



A COMPARATIVE STUDY OF FINITE-DIFFERENCE METHODS FOR RADIATIVE TRANSFER PROBLEMS

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Abstract—We have compared the numerical results of two widely used difference methods for the radiative transfer equation in plane-parallel medium. The Discrete Space theory (DS) is based on the direct first-order differential equation for the specific intensity whereas Auer's Hermitian (AH) method used the second order form for the mean-intensity and flux-like variables. The numerical results of these two methods are compared with analytical solutions under the two-stream approximation in a semi-infinite atmosphere. For the multi-stream case, the numerical errors are estimated using the solution of Chandrasekhar's discrete ordinate method. It is found that DS method is stable with respect to the logarithmic spacing of optical depth and gives less error for the specific intensity at the surface than that of AH method. The maximum relative error for the mean intensity variable is less for AH method. Analytical solution of the difference equation of DS method is studied and it is found that the solution gives the correct surface value and the diffusion limit in a semi-infinite atmosphere.

1. INTRODUCTION

The transfer of energy by radiation is an important process in most of the astrophysical objects. Many computational techniques are developed in the past to solve the transfer equation in plane-parallel medium. They can be classified broadly into two groups: (1a) Escape probability methods: these methods may be used to solve the time-dependent gas dynamics in which radiative transfer plays an important role. In these approaches high accuracy is not needed but one needs great computational speed.¹ (b) Operator perturbation techniques: these are fairly recent in origin and can be used for solving the non-LTE line blanketing problems.² (2) Methods based on discretization of the differential equation of radiative transfer: they are very accurate and can be used in the study of various physical processes in astronomical situations. In this paper, we have concentrated on these finite-difference techniques in plane-parallel medium.

There are two approaches to solve the transfer equation by discretization methods. One is based on the direct solution of the first order differential equation form of the transfer equation. This method was developed by Grant and Hunt^{3,4} and they called it as "Discrete Space theory of Radiative Transfer" (DS). They used "interaction principle" to derive the reflection and transmission operators of the medium and gave an algorithm to calculate the internal and emergent radiation fields. The form of difference equation for "step" and "diamond" scheme is given by Grant and Hunt.⁵ The "diamond" scheme uses mid-point values as the cell averages. Peraiah and Grant⁶ (PG) used this method to solve the transfer equation in spherical symmetry. One can obtain the plane-parallel limit from their method by taking the ratio of inner to outer radii of the medium as unity. Peraiah^{7,8} used the diamond scheme extensively to solve line formation problems in expanding medium in the rest frame and in the comoving frame. Recently DS was used to solve the problem of polarized radiation field.^{9,10}

Feautrier¹¹ transformed the transfer equation into second order differential equation by introducing the mean-intensity and flux-like variables. He proposed a central difference scheme which is of second order accuracy. Auer¹² extended this method to fourth-order accuracy by using the Hermitian scheme (AH). This method is applied extensively for various applications for e.g., model atmospheres.¹³ Feautrier form is also used in other applications like polarized line transfer.¹⁴

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The computer memory requirements for AH are less and also the method is faster compared to DS. But the first order form is advantageous in problem with complicated phase functions and anisotropic velocity fields. It is reported in the literature that the solution of their first-order equation may be inaccurate and instabilities occur.^{15,16} But our experience shows that DS method is always stable and accurate in a wide variety of applications. The step size restriction of DS is applicable only to the very outer layers. To verify our claim we incorporated logarithmic optical depth scale for semi-infinite atmosphere in DS and obtained the correct diffusion limit and the surface values. The stability analysis of difference equations of DS is performed. We compared the two methods, i.e., AH and DS methods, and estimated the errors using the analytical solutions wherever possible.

In Sect. 2, we briefly describe the mathematical schemes of these methods. The computational results are described in Sect. 3. In Sect. 4, we give analytical solution of DS method. In Sect. 5, we give the conclusions.

2. A BRIEF DESCRIPTION OF THE DIFFERENCE METHODS

(a) The Discrete Space theory

The monochromatic transfer equation for the isotropic scattering problem for constant ϵ and B is

$$\pm \mu \frac{dI^\pm(\tau, \mu)}{d\tau} = I^\pm(\tau, \mu) - 0.5(1 - \epsilon) \int_0^1 [I^+(\tau, \mu') + I^-(\tau, \mu')] d\mu' - \epsilon B, \quad (1)$$

with the boundary conditions

$$I^-(\tau = 0, \mu) = f(\mu) \quad \text{and} \quad I^+(\tau = T, \mu) = g(\mu). \quad (2)$$

Here $I^+(\tau, \mu)$ and $I^-(\tau, \mu)$ are, respectively, the upward and downward intensities at the optical depth τ along the direction μ , where μ is the cosine of the angle made by the ray to the plane of stratification. ϵ is the collision parameter and B is the Planck function. $f(\mu)$ and $g(\mu)$ are the given functions. The scattering integral is discretized using Gauss-Legendre formula of order J in the interval $\mu \in [0, 1]$. By integrating Eq. (1) from τ_n to τ_{n+1} gives,

$$\pm M[U_{n+1}^\pm - U_n^\pm] = U_{n+1/2}^\pm - 0.5(1 - \epsilon)C[U_{n+1/2}^+ + U_{n+1/2}^-] - \epsilon B, \quad (3)$$

where

$$U_{n+1/2}^\pm = 0.5[U_n^\pm + U_{n+1}^\pm], \quad (4)$$

which is called "the diamond" scheme and

$$M = [\mu_j \delta_{jj'}]_{J \times J},$$

$$C = \begin{bmatrix} c_1 & c_2 & \cdots & c_J \\ c_1 & c_2 & \cdots & c_J \\ \vdots & \vdots & \ddots & \vdots \\ c_1 & c_2 & \cdots & c_J \end{bmatrix}$$

$$U(\tau) = [I(\tau, \mu_1), \dots, I(\tau, \mu_J)]^T. \quad (5)$$

The resulting system of equations are solved using the interaction principle and star product. This semi-implicit method is more accurate compared to the explicit and fully-implicit schemes. Details of the methods can be seen in Ref. 6.

(b) Auer's Hermitian scheme

Feautrier¹¹ introduced the variables

$$U(\tau, \mu) = \frac{I(\tau, \mu) + I(\tau, -\mu)}{2} \quad \text{and} \quad V(\tau, \mu) = \frac{I(\tau, \mu) - I(\tau, -\mu)}{2}, \quad (6)$$

which have respectively, a mean-intensity and flux-like character. By adding and subtracting Eq. (1), we have

$$\mu^2 \left(\frac{d^2 U(\tau, \mu)}{d\tau^2} \right) = U(\tau, \mu) - (1 - \epsilon) \int_0^1 U(\tau, \mu') d\mu' - \epsilon B. \tag{7}$$

The boundary conditions can be written as

$$\mu \left(\frac{dU}{d\tau} \right) = U(0, \tau) - f(\mu) \quad \text{at } \tau = 0$$

and

$$\mu \left(\frac{dU}{d\tau} \right) = g(\mu) - U(\tau, \mu) \quad \text{at } \tau = T. \tag{8}$$

The scattering integral is discretized using Gauss–Legendre quadrature. Feautrier¹¹ proposed a second order discretization scheme to solve Eq. (7) and Eq. (8). Auer¹² introduced Hermitian scheme which is fourth order accurate. The resulting system of equations is tridiagonal in form and can be solved by standard techniques.

3. A COMPARATIVE STUDY OF THE NUMERICAL RESULTS

In order to compare the accuracy of these methods, we consider the solution of radiative transfer equation for three simple cases.

- (1) The first case is monochromatic conservative scattering under the two-stream approximation in a semi-infinite atmosphere with $\epsilon = 1, 10^{-2}$ and 10^{-4} and for $B = 1, \tau$ and τ^2 . For the numerical evaluation, we have considered only the cases given by Auer,¹² so that we can compare DS method with other methods discussed in this paper. We have chosen the logarithmic spacing $\Delta\tau_d = f\Delta\tau_{d-1}, \tau = K(f^{d-1} - 1)$ with $K = 0.01$ and $f = 10^{1/N}$, where N is the number of points per decade. We have chosen $N = 5$ and $\mu = 1.0$. The source function for this problem is given by

$$S = (1 - \epsilon)U(\tau) + \epsilon B(\tau). \tag{9}$$

We compared the results of DS and AH with the analytical solution for this problem which can be easily obtained. We have tabulated the results in Table 1. At the surface DS method is more accurate whereas maximum relative error (MRE) is less for AH method.

- (2) We have considered another problem which is similar to the first one but solved under the multi-approximation. We have and $B = 1$ and $\epsilon = 1, 10^{-2}, 10^{-4}$. Now the source function is given by

$$S = (1 - \epsilon) \int_0^1 U(\tau, \mu') d\mu' + \epsilon B. \tag{10}$$

One can obtain the solution for this case using Chandrasekhar's¹⁷ discrete ordinate method. We compared the results of DS and AH methods with this solution and the results are tabulated in Table 2 for the four Gaussian angles. At all the angles, surface relative error (SRE) is less for DS and in the interior, MRE is less for AH method.

Table 1. Surface relative error (SRE) and maximum relative errors (MRE) for DS and AH methods in a semi-infinite atmosphere under the two-stream approximation.

$B(\tau)$ ϵ	1			τ			τ^2		
	1	10^{-2}	10^{-4}	1	10^{-2}	10^{-4}	1	10^{-2}	10^{-4}
DS (PG) Method									
SRE	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.8E-05	7.1E-05	7.5E-05
MRE	4.0E-03	7.5E-03	8.3E-03	1.5E-03	2.7E-04	3.2E-05	1.5E-03	2.6E-03	2.9E-03
AH method									
SRE	3.4E-04	6.1E-04	6.6E-04	5.4E-04	2.6E-04	2.0E-04	4.2E-05	3.0E-04	3.6E-04
MRE	9.2E-04	1.7E-03	1.9E-03	5.8E-04	2.6E-04	2.4E-04	4.4E-04	4.0E-04	4.0E-04

Table 2. Same as in Table 1 but under the multi-stream approximation for the four Gaussian angles.

ϵ	10^{-2}				10^{-4}				
	μ	0.069	0.33	0.66	0.93	0.069	0.33	0.66	0.93
DS (PG) Method									
SRE	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
MRE	7.4E-03	7.4E-03	7.5E-03	7.6E-03	8.4E-03	8.4E-03	8.4E-03	8.4E-03	8.4E-03
AH Method									
SRE	9.0E-04	6.9E-04	5.9E-04	5.5E-04	1.0E-03	7.7E-04	6.5E-04	6.0E-04	6.0E-04
MRE	1.6E-03	1.6E-03	1.6E-03	1.7E-03	1.8E-03	1.8E-03	1.8E-03	1.8E-03	1.8E-03

(3) We have considered finite atmosphere with total optical thickness $T = 1, 2$ and 10 , with $\epsilon = 0$, and $g(\mu) = 1$ at the lower boundary. The medium is divided into 20 shells with equal optical thickness except for the case $T = 1$, where only 10 shells are considered. The solutions are compared again with Chandrasekhar's discrete ordinate method. From Table 3, we see for AH method, SRE and MRE coincide. For DS method, SRE is less than MRE.

4. ANALYTICAL SOLUTION OF DIFFERENCE EQUATIONS FOR DS METHOD

Grant and Hunt³ derived the step size requirement for a stable solution of DS method by considering the non-negativity of the transmission matrix. The stability condition is

$$\Delta\tau \leq \min_j \left[\frac{2\mu_j}{1 - (1 - \epsilon)c_j} \right]$$

For the two stream approximation, $\Delta\tau \leq 2/\epsilon$. For optically thick atmospheres they suggested doubling method where one subdivides the shell until the stability condition is satisfied.

Since we could use a large step size (i.e., for logarithmic spacing of optical depth) for $\epsilon = 1$ in the two-stream approximation, we reexamined the stability criterion using the analytical solution of the difference equations of DS method. A similar analysis was done for the step scheme of the first order differential equation by Kalkofen and Wehrse.¹⁸ They showed that for sufficiently large

Table 3. Same as in Table 2 but for finite atmospheres.

T	1				
	μ	0.069	0.33	0.66	0.93
DS (PG) Method					
SRE		1.1E-04	3.8E-04	2.4E-05	7.7E-05
MRE		2.6E-02	3.8E-04	5.8E-05	7.7E-05
AH Method					
SRE		2.1E-02	3.3E-04	1.3E-04	6.8E-05
MRE		2.1E-02	3.3E-04	1.3E-04	6.8E-05
T	2				
	μ	0.069	0.33	0.66	0.93
DS (PG) Method					
SRE		2.1E-05	6.9E-05	1.0E-05	3.4E-05
MRE		2.6E-02	3.1E-04	9.6E-05	3.4E-05
AH Method					
SRE		2.1E-02	3.6E-04	1.7E-04	9.8E-05
MRE		2.1E-02	3.6E-04	1.7E-04	9.8E-05
T	10				
	μ	0.069	0.33	0.66	0.93
DS (PG) Method					
SRE		0.0E+00	0.0E+00	0.0E+00	0.0E+00
MRE		1.3E-01	8.5E-03	1.1E-03	1.4E-03
AH Method					
SRE		3.1E-01	3.1E-04	4.7E-03	3.4E-03
MRE		3.1E-01	8.3E-04	4.7E-03	3.4E-03

value of $\Delta\tau$, the solution diverges instead of reaching the constant value $I_k^+ = I_k^- = B$, for large K . We extend the same analysis in this paper for the most important case of semi-implicit difference scheme and show that the solution reaches the correct limit.

In another paper, Kalkofen and Wehrse¹⁹ compared the finite difference equations in various formulations of radiative transfer. They discussed the stability of semi-implicit difference scheme only for the restricted case where the source function is $S = 1$. In this paper the stability analysis is done for the general case where the source function is given by the form

$$S = 0.5(1 - \epsilon) \int_{-1}^{+1} I(\tau, \mu') d\mu' + \epsilon B.$$

We first consider the case for $\epsilon = 1.0$.

(a) *True absorption*

The transfer equation for the outward intensity in the case of “diamond scheme” is

$$\frac{1}{\Delta\tau} (E - 1)I_k^+ = \frac{(E + 1)}{2} I_k^+ - B, \quad k = 0, 1, 2, \dots \tag{11}$$

where $I_k = I(\tau_k, \mu)$ and the shift operator $E I_k = I_{k+1}$. The boundary condition is

$$I_N^+ = B, \quad \text{for very large } N. \tag{12}$$

The solution for this equation is

$$I_k^+ = B. \tag{13}$$

The transfer equation for the inward intensity is

$$-\frac{1}{\Delta\tau} (E - 1)I_k^- = \frac{(E + 1)}{2} I_k^- - B, \quad k = 0, 1, 2, \dots \tag{14}$$

The boundary condition is

$$I_0^- = 0. \tag{15}$$

The solution for this equation is

$$I_k^- = B(1 - r^k), \quad r = \frac{(1 - 0.5\Delta\tau)}{(1 + 0.5\Delta\tau)}.$$

For very large K , $r^k \rightarrow 0$ (even for very large values of $\Delta\tau$), we have

$$I_k^- = B. \tag{16}$$

(b) *The two-stream approximation*

Here we describe the analytical solution of difference equations of DS under the two-stream approximation for constant ϵ and B .

$$\pm \gamma(E - 1)I_k^\pm = \frac{(E + 1)}{2} I_k^\pm - \frac{(1 - \epsilon)}{4} (E + 1)[I_k^+ + I_k^-] - \epsilon B \tag{17}$$

where $\gamma = 1/\Delta\tau$. Let

$$a_1 = \gamma(E - 1) - \frac{(1 + \epsilon)(1 + E)}{4}, \quad b_1 = -\frac{(1 - \epsilon)(1 + E)}{4},$$

$$a_2 = -\gamma(E - 1) - \frac{(1 + \epsilon)(1 + E)}{4}. \tag{18}$$

Equation (17) can be written as

$$a_1 I_k^+ = b_1 I_k^- - \epsilon B,$$

$$a_2 I_k^- = b_1 I_k^+ - \epsilon B. \tag{19}$$

The particular solution is given by

$$I_k^+ = -\frac{(a_2 + b_1)}{(a_1 a_2 - b_1^2)} cB$$

From this expression one can show that $I_k^+ = B$ by considering only the first order terms in $\Delta = E - 1$. Similarly,

$$I_k^- = -\frac{(a_1 + b_1)}{(a_1 a_2 - b_1^2)} cB = B. \quad (20)$$

To find the homogeneous solutions, we obtain the roots of the equation

$$(a_1 a_2 - b_1^2) = 0, \quad \text{which are } r_1 = \frac{(1 + 0.5\sqrt{\epsilon\Delta\tau})}{(1 - 0.5\sqrt{\epsilon\Delta\tau})}, \quad r_2 = \frac{1}{r_1}. \quad (21)$$

The general solution of the homogeneous equation can be written as

$$I_k^{\pm \text{hom}} = A_1^{\pm} r_1^k + A_2^{\pm} r_2^k. \quad (22)$$

Two of the four arbitrary constants are redundant. We obtain a relation between them by introducing Eq. (22) into either one of the Eqs. (17). It follows that

$$A_1^- = r A_1^+ \quad \text{and} \quad A_2^- = \frac{1}{r} A_2^+, \quad \text{where } r = \frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}}. \quad (23)$$

Now the general solution of Eqs. (17) can be written as

$$\begin{aligned} I_k^+ &= A_1^+ r_1^k + A_2^+ r_2^k + B \\ I_k^- &= r A_1^+ r_1^k + \frac{1}{r} A_2^+ r_2^k + B. \end{aligned} \quad (24)$$

By imposing the boundary condition $I_0^- = 0$ and $I_N^+ = B$, we obtain

$$A_1^+ = \frac{-B r r_2^N}{(r^2 r_2^N - r_1^N)} \quad \text{and} \quad A_2^+ = \frac{B r r_1^N}{(r^2 r_2^N - r_1^N)}$$

At the boundary, we have,

$$I_0^+ = B \left[\frac{-r}{r^2 - \left(\frac{r_1}{r_2}\right)^N} + \frac{r}{r^2 \left(\frac{r_2}{r_1}\right)^N - 1} + 1 \right]. \quad (25)$$

For very large N , $(r_1/r_2)^N = r_1^{2N} \rightarrow \infty$, and $(r_2/r_1)^N = r_2^{2N} \rightarrow 0$, we obtain

$$I_0^+ = B(1 - r) = B \left(1 - \frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \right) = B \left(\frac{2\sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \right), \quad (26)$$

which gives the correct surface value for the mean intensity $J(0) = 0.5I^+(0) = B\sqrt{\epsilon}/(1 + \sqrt{\epsilon})$.

Away from the boundary, we have

$$I_k^+ = B \left[\frac{-r r_1^k}{r^2 - \left(\frac{r_1}{r_2}\right)^N} + \frac{r r_2^k}{r^2 \left(\frac{r_2}{r_1}\right)^N - 1} + 1 \right] = B(1 - r r_2^k). \quad (27)$$

For large values of k , $r_2^k \rightarrow 0$, we have

$$I_k^+ = B. \quad (28)$$

Similarly, we have

$$I_k^- = B(1 - r_2^k) = B. \quad (29)$$

In comparison, for step scheme, the roots r_1 and r_2 are $r_1 = 1 + \sqrt{\epsilon\tau}$ and $r_2 = 1 - \sqrt{\epsilon\tau}$.¹⁸ For large K , the expressions for I_k^+ and I_k^- oscillate in sign and do not converge to B is $\sqrt{\epsilon\tau} > 1$.

We have performed the above analysis for the two-stream approximation. We find that we need to take small step size only in the outer layers for getting an accurate solution. The diffusion limit is obtained irrespective of the step size as we go deep into the medium. This analysis holds good even in the multi-stream case, as the two-stream approximation is valid inside the medium (i.e., radiation field is nearly isotropic). In the very outer layers, where the radiation field is anisotropic, one has to restrict the step size to $\approx 2\mu$. The logarithmic optical depth scale always satisfy the above conditions.

5. CONCLUSIONS

We have compared the methods of DS and AH for few idealized models. We find that at the surface DS is more accurate compared to AH, whereas in the interior AH is more accurate. The error of both the methods are insignificant. We performed the stability analysis of the DS method under the "diamond scheme" and found that it gives the correct diffusion limit. The logarithmic depth scale also ensures the correct step restriction for DS method. We conclude that the methods based on the first transfer equation need not be less stable compared to the difference schemes for the second order form.

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