].

Another idea for improving the diffusion equation may be to go beyond the zeroth order solution. The zeroth order angular distribution $\phi^{(0)}$ is constructed from R's, and is used to construct the first order distribution, which in turn can be used to improve the expression for the flux. One may find a way to use the higher order expression for the flux to improve the solution. Two results might contribute to such possible work: 1) In (5.20) we show a discretized functional equation that has some additional terms that do not appear in the analytic functional transport

equation. 2) A more well defined numerical set of R's may make an iteration on the next order diffusion equation more efficient or feasible.

Other further work would be to perform more qualitative tests and benchmarks with different thermal setups (such as with temperature dependent cross-sections). Szilard and Pomraning [7] warn of one situation where a radiative shock wave into a cold slab (which has large σ_A at low T) can get trapped. The thermal wave may propagate too slowly, or not at all, unless certain steps are taken (averaging for T and R).

Important future research would be to extend the current work to two, and and eventually three dimensions.

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