Short Characteristic Solution to Neutral and Photon Transport

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Short Characteristic Solution to Neutral and Photon Transport

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Neutral particle transport is described by an integral form, which will lead to an inherently stable simple numerical solution, of the Boltzmann equation with BGK collision operator. Our governing equation possesses one part depicting an initial (or boundary) condition and another describing the causal nature of the. Using the short characteristic method, and retaining all terms to order of the mesh spacing squared, discretization is performed via a very plane second-degree Taylor polynomial with second-order difference formulas. Acclimating the numerical result to areas outside neutral particle transport the discretized solution is morphed into one describing the transport of photons and compared with results taken from the astrophysics community. What this paper brings to the literature is a new, accurate, unembellished finite difference numerical solution to the transport of neutrals and photons.

I. INTRODUCTION

If our system contains identical neutral particles, possesses no external forces and we may claim that the dominant effect of collisions is to restore local equilibrium, then a suitable governing equation is the Boltzmann equation with BGK collision operator:

\[
\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \frac{1}{\tau} (f^M - f).
\]

(1)

\(\tau\) represents a collision interval and \(f^M\) is the highly nonlinear Maxwellian velocity-distribution function. [1,2] By introducing the total derivative \(\left(\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla\right)\) on the left-hand-side (LHS) of Eq. 1, a seemingly first-order differential equation is formed:

\[
\frac{df}{dt} + \frac{1}{\tau} f = \frac{1}{\tau} f^M.
\]

(2)

where the parameter \(t\) now describes a characteristic path in phase space and time.

Integral equations allow for stable finite difference numerical solutions. Solving Eq. 2 by use of an exponential antiderivative \(\exp(\int_0^t \frac{1}{\tau} dt')\) leads to the following integral equation:

\[
f(t) = e^{-\int_0^t \frac{1}{\tau} dt'} f(0) + \int_0^t e^{-\int_0^t \frac{1}{\tau} dt''} f^M dt'.
\]

(3)

On the right-hand-side (RHS), the first term is dependent on our initial (or boundary) condition and the second term appears to sum the contributions of the Maxwellian in such a manner as to include no source effect before its time. The essence of this solution is captured in Duhamel’s principle.

In most of this paper we parry the physics and focus on establishing a discretization method. Section II will delineate a general short characteristic method that may be used for central and boundary regions of a system; Section III acclimates the discretization method to the description of photon transport; and Section IV contains thoughts of interest for the reader concerned with applying this research.

II. DISCRETIZATION

Seeking a balance between removing addle feelings and beginning to grate the reader with details, this section is dense with information contained within an exterior shell. Our integral equation will be discretized using a second-degree Taylor polynomial with second-order difference formulas (center for interior regions and backward for boundaries). Much of the detail is directed toward the central region results, the boundary region results are presented for completeness.
A. Interior Discretization

The short characteristic solution takes a point of focus and considers the influence of local neighbors. To begin, we establish a local coordinate (indexed by ‘\(i\)’ in Fig. 1) and write our integral equation in the from:

\[
f_i = \int_{t_{i-1}}^{t_i} \frac{1}{\tau(t)} \exp \left\{ -\int_{t}^{t_i} \frac{1}{\tau(s)} ds \right\} f^M(t) dt + \int_{t_{i-1}}^{t_i-1} \frac{1}{\tau(t)} \exp \left\{ -\int_{t}^{t_{i-1}} \frac{1}{\tau(s)} ds \right\} dt.
\] (4)

**FIG. 1. Mesh Spacing for Interior Discretization Formulas**

Then we approximate the Maxwellian as a second-degree Taylor polynomial:

\[
f^M(t) \approx f^M|_{t=t_i} + \frac{df^M}{dt}|_{t=t_i} (t-t_i) + \frac{1}{2} \frac{d^2 f^M}{dt^2}|_{t=t_i} (t-t_i)^2 + \cdots
\] (5)

and use the following centered second-order difference formulas for Maxwellian derivatives:

\[
\frac{df^M}{dt}|_{t=t_i} = \frac{f^M(t_{i+1}) - f^M(t_{i-1})}{2(\Delta t)} - \frac{1}{6} f^{M(iv)}(\xi)(\Delta t)^2
\] (6)

\[
\frac{d^2 f^M}{dt^2}|_{t=t_i} = \frac{f^M(t_{i+1}) - 2f^M(t_i) + f^M(t_{i-1})}{(\Delta t)^2} - \frac{1}{12} f^{M(iv)}(\xi)(\Delta t)^2
\] (7)

After placing Eqs. 6 and 7 into Eq. 5, inserting the latter into Eq. 4 and simplifying notation by letting \(f^M|_{t=t_i} = f_i^M\) we may write:

\[
f_i = \int_{t_{i-1}}^{t_i} \frac{1}{\tau(t)} \exp \left\{ -\int_{t}^{t_i} \frac{1}{\tau(s)} ds \right\} \left[ f_i^M + \frac{1}{2} \frac{f_{i+1}^M - f_{i-1}^M}{\Delta t} (t-t_i) + \frac{1}{2} \frac{f_{i+1}^M - 2f_i^M + f_{i-1}^M}{(\Delta t)^2} (t-t_i)^2 \right] dt + f_{i-1} \exp \left\{ -\int_{t_{i-1}}^{t_i} \frac{1}{\tau(t)} ds \right\}
\] (8)

The RHS of this equation consists of four separate integrals. Each term will be investigated apart from the rest and collected at the end of this section, thus obtaining our desired solution.

**I) Term One**

This term may be easily solved after a change of variables. To perform the change of variables we define \(z\) and a few properties:

\[
z \equiv -\int_{t_i}^{t_{i-1}} \frac{1}{\tau(s)} ds
\] (9)

\[
\frac{dz}{dt} = \frac{d}{dt} \int_{t_i}^{t} \frac{1}{\tau(s)} ds = \frac{1}{\tau(t)}
\] (10)

\[
z_{i-1} \equiv -\int_{t_{i-1}}^{t_i} \frac{1}{\tau(s)} ds
\] (11)
Then the first integral clearly becomes:

\[ \Rightarrow f_i^M \int_{z_{i-1}}^{0} \exp^z dz = f_i^M(1 - \exp^{z_{i-1}}) \quad (12) \]

(While investigating individual terms we denote a step of evolution by “\( \Rightarrow \)” , equations that represent a definition or some other type of simplification appear with no arrow.)

II) Term Two

After the following change of variables:

\[ \Rightarrow -\left\{ \frac{f_{i+1}^M - f_{i-1}^M}{2(\Delta t)} \right\} \int_{t_{i-1}}^{t_i} \frac{1}{\tau(t)} \exp - f_i^M \int_{t-i}^{t-i+1} ds (t_i - t) dt \]

\[ = -\left\{ \frac{f_{i+1}^M - f_{i-1}^M}{2(\Delta t)} \right\} \int_{z_{i-1}}^{0} (t_i - t) \exp^z dz, \quad (13) \]

and then integrating by parts we may write:

\[ \Rightarrow -\left\{ \frac{f_{i+1}^M - f_{i-1}^M}{2(\Delta t)} \right\} [ - \Delta t \exp^{z_{i-1}} + \int_{z_{i-1}}^{0} \tau(t) \exp^z dz]. \quad (14) \]

The collision interval is treated in a fashion identical to the Maxwellian velocity-distribution function; it is expanded as a second-degree Taylor polynomial with centered second-order difference formulas for the derivatives. Expanding the collision interval in Eq. 14 allows us to write:

\[ \Rightarrow -\left\{ \frac{f_{i+1}^M - f_{i-1}^M}{2(\Delta t)} \right\} [ - \Delta t \exp^{z_{i-1}} + \tau_i(1 - \exp^{z_{i-1}}) - \left\{ \frac{\tau_{i+1} - \tau_{i-1}}{2(\Delta t)} \right\} \int_{z_{i-1}}^{0} (t_i - t) \exp^z dz + \left\{ \frac{\tau_{i+1} - 2\tau_i + \tau_{i-1}}{2(\Delta t)^2} \right\} \int_{z_{i-1}}^{0} (t_i - t)^2 \exp^z dz] \quad (15) \]

To finish the discretization, we need to address the last term on the RHS and ensure that our order of accuracy is retained. Consistent with the series expansions used thus far, we choose to drop terms of order \((t_i - t)^3\). Working on this last term, we use integrating by parts and our collision interval series expansion to arrive at the following equation:

\[ \int_{z_{i-1}}^{0} (t_i - t)^2 \exp^z dz = \]

\[ -(\Delta t)^2 \exp^{z_{i-1}} + \int_{z_{i-1}}^{0} 2(t_i - t) \exp^z \frac{dt}{dz} dz = \]

\[ -(\Delta t)^2 \exp^{z_{i-1}} + 2\tau_i \int_{z_{i-1}}^{0} (t_i - t) \exp^z dz \]

\[ 1 + 2 \left\{ \frac{\tau_{i+1} - \tau_{i-1}}{2(\Delta t)} \right\} \]

\[ \quad (16) \]

And then we need to address the penultimate term on the RHS of Eq. 15 by using integration by parts. Instead of dropping terms we substitute the result of Eq. 16 where necessary. So the fully discretized from of this integral is found to be:

\[ \int_{z_{i-1}}^{0} (t_i - t) \exp^z dz = \]

\[ \frac{-\exp^{z_{i-1}}(\tau_i + \Delta t) \left\{ \frac{\tau_{i+1} - 2\tau_i + \tau_{i-1}}{2(\Delta t)} \right\} (\Delta t)^2 + \tau_i}{1 + 2 \left\{ \frac{\tau_{i+1} - \tau_{i-1}}{2\Delta t} \right\} - 2\tau_i \left\{ \frac{\tau_{i+1} - \tau_{i-1}}{2(\Delta t)^2} \right\}} \quad (17) \]
Before collecting the terms above it is important to note that the above integral is the solution of Term Two without the appropriate global factor in front. Adding this factor leads to the final discretized second integral term:

\[ \implies -\left( \frac{f^M_{i+1} - f^M_i}{2(\Delta t)} \right) \cdot \left[ \frac{- \exp^{z_i^{-1}}(\tau_i + \Delta t) + \left( \frac{\tau_{i+1} - \tau_i}{2(\Delta t)^2} \right)(\Delta t)^2 + \tau_i}{1 + \left( \frac{\tau_{i+1} - \tau_i}{2(\Delta t)} \right) - 2\tau_i \left( \frac{\tau_{i+1} - \tau_i - 1}{2(\Delta t)^2} \right) + \frac{1 + 2(\Delta t)}{1 + 2(\Delta t) - 2\tau_i}} \right] \]  

(18)

### III) Term Three

All the ingredients necessary to solve this integral are contained within the previous terms. Here we define the following terms to simplify future notation:

\[ M1 \equiv \tau_{i+1} - 2\tau_i + \tau_{i-1} \]  

(19)

\[ M2 \equiv \tau_{i+1} - \tau_i - \Delta t \]  

(20)

then use these definitions to clean up the following messy fraction:

\[ \int_{z_{i-1}}^{0} (t_i - t) \exp^z dz = \frac{-2(\Delta t) \exp^{z_i^{-1}}(\tau_i + \Delta t + \frac{\Delta t M1}{M2}) + 2(\Delta t)\tau_i}{\Delta t + M2 - 2\tau_i M1} \]  

(22)

and finally work the new definitions into Eq. 16:

\[ \int_{z_{i-1}}^{0} (t_i - t)^2 \exp^z dz = \frac{-(\Delta t)^3 \exp^{z_i^{-1}}}{M2} + \frac{-4(\Delta t)^2 \tau_i \exp^{z_i^{-1}}(\tau_i + \Delta t + \frac{\Delta t M1}{2M2}) + 2(\Delta t)\tau_i)^2}{M2^2 + (\Delta t)M2 - 2\tau_i M1} \]  

(23)

Eq. 23 is the essence of Term Three. Adding the necessary global factor to this integral yields the following discretized term:

\[ \implies \frac{1}{2} \left( f^M_{i+1} - 2f^M_i + f^M_{i-1} \right) \cdot \left[ \frac{-(\Delta t)^3 \exp^{z_i^{-1}}}{M2} + \frac{-4(\Delta t)^2 \tau_i \exp^{z_i^{-1}}(\tau_i + \Delta t + \frac{\Delta t M1}{2M2}) + 2(\Delta t)\tau_i)^2}{M2^2 + (\Delta t)M2 - 2\tau_i M1} \} \]  

(24)

### IV) Term Four

The fourth term has already been discretized via our definition of \( z_{i-1} \):

\[ \implies \exp^{z_i^{-1}} f_{i-1} \]  

(25)

Before collecting the terms above it is important to note that \( z_{i-1} \) itself contains an unevaluated integral. Using our collision interval approximation this term may be written:

\[ z_{i-1} = \Delta t \left( \frac{1}{12\tau_{i+1}} - \frac{2}{3\tau_i} - \frac{5}{12\tau_{i-1}} \right) \]  

(26)

Collecting the terms in Eq. 8 ( Eqs. 12, 18 (with slight modifications), 24 and 25) leads to our discretized integral Boltzmann equation solution:
\[ f_i = f_i^M (1 - \exp^{z_{i-1}}) \]
\[ -\frac{f_i^{M} - f_i^{M-1}}{2(\Delta t)} \left[ -\exp^{z_{i-1}}(\tau_i + \Delta t + \frac{M_1}{2(\Delta t)M_2}(\Delta t)^2 + \tau_i) \right. \]
\[ + \frac{1}{2} \left( f_i^{M-1} - 2f_i^{M} + f_i^{M+1} \right) \left\{ \frac{-(\Delta t)^3 \exp^{z_{i-1}}}{M_2} \right. \]
\[ - 4(\Delta t)^2 \tau_i \exp^{z_{i-1}}(\tau_i + \Delta t + \frac{(\Delta t)M_1}{M_2}) + \frac{(2(\Delta t)\tau_i)^2}{M_2^2 + (\Delta t)M_2 - 2\tau_i M_1} \}
\[ \left. \right\} + \exp^{z_{i-1}} f_{i-1}, \quad (27) \]

where \( M_1, M_2 \) and \( z_{i-1} \) are defined by Eqs. 19, 20 and 26, respectively.

B. Boundary Discretization

Imagine a gas contained within a solid box. For this system our central discretization formula will be useful throughout the interior of the box, however when considering a trajectory that is incident on a side of the box our central formula becomes invalid. To see this, consider a trajectory whose location \((t_i)\) is on the solid-gas interface (side of the box) and directed into the solid. The value of \( f_i \) depends on knowledge of locations inside the box \((t_{i+1})\) which are assumed to be in local equilibrium and described by a Maxwellian velocity-distribution. It is clear that the ordered lattice of the box is not represented by a Maxwellian. (A less interesting argument could be based on the improbable occurrence of a system with a solid box containing a gas of the same species.) Thus, for systems such as these, we have developed a backward finite-difference discretized solution which only considers locations within the gas — see Fig. 2 for a description of the new mesh.

**FIG. 2. Mesh Spacing for Boundary Discretization Formulas**

To arrive at the boundary discretization formula our technique of the previous subsection is still valid; new definitions and those that have been changed are now presented before the boundary discretized solution. The central second-order difference formulas are replaced by the following backward second-order difference formulas:

\[ \frac{dg}{dt} \bigg|_{t=t_i} = \frac{g_{i-2} - 4g_{i-1} + 3g_{i}}{2(\Delta t)} + \frac{1}{3} g^{(iii)}(\xi)(\Delta t)^2 \]  
\[ \quad (28) \]

\[ \frac{d^2 g}{dt^2} \bigg|_{t=t_i} = \frac{-g_{i-3} + 4g_{i-2} - 5g_{i-1} + 2g_{i}}{(\Delta t)^2} + \frac{11}{12} g^{(iv)}(\xi)(\Delta t)^2, \]  
\[ \quad (29) \]

where \( g \to \{ f^M, \tau \} \). New \( M \) definitions are used:

\[ M_3 = -\tau_{i-3} + 4\tau_{i-2} - 5\tau_{i-1} + 2\tau_i \]  
\[ \quad (30) \]

\[ M_4 = \Delta t + \tau_{i-2} - 4\tau_{i-1} + 3\tau_i \]  
\[ \quad (31) \]

\[ \frac{M_1}{2(\Delta t)M_2} \rightarrow \frac{M_3}{2(\Delta t)M_4} \]  
\[ \quad (32) \]

and \( z_{i-1} \) takes the form:
z_{i-1} = -\frac{\Delta t}{12} \left( \frac{7}{\tau_i} + \frac{2}{\tau_{i-1}} + \frac{5}{\tau_{i-2}} - \frac{2}{\tau_{i-3}} \right) \quad (33)

Aware of these changes, one may derive the following boundary discretized integral Boltzmann equation solution:

\[ f_i = f_i^M (1 - \exp^{z_{i-1}}) \]

\[ -(f_i^M - 4f_{i-1}^M + 3f_i^M) \frac{\exp^{z_{i-1}}(\tau_i + \Delta t + \frac{(\Delta t)M3}{2M4}) + \tau_i}{\Delta t + M4 - \frac{2\tau_iM2}{M4}} \]

\[ + \frac{1}{2(\Delta t)^2} (-f_{i-3}^M + 4f_{i-2}^M - 5f_{i-1}^M + 2f_i^M) \]

\[ \times \left[ -\frac{(\Delta t)^3 \exp^{z_{i-1}}}{M4} + \frac{-4(\Delta t)^2 \tau_i \exp^{z_{i-1}}(\tau_i + \Delta t + \frac{(\Delta t)M3}{2M4}) + (2(\Delta t)\tau_i)^2}{M4^2 + (\Delta t)M4 - 2\tau_iM3} \right] \]

\[ + \exp^{z_{i-1}} f_{i-1} \quad (34) \]

III. DISCRETIZATION OF THE RADIATION TRANSFER EQUATION

Taking advantage of similarities between the Boltzmann equation with BGK collision operator and the radiation transfer equation, we morph our neutral transport numerical solution into a photon transport numerical solution. Although this makes it easy to understand the procedure for discretization of photons, comparison with existing astrophysics literature \[3-5\] is very difficult. Confronting this quandary, an effort is made to allow future comparisons between the solution developed here and those exist in astrophysics literature.

A. Radiation Transfer Equation

Photon transport may be characterized by an equation of the form:

\[ \frac{df_R}{dt} = (Df_R)_{\text{coll}} \quad (35) \]

where \( f_R \) represents the photon distribution function. Most radiation transfer literature discusses the evolution of specific intensity, defined by the relation \( I(\vec{r}, \hat{n}, \nu, t) \equiv c h \nu f_R(\vec{r}, \hat{n}, \nu, t) \), rather than the photon distribution function; the specific intensity is more useful in descriptions of energy transport. In the case where the direction of observation and radiation propagation are along the same line, our governing radiation transfer equation takes the form:

\[ \frac{dI}{dt} + \chi I = \chi S \quad (36) \]

By comparison with Eq. 2 it is easy to see that the dominant inhomogeneity is now the source function \( S \), where to zero-order this term is behaves like the Planck distribution function.

B. Discretization

To arrive at a numerical radiation transfer equation, and hence solve for the transport of photons, a quick variable re-identification is performed. The notation gets a little confusing here since in the previous section we used \( \tau \) to represent the collision interval and here we define the optical depth \( (\tau) \) as \( d\tau = -\chi dz \).

We change notation by letting: \( f \rightarrow I, \frac{1}{\chi} \rightarrow \chi, f^M \rightarrow S \) and \( z_{i-1} \rightarrow -\Delta \tau_{i-1} \). Placing the new notation into Eq. 27 leads to the following central numerical radiation transfer equation solution (Finding the boundary region discretized solution is trivial.):
Although the equation above allows for one to understand how to acclimate our neutral particle transport solution to photon transport it is not useful for comparison with the literature. In astrophysics the short characteristic solution of radiation transfer will typically appear in the form:

\[
I_i = S_i (1 - \exp^{-\Delta \tau_{-1}})
\]

\[
-\left\{ \frac{S_{i+1} - S_{i-1}}{2(\Delta t)} \right\} - \exp^{-\Delta \tau_{-1}} \left( \frac{1}{\chi_i} + \Delta t + \frac{M_1}{4(\Delta t)M_2} (\Delta t)^2 + \frac{1}{\chi_i} \right)
\]

\[
+ \frac{1}{2} \left\{ \frac{S_{i+1} - 2S_i + S_{i-1}}{(\Delta t)^2} \right\} - \frac{(\Delta t)^3}{M_2} \exp^{-\Delta \tau_{-1}}
\]

\[
-4(\Delta t)^2 \left( \frac{1}{\chi_i} \right) \exp^{-\Delta \tau_{-1}} \left( \frac{1}{\chi_i} + \Delta t + \frac{(\Delta t)M_1}{2M_2} + (2(\Delta t)(\frac{1}{\chi_i})^2 \right)
\]

\[
\frac{M_2 + (\Delta t)M_2 - 2(\frac{1}{\chi_i})M_1}{CD}
\]

\ [+ \exp^{-\Delta \tau_{-1}} I_{i-1}
\]

(37)

After some algebra, Eq. 37 takes the above form with the following coefficient:

\[
CD = 4\chi^2_1 - 2\chi_1(\chi_1 + 1) + \chi_1^2 \chi_1 (\chi_1 - 1 + \chi_1 + 2(\Delta t)(\chi_1 - 1))
\]

\[
\alpha \times CD = \chi_1 (\chi_1 - 1 + 2(\Delta t)(\chi_1 - 1))
\]

\[
\gamma \times CD = \chi_1 \chi_1 (\chi_1 - 1 + 2(\Delta t)(\chi_1 - 1))
\]

where \( CD \) is just a common denominator. No further comparisons will be made at this time.

IV. DISCUSSION

This paper delineates a procedure for the discretization of general transport equations in a manner ductile enough to be applied to both neutral and photon transport. The procedure is based on the short characteristic method and uses a simple second-degree Taylor polynomial with second-order difference formulas. It this section we discuss some details of the neutral solution as well as the photon solution.

A. Neutral Transport

To begin, it is instructive to look at the limits, both collisional (\( \frac{\Delta t}{\tau} \to \infty \)) and collisionless (\( \frac{\Delta t}{\tau} \to 0 \)), of the central discretization solution for neutrals. In the collisional limit we find:

\[
f_i = f_i^M \left[ -2 \left( \frac{\tau}{\Delta t} \right)^2 + 1 \right] + \cdots \sim f_i^M
\]

(43)

and in the collisionless we find:

\[
f_i = f_{i-1} + \left( f_i^M - f_{i-1}^M \right) - \frac{\tau}{\Delta t} \left( f_{i+1}^M - 2f_i^M + f_{i-1}^M \right)
\]

(44)

These compare very well with the known first-order limits of:
\[ f_i = f_i^M \]  
(45) 
\[ f_i = f_{i-1} + (f_i^M - f_{i-1}^M) \]  
(46)

for the collisional and collisionless limits, respectively.

Another comment, one that is probably obvious to most readers, is that our solution has the ability to handle multi-species systems. Nothing prevents us from defining effective variables and updating their value between iterations or applying a linearization technique as will be discussed in the next subsection.

B. Radiation Transfer

In the introduction we mentioned that the Boltzmann equation with BGK collision operator is valid when the dominant effect of collisions is to restore local equilibrium. Due to photon scattering, a process defined as a photon-matter interaction with the net effect being a change in photon direction, radiation transfer is frequently non-local. In this case the short characteristic method breaks down in the sense that convergence may take an infinite amount of time. Many techniques have been developed to solve this problem and the interested reader is referred to the literature. [6,7]

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